

University of California, Irvine

July 24-29, 2011



23rd International Colloquium on the  
Dynamics of Explosions and Reactive Systems

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# 23<sup>rd</sup> ICDERS

**Organizer**

Institute of Dynamics of Explosions and Reactive System (IDERS), Seattle, USA.

**Recognized by**

The Combustion Institute as a Specialists Meeting on the fluid dynamics of combustion.

**IDERS Board Members**

L. Bauwens, Y.-C. Chao, G. Continillo (*President*), D. Dunn-Rankin, G. Dupre, V. Gamezo, A.K. Hayashi, A. Higgins, A.L. Kuhl, J.H.S. Lee, U. Maas, A. Matsuo, E.L. Petersen, M.I. Radulescu, J.E. Shepherd, S.S. Shy, W.A. Sirignano, F. Williams, P. Wolanski.

**Program Committee**

Y.-C. Chao (Chair), M.I. Radulescu (Vice Chair), J.-Y. Choi, A. Higgins, U. Maas, F.S. Marra, A. Matsuo, S.P. Medvedev, E.L. Petersen, S.S. Shy, H.-G. Sung, J. X. Wen, V. Yang and F. Zhang

**Host Committee**

D. Dunn-Rankin (Chair), W.A. Sirignano, G.S. Samuelsen, R.H. Rangel, J.C. LaRue, S.E. Elghobashi, V.G. McDonell, D. Dabdub, and J.M. McCarthy

## CONFERENCE SPONSORS

The organizers of the 23<sup>rd</sup> ICDERS are most grateful to the following organizations for their kind material and financial support.

 Office of Naval Research	Office of Naval Research
 National Science Foundation WHERE DISCOVERIES BEGIN	National Science Foundation
 UNIVERSITY of CALIFORNIA · IRVINE	University of California, Irvine
	Elsevier Publishing
	Taylor and Francis Publishing
	Vision Research
	The Combustion Institute

## Message from the Host Committee Chair

On behalf of the host committee and The Henry Samueli School of Engineering, I welcome you to the University of California, Irvine (UCI). While a fairly young campus of the University of California system, UCI has grown rapidly to become the premier research university in Orange County. We hope very much that you will enjoy UCI's combination of a beautiful Southern California location and the intellectual vibrancy of an academic institution.

Our goal as local hosts is to make sure that your experience at this meeting is excellent in all respects. The technical program of the 23<sup>rd</sup> ICDERS is outstanding. We will strive to provide an equally outstanding environment for discussion and exploration. If you have any questions or need any assistance, please do not hesitate to ask any of the local staff or students. Student assistants from UCI will be easily identifiable by their 23<sup>rd</sup> ICDERS t-shirts.

In addition to the Sunday welcome reception, the Wednesday excursion, the Thursday conference dinner, and the Friday farewell reception, we have a special Monday evening event arranged for young researchers in the ICDERS community. My colleague, Professor Donald Dabdub, graciously provided his wine expertise in the selection of the California selections we will enjoy at the Welcome reception and the Thursday dinner. The Monday event is for graduate students and recent post-doctoral researchers only (without senior advisors) to get to know each other and share their experiences with a special presentation followed by a pub night at the Anteatr Pub. We hope that this will be an opportunity for a free flow of ideas among the energetic youth.

The Wednesday excursion is to the beach at Dana Point with plenty of time for you to swim, surf, play volleyball, bike, or just explore. It is a true Southern California experience that I am sure you will enjoy.

As every host knows, an event of this magnitude requires the dedication and enthusiasm of a great number of people. In addition to the identified local host committee, I would like to add my appreciation for the hard work of Dr. Edward Ho-Chuan Lin in creating this program booklet and the program documentation. I also appreciate the advice and information provided by Program Chair Professor Yei-Chin Chao. It has been a pleasure working with these two individuals. Ms. Barbara Waronek of the International Combustion Institute saved us untold difficulties in handling the registrations for this meeting. Her contributions to the meeting itself are also a great benefit. The UCI Conference Services people, particularly Lisa Nakamura and Erin Lane, provided us with a lot of flexibility in creating this event.

Much of the graphical aspects of this meeting are due to the unsolicited effort and dedication of my colleague Professor J. Michael McCarthy. Though he is not a combustion person, the concept of a conference on explosions proved irresistible. I also appreciate the graphical expertise of Ms. Sara McCarthy, whose skills gave us many of the designs for the meeting.

Most importantly, a very special recognition is due Ms. Tanya Eberhard. With infinite good humour, she maintained all of the meeting details, including mailing out letters of invitation, ordering all of the materials, coordinating meetings with all parties, and organizing the volunteers. While it might have been possible to put this meeting on without her, I cannot imagine it.

Derek Dunn-Rankin  
Local Host (Chair)

## Message from the Program Committee Chairs

The Scientific Program of ICDERS 2011 was prepared with two main objectives: the involvement of younger researchers in the ICDERS activities and the encouragement of active discussion among all participants. Younger members of the ICDERS community were encouraged to serve as Program Committee members, reviewers, and session chairs. A novel introduction to the ICDERS technical program is the inclusion of special topical sessions organized to provide discussion forums on topics of popular interest and timely importance.

Of the contributed papers, 168 were selected for oral presentation, 56 for special topical sessions, 83 for poster presentation, and 22 for Work-In-Progress posters. The Scientific Program includes:

- The Plenary Lecture following the Welcome session, given by Dr. Sergey P. Medvedev
- 7 special topical sessions organized in parallel to the regular technical sessions
- 51 technical sessions for contributed oral papers, split into three parallel schedules
- 2 sessions on Tuesday and Thursday for contributed and Work-In-Progress Posters

The plenary lecture is dedicated to the memory of Professor Boris Gelfand, an active member of the IDERS Board of Directors, member of the Russian Academy of Natural Sciences. Professor Boris Gelfand made prominent contributions in various fields of shock wave, combustion and detonation science, especially with his joint work with Academician Ya.B. Zel'dovich. His further development of Zel'dovich's gradient mechanism for detonation initiation is now a cornerstone in most theoretical investigations on the subject.

Seven special topical sessions were organized by members of the Program Committee. Each special session is organized by a grouping of papers, invited or selected among the submitted papers, addressing a topic of popular interest and timely importance. The special session is led by a topical review of the current status and challenges. The special sessions are designed to provide extensive comparison of results and intensive discussions.

The Program Committee Chairs encourage authors to submit full-length versions of their papers to one of the three archival journals recommended as targets: (1) *Combustion Science and Technology*, (2) *Combustion Theory and Modelling* and (3) *Shock Waves*. Details for the submission to these journals will be emailed to all ICDERS paper authors at the end of the meeting. To ensure a timely and organized publication of work from the meeting, the deadline for submission is October 15th.

The Program Committee Chairs thank all authors, all 14 Program Committee Members and the over 200 reviewers for their contribution to the program and the paper selection process. We also thank the 7 special session organizers for their dedicated efforts to create the special topical sessions. The Program Committee Chairs would like to express their appreciation for the guidance and advice given by Gaetano Continillo and Derek Dunn-Rankin throughout the course of paper selection and program preparation. The Program Committee Chairs wish to acknowledge Dr. Edward Ho-Chuan Lin for his contributions in administering the online *Confmaster* system, handling the paper submission and review process, and preparing the program booklet and CD. His help was invaluable.

We wish you an excellent and fruitful conference.

Yei-Chin Chao (Chair) and Matei I. Radulescu (Vice Chair)

## **GENERAL INFORMATION**

### **Registration Desk**

The Registration Desk on the first day will be located in the Emerald Bay room AB and will be open from 4:00 PM – 8:00 PM. Subsequent days the desk will be open in the Pacific Ballroom Lobby area beginning at 8:00 AM each day, and closing at the end of the technical sessions. The ICDERS 2011 team will be available throughout the week to assist you and your guests.

### **Name Badges**

Please, wear your name badge at all times. Badges are required for admission to technical session and social events.

### **No Smoking**

Please, observe the no smoking regulation inside buildings and in the Student Center area.

### **Computer Access**

Computers with internet access will be available for Colloquium attendees at the Student Center computer rooms. There is also wireless access throughout the Center. Details for login will be available at the Registration Desk. If you are staying in the on-campus dormitories, you will be better off with a hard wire connection. Again, the details of login will be available at the Registration Desk.

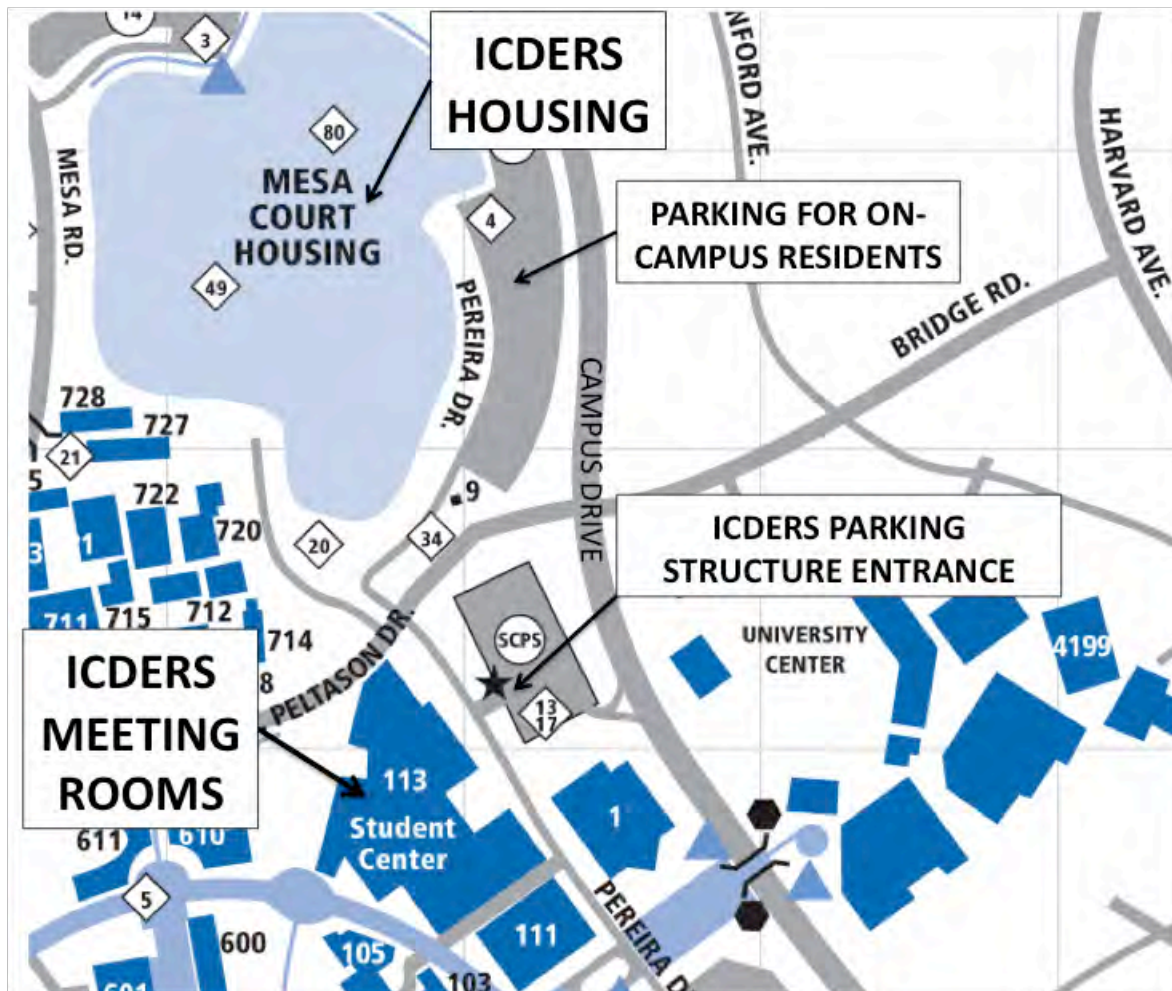
### **Refreshment Breaks**

Refreshment will be served every morning and afternoon during breaks in the Technical Sessions. Coffee, tea, and water will be available at all times during the meeting.

### **Lunch**

Lunch for Colloquium delegates who are staying in on-campus accommodations is included in the room charge and will be served in the Mesa Court Commons. See your information packet for details of the Commons. Other delegates are on their own for lunch; there are many options in the Student Center and directly across Campus Drive in the University Center. The University Center contains restaurants, a micro-brewery, and other shops, It is just over the bridge that crosses Campus drive, a short walk from the Student Center. There are many restaurants in the area for people with cars. A partial listing of restaurants is available at the Registration Desk or ask one of the UCI volunteers for suggestions.

## GENERAL INFORMATION



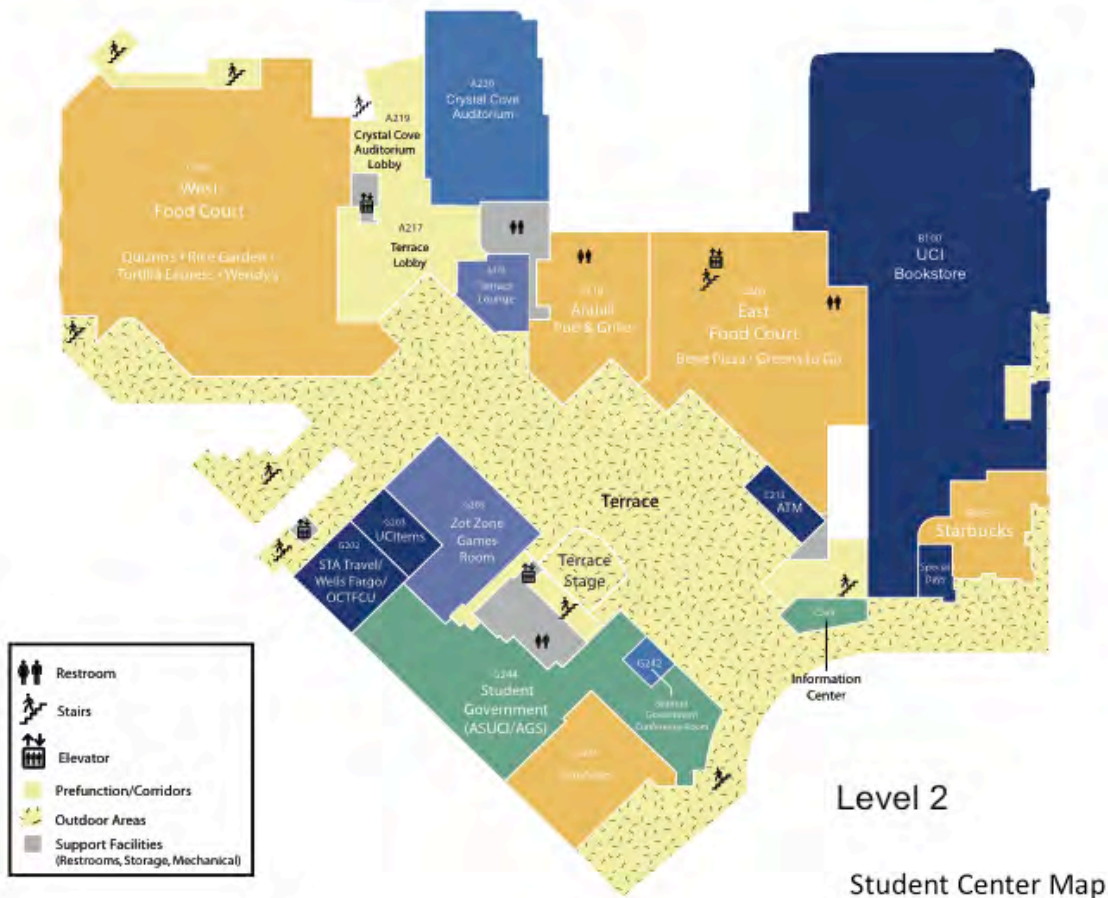
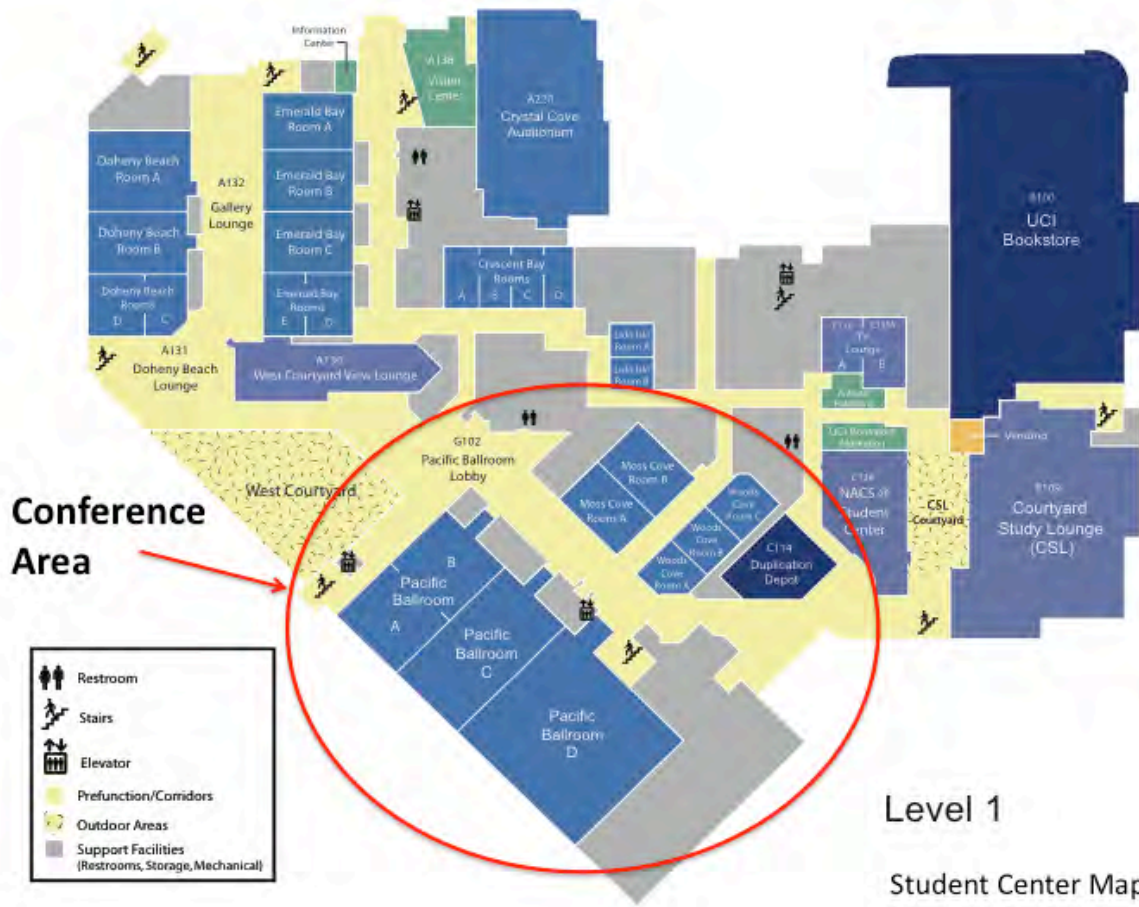
The above map is a close up of the portion of the UCI campus where most of the ICDERS activities will be held.

The meeting rooms in the Student Center will house all the Technical Sessions, the Poster Sessions, the Receptions, and the Conference Dinner.

The on-campus housing option is Mesa Court Housing, which is just across Peltason Drive from the Student Center. Only those in on-campus housing with cars will park in the housing parking lot just beside the complex.

Parking for the off-campus residents of the conference is conveniently located in the parking structure identified SCPS (Student Center Parking Structure). Parking is \$8/day. You may buy your pass at the kiosk as you enter the structure.

The next page shows a map of the Student Center; Level 1 is where the conference will be held. Level 2 has two food courts, the University bookstore, Starbuck's, and the Anteatr Pub. There are also banking services, UCItems for discounts at local attractions, and a terrace for an outdoor break.



# Social Program

Details are provided in an separate addendum sheet; below is just a general timetable

## ***Sunday, July 24th, 2011***

18:00 - 20:00 Welcome reception Emerald Bay AB

## ***Monday, July 25th, 2011***

NSF Young Researcher Night (grad students and post-doctoral scholars ONLY)

17:45 - 18:30 Special Young Researcher presentation Moss Cove AB

18:30 - 23:00 UCI Pub Night Anteater Pub

For others -- Evening free to explore the area

## ***Tuesday, July 26th, 2011***

Evening free to explore on your own

## ***Wednesday, July 27th, 2011***

15:00 - 21:00 Doheny State Beach BBQ Dana Point

## ***Thursday, July 28th, 2011***

17:30 - 18:45 Cocktail Hour Ballroom Lobby

18:45 - 23:00 ICDERS Conference Dinner Pacific Ballroom

## ***Friday, July 29th, 2011***

17:00 - 19:00 Farewell Reception Pacific Ballroom





## **ICDERS 2011 -- WEDNESDAY EXCURSION**

### **Doheny Beach Park**

### **Dana Point, California**

#### **Summary**

The 2011 ICDERS excursion is a California beach party at the Doheny State Beach Park in Dana Point, a little south of Irvine. You will have some time to surf, bike, play volleyball, or just explore. Please remember that it can be cool in the evening even in the summer, and coastal fog is always possible. You may need a sweater or light jacket. If you plan to take an ocean dip, bring a towel and change of clothes; there are changing rooms and outdoor (cold water) showers at the park.

We will have a DJ playing music throughout the party, and then at the end of the evening you will be entertained by Einstein Brown and the Carribean Jems.

#### **Itinerary**

3:00 pm	Motorcoaches arrive at U.C.I. and Radisson
3:15 pm	Guests board motorcoaches and depart for Doheny
4:00 pm	Guests arrive at Doheny
4:00 pm - 7:30 pm	DJ plays background music
4:00 pm - 8:00 pm	Bar is open
5:00 pm - 7:30 pm	Dinner buffet is available
7:30 pm - 8:30 pm	Einstein Brown & the Caribbean Jems perform
8:30 pm	Guests depart Doheny for U.C.I.
9:15 pm - 9:30 pm	Approximate return time of the motorcoaches

#### **Some Beach Activities**

Volleyball Courts #6 & #7 will be available for UCI use. Volleyballs will be available.

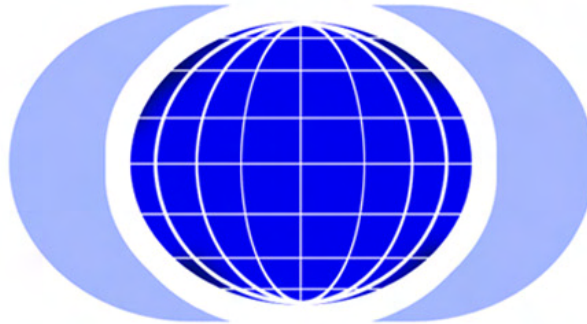
Items available to rent on-site include:

Boogie Boards	\$8 hour
Surfboards	\$12 hour
Cruiser Bikes	\$10 hour
Tandem Bikes	\$12 hour
Surrey Bike (Single)	\$20 hour
Double Surrey Bike	\$30 hour



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**23rd International Colloquium on the  
Dynamics of Explosions and Reactive Systems**

**TECHNICAL PROGRAM**

**AND**

**ABSTRACTS**

Jul. 25 (Mon)		Jul. 26 (Tue)		Jul. 27 (Wed)		Jul. 28 (Thu)		Jul. 29 (Fri)	
8:00	Registration	8:30	S3-I Mini Plenary	8:30	Special S4-I	9:00	Special S5-I	9:00	Special S7-I
8:45	Welcome	9:10	Regular R5	9:10	Regular R9	9:25	Regular R11	9:25	Regular R14
9:15	Plenary	9:35		9:35		9:50	Topical Review	9:50	
10:00	Regular R1	10:00	Poster-I	10:00	Break	10:15		10:15	Break
10:25	Special S1-I	10:25		10:25	Regular R10	10:40	Break	10:45	Regular R15
10:50	Break	10:50		10:55	Special S4-II	11:10	Poster-II and WIP	11:10	Special S7-II
11:15	Break	11:15	Break	11:20		11:35		11:35	
11:45	Regular R2	11:45	Regular R6	11:45		12:00	Lunch	12:00	Lunch
12:10	Special S1-II	12:10	Special S3-I			13:30	Regular R12	13:30	Regular R16
12:35		12:35				13:55		13:55	
13:00	Lunch	13:00	Lunch			14:20	Topical Review	14:20	Topical Review
14:30	Regular R3	14:30	Regular R7			14:45		14:45	
14:55	Special S2-I	14:55	Special S3-II			15:10	Break	15:10	Break
15:20		15:20				15:40	Regular R13	15:40	Regular R17
15:45	Break	15:45	Break			16:05		16:05	
16:15	Regular R4	16:15	Regular R8			16:30		16:30	
16:40	Special S2-II	16:40	Special S3-IV			16:55		16:55	
17:05		17:05							
Young Researcher Pub Night				Excursion to Doheny Beach and BBQ Picnic		Conference Dinner		Farewell Party	
				Return 9:00 PM					

# Technical Program Information

## Audio-Visual Equipment

All of the presentation rooms are equipped with a computer, a projector and screen. Authors may use their own computer if they prefer. As always, it is the author's responsibility to be sure that their presentation runs smoothly. Either load the presentation before the session and test the conference computer or test your own computer. Host students and technical staff will be available to assist in a limited way, if needed, but please make sure your presentation operates as you expect ahead of time.

## Practice Rooms

There are no formal practice rooms set aside at the conference, but if you are concerned about your connection to the Audio Visual equipment, please test the connection at the breaks, or before and after the technical sessions.

## Poster Sessions

Two poster sessions will be presented in Pacific Ballroom D; the posters will be up for most of the day, but authors are asked to please be available for questions and comments during the formal poster session periods:

Poster I  
Tuesday, July 26, 10:25 - 11:45 AM

Poster II and WIP  
Thursday, July 28, 10:40 – 12:00

Instructions regarding the size of the posters are available on the website. The appropriate material for hanging the posters will be provided. We are planning mostly on clipping single sheets to 36" x 48" vertical poster board, but you may use other methods if you need them. Please let the information desk know if you have any special needs.

Posters should be installed by 9:00 AM. Tuesday posters need to be removed at the end of the afternoon break (16:15). The Thursday posters should be installed again by 9:00 AM but they will need to be removed a bit earlier (14:30) to allow preparation of the Ballroom for the conference dinner that will be in the same room.

08:00	<b>Registration</b>			
08:45	<b>Welcome and Plenary</b> (Gaetano Continillo)			
09:15	<b>(PL1)</b> 357 Dynamics of Physical Explosion: A Tribute to Professor Boris Gelfand (Sergey P. Medvedev)			
	<b>(S1) – Toward a Better Understanding of Shock-Tube Flows and Ignition Behaviors – I</b> (Eric L. Petersen)	<b>(R1A) – DDT – I</b> (V. N. Gamezo)	<b>(R1B) – Heterogeneous / Multiphase Reactive System–I</b> (Allen L. Kuhl)	<b>(R1C) – Premixed Flames – I</b> (Steven S. Shy)
10:00	9 R. Cook, ...	74 G. Ciccarelli, ...	329 K. Balakrishnan,	61 H. Zhang, ...
10:25	10 W. Ren, ...	234 R. Porowski, ...	246 Y. Gan, ...	70 T. Cheng, ...
10:50	81 D. Ignatenko, ...	313 A. Susa, ...	150 S. Goroshin, ...	159 M. Hori, ...
11:15	<b>Break</b>			
	<b>(S1) – Toward a Better Understanding of Shock-Tube Flows and Ignition Behaviors – II</b> (Eric L. Petersen)	<b>(R2A) – DDT – II</b> (A. Koichi Hayashi)	<b>(R2B) – Heterogeneous / Multiphase Reactive System–II</b> (Allen L. Kuhl)	<b>(R2C) – Premixed Flames – II</b> (B. Fiorina)
11:45	110 C. Aul, ...	27 M. Liberman, ...	53 V. Leschevich, ...	260 M. Magar, ...
12:10	163 K. Heufer, ...	76 K. Vollmer, ...	265 D. Frost, ...	328 G.B. Chen, ...
12:35	231 S. Medvedev, ..	310 M. Kuznetsov, .	43 B. Shaw, ...	127 M. Goswami, ...
13:00	<b>Lunch</b>			
	<b>(S2) – Shock Induced Ignition –I</b> (Eric L. Petersen)	<b>(R3A) – DDT – III</b> (A. Koichi Hayashi)	<b>(R3B) – Flame Instability and Acceleration</b> (M. Kuznetsov)	<b>(R3C) – Premixed Flames – III</b> (Paul Ronney)
14:30	31 I. Stranic, ...	41 V. Karlin, ...	288 T. Ikawa, ...	256 G. Gauthier, ...
14:55	54 B. Akih-Kumgeh,	207 M. Fukuda, ...	119 Y. -J. Zhu, ...	227 C. C. Liu, ...
15:20	104 J. Herzler, ...	330 V. Gamezo, ...	28 M. Ivanov, ...	269 M. Short, ...
15:45	<b>Break</b>			
	<b>(S2) – Shock Induced Ignition–II</b> (Eric L. Petersen)	<b>(R4A) – DDT – IV</b> (Luc Bauwens)	<b>(R4B) – Criticality of Diffusion Flames</b> (Arnaud Mura)	<b>(R4C) – Premixed Flames and Laminar Flame Speeds</b> (R. K. Cheng)
16:15	188 O. Mathieu, ...	56 T. Ogawa, ...	50 R. Nozaki, ...	152 N. Malik, ...
16:40	203 M. Fikri, ...	270 S. Jackson, ...	182 J. S. Park, ...	210 T. Szabó
17:05	342 C. Tobin, ...	261 M. C. Gwak, ...	131 A. Fartouk, ...	298 E. Varea, ...
17:30	<b>End of Technical Sessions</b>			
18:00	<b>Special Young Researcher Session</b>			

**08:00 Registration****08:45 (PL1) Welcome and Plenary Lecture****Pg. 45***Session Chair : Gaetano Continillo***Pacific Ballroom D**

09:00 Welcome

09:15 357 Dynamics of Physical Explosions: A Tribute to Professor Boris Gelfand  
*Sergey P. Medvedev***10:00 (S1) – Toward a Better Understanding of Shock-Tube Flows and Ignition Behaviors – I Pg. 45***Session Chair : Eric L. Petersen***Pacific Ballroom C**10:00 9 MMH Pyrolysis and Oxidation: Species Time-History Measurements behind Reflected Shock Waves  
*R. D. Cook, S. H. Pyun, D. F. Davidson and R. K. Hanson*10:25 10 Temperature Time-History Measurements in a Shock Tube Using Diode Laser Absorption of CO<sub>2</sub> near 2.7 $\mu$ m  
*Wei Ren, Sijie Li, David F Davidson and Ronald K Hanson*10:50 81 Auto-ignitions of Methane at Intermediate and High Temperatures  
*D.G. Ignatenko, N. Joshi, V.V. Leschevich, V.V. Martynenko, O.G. Penyazkov, K.L. Sevrouk, S.I. Shabunya, A.V. Skilondz and V. Tangirala***10:00 (R1A) – DDT – I****Pg. 46***Session Chair : V. N. Gamezo***Pacific Ballroom AB**10:00 74 Role of Transverse Shock Waves on DDT in a Very Rough-Walled Channel  
*G. Ciccarelli, C. Johansen and M. Kellenberger*10:25 234 Experimental and Computational Study on DDT for Hydrogen-Methane-Air Mixtures in Tube with Obstacles  
*Rafal Porowski Andrzej Teodorczyk, Knut Vaagsaether and Dag Bjerketvedt*10:50 313 Oscillating Propagation of Near-limit Detonations of CH<sub>4</sub>/O<sub>2</sub> System in a Small Diameter Tubes  
*A. SUSA, S. Hasegawa, H. Yokoyama, T. Endo, Y. Ogawa, Y. Morii and N. Tsuboi***10:00 (R1B) – Heterogeneous / Multiphase Reactive System – I****Pg. 46***Session Chair : Allen L. Kuhl***Moss Cove AB**10:00 329 Ignition of Aluminum Particle Clouds Behind Reflected Shock Waves  
*Kaushik Balakrishnan, Allen L. Kuhl, John B. Bell, and Vincent E. Beckner*10:25 246 Effects of Addition of Energetic Nanoparticles on Fuel Droplet Combustion at Dilute and Dense Particle Loading  
*Yanan Gan and Li Qiao*10:50 150 Flame Fronts in Iron Suspensions Dominated by the Effect of Discreteness  
*Sam Goroshin, Francois-David Tang and Andrew J. Higgins*

**10:00 (R1C) – Premixed Flames – I**

Pg. 47

Session Chair : Steven S. Shy

Woods Cove ABC

- 10:00 61 Outwardly Propagating Spherical Flames with Thermally Sensitive Intermediate Kinetics and Radiative Loss  
*Huangwei Zhang, Xialing Zhang and Zheng Chen*
- 10:25 70 Characteristics of Laminar Premixed H<sub>2</sub>/CO/CH<sub>4</sub>/Air Opposed-jet Flames  
*T. S. Cheng, Y.-C. Chang, Y.-C. Chao, G.-B. Chen, Y.-H. Li and C.-Y. Wu*
- 10:50 159 Weak Flame Responses to Octane Number and Pressure in a Micro Flow Reactor with a Controlled Temperature Profile  
*Mikito Hori, Akira Yamamoto, Hisashi Nakamura, Takuya Tezuka, Susumu Hasegawa and Kaoru Maruta*

**11:15 (B) – Coffee Break****11:45 (S1) – Toward a Better Understanding of Shock–Tube Flows and Ignition Behaviors – II** Pg. 48

Session Chair : Eric L. Petersen

Pacific Ballroom C

- 11:45 110 Interpretation of Low-Temperature, High-Pressure Ignition Data from a Shock Tube with Significant Pre-Ignition Pressure Rise  
*Christopher J. Aul, Eric L. Petersen, Henry Curran, Mustapha Fikri and Christof Schulz*
- 12:10 163 Optical Investigation of Shock Induced Ignition of Different Biofuels  
*K.A. Heufer, H. Olivier, S.P. Medvedev, S.V. Khomik*
- 12:35 231 Towards Consolidation of Hydrogen-Air Ignition Data from Shock Tube and Flow Reactor Experiments  
*Sergey P. Medvedev, Sergey V. Khomik, Aleksander K. Heufer and Herbert Olivier*

**11:45 (R2A) – DDT– II**

Pg. 49

Session Chair : A. Koichi Hayashi

Pacific Ballroom AB

- 11:45 27 Deflagration-to-Detonation Transition in Highly Reactive Combustible Mixtures  
*M. A. Liberman, M. F. Ivanov, A. D. Kiverin, M. S. Kuznetsov, A. A. Chukalovsky, T. V. Rakhimova*
- 12:10 76 Deflagration-to-Detonation Transition in Hydrogen-Air Mixtures with Concentration Gradients  
*K.G. Vollmer, F. Ettner and T. Sattelmayer*
- 12:35 310 Effects of Shock Waves, Boundary Layer and Turbulence on Flame Acceleration and DDT in Highly Reactive Mixtures  
*M. Kuznetsov, J. Grune and I. Matsukov*

**11:45 (R2B) – Heterogeneous / Multiphase Reactive System – II**

Pg. 50

Session Chair : Allen L. Kuhl

Moss Cove AB

- 11:45 53 Auto-ignition Conditions of Iron Micro Powders in Heated Oxygen  
*Vladimir V. Leschevich, Oleg G. Penyazkov and Jean-Christophe Rostaing*
- 12:10 265 Interfacial Instabilities in Explosive Gas-Particle Flows  
*David L. Frost, Yann Gregoire, Samuel Goroshin and Fan Zhang*

- 12:35 43 Models for Fast Combustion Waves in Nanocomposite Thermite Powders  
*Benjamin D. Shaw, Birce Dikici, & Michelle L. Pantoya*

**11:45 (R2C) – Premixed Flames – II****Pg. 51***Session Chair : B. Fiorina***Woods Cove ABC**

- 11:45 260 Premature Flame Initiation in SI Engines: Modeling Studies on the Role of Residual Gas  
*M. Magar, R. Schießl and U. Maas*
- 12:10 328 Effects of Hydrogen Peroxide on Methane Premixed Flames  
*Guan-Bang Chen, Yueh-Heng Li, Tsarng-Sheng Cheng, Hung-Wei Hsu and Yei-Chin Chao*
- 12:35 127 Effect of Elevated Pressures on Laminar Burning Velocity of Methane+Air Mixtures  
*M. Goswami, S. Derks, K. Coumans, M.H. de Andrade Oliveira, A.A. Konnov, R.J.M Bastiaans, C.C.M Luijten and L.P.H de Goey*

**13:00 (L) – Lunch****14:30 (S2) – Shock Induced Ignition – I****Pg. 51***Session Chair : Eric L. Petersen***Pacific Ballroom C**

- 14:30 31 Shock Tube Measurements of Ignition Delay Times for the Butanol Isomers  
*I. Stranic, D. P. Chase, J. T. Harmon, S. Yang, D. F. Davidson, R. K. Hanson.*
- 14:55 54 Methyl and Ethyl Esters as Biodiesel Surrogates: Observations on Trends in Ignition Behavior  
*Benjamin Akih-Kumgeh, Jeffrey M. Bergthorson*
- 15:20 104 Shock Tube Study of the Influence of NO<sub>x</sub> on the Ignition Delay Times of Natural Gas at High Pressure  
*J. Herzler, C. Naumann*

**14:30 (R3A) – DDT – III****Pg. 52***Session Chair : A. Koichi Hayashi***Pacific Ballroom AB**

- ~~14:30 41 Effect of Radiation Preheating on Dynamics of Wrinkled Flames  
*Vladimir Karlin*~~
- 14:55 207 Effect of Wall Conditions on DDT in Hydrogen-Oxygen Mixture  
*Motoki Fukuda, Edyta Dzieminska, A.Koichi Hayashi, Eisuke Yamada and Nobuyuki Tsuboi*
- 15:20 330 One-dimensional Evolution of Fast Flames  
*V. N. Gamezo, A. Y. Poludnenko and E. S. Oran*

**14:30 (R3B) – Flame Instability and Acceleration****Pg. 53***Session Chair : M. Kuznetsov***Moss Cove AB**

- 14:30 288 Short-term Prediction of Combustion Instability in a Lean Premixed Gas-turbine Combustor Using Nonlinear Time Series Analysis  
*Takuya Ikawa, Masahito Amano, Hiroshi Gotoda, Takaya Miyano, Shigeru Tachibana*
- 14:55 119 3D Numerical Simulations of Spherical Flames Instability and Acceleration in Shock Accelerated Flows  
*Yuejin Zhu, Gang Dong, Baochun Fan, Yixin Liu*



- 15:20 28 Hydrogen-Oxygen Flame Acceleration in Channels of Different Widths and Deflagration-to-Detonation Transitions for a Detailed Chemical Reaction Models  
*M. F. Ivanov, A. D. Kiverin, M. A. Liberman*

**14:30 (R3C) – Premixed Flames – III****Pg. 54***Session Chair : Paul Ronney***Woods Cove ABC**

- 14:30 256 Numerical Investigation of Premixed Flames Stabilized in a Narrow Duct with a Wall Temperature Gradient  
*G.P. Gauthier, G.M.G. Watson and J.M. Bergthorson*
- 14:55 227 High-Pressure Turbulent Burning Velocity Measurements at Constant Reynolds Numbers  
*C. C. Liu, S. S. Shy, M. W. Peng, C. W. Chiu, Y. C. Dong*
- 15:20 269 Variable Density Premixed Thick Flame Propagation in a Microchannel with Heat Conducting Walls  
*Mark Short and David A. Kessler*

**15:45 (B) – Coffee Break****16:15 (S2) – Shock Induced Ignition – II****Pg. 55***Session Chair : Eric L. Petersen***Pacific Ballroom C**

- 16:15 188 Oxidation of Selected Aromatics Behind Shock Waves  
*O. Mathieu, G. Pengloan, N. Chaumeix and C. -E. Paillard*
- 16:40 203 High-pressure Shock Tube experiments of the ignition of 3-pentanone-doped n-heptane and iso-octane/air mixtures  
*Mustapha Fikri, Leonel R. Cancino, Michaela Hartmann and Christof Schulz*
- 17:05 342 A High Temperature Shock Tube Study of n-Butylbenzene Oxidation  
*Colin Tobin, Kenji Yasunaga, John Simmie, Judith Würmel, Henry Curran, Olivier Mathieu*

**16:15 (R4A) – DDT– IV****Pg. 55***Session Chair : Luc Bauwens***Pacific Ballroom AB**

- 16:15 56 Flame Acceleration and Transition to Detonation in an Array of Cylinders  
*Takanobu Ogawa, Vadim N. Gamezo, Elaine S. Oran*
- 16:40 270 Geometry-Specific Scaling of Detonation Parameters from Front Curvature  
*Scott I. Jackson and Mark Short*
- 17:05 261 Numerical Simulation of Deflagration to Detonation Transition with Wall Cooling Effect in Ethylene-air Mixture  
*Min-cheol Gwak, Ki-hong Kim and Jack J. Yoh*

**16:15 (R4B) – Criticality of Diffusion Flames****Pg. 56***Session Chair : Arnaud Mura***Moss Cove AB**

- 16:15 50 Study on Ignition-like Behavior Caused by Interaction of Curved Diffusion Flames  
*Ryosuke Nozaki, Yuji Nakamura, Akio Kitajima*
- 16:40 182 Determination of the Transition Threshold from Laminar Flat Flames to Turbulent Flames by a CO<sub>2</sub> Laser Irradiation Method  
*June Sung Park, Osamu Fujita, Yoshikazu Taniyama*

- 17:05 131 A Multi-mixture Fraction Closure for Dilute Turbulent Diffusion Flame  
*Avner Fartouk, Pierre Plion, Arnaud Mura*

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**16:15 (R4C) – Premixed Flames and Laminar Flame Speeds****Pg. 56***Session Chair : R. K. Cheng***Woods Cove ABC**

- 16:15 152 Premixed Flame Response to Disturbances in Pressure and Fuel Distributions  
*Nadeem A. Malik, R.P Lindstedt*
- 16:40 210 Parameterization of Laminar Flame Speed Dependence on Pressure and Temperature in Hydrogen-air Mixtures  
*T. Szabó, J. Yáñez, A. Kotchourko, M. Kuznetsov, T. Jordan*
- 17:05 298 Laminar Burning Velocity and Markstein Length Relative to Fresh Gases Determination for Isooctane-Ethanol Air Flames  
*E. Varea, A. Vandiel, V. Modica, B. Renou*

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**17:30 End of Technical Sessions**

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**18:00 Special Young Research Session and Pub Night***Session Chair : D. Dunn-Rankin***Moss Cove AB**

	<b>(S3) – Dynamics of Large Scale Fire and Explosions – I</b> <i>(C. Fernandez-Pello, &amp; J. Puttock)</i>	<b>(R5A) – Detonation Limits and Engine</b> <i>(Piotr Wolanski)</i>	<b>(R5B) – Shock Induced Combustion and Detonation</b> <i>(O. Penyazkov)</i>	<b>(R5C) – Blow-off and Extinction</b> <i>(F. Baillot)</i>
08:30	333 <i>T. Blanchat, ...</i>			
09:10	221 <i>B. Magnussen,</i>	268 <i>M. Okamura, ..</i>	13 <i>J. Verreault, ...</i>	195 <i>M. Hirota, ...</i>
09:35	236 <i>A. Osorio, ...</i>	187 <i>N. Tsuboi, ...</i>	243 <i>S. Ilya, ...</i>	264 <i>K. Fujiwara, ...</i>
10:00	103 <i>H. Y. Wang, ...</i>	106 <i>D. Schwer, ...</i>	274 <i>T. Segawa, ...</i>	299 <i>M. Nishioka, ...</i>
10:25	132 <i>F. Ferrero, ...</i>	Poster-I: (D) 20, 25, 47, 64, 69, 86, 95, 100, 107, 114, 120, 121, 125, 130, 173, 190, 196, 217, 222, 228, 232, 258, 262, 266, 282, 286, 322, 331, 336; (E) 46, 72, 118, 189, 239, 281; (F) 12, 21, 30, 55, 82, 94, 109, 111, 169, 171, 183, 185, 200, 202, 204, 223, 290, 300, 323, 325, 332, 334, 340		
10:50	68 <i>Z. B. Chen, ...</i>			
11:15	<b>Break</b>			
	<b>(S3) – Dynamics of Large Scale Fire and Explosions– II</b> <i>(J.Wen &amp; S.Dorofeev)</i>	<b>(R6A) – Detonation Dynamics and Structure – I</b> <i>(L. Bauwens)</i>	<b>(R6B) – Gas Turbine Combustors</b> <i>(Steven S. Shy)</i>	<b>(R6C) – Electric Aspects of Combustion</b> <i>(Paul Ronney)</i>
11:45	138 <i>J. Puttock, ...</i>	112 <i>M. Gui, ...</i>	102 <i>A. Ruiz, ...</i>	206 <i>A. Chukalovsky,</i>
12:10	250 <i>A. Poludnenko, .</i>	116 <i>S. Maeda, ...</i>	233 <i>P. Therkelsen, .</i>	302 <i>S. Karnani, ...</i>
12:35	247 <i>H. Pedersen, ..</i>	136 <i>C. Leung, ...</i>	314 <i>M. Akbarzadeh,</i>	201 <i>M. Belhi, ...</i>
13:00	<b>Lunch</b>			
	<b>(S3) – Dynamics of Large Scale Fire and Explosions – III</b> <i>(J.Wen &amp; S.Dorofeev)</i>	<b>(R7A) – Detonation Dynamics and Structure – II</b> <i>(A. Matsuo)</i>	<b>(R7B) – Dynamics of Ignition</b> <i>(Detlef Markus)</i>	<b>(R7C) – Laser Diagnostics</b> <i>(R. Schießl)</i>
14:30	226 <i>M. Hadjipanayis,</i>	146 <i>J. Verreault, ..</i>	32 <i>J. Regele, ...</i>	77 <i>C. Letty</i>
14:55	14 <i>P. Middha, ...</i>	242 <i>J. H.S. Lee, ...</i>	218 <i>O. Penyazkov, ..</i>	90 <i>W. Meier</i>
15:20	44 <i>A. Kuhl, ..</i>	63 <i>K. Mazaheri, ...</i>	122 <i>C. Cardin, ...</i>	166 <i>N. Nakatsuka, .</i>
15:45	<b>Break</b>			
	<b>(S3) – Dynamics of Large Scale Fire and Explosions–IV</b> <i>(J.Wen &amp; S.Dorofeev)</i>	<b>(R8A) – Detonation Cell Structure – I</b> <i>(Hoi Dick Ng)</i>	<b>(R8B) – Detonation Initiation</b> <i>(S. Medvedev)</i>	<b>(R8C) – Diagnostics</b> <i>(R. Schießl)</i>
16:15	148 <i>J. Chao, ...</i>	162 <i>B. Borzou, ...</i>	147 <i>B. Zhang, ...</i>	83 <i>M. Harker, ...</i>
16:40	149 <i>C. Bauwens, ..</i>	275 <i>K. Ishii, ...</i>	279 <i>A. Jesuthasan, ..</i>	179 <i>D. Markus, ...</i>
17:05	283 <i>A. Heidari, ...</i>	280 <i>R. Mével, ...</i>	199 <i>H. Yamashita, .</i>	216 <i>J. Hayashi, ...</i>
17:30	301 <i>B. Fakandu, ..</i>	324 <i>M. Asahara, ..</i>	96 <i>Q. Wang, ...</i>	80 <i>C. Arndt, ...</i>
17:55	327 <i>R. K. Zipf, Jr., ..</i>	326 <i>M. Short, ...</i>	272 <i>S. Ishihara, ...</i>	139 <i>G. Agafonov, ...</i>
18:20	<b>End</b>			

**08:30 (S3) – Dynamics of Large Scale Fire and Explosions – I****Pg. 59***Session Chair : Carlos Fernandez-Pello and Jonathan Puttock***Pacific Ballroom C**

- 08:30 333 (Mini Plenary: 40 min) Summary of the Phoenix Series Large Scale LNG Pool Fire Experiments  
*Thomas Blanchat, Paul Helmick, Richard Jensen, Anay Luketa, Regina Deola, Jill Suo-Anttila, Jeffery Mercier, Timothy Miller, Allen Ricks, Richard Simpson, Byron Demosthenous, Sheldon Tieszen, Michael Hightower*
- 09:10 221 (Invited Talk) Computation of Large Scale Fires in Complex Geometries - a Means to Safeguard People and Structural Integrity in the Oil and Gas Industry  
*Bjørn F. Magnussen*
- 09:35 236 Flame Spread Characteristics of Fire Retardant Fabrics  
*Andres F. Osorio, Chris Lautenberger, Carlos Fernandez-Pello, David Urban, Gary Ruff*
- 10:00 103 Mathematical Modelling of a Large-Scale Ventilated Tunnel Fire  
*Hui Ying Wang*
- 10:25 132 Prevention of the Explosion of Acetylene Cylinders Involved in Fire: Experiments and Simulations  
*F. Ferrero, M. Beckmann-Kluge, M. Kreißig, U. Schmidtchen, K. Holtappels*
- 10:50 68 The Extension of Eddy Dissipation Concept in the Framework of Large Eddy Simulation and the Subsequent Modification  
*Z.B.Chen, J.X.Wen, B.P.Xu and S.Dembele*

**09:10 (R5A) – Detonation Limits and Engine****Pg. 60***Session Chair : Piotr Wolanski***Pacific Ballroom AB**

- 09:10 268 Numerical Investigation of H<sub>2</sub>-O<sub>2</sub> Layered Detonation in Narrow Channel  
*Masatsugu Okamura, Akiko Matsuo*
- 09:35 187 Numerical Simulation on Two-Dimensional Detonation Including Boundary Layer Effects  
*Nobuyuki Tsuboi, Youhi Morii, A. Koichi Hayashi, Mitsuo Koshi*
- 10:00 106 Fuel Effects on Rotating Detonation Engines  
*Douglas A. Schwer, Kailas Kailasanath*

**09:10 (R5B) – Shock Induced Combustion and Detonation****Pg. 61***Session Chair : Oleg G. Penyazkov***Moss Cove AB**

- 09:10 13 Cellular Structure in an Oblique Detonation Wave  
*Jimmy Verreault, Matei I. Radulescu, Andrew J. Higgins*
- 09:35 243 Numerical Modelling of Shock-to-Detonation Transition in Methane - Air Mixture  
*Ilya Semenov, Pavel Utkin, Nikita Demidov, Ilda Akhmedyanov*
- 10:00 274 Numerical Investigation of Shock-Induced Combustion around a Cylindrical Body  
*Taku Segawa, Akiko Matsuo*

**09:10 (R5C) – Blow-off and Extinction****Pg. 62***Session Chair : Françoise Baillot***Woods Cove ABC**

- 09:10 195 Influences of Ultrasonic Waves on Blow-off Limits of Lifted Jet Flames  
*Mitsutomo Hirota, Takuya Tsuji, Yuji Nakamura, Tsutomu Saito*

- 09:35 264 Experimental Study on near Extinction Behavior of Microflame in Preheated Air  
*Kakeru Fujiwara, Yuji Nakamura*
- 10:00 299 Study on the Effect of Premixed Gas Addition on the Anti-Blow-Off Performance of Jet Diffusion Flame  
*Makihito Nishioka, Kosuke Miyazaki, Hiroki Takayama, Akane Uemichi*

**10:25 Poster Session I****Pg. 108***Session Chair : C. Regis Bauwens***Pacific Ballroom D****11:15 (B) – Coffee Break****11:45 (S3) – Dynamics of Large Scale Fire and Explosions – II****Pg. 63***Session Chair : Jennifer Wen and Sergey Dorofeev***Pacific Ballroom C**

- 11:45 138 (Invited Talk) DDT in Highly-congested Environments-the Buncefield Vapour Cloud Explosion  
*J.S. Puttock, A. Pekalski*
- 12:10 250 (Invited Talk) Deflagration-to-Detonation Transition in Unconfined Media  
*A.Y. Poludnenko, T.A. Gardiner, E.S. Oran*
- 12:35 247 Modelling of Flame Acceleration due to Intrinsic Instabilities in Industrial Scale Explosions  
*Helene H. Pedersen, Prankul Middha, Trygve Skjold, Kees van Wingerden, Bjørn J. Arntzen*

**11:45 (R6A) – Detonation Dynamics and Structure – I****Pg. 64***Session Chair : Luc Bauwens***Pacific Ballroom AB**

- 11:45 112 Periodic Oscillation and Fine Structure of Wedge-Induced Oblique Detonation Waves  
*Mingyue Gui, Baochun Fan, Zhihua Chen*
- 12:10 116 Visualization of the Initiation and Stabilization Process of an Oblique Detonation Wave Around a Projectile  
*Shinichi Maeda, Jiro Kasahara, Akiko Matsuo*
- 12:35 136 Coherent High Frequency Instabilities of Detonations  
*C. Leung, M.I. Radulescu, G.J. Sharpe*

**11:45 (R6B) – Gas Turbine Combustors****Pg. 65***Session Chair : Steven S. Shy***Moss Cove AB**

- 11:45 102 Effects of the Recess Length of a Coaxial Injector on a Transcritical LO<sub>2</sub>/H<sub>2</sub> Jet Flame  
*A. Ruiz, T. Schmitt, L. Selle, B. Cuenot and T. Poinsot*
- 12:10 233 Extension of LSI Functionality for Gas Turbine Applications  
*P. L. Therkelsen, D. Littlejohn, R. K. Cheng*
- 12:35 314 Effect of Fuel Nozzle Geometry on the Stability of Non-premixed Turbulent Methane Flame  
*Mohsen Akbarzadeh and Madjid Birouk*

**11:45 (R6C) – Electric Aspects of Combustion****Pg. 66***Session Chair : Paul Ronney***Woods Cove ABC**

- 11:45 206 Two-dimensional Modeling of the Ignition Length Decrease in Hydrogen Mixture with Oxygen Excited in Electric Discharge  
*A.A.Chukalovsky, K.K.Klopovsky, M.A.Liberman, Yu.A.Mankelevich, N.A.Popov, O.V.Proshina and T.V.Rakhimova*
- 12:10 302 Simulated Gravity Using Electric Fields in Microgravity Combustion  
*S. Karnani, D. Dunn-Rankin, F. Takahashi, Z-G. Yuan, D. Stocker*
- 12:35 201 Numerical Simulation of the Effect of the Ion-driven Wind on Flame Stability  
*Memdouh Belhi, Pascale Domingo, Pierre Vervisch*

**13:00 (L) – Lunch****14:30 (S3) – Dynamics of Large Scale Fire and Explosions – III****Pg. 67***Session Chair : Jennifer Wen and Sergey Dorofeev***Pacific Ballroom C**

- 14:30 226 Radiation Based Initiation of Vapour Cloud Explosions  
*M. A. Hadjipanayis, F. Beyrau and R. P. Lindstedt*
- 14:55 14 Effect of Initial Temperature on FA and DDT in H<sub>2</sub>-air Mixtures: CFD Simulations & Validation against Experimental Data  
*Prankul Middha*
- 15:20 44 Spherical Combustion Clouds in Explosions  
*Allen L. Kuhl, John B. Bell, Vincent E. Beckner and Kaushik Balakrishnan*

**14:30 (R7A) – Detonation Dynamics and Structure – II****Pg. 68***Session Chair : Akiko Matsuo***Pacific Ballroom AB**

- 14:30 146 Oscillations in Shock-Induced Combustion near Conical Projectiles  
*Jimmy Verreault, Andrew J. Higgins*
- 14:55 242 Response of Cellular Detonations of Finite Perturbations  
*John H.S. Lee, Yannick Fortin*
- 15:20 63 Numerical Study of Detonation Structure in a Channel with Porous Wall  
*K. Mazaheri, M. Sabzpooshani, Y. Mahmoudi, M. I. Radulescu*

**14:30 (R7B) – Dynamics of Ignition****Pg. 68***Session Chair : Detlef Markus***Moss Cove AB**

- 14:30 32 Acoustic Timescale Detonation Initiation in 2-D and its Relationship with the 1-D Description  
*Jonathan D. Regele, David R. Kassoy, Oleg V. Vasilyev*
- 14:55 218 Auto-ignition at Shock-Wave Collisions in Hydrogen-Air Detonation  
*Oleg G. Penyazkov, Kirill L. Sevrouk, Khaled Alhusan*
- 15:20 122 Experimental Analysis of Laser-Induced Spark Ignition of Lean Turbulent Premixed Flames  
*C. Cardin, B. Renou, G. Cabot, A. Boukhalfa*

**14:30 (R7C) – Laser Diagnostics****Pg. 69***Session Chair : R. Schießl***Woods Cove ABC**

- 14:30 77 Laser Spark Ignition and Flame Expansion in Swirl Burners Fuelled with n-heptane Sprays  
*C. Letty, E. Mastorakos, M. Juddoo, W. O'Loughlin, A. R. Masri*
- 14:55 90 High-Speed Imaging Diagnostics Applied to the Study of Auto-Ignition of Methane Jets in a Hot Coflow  
*W. Meier, C.M. Arndt, J. Gounder, I. Boxx, K. Marr*
- 15:20 166 Detection of Soot Incandescence and PAHs Fluorescence at the Proximity of the Inverse Diffusion Flames by Using Laser Diagnostics  
*Noriaki Nakatsuka, Yasushi Imoto, Jun Hayashi, Miki Taniguchi, Kenichi Sasauchi, Fumiteru Akamatsu*

**15:45 (B) – Coffee Break****16:15 (S3) – Dynamics of Large Scale Fire and Explosions – IV****Pg. 70***Session Chair : Jennifer Wen and Sergey Dorofeev***Pacific Ballroom C**

- 16:15 148 Estimating Blast Effects from an Accidental Release of High-Pressure Silane  
*J. Chao, C.R. Bauwens, S.B. Dorofeev*
- 16:40 149 Effect of Vent Deployment Pressure and Panel Inertia on Vented Gaseous Explosions  
*C. Regis Bauwens, Sergey B. Dorofeev*
- 17:05 283 Numerical Simulations of Large Scale Hemispherical and Pancake Cloud Detonation  
*A. Heidari, J.X. Wen*
- 17:30 301 Explosion Venting and Mixture Reactivity Influences in a Small Vessel  
*B.M. Fakandu, R.M. Kasmani, G.E. Andrews, H.N. Phylaktou*
- 17:55 327 Preliminary Large-scale DDT Experiments at NIOSH Lake Lynn Laboratory  
*R. K. Zipf, Jr., V. N. Gamezo, M. J. Sapko, W. P. Marchewka, K. M, Mohamed, E. S. Oran, D. A. Kessler, E. S. Weiss, J.D. Addis, F.A. Karnack, D.D. Sellers*

**16:15 (R8A) – Detonation Cellular Structure – I****Pg. 72***Session Chair : Hoi Dick Ng***Pacific Ballroom AB**

- 16:15 162 Influence of the Reaction-to-Induction Length Ratio on the Stability of Cellular Detonations  
*Bijan Borzou, Brian Maxwell, Matei I. Radulescu*
- 16:40 275 On Cellular Pattern Formation in Detonation Propagation  
*Kazuhiro Ishii, Yuta Okitsu, Koji Morita, Shogo Sayama*
- 17:05 280 Application of a Laser Induced Fluorescence Model to the Numerical Simulation of Detonation Waves  
*Rémy Mével, Dmitry Davidenko, Florian Pintgen, Joanna Austin, Joseph Shepherd*
- 17:30 324 Detailed Shock Configuration of Cylindrical Cellular Detonation  
*Makoto Asahara, Nobuyuki Tsuboi, A. Koichi Hayashi, Eisuke Yamada*
- 17:55 326 The Role of Cellular Structure on Increasing the Detonability Limits of Three-Step Chain-Branching Detonations  
*Mark Short, Charles B. Kiyanda, James J. Quirk, Gary J. Sharpe*

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**16:15 (R8B) – Detonation Initiation****Pg. 73***Session Chair : Sergey P. Medvedev***Moss Cove AB**

- 16:15 147 Direct Measurement and Relationship between Critical Tube Diameter and Critical Energy for Direct Detonation Initiation  
*Bo Zhang, Hoi Dick Ng and John H.S. Lee*
- 16:40 279 Near-limit Propagation of Detonations in Annular Channels  
*Anne Jesuthasan, Aloïs Joassard, Hoi Dick Ng, John H.S. Lee*
- 17:05 199 Visualization Study of Detonation Initiations Behind Reflected Shock Waves Using a High Speed Video Camera  
*Hiroki Yamashita, Jiro Kasahara, Akiko Matsuo*
- 17:30 96 High Speed Stereoscopic Shadowgraph and Its Digital 3D Reconstruction  
*Q. Wang, Y. Zhang*
- 17:55 272 Onset of Detonation by Forced Ignition behind an Incident Shock Wave  
*S. Ishihara, T. Kojima, K. Ishii, H. Kataoka*

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**16:15 (R8C) – Diagnostics****Pg. 74***Session Chair : R. Schießl***Woods Cove ABC**

- 16:15 83 Measurements of the Three Dimensional Structure of Flames at Low Turbulence  
*M.R. Harker, M. Lawes, C.G.W. Sheppard, N. Tripathi and R. Woolley*
- 16:40 179 Investigation of the Ignition by Repetitive Streamer Discharges Using Time-resolved OH LIF Measurements  
*Detlef Markus, Aljoscha Hallermann, Tim Langer, Frank Lienesch, Ulrich Maas*
- 17:05 216 Effects of the Width of Droplet Size Distribution on Soot Formation in Spray Flame  
*Jun Hayashi, Junichi Fukui, Noriaki Nakatsuka, Fumiteru Akamatsu*
- 17:30 80 Influence of Heat Release on Swirl Flow Dynamics From High Speed Laser Measurements in a Gas Turbine Model Combustor  
*Christoph M. Arndt, Adam M. Steinberg, Isaac G. Boxx, Wolfgang Meier, Manfred Aigner*
- 17:55 139 Effect of Iron Pentacarbonyl on Soot Formation behind Shock Waves  
*G. L. Agafonov, V. N. Smirnov and P. A. Vlasov*

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**18:20 End**

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	<b>(S4) – Supercritical Combustion – I</b> <i>(J. Oefelein)</i>	<b>(R9A) – Detonation Cellular Structure–II</b> <i>(Mark Short)</i>	<b>(R9B) – Flame Ignition and Quenching – I</b> <i>(E. Mastorakos)</i>	<b>(R9C) – Premixed Flames Structures</b> <i>(F. Baillot)</i>
08:30	213 <i>S. Candel, ...</i>			
09:10	244 <i>I. Leyva, ...</i>	67 <i>C. Johansen, ..</i>	11 <i>S. Ahmed, ...</i>	22 <i>H. C. Lin, ...</i>
09:35	335 <i>G. Ribert, ...</i>	73 <i>F. Ettner, ...</i>	60 <i>S. Bane, ...</i>	93 <i>G. Garcia-Soriano</i>
10:00	338 <i>K. J. Kim, ...</i>	145 <i>H. D. Ng, ...</i>	172 <i>C. C. Liu, ...</i>	307 <i>M. Shimura, ...</i>
10:25	<b>Break</b>			
	<b>(S4) – Supercritical Combustion – II</b> <i>(H. G. Sung)</i>	<b>(R10A) – Detonation with Confinement</b> <i>(B. C. Fan)</i>	<b>(R10B) – Flame Ignition and Quenching – II</b> <i>(E. Mastorakos)</i>	<b>(R10C) – Flame Structures</b> <i>(R. K. Cheng)</i>
10:55	341 <i>J. Bellan</i>	37 <i>A. Chinnayya, ...</i>	92 <i>Q. Wang, ...</i>	194 <i>K. Takase,</i>
11:20	284 <i>J. Oefelein, ...</i>	51 <i>L. Munier</i>	339 <i>B. Colcord, ...</i>	66 <i>T. Dunstan, ...</i>
11:45	181 <i>L. Hakim, ..</i>	59 <i>N. Polley, ...</i>	319 <i>P. Sharma,...</i>	178 <i>A. Uemichi, ...</i>
12:10	<b>End</b>			

**08:30 (S4) – Supercritical Combustion – I****Pg. 76***Session Chair : Joseph C. Oefelein***Pacific Ballroom C**

- 08:30 213 (Topical Review: 40 min) Progress in Transcritical Combustion : Experimentation, Modeling and Simulation  
*S. Candel, T. Schmitt, N. Darabiha*
- 09:10 244 Shear Coaxial Jets Subjected to an External Acoustic Field  
*Ivett A. Leyva, Doug Talley, Sophonias Teshome, Juan Rodriguez, Jeffrey Graham*
- 09:35 335 Supercritical Fluid Flow in Rocket Motor Engines  
*Guillaume Ribert, Hongfa Huo, Vigor Yang*
- 10:00 338 Theoretical and Numerical Investigation for Kerosene Mixing in a Swirl Injector at Supercritical Conditions  
*Kuk-Jin Kim, Jun-Young Heo, Hong-Gye Sung, Vigor Yang*

**09:10 (R9A) – Detonation Cellular Structure – II****Pg. 77***Session Chair : Mark Short***Pacific Ballroom AB**

- 09:10 67 Large Eddy Simulation of Flame Acceleration in an Obstructed Channel  
*Craig Johansen and Gaby Ciccarelli*
- 09:35 73 Mach Reflection in Detonations Propagating through a Gas with a Mixture Gradient  
*F. Ettner, K.G. Vollmer and T. Sattelmayer*
- 10:00 145 Geometrical Characterization of the Reaction Front in Gaseous Detonations Using Fractal Theory  
*Hoi Dick Ng, Hamid Ait Abderrahmane, Kevin R. Bates, Nikos Nikiforakis*

**09:10 (R9B) – Flame Ignition and Quenching – I****Pg. 77***Session Chair : E. Mastorakos***Moss Cove AB**

- 09:10 11 Ignition Probability of Lean Premixed Bluff-Body Flames  
*S. F. Ahmed, E. Mastorakos*
- 09:35 60 Spark Ignition of Kerosene-Air Mixtures  
*Sally P. M. Bane, Stephanie A. Coronel, Philipp A. Boettcher, Joseph E. Shepherd*
- 10:00 172 A New Look at Global Quenching of Premixed Flames by Turbulence  
*C. C. Liu, S. S. Shy, M. W. Peng, Y. C. Dong*

**09:10 (R9C) – Premixed Flames Structures****Pg. 78***Session Chair : K. Maruta***Woods Cove ABC**

- 09:10 22 A Stable Premixed Methane/Air Sub-Lean Flame Stabilized by Lean Sandwich Flames  
*Ho-Chuan Lin, Yueh-Heng Li and Yei-Chin Chao*
- 09:35 93 Burning Velocity of Premixed Flame Tips: Experimental and Numerical Study  
*G. Garcia-Soriano, F. J. Higuera, J. L. Castillo, P. L. Garcia-Ybarra*
- 10:00 307 Measurement of Flame and Flow Structures of Turbulent Jet Premixed Flame by Simultaneous Triple-Plane PLIF and Dual-Plane Stereoscopic PIV  
*Masayasu Shimura, Ayane Johchi, Gyung-Min Choi, Kaoru Iwamoto, Mamoru Tanahashi, Toshio Miyauchi*

**10:25 (B) – Coffee Break**

**10:55 (S4) – Supercritical Combustion – II****Pg. 79***Session Chair : H. G. Sung***Pacific Ballroom C**

- 10:55 341 Species Mixing under Supercritical Pressure Conditions  
*Josette Bellan*
- 11:20 284 Low Temperature Injection Dynamics and Turbulent Flame Structure in High-Pressure Supercritical Flows  
*Joseph C. Oefelein, Guilhem Lacaze*
- 11:45 181 Numerical Simulation of Cryogenic Flames under High Frequency Acoustic Modulation  
*L. Hakim, T. Schmitt, S. Ducruix and S. Candel*

**10:55 (R10A) – Detonation with Confinement****Pg. 80***Session Chair : Baochun Fan***Pacific Ballroom AB**

- 10:55 37 Computational Study of Detonation-wave Propagation in Narrow Channels  
*Ashwin Chinnayya and Abdellah Hadjadj*
- 11:20 51 Experimental Study of Closed Volume Detonation  
*Laurent Munier*
- 11:45 59 Experimentally Observed Methods of Re-initiation During Detonation Diffraction into a Confined Volume  
*Nolan Polley, Miles Q. Egbert, Eric L. Petersen*

**10:55 (R10B) – Flame Ignition and Quenching – II****Pg. 81***Session Chair : E. Mastorakos***Moss Cove AB**

- 10:55 92 3D Visualisation of Diffusion Flame Structure and Dynamics under Acoustic Excitation  
*Qian Wang, Yang Zhang, Hao Jie Tang, Min Zhu*
- 11:20 339 Flame Stabilization with Fuel Injection into a Cavity Adjacent to a Curved, Converging Air-flow Channel  
*Ben J. Colcord, Feng Liu and William A. Sirignano*
- 11:45 319 Parametric Numerical Studies on Auto-Ignition around a Single Fuel Droplet  
*Pratyush Sharma, Robert Schießl, Ulrich Maas*

**10:55 (R10C) – Flames Structures****Pg. 82***Session Chair : R. K. Cheng***Woods Cove ABC**

- 10:55 194 Radiative Extinction Characteristics of Low-Lewis-Number Counterflow Premixed Flame in Microgravity and Its Correlation with Flame Ball  
*Koichi Takase, Hisashi Nakamura, Takuya Tezuka, Susumu Hasegawa, Xing Li, Philip Wang, Kaoru Maruta*
- 11:20 66 Flame Surface Density Measurements in Interacting Premixed Flames Using Experiment and DNS  
*T.D. Dunstan, F. T. C. Yuen, E. Mastorakos, N. Swaminathan, K. N. C. Bray*
- 11:45 178 Numerical Study on Ultra-Lean Premixed Flame in Swirl Flow with Recirculating of Burned Gas including Active Radicals  
*Akane Uemichi, Yasuo Kondo, Makihito Nishioka*

**12:10 End**

	<b>(S5) – Detonation Analog – I</b> (A. Higgins)	<b>(R11A) – Detonation Propagation</b> (J. Chao)	<b>(R11B) – Detonation Structure: General</b> (V. N. Gamezo)	<b>(R11C) – Turbulent Premixed Flames</b> (V. McDonell)
09:00	289 Aslan Kasimov	71 X. -D. Zhang, ...	108 M. Liu, ..	184 W.Ramaekers,
09:25		98 M. Wakita, ..	58 T. Honda, ...	126 V. Robin, ...
09:50	277 C. Kiyanda, ...	193 H. Nakayama, .	219 G. Cheng, ...	273 I. Ahmed, ...
10:15	137 M. Radulescu, .	278M.Lopez-Aoyagi	259 D. -R. Cho, ...	186 P. Auzillon, ...
10:40	<b>Break</b>			
	<b>(S5) – Detonation Analog – II</b> (A. Higgins)	<b>Poster Session II with WIP</b> (Francesco S. Marra)		
11:10	251 N. Sirmas, ...	Poster-II: (D) 52, 160, 208, 225, 295; (F) 6, 7, 15, 35, 36, 39, 40, 48, 75, 87, 170, 175, 191, 212, 215, 241, 263, 294, 311, 321 WIP: (D) 353, 360, 363, 366, 368; (E) 347, 349; (F) 343, 344, 345, 346, 348, 355, 358, 361, 362, 364, 365, 367, 369, 374, 380		
11:35	320 A. Higgins, ...			
12:00	<b>Lunch</b>			
	<b>(S6) – Verification and Validation of Detonation Simulation – I</b> (M. Radulescu and J. Powers)	<b>(R12A) – Detonation Front Structure</b> (E. S. Oran)	<b>(R12B) – Detonation Initiation and Transmission</b> (A. Matsuo)	<b>(R12C) – Turbulent Non-Premixed and Stratified Flames</b> (F. Baillot)
13:30	Topical Review J. Powers	134 B. Khasainov, ..	65 J.-S. Grondin, ..	235 R. Vicquelin, ..
13:55	156R.Bhattacharjee	214 B. Khasainov, ..	99 W. -C. Kuo, ...	168 M. Pasternak, ..
14:20	293 J. Ziegler, ...	267 D. Kessler, ...	115 B. Maxwell, ...	142 S. Malkeson, ..
14:45	62 K. Mazaheri, ..	240 L. Maley, ...	128 S. Khomik, ...	123 J. Tillou, ...
15:10	<b>Break</b>			
	<b>(S6) – Verification and Validation of Detonation Simulation – II</b> (M. Radulescu and J. Powers)	<b>(R13A) – High Speed Flames</b> (J. Chao)	<b>(R13B) – Chemical Kinetics and Reaction Dynamics – I</b> (U. Mass)	<b>(R13C) – Hydrogen Combustion</b> (O. Penyazkov)
15:40	89 L. Cole, ...	165 R. Porowski, ...	276 J. Melguizo-Gavilanes, ...	174 H. Lee, ...
16:05	29 M. Papalexandris, ...	167 W. -K. Kim, ...	285 Bert Debusschere,.	249 N. Rezaeyan, ..
16:30	33 C. Romick,...	291 G. Cheng, ...	304 F. Marra, ...	238 U. Niemann, ...
16:55		229 S. Golovastov, .	198 V. Bykov, ...	248 F. Welzel, ...
17:20	<b>End</b>			

**09:00 (S5) – Detonation Analog – I****Pg. 84***Session Chair : John H. S. Lee***Doheny Beach AB**

- 09:00 289 *(Topical Review: 50 min) On Detonation Analogs*  
*Aslan Kasimov*
- 09:50 277 *Dynamic Behaviour of Analog Detonation Systems*  
*C.B. Kiyanda, H.D. Ng*
- 10:15 137 *Non-linear Dynamics and Route to Chaos in Fickett's Detonation Analogue*  
*Matei I. Radulescu, Justin Tang*

**9:00 (R11A) – Detonation Propagation****Pg. 84***Session Chair: J. Chao***Pacific Ballroom AB**

- 09:00 71 *Experimental and Numerical Study on Detonation Propagating in an Annular Cylinder*  
*Xudong Zhang, Baochun Fan, Zhenhua Pan, Mingyue Gui, Zhihua Chen*
- 09:25 98 *Planar Toroidal Detonation Propagation through Gradual Expanding Channel*  
*Masashi Wakita, Masayoshi Tamura, Akihiro Terasaka, Kazuya Sajiki, Tsuyoshi Totani and Harunori Nagata*
- 09:50 193 *Study on Detonation Waves Propagating through Curved Channels*  
*H. Nakayama, T. Moriya, J. Kasahara, A. Matsuo, Y. Sasamoto and I. Funaki*
- 10:15 278 *Stability of Chain Branched Detonation Waves with Slow Initiation*  
*Megumi Lopez-Aoyagi, Josue Melguizo-Gavilanes and Luc Bauwens*

**9:00 (R11B) – Detonation Structure: General****Pg. 85***Session Chair : V. N. Gamezo***Moss Cove AB**

- 09:00 108 *Three Dimensional Simulation for the Effects of Fuel Injection Patterns in Rotating Detonation Engine*  
*Meng Liu, Jian-Ping Wang*
- 09:25 58 *Experiments on Hydrodynamic Stability of Laser-Driven Detonations in Nitrogen and Helium Gases*  
*Tomohisa Honda, Akira Kawaguchi, Yoshiki Hanta, Akio Susa, Shinichi Namba, Takuma Endo, Hiroyuki Shiraga, Keisuke Shigemori and Mayuko Koga*
- 09:50 219 *Detonation Characteristics in Tube Filled with the Binary Fuels H<sub>2</sub>/C<sub>3</sub>H<sub>8</sub>-Air Mixtures*  
*Guanbing Cheng, Ratiba Zitoun, Pascal Bauer*
- 10:15 259 *Reynolds Number Effects on the Structure and Stability of Highly Unstable Detonation Wave*  
*Deok-Rae Cho, Kiha kang, Jae-Ryul Shin, Jeong-Yeol Choi*

**9:00 (R11C) – Turbulent Premixed Flames****Pg. 86***Session Chair : V. McDonell***Woods Cove ABC**

- 09:00 184 *Subgrid Analysis of DNS of Stratified Bunsen Flames*  
*W.J.S. Ramaekers, J.A. van Oijen, L.P.H. de Goey*
- 09:25 126 *Algebraic Models for Turbulent Transports in Flames : Applications to Stagnating and 2D Premixed Flames*  
*Vincent Robin, Arnaud Mura, Michel Champion*
- 09:50 273 *Effects of Mean Curvature on Flame Propagation*  
*I. Ahmed, N. Swaminathan*

- 10:15 186 A Filtered Tabulated Chemistry Model for LES of Partially-premixed Flames  
*P. Auzillon, O. Gicquel, N. Darabiha, D. Veynante, B. Fiorina*

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**10:40 (B) – Coffee Break**

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**11:10 (S5) – Detonation Analog – II**

**Pg. 87**

*Session Chair : John H. S. Lee*

**Doheny Beach AB**

- 11:10 251 Molecular Dynamics Simulations of Detonations  
*Nick Sirmas, Matei Radulescu*
- 11:35 320 Shock-like and Detonation-like Waves in One-dimensional Lattice Chains  
*Andrew Higgins*

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**11:10 Poster Session II and WIP**

**Pg. 126**

*Session Chair : Francesco S. Marra*

**Pacific Ballroom D**

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**12:00 Lunch**

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**13:30 (S6) – Verification and Validation of Detonation Simulation – I**

**Pg. 87**

*Session Chair : M. Radulescu and J. Powers*

**Doheny Beach AB**

- 13:30 (Topical Review) Outstanding Issues in Verification and Validation of Compressible Reacting Flow Calculations  
*J.M. Powers*
- 13:55 156 Detonation Wave Attenuation by a Cylinder and the Subsequent Re-initiation Regimes  
*R. Bhattacharjee, G. Maines, L. Maley and M.I. Radulescu*
- 14:20 293 Verification and Direct Numerical Simulation of Irregular Hydrocarbon Detonations  
*Jack L. Ziegler, Ralf Deiterding, Joseph E. Shepherd, D. I. Pullin, G. Blanquart*
- 14:45 62 Diffusion in Gaseous Detonations  
*K. Mazaheri, Y. Mahmoudi, M. I. Radulescu*

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**13:30 (R12A) – Detonation Front Structure**

**Pg. 88**

*Session Chair : E. S. Oran*

**Pacific Ballroom AB**

- 13:30 134 Three-Dimensional Structure of Detonations in Suspensions of Aluminum Particles  
*B. Khasainov, F. Viro, B. Veyssiere*
- 13:55 214 Parametric Study of Double Cellular Detonation Structure  
*B.A. Khasainov, F. Viro, H.-N. Presles, D. Desbordes*
- 14:20 267 Detonation Propagation through a Gradient in Fuel Composition  
*D.A. Kessler, V.N. Gamezo, E.S. Oran*
- 14:45 240 Experimental Implementation of a Converging Diverging Nozzle Technique to Study Shock Reflections in Reactive Gases  
*L. Maley, J. Armstrong and M.I. Radulescu*

**13:30 (R12B) – Detonation Initiation and Transmission****Pg. 89***Session Chair : Akiko Matsuo***Moss Cove AB**

- 13:30 65 The Onset of Detonation in Mixtures with Regular and Irregular Detonation Cellular Structures  
*J.-S. Grondin, J.H.S. Lee*
- 13:55 99 Effects of Nitrogen Dilution on Detonation Transmission across a Sudden Expansion in a Millimeter-scale Channel  
*Wei-Chun Kuo, Po-Yuan Chiu, Ming-Hsun Wu*
- 14:20 115 Critical Ignition in Rapidly Expanding Flows Described by a Power Law  
*B.M. Maxwell, M.I. Radulescu*
- 14:45 128 On Some Conditions of Detonation Initiation behind a Multi-Orifice Plate  
*S.V. Khomik, B. Veyssiere, V. Montassier, S.P. Medvedev, G.L. Agafonov*

**13:30 (R12C) – Turbulent Non-Premixed and Stratified Flames****Pg. 90***Session Chair : F. Baillot***Woods Cove ABC**

- 13:30 235 A Turbulent Combustion Model for Jet Flames Issuing in a Vitiated Coflow  
*Ronan Vicquelin, Benoit Fiorina and Olivier Gicquel*
- 13:55 168 Time Dependent Based Mixing Time Modelling for Diesel Engine Combustion Simulations  
*M. Pasternak, F. Mauss, F. Lange*
- 14:20 142 Statistical Analysis and Modelling of Turbulent Fuel Mass Fraction Flux in Turbulent Stratified Flames Using Direct Numerical Simulations  
*Sean P. Malkeson, Nilanjan Chakraborty*
- 14:45 123 Large-Eddy Simulation of an Auto-Igniting Liquid Diesel-Type Spray  
*J. Tillou, C. Angelberger, J. B. Michel, A. Robert, L. Martinez, S. Richard, D. Veynante*

**15:10 (B) – Coffee Break****15:40 (S6) – Verification and Validation of Detonation Simulation – II****Pg. 91***Session Chair : M. Radulescu and J. Powers***Doheny Beach AB**

- 15:40 89 Stability of Flame-Shock Coupling in Detonation Waves: 1D Dynamics  
*Lord K. Cole, Ann R. Karagozian, Jean-Luc Cambier*
- 16:05 29 Numerical Study of Detonation Suppression with Chemical Inhibitors  
*Miltiadis V. Papalexandris and Quentin Steisel*
- 16:30 33 Verified Calculation of Nonlinear Dynamics of Viscous Detonation  
*Christopher M. Romick, Tariq D. Aslam and Joseph M. Powers*

**15:40 (R13A) – High Speed Flames****Pg. 92***Session Chair : J. Chao***Pacific Ballroom AB**

- 15:40 165 Experimental Study on Premixed Flame Propagation in Small Channel  
*Rafal Porowski, Andrzej Dabkowski, Andrzej Teodorczyk, Felipe Alfonso Galvis Millan*
- 16:05 167 Effects of Hydrogen Addition on Flame Propagation and Blast Wave Generation during Explosion of Methane-air Mixtures  
*Woo-Kyung Kim, Toshio Mogi, Ritsu Dobashi*

- 16:30 291 High-speed Camera Visualizations of Flame Acceleration in a Square Channel with Obstacles: the Case of Binary Fuels  $H_2/C_3H_8$ -Air mixture  
*Guanbing Cheng, Ratiba Zitoun, Yves Sarrazin, Alain Claverie, Pierre Vidal, Bernard Veyssiere, Pascal Bauer*
- 16:55 229 Influence of Diaphragm on Self-Ignition of Hydrogen at Spontaneous Release into Air  
*Sergey Golovastov, Victor Golub, Dmitry Baklanov, Vladimir Bocharnikov*

**15:40 (R13B) – Chemical Kinetics and Reaction Dynamics – I****Pg. 93***Session Chair : Ulrich Mass***Moss Cove AB**

- 15:40 276 Shock-induced Ignition for Simplified Chain-branching Kinetics  
*Josue Melguizo-Gavilanes, Mingjun Tian, Luc Bauwens, Zhenhua Pan*
- 16:05 285 Computational Singular Perturbation with Non-Parametric Tabulation of Slow Manifolds for Time Integration of Stiff Chemical Kinetics  
*Bert Debusschere, Youssef Marzouk, Habib Najm, Dimitris Goussis, Mauro Valorani*
- 16:30 304 Non-linear Response to Periodic Forcing of Methane-air Global and Detailed Kinetics in Perfectly Stirred Reactors  
*Francesco Saverio Marra, Emanuele Martelli*
- 16:55 198 An Analysis of the Attractive Properties of REDIM Manifolds for Model Reduction  
*Viatcheslav Bykov, Ulrich Maas*

**15:40 (R13C) – Hydrogen Combustion****Pg. 94***Session Chair : Oleg G. Penyazkov***Woods Cove ABC**

- 15:40 174 Self-ignition and Flame Propagation of Pressurized Hydrogen by Sudden Release through a Tube  
*Hyoungh Jin Lee, Sei Hwan Kim, Yeong Ryeon Kim, In-Seuck Jeung*
- 16:05 249 Influence of Lewis Number and Expansion on Jet Ignition  
*N. Rezaeyan, L. Bauwens, M. Radulescu, F.F. Fachini*
- 16:30 238 Extinction and Auto-Ignition of  $C_3$  and  $C_4$  Alcohols in Laminar Nonpremixed Flows  
*Ulrich Niemann, Kalyanasundaram Seshadri, Forman A. Williams*
- 16:55 248 Limiting Values for the Ignition of Hydrogen/Air Mixtures by Mechanically Generated Ignition Sources  
*F. Welzel, M. Beyer, C. -P. Klages*

**17:20 End**



	<b>(S7) – Supersonic Combustion – I</b> (A. Higgins)	<b>(R14A) – Detonation and High Speed Flames: Applications</b> (T. Endo)	<b>(R14B) – Chemical Kinetics and Reaction Dynamics – II</b> (U. Riedel)	<b>(R14C) – Reacting Flow Dynamics – I</b> (T. Dunstan)
09:00	296 V. Yang, ...	88 R. Zhou, ...	16 K. Urness, ...	79 M. Akram, ...
09:25	318 C. Segal, ..	211 P. Wolański	57 Y. Mizobuchi, ...	91 H. -W. Ge, ...
09:50	117 K. Takita	158 S. -W. Lo, ...	176 O. Skrebkov, ..	105 S. Amzin, ...
10:15	<b>Break</b>			
	<b>(S7) – Supersonic Combustion – II</b> (J.Y. Choi and V. Yang)	<b>(R15A) – Explosion and Blast</b> (S. Medvedev)	<b>(R15B) – Chemical Kinetics and Reaction Dynamics – III</b> (O. Mathieu)	<b>(R15C) – Reacting Flow Dynamics – I</b> (T. Dunstan)
10:45	155 K. -C. Lin, ...	38 E. Del Prete,...	312 Y. -H. Li, ..	135 C. Merlin, ...
11:10	45 S. Tomioka, ...	42 E. Fedina, ...	26 T. Kathrotia, ...	164 P. Gillon, ...
11:35	161 S. Yang,	305 S. Jackson, ...	252 M. Hilbig,	224 T. Hirasawa, ..
12:00	<b>Lunch</b>			
	<b>(S7) – Supersonic Combustion – III</b> (J.Y. Choi and V. Yang)	<b>(R16A) – Accidental Explosions and Energetic Materials</b> (C. R. Bauwens)	<b>(R16B) – Multiphase Detonation</b> (M. Short)	<b>(R16C) – Numerical Development</b> (F. S. Marra)
13:30	34 C. Fureby, ..	253 D.Castellanos,	18 K. Balakrishnan,.	101 C. Safta, ...
13:55	97 L. Gomet, ..	257 J. Damazo, ...	205T. Shimada, ..	78 C. Schrödinger, .
14:20	154 J. -Y.Choi, ...	8 R. Ball, ...	17 A. Ishihara, ...	192 D. Tudorache,..
14:45		297 Y. Charron-Tousignant,	315 R. C. Ripley	197 M. Folusiak, ...
15:10	<b>Break</b>			
		<b>(R17A) – Meso - scale Combustion</b> (M. -H. Wu)	<b>(R17B) – Flame Extinction</b> (A. Mura)	<b>(R17C) – Numerical Simulations</b> (F. S. Marra)
15:40		237 G.Watson, ...	84 J. Min, ...	19 A. Teraji, ...
16:05		306 C. -H. Chen, ...	316 K. Seshadri, ...	151 N. Malik, ...
16:30	<b>End</b>			

**09:00 (S7) – Supersonic Combustion – I****Pg. 96***Session Chair : J.Y. Choi and V. Yang***Pacific Ballroom C**

- 09:00 296 Hypersonic Proulsion and Supersonic Combustion: Review on Current Status for the Future  
*Vigor Yang and Jeong-Yeol Choi*
- 09:25 318 Injection Schemes for Improved Flameholding in Supersonic Flow  
*Corin Segal and Qiuya Tu*
- 09:50 117 Ignition by Plasma Jet in Supersonic Flow  
*Kenichi Takita*

**9:00 (R14A) – Detonation and High Speed Flames: Applications****Pg. 96***Session Chair: Takuma Endo***Pacific Ballroom AB**

- 09:00 88 Thermodynamic Performance Numerical Simulation of Rotating Detonation Engine  
*Rui Zhou and Jian-ping Wang*
- 09:25 211 Rotating Detonation Wave Stability  
*Piotr Wolański*
- 09:50 158 Numerical Study of the Noise Generation by a Rifle Shooting with Suppressor  
*Shi-Wei Lo, Chang-Hsien Tai, Jyh-Tong Teng and Yong-Jhou Lin*

**9:00 (R14B) – Chemical Kinetics and Reaction Dynamics – II****Pg. 97***Session Chair : Uwe Riedel***Moss Cove AB**

- 09:00 16 Hydrogen Rich Syngas Oxidative Catalytic Activity of Nickel and Inconel  
*Kimberly N. Urness, John W. Daily and G. Barney Ellison*
- 09:25 57 Effects of Flame Curvature on Chemical Reactions in Rich Hydrogen-Air Premixed Flame  
*Yasuhiro Mizobuchi, Tadao Takeno, Shingo Matsuyama, Junji Shinjo, Satoru Ogawa*
- 09:50 176 Vibrational Nonequilibrium and Electronical Excitation in the Hydrogen-Oxygen Reaction  
*Oleg V. Skrebkov*

**9:00 (R14C) – Reacting Flow Dynamics – I****Pg. 98***Session Chair : T. D. Dunstan***Woods Cove ABC**

- 09:00 79 Experimental Studies on the Dynamics of Premixed Methane-Air Flames in Various Aspect Ratio Channels  
*Mohammad Akram, Sudarshan Kumar*
- 09:25 91 Joint Velocity-Scalar PDF Modeling of Turbulent Spray Flows  
*Hai-Wen Ge and Eva Gutheil*
- 09:50 105 Conditional Moment Closure for Turbulent Premixed Flames  
*S. Amzin, N. Swaminathan, J. W. Rogerson, J. H. Kent*

**10:15 (B) - Coffee Break**

**10:45 (S7) – Supersonic Combustion – II****Pg. 99***Session Chair : J.Y. Choi and V. Yang***Pacific Ballroom C**

- 10:45 155 Exploration on Unsteady and Transient Combustion Phenomena in High-Speed Air-Breathing Propulsion  
*Kuo-Cheng Lin, Vigor Yang*
- 11:10 45 Interaction Phenomena in Supersonic Combustors  
*Sadatake Tomioka, Ryo Masumoto*
- 11:35 161 Scramjet Engine Research of KARI : Ground Tests of Engines and Components  
*Soo Seok Yang, Sang Hun Kang, Yang Ji Lee*

**10:45 (R15A) – Explosion and Blast****Pg. 100***Session Chair : Sergey P. Medvedev***Pacific Ballroom AB**

- 10:45 38 Numerical Simulation and Experimental Investigation of Blast Wave Mitigation in Dry Aqueous Foams  
*E. Del Prete, L. Domergue, J.-F. Haas, A. Chinnayya, A. Hadjadj*
- 11:10 42 Investigating Ground Effects on Mixing and Afterburning During a TNT Explosion  
*Ekaterina Fedina and Christer Fureby*
- 11:35 305 Planar Blast Scaling with Condensed-Phase Explosives in a Shock Tube  
*Scott I. Jackson*

**10:45 (R15B) – Chemical Kinetics and Reaction Dynamics – III****Pg. 100***Session Chair : Oliver Mathieu***Moss Cove AB**

- 10:45 312 Effect of Catalyst Segmentation with Cavities on Combustion Enhancement of Multi-Fuels in a Micro Channel  
*Yueh-Heng Li, Guan-Bang Chen, Tsarng-Sheng Cheng, Yei-Chin Chao*
- 11:10 26 Reaction Kinetics Mechanism for Chemiluminescent Species  
*Trupti Kathrotia, Uwe Riedel*
- 11:35 252 Computer Aided Detailed Mechanism Generation for Large Hydrocarbons: n-Decane  
*Martin Hilbig, Lars Seidel, Xiaoxiao Wang, Fabian Mauss and Thomas Zeuch*

**10:45 (R15C) – Reacting Flow Dynamics – II****Pg. 101***Session Chair : T. D. Dunstan***Woods Cove ABC**

- 10:45 135 Large Eddy Simulation and Experimental Study of a Trapped Vortex Combustor  
*C. Merlin, P. Domingo, L. Vervisch, J. Burguburu, G. Cabot, B. Renou*
- 11:10 164 Stability of Laminar Diffusion Flames of Methane in an Oxygen-enriched Air Co-jet  
*P. Gillon, M. Chahine, B. Sarh, V. Gilard, J.N. Blanchard*
- 11:35 224 Impact of Flame-Flame Interaction in Identical Two Non-premixed Microflames  
*Taro Hirasawa, Kunihiko Gotanda, Hiroki Masuda, Yuji Nakamura*

**12:00 Lunch**

**13:30 (S7) – Supersonic Combustion – III****Pg. 102***Session Chair : J.Y. Choi and V. Yang***Pacific Ballroom C**

- 13:30 34 Modeling Supersonic Combustion  
*C. Fureby and V. Sabel'nikov*
- 13:55 97 Influence of the Residence and Scalar Mixing Time Scales in Non Premixed Combustion in Supersonic Turbulent Flows  
*Laurent Gomet, Vincent Robin, Arnaud Mura*
- 14:20 154 Numerical Study of H<sub>2</sub>+CO Turbulent Combustion with Supersonic Coflow in Confined Geometries  
*Jeong-Yeol Choi and Vigor Yang*

**13:30 (R16A) – Accidental Explosions and Energetic Materials****Pg. 103***Session Chair : C. Regis Bauwens***Pacific Ballroom AB**

- 13:30 253 Simulating Dust Explosion Venting Through Ducts  
*Diana Castellanos, Trygve Skjold, Kees van Wingerden, Rolf K. Eckhoff and Sam Mannan*
- 13:55 257 Deformation of Coated Stainless Steel Tubes from Reflected Detonation  
*J. Damazo, J.E. Shepherd, K. Chow-Yee, J. Karnesky*
- 14:20 8 Nonclassical Thermal Runaway: The Bhopal Disaster and Liquid Hydroperoxide Explosives  
*R. Ball*
- 14:45 297 Activation Effects on the Deflagration Speeds in Ni-Al  
*Y. Charron-Tousignant, B. Barrett, M. Yandouzi, M. Radulescu, A. Weck, J.J. Lee*

**13:30 (R16B) – Multiphase Detonation****Pg. 104***Session Chair : Mark Short***Moss Cove AB**

- 13:30 18 An Empirical Model for the Ignition of Aluminum Particle Clouds Behind Blast Waves  
*Kaushik Balakrishnan, Allen L. Kuhl, John B. Bell, Vincent E. Beckner*
- 13:55 205 Numerical Study on the Ethanol/Air Two-phase Detonation  
*Takashi Shimada, Eisuke Yamada, A.Koichi Hayashi and Nobuyuki Tsuboi*
- 14:20 17 The Burning Surface Temperature and Boiling Point of Ammonium Nitrate  
*Atsushi Ishihara*
- 14:45 315 Effect of Aerodynamic Breakup on Combustion of Aluminum Particles from Heterogeneous Explosives  
*Robert C. Ripley and Fan Zhang*

**13:30 (R16C) – Numerical Development****Pg. 105***Session Chair : Francesco Saverio Marra***Woods Cove ABC**

- 13:30 101 A High-Order AMR Algorithm for Chemically Reacting Flows  
*Cosmin Safta, Jaideep Ray, Habib N. Najm*
- 13:55 78 Numerical Studies of the Influence of Turbulence and Coherent Structures on Flame and Emission Characteristics in Lean Premixed Combustion  
*C. Schrödinger, C. O. Paschereit, M. Oevermann*
- 14:20 192 Development of a Chemical Kinetics Tabulation Method for the Prediction of Diesel Engine Pollutants  
*D.E.Tudorache, P. Auzillon, L. Thobois, N. Darabiha, R. Vicquelin, O. Gicquel, B. Fiorina*

- 14:45 197 Graphics Processors as a Tool for Rotating Detonation Simulations  
*Michal Folusiak, Karol Swiderski, Arkadiusz Kobiera, Piotr Wolanski*

**15:10 (B) – Coffee Break**

**15:40 (R17A) – Mesoscale Combustion**

**Pg. 106**

*Session Chair : Ming-Hsun Wu*

**Pacific Ballroom AB**

- 15:40 237 The Effect of Mixture Composition on Stabilized Flames in a Meso-scale Channel with a Wall Temperature Gradient  
*Graeme M.G.Watson, Jeffrey M. Bergthorson*
- 16:05 306 Effects of Scale on Non-Adiabatic Swiss-roll Heat-Recirculating Combustors  
*Chien-Hua Chen and Paul Ronney*

**15:40 (R17B) – Flame Extinction**

**Pg. 106**

*Session Chair : Arnaud Mura*

**Moss Cove AB**

- 15:40 84 Experimental Investigation on Flame Extinction Process of Non-premixed CH<sub>4</sub>/air Flames in an Air-diluted Coflow by CO<sub>2</sub>, N<sub>2</sub> or Ar  
*Jiesheng Min, Françoise Baillet*
- 16:05 316 Rate Ratio Asymptotic Analysis of the Structure and Mechanisms of Extinction of Nonpremixed CH<sub>4</sub>/N<sub>2</sub>-O<sub>2</sub>/N<sub>2</sub>O/N<sub>2</sub> Flames  
*Kalyanasundaram Seshadri, Xue-Song Bai, Forman A. Williams*

**16:20 (R17C) – Numerical Simulations**

**Pg. 107**

*Session Chair : Francesco Saverio Marra*

**Woods Cove ABC**

- 15:40 19 2D Direct Numerical Simulation of Intermediate Species Diffusion in Low Temperature Oxidation Process  
*Atsushi Teraji, Takahiro Morikawa, Takashi Ishihara, Yukio Kaneda*
- 16:05 151 A Numerical Study of the Markstein Hypothesis in Finite Thickness Flames with Realistic Chemistry  
*Nadeem A. Malik*

**16:30 End**

**Paper #20: Kinetics of Drop Shattering Behind Detonation Wave***A. G. Girin***Paper #25: Detonation Initiation by a Temperature Gradient for a Detailed Chemical Reaction Models***A. D. Kiverin, A. A. Chukalovsky, M. F. Ivanov, M. A. Liberman***Paper #47: The Influence of Initial Temperature on Detonation Structure***Lin Zhi-yong, Liu Shi-jie, Liu Wei-dong, Zhou Jin***Paper #64: Triple Points Collision in Unstable Detonations***Y. Mahmoudi, K. Mazaheri, M. I. Radulescu***Paper #69: A Dataset of Critical Energy for Direct Initiation of Spherical Detonations in Some Hydrocarbon-Oxygen Mixtures***Bo Zhang, Hoi Dick Ng and John H.S. Lee***Paper #86: Experimental Demonstration of a Multi-Tube Pulse Detonation Engine with a Rotary Valve***Han Qixiang, Zhang Yadong, Zhang Qi, Wang Jiahua***Paper #95: Experimental Study of DDT in Hydrogen-Air behind a Single Obstacle***Gaathaug A. V., Bjerketvedt D. and Vaagsaether K.***Paper #371 (was 100): Numerical Simulation of Deflagration and Initiation of Detonation***S. N. Martyushov, T. Elperin, O. Igra***Paper #107: Three Dimensional Simulation of Rotating Detonation Engine without Inner Wall***Shao Ye-Tao, Wang Jian-Ping***Paper #114: Spontaneous Ignition of Hydrogen Jets in the Presence of Reflected Shock Waves***Maxwell, B. M., Tawagi, P., Radulescu, M. I.***Paper #120: A Study on Deflagration to Detonation Transition in Injected Hydrogen/Air Mixtures***Masanori Yabe, Masaki Naitoh, Teruo Yoshihashi, Tetsuro Obara and Shigeharu Ohyagi***Paper #121: Numerical Simulation of Pulse Detonation Engine Working Process Initiated by Small Energy***WANG Wei, FAN Wei, Qiu Hua, YUAN Cheng, PENG Changxin, YAN Chuanjun***Paper #125: Simulation of Detonation Wave Passage through Cloud of Chemically Inert Solid Particles***Fedorov A.V., Tropin D.A.***Paper #130: Experimental Study of Flame Acceleration and Deflagration-To-Detonation Transition***Kong-Qian SUN, Yi-Ning ZHANG, Kun GUO***Paper #173: Physics of Detonation Propagation in Rotating Detonation Engine***Takayuki Yamada, Yuho Uemura, Nobuyuki Tsuboi, A. Koichi Hayashi and Eisuke Yamada***Paper #190: Moving-Component-Free Pulse-Detonation Combustors and Their Use in Ground Applications***T. Endo, A. Susa, T. Akitomo, T. Okamoto, K. Kanekiyo, Y. Sakaguchi, H. Yokoyama, S. Kato, A. Mitsunobu and T. Takahashi***Paper #196: Surface Chemical Reaction of Laser Ablated Aluminum Sample for Detonation Initiation***Chang-hwan Kim, Ardian B. Gojani and Jack J. Yoh*

Paper #217: **Comparison of Conditions of Direct Detonation Initiation by Spark with one by Pulsed Arc According to the Gradient Mechanism of Ya.B. Zeldovich**  
*Korytchenko K. V., Poklonskiy E. V., Galak O. V.*

Paper #222: **Effect of an Axial Electric Field on Detonations**  
*Vsevolods Kamenskihs and John H.S. Lee*

Paper #228: **Effect of Transmission of Detonation from Smaller to Larger Tube on the Performance of PDE**  
*Abhishek R. Bhat, N Harish, P. J. Paul*

Paper #232: **On the Detonation Structure in Ozone**  
*Aslan Kasimov, Vladimir Shargatov*

Paper #258: **Formation of Detonation in Confined Moving Regions**  
*V.A. Levin, I.S. Manuylovich, V.V. Markov*

Paper #262: **Numerical Simulation of the Oblique Detonation Waves in Different Regimes Initiated by Conical Projectile**  
*Jeong-Yeol Choi, Jimmy Verreault, Andrew J Higgins*

Paper #266: **Generation of Detonation Due to Kinetic Energy of the Supersonic Flow**  
*V.A. Levin, I.S. Manuylovich, V.V. Markov*

Paper #282: **Drag Coefficients of Hypervelocity Spherical Projectile Initiating Oblique Detonation Wave**  
*Jeong-Yeol Choi, Shinichi Maeda, Jiro Kasahara, Akiko Matsuo*

Paper #286: **Deflagration to Detonation Transition in Narrow Channel with For-chamber**  
*Golub V.V, Baclanov D.I., Ivanov K.V., Krivokoritov M.S*

Paper #322: **The Transmission Behavior of the Over-driven Detonation across the Mixture with the Abrupt Area Change**  
*Yao-Chung Hsu, Kung-Ming Chung, Yei-Chin Chao*

Paper #331: **Detonation Initiation by Gradient Mechanism in Propane-Oxygen and Propane-Air Mixtures**  
*A.E. Rakitin, I.B. Popov, A.Yu. Starikovskiy*

Paper #336: **Numerical Simulation of Detonation Propagation in Ducts with Obstacles**  
*Cheng Wang, Wenhui Han, Jianguo Ning*

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**10:25 Poster Session I - Explosion/Fire****Pg. 117**

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Paper #46: **Numerical Study of Interactions between Blast Wave and Moving Bodies in Ambient and Indoor Areas**  
*Lo, Shi-Wei, Tai, Chang-Hsien, Teng, Jyh-Tong and Lai, Ching-Chung*

Paper #72: **Buncefield: Reconciliation of Evidence with Mechanisms of Blast**  
*James Venart*

Paper #118: **Mitigation of Vapour Cloud Explosions - A Review**  
*Kees van Wingerden*

Paper #189: **Limiting Oxygen Concentrations - Process Safety by Oxygen Monitoring**  
*K. Holtappels, V. Schröder, A. Pekalski, H.-P. Schildberg*

Paper #239: **Analysis of Mobilisation and Explosion Problems in Gas and Dust Mixtures**  
*JR García-Cascales, F Vera García, R Otón-Martínez, A Bentaib, N Meynet*

Paper #373 (was281): **Vented Gas Explosion in Small Vessels of L/D of 2.4**  
*Fakandu, B.M., Sattar, H., Phylaktou, H.N. and Andrews, G.E.*

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**10:25 Poster Session I - Flame****Pg. 118**

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Paper #12: **Studies on Methanol, Ethanol and Biomethanol Flame Structure**  
*Akimasa Tsutsumi, Makihito Nishioka and Keiichi Hori*

Paper #21: **Two-Phase Spray in a Wake of Shattering Fuel Drop**  
*A. G. Girin*

Paper #30: **Polydispersed Initiation of a Dust Suspension in a Partitioned Structure**  
*J.M. Pascaud*

Paper #55: **Soot Formation from Laminar Ethylene/Air Diffusion Flames at Pressures from 1 to 8 atm**  
*Hongsheng Guo, Zhongzhu Gu, Kevin A. Thomson, Gregory J. Smallwood*

Paper #82: **The Investigation of the N<sub>2</sub>O Catalytic Decomposition for Hybrid Rocket Ignition**  
*Hung-Wei Hsu, Meng-Chun Hsu, Tsung-Sheng Lee, Guan-Bang Chen, Yei-Chin Chao*

Paper #94: **The Structure of Nonpremixed Ethanol Flames**  
*Tej Newman-Lehman, Vaibhav Kumar Sahu, Vasudevan Raghavan Kalyanasundaram Seshadri and Forman A. Williams*

Paper #109: **An Approach to Construction of Universal Global Kinetic Mechanisms of Hydrocarbons Combustion**  
*Ivan A. Zaev, Igor V. Prokopovich*

Paper #111: **High-Temperature Decomposition of Nitromethane in the Shock Waves at Pressures 0.15-36 atm and Hypothesis of the Isomerisation in Its Decomposition Mechanism**  
*Nikolai M. Kusnetsov, Yuri P. Petrov, Stanislav V. Turetskii*

Paper #169: **Empirical Reduction of Dynamical Reactor Models via Chaos Sampling: Comparison with Classic Reduction Methods**  
*Katarzyna Bizon, Joanna Smuła and Gaetano Continillo*

Paper #171: **Hydrogen Peroxide Thermal Decomposition: new Features**  
*Nabiha Chaumeix, Servane Pichon, Laurent Catoire, Claude Paillard*

Paper #183: **On the Critical Conditions of Hybrid Dusts Ignition**  
*Regul'skaya O. S., Vovchuk Ya. I.*

Paper #185 (372): **Fast Deflagration in the Smooth Tube in Hydrogen-Oxygen Mixture**  
*Dziemińska, E., Fukuda, M., Hayashi, A.K., Tsuboi, N. and Yamada, E.*

Paper #200: **Ignition by Electric Spark and by Laser-Induced Spark of Ultra-lean CH<sub>4</sub>/air and CH<sub>4</sub>/CO<sub>2</sub>/air mixtures**  
*Joffrey Biet, Marie Ndem, Mahmoud Idir, Nabiha Chaumeix*

Paper #202: **Transient Interactive Flamelets with Tabulated Chemistry**  
*Anders Borg, Harry Lehtiniemi and Fabian Mauss*

Paper #204: **Chemically Unstable Gases - MITD of Ethylene Oxide Mixtures**  
*Enis Askar, Aydan Acikalin and Volkmar Schroeder*

Paper #223: **Performance, Fuel-Flexibility and Emissions Characteristics of a 4.97cc Wankel Rotary Engine for Portable Power**



*Chris D. McCoy, Nicholas Maiden, Mario Sánchez Sanz, Juan Ramón Arias, Ángel Velázquez, Carlos Fernandez-Pello and Albert P. Pisano*

**Paper #290: Experimental Investigation of Flame Propagation in Turbulent Propane-Air Mixtures and Dust-Air Suspensions**

*Trygve Skjold and Diana Castellanos*

**Paper #300: Computational Model of a Biomass Cookstove**

*Jennifer L. Jones, Ashok Gadgil, Carlos Fernandez-Pello*

**Paper #323: Turbulent Premixed Methane-Air Jet Flames: A Numerical Study**

*M. Chekired, M.S. Boulahlib, Z. Nemouchi*

**Paper #325: Predictive Flame Propagation Model for Stochastic Reactor Model Based Engine Simulations**

*Simon Bjerkborn, Cathleen Perlman, Karin Fröjd and Fabian Mauss*

**Paper #332: Plasma Assisted Ignition below Self-Ignition Threshold in Hydrogen-Air and Hydrocarbon-Air Mixtures**

*L.Wu, J. Lane, N.P. Cernansky, D.L. Miller, A.A. Fridman, A.Yu. Starikovskiy*

**Paper #334: Solid Rocket Motor Internal Ballistics Using a Least-Distance Surface-Regression Method**

*C. H. Chiang, Y. H. Hwang*

**Paper #340: Numerical Investigation of Supersonic Combustion of the Hyshot II in the Shock Tunnel**

*Chih-Peng Chen, Dun C. Liu, Guan-Bang Chen and Ruey-Hung Chen*

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**11:10 Poster Session II - Detonation****Pg. 126**

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**Paper #52: Numerical Study of Shock-Flame Interaction and Deflagration-to-Detonation Transition in H<sub>2</sub>-O<sub>2</sub> Mixtures Using a Detailed Chemical Reaction Model**

*A. D. Kiverin, M. F. Ivanov, M. A. Liberman*

**Paper #160: The Determination of Atmospheric Pressure Linear Burning Rates of Solid Propellants Formulations**

*Frederick Paquet, Hoi Dick Ng*

**Paper #208: Experiment Research on Continuous Detonation Engine**

*Jianping Wang, Tianyi Shi, Yuhui Wang, Yusi Liu, Yongsheng Li*

**Paper #225: Study of Nitrogen Dilution, Pressure and Temperature Effects on Spherical Flames Propagation of H<sub>2</sub>/O<sub>2</sub>/N<sub>2</sub> Mixtures**

*SABARD Jérémy, CHAUMEIX Nabih, CATOIRE Laurent, BENTAIB Ahmed*

**Paper #295: Asymptotic Study of Pulsating Evolution of Overdriven and CJ Detonation with a Chain-Branching Kinetics Model**

*Carlos Chiquete and Mark Short*

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**11:10 Poster Session II - Flame****Pg. 128**

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**Paper #6: Combustion and Evolution of the Polycyclic Aromatic Hydrocarbons in Diesel Engine**

*Ju Hongling, Cheng Xiaobei*

**Paper #7: A Study on Flame Propagation through a Narrow Channel**

*Shigeharu Ohyagi, Teruo Yoshihashi, Tetsuro Obara and Jifeng Du*

**Paper #356 (was 15): Characteristics of Combustion of a Rich-Lean Flame Burner with Controlled Boundary Zone between Rich and Lean Flames**

*Katsuo Asato, Hirofumi Yasuda, Takeshi Miyasaka, Hiroshi Eguchi, Kazusa Kondo, Hiroshi Yamashita*

**Paper #35: Structural Differences between the Non-Reacting and Reacting Supersonic Planar Mixing Layer**

*Huanhao Zhang, Zhihua Chen, Baochun Fan, Xiaohai Jiang*

**Paper #36: Horizontal Flame Spread Along Paper Sheet with a Backing Board**

*Takashi Tsuruda*

**Paper #354 (was 39): Gasdynamics in Turbulent Premixed Combustion: Conditionally Averaged Unclosed Equations and Analytical Formulation of the Problem**

*Vladimir L. Zimont*

**Paper #40: Determination of  $\alpha$ -Pinene/Air Premixed Flame Speeds Involved in Accelerating Forest Fires and Real Accidents**

*Courty, L., Chetehouna, K, Halter, F., Foucher, F., Garo, J.P. and M. Rousselle, C.*

**Paper #48: Local Quenching Recovery Mechanisms and Flamelet Structures in a Heterogeneous Combustion**

*Yuji Yahagi, Takayuki Kawanami, Hirokazu Takeda*

**Paper #378 (was 75): Heat Transfer Parameters During Limit Flame Propagation in Small Tubes**

*Artur Gutkowski*

**Paper #87: Experimental Investigations on Pressure Swirl Atomized Lifted Flames in a Co-flow Field**

*V Mahendra Reddy, Darshan Trivedi and Sudarshan Kumar*

Paper #170: **Numerical Study on Combustion Stability of n-Heptane /Air in a Micro Tube Combustor**  
*LI Junwei, WEI Zhijun, WANG Ningfei*

Paper #175: **Ignition Transition in Turbulent Premixed Combustion at Elevated Pressure**  
*C. C. Liu, S. S. Shy, M. W. Peng, H. J. Chung, Y. W. Hsiu*

Paper #191: **Stability of Premixed Flames in Narrow Channels**  
*Diego Alonso and Mario Sánchez-Sanz*

Paper #212: **Experimental Study about Instability in Global Lean Combustion**  
*Marcel Martins Alves, Rogério Corá, Pedro Teixeira Lacava*

Paper #215: **Laminar Flame Velocities and Fundamental Properties for Two Methane Based Mixtures: G27 and G222**  
*Kodjo Coudoro, Nabiha Chaumeix, Bentaib Ahmed, C-E Paillard*

Paper #241: **Multi-physics Modeling of Coal Gasification Processes in a Well-Stirred Reactor with Detailed Chemistry**  
*Jian Xu, Li Qiao and Jay Gore*

Paper #263: **Hydrogen Explosion Suppression in Experiments of Different Scale**  
*Gavrikov A.I., Chernenko E.V., Efimenko A.A., Mayorov A.S., Privezentsev S.S., Schepetov N.G., Zaretskiy N.P.*

Paper #294: **Analysis of Combustion Problems in Highly Dilute Dust and Gas Mixtures**  
*R.A. Otón Martínez, J.R. García Cascales, F. Vera García, A. Bentaib, N. Meynet*

Paper #311: **Characteristics of Propagation of CH<sub>4</sub>/CO Flames in a Confined Quartz Tube**  
*C.-Y. Wu, T. -W. Chang, Y.-H. Li, Y.-C. Chao*

Paper #321: **Combustion of Methane Hydrate**  
*Melika Roshandell, Jordan Glassman, Matt Khalil, Peter Taborek and Derek Dunn-Rankin*

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**11:10 WIP - Detonation****Pg. 133**

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Paper #353: **Experimental and Numerical Investigation Into the Dynamics of Dust Dispersion From the Layer Behind the Propagating Shock Wave**

*Rudolf Klemens, Pawel Oleszczak, Przemyslaw Zydak*

Paper #360: **Detonation Properties of Ethylene/ Hydrogen Blended Fuels**

*Hidefumi Kataoka, Yutaka Asai, Atsuhiko Kawamura, Koji Fumoto, Kazuhiro Ishii*

Paper #363: **Effect of Piping Shape on Self-ignition of High-pressure Hydrogen during Sudden Discharge**

*Toshio Mogi, Takayuki Tomizuka, Ritsu Dobashi, Yuji Wada*

Paper #366: **Pulse Detonation Engines in the Choked Flame Regime**

*Jim Karnesky, John Hoke, Fred Schauer*

Paper #368: **Measurement of Detonation Cell Size in Ammonia Based Mixtures**

*Remy Mével, Nabih Chaumeix, Joseph Shepherd*

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**11:10 WIP - Explosion/Fire****Pg. 135**

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Paper #347: **Mine Explosion Simulation at ULMIS Large-Scale Facility**

*Victor S. Shalaev, Alexander V. Gerasimov, Sergey V. Khomik, Sergey P. Medvedev*

Paper #349: **Pool Fire Suppression by Blankets**

*Fumiaki Takahashi, Jason P. Williams, Clay B. Criss, Sandra L. Olson, James S. T'ien*

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**11:10 WIP - Flame****Pg. 136**

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Paper #343: **Group Combustion Characteristics inside a Motorcycle Gasoline Direct Injection Engine**

*Hsin-Luen Tsai, J.-Y. Chen and Gregory T. Chin*

Paper #344: **A Study of the Influence by Diluting Carbon Dioxide to Methane Counterflow Flame**

*Yung-Sheng Lien, Yueh-Heng Li, Guan-Bung Chen, Yei-Chin Chao*

Paper #345: **Enhancement of Hydrogen Reaction in A Meso-Scale Burner Using Innovative Catalyst Segmentation and Cavity**

*Fang-Hsien Wu, Yueh-Heng Li, Guan-Bang Chen, Yei-Chin Chao*

Paper #346: **An Experimental Study on Influence of Markstein Number on Local Burning Velocity of Two-component Fuel Premixed Turbulent Flames**

*Masaya Nakahara, Fumiaki Abe, Jun Hashimoto, Atsushi Ishihara*

Paper #348: **Extinguishment of Cup Burner Flames of Propane and the FAA Aerosol Can Simulator Fuel by  $CF_3Br$  and  $C_2HF_5$**

*Fumiaki Takahashi, Viswanath R. Katta, Gregory T. Linteris, Harsha Chelliah, Oliver C. Meier*

Paper #355: **High Pressure and Temperature Lean Premixed Combustor Studies of Alternative Gas Fuels**

*David Beerer, Joe Velasco, Merna Ibrahim, Guillermo Gomez, Rich Hack, Adrian Narvaez, Prof. G. S. Samuelsen and Dr. V. G. McDonell*

Paper #358: **Study on Micromix Concept Based Combustors for Higher Flame Stability Limits and Low Emission**

*Bhupendra Khandelwal, Priyadarshini Murthy, Vishal Sethi*

**Paper #361: Comparison of Axial Forcing Effect on A Strongly Swirling Jet and Lifted Propane-Air Flame**

*S.V. Alekseenko, V.M. Dulin, Yu.S. Kozorezov, D.M. Markovich*

**Paper #362: Ignition Delay in Hydrogen-Air Mixtures: Low-Temperature Data Interpretation via Reaction Mechanism with Quantum Corrections**

*Andrey N. Starostin, Mikhail D. Taran, Yuri V. Petrushevich, Sergey P. Medvedev, Gennady L. Agafonov, Sergey V. Khomik*

**Paper #364: The Effect of Heating Rates on Low Temperature Hexane Air Combustion**

*P.A. Boettcher, R. Mével, V. Thomas and J.E. Shepherd*

**Paper #365: Forming Stability of Biodiesel/Water, /Water+Alcohol Emulsions, and the Burning Behavior of Droplets**

*C.H. Wang, G.J. Ueng, K.L. Pan, H.S. Su-Chen, J.Y. Yang*

**Paper #367: Prediction of Markstein Lengths for Hydrogen-Air and Hydrogen-Nitrous oxide Mixtures**

*Remy Mével, Jonathan Regele, Sally Bane, Guillaume Blanquart, Joseph Shepherd*

**Paper #369: Microgravity Combustion of Blended Fuels with Alcohol and Biodiesel/Diesel**

*Kuo-Long Pan and Ming-Chun Chiu*

**Paper #374: Explicit Analytic Prediction for Hydrogen-Oxygen Ignition Time at Temperatures Below Crossover**

*P. Boivin, A. L. Sánchez, F.A. Williams*

**Paper #380: Probing Dense Sprays with Gated, Picosecond, Digital Particle Field Holography**

*James Trolinger, Ivan Tomov, Wytze Van der Veer, Dunn-Rankin Derek and John Garman*

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**09:00 Welcome and Plenary Lecture**

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Paper #357

**Dynamics of Physical Explosions: A Tribute to Professor Boris Gelfand***Sergey P. Medvedev*

Professor Boris Efimovich Gelfand passed away on the 4<sup>th</sup> of October 2010 in Odintsovo (a small town near Moscow), at the age of 69 after long suffering from cancer. Professor Boris Gelfand made prominent contribution in various fields of shock wave, combustion and detonation science. He was a member of the Russian Academy of Natural Sciences, Doctor of Physical and Mathematical Sciences, Professor in Chemical Physics, Professor of Saint-Petersburg University of State Fire Service Ministry of Russian Federation for Civil Defense, Emergencies and Elimination of Consequences of Natural Disasters (EMERCOM), member of the Scientific Counsel on Combustion and Explosion (Russian Academy of Sciences), head of Laboratory of the N.N. Semenov Institute of Chemical Physics, Russian Academy of Sciences. He was involved into international scientific activity as a member of numerous committees at the International Colloquiums on Dynamics of Explosion and Reactive Systems and International Shock Wave Symposiums, and many other meetings. In the last years he was a member of the ICDERS Board of Directors. Scientific interests of Professor Boris Gelfand were extremely wide. He started research work from the study of self-ignition and detonation in two-phase gas-droplets and gas-particles systems. In parallel, he achieved a great success in the investigation of propagation of shock waves in liquids with gaseous bubbles. A lot of his works were devoted to the study of the interaction of shock waves with structures, dusty and porous systems. Boris Gelfand always appreciated friendship and joint work with Academician Ya.B. Zel'dovich. Starting from 1984 he developed further insight into the Zel'dovich's gradient mechanism of detonation initiation that currently became a standard of most relevant theoretical investigations. Special mention should be given to the profound research of hydrogen combustion and detonation that was initiated by Professor Boris Gelfand after Chernobyl accident at the end of the 1980s. The results of these long-term investigations were summarized in his recent monographs that represent part of totally ten monographs and textbooks where he is a title coauthor. In this memorial lecture we present a review of the works performed by the group of Professor Gelfand on dynamics of physical explosions. A physical explosion is considered as an accidental rupture of a pressurized vessel that can create shock waves in the environment. Professor Boris Gelfand extended examination of physical explosion sources from high-pressure gas to the two-phase systems such as dusty media and boiling liquids. Basing on the comparative study of different types of explosions the generalized description of the shock waves parameters is suggested.

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**10:00 (S1) Toward a Better Understanding of Shock-Tube Flows and Ignition Behaviors – I**

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Paper #9

**MMH Pyrolysis and Oxidation: Species Time-History Measurements behind Reflected Shock Waves***R. D. Cook, S. H. Pyun, D. F. Davidson, R. K. Hanson*

Species time-histories were measured by laser absorption during monomethyl hydrazine (MMH) pyrolysis and oxidation behind reflected shock waves. Species measured included OH, NH<sub>2</sub>, NH<sub>3</sub>, CH<sub>4</sub>, and MMH. Reflected shock conditions covered mixtures of 1% MMH in argon and 2.5% O<sub>2</sub> in argon ( $\phi=1$ ) over a temperature range of 1000 to 1300 K and pressures near 2.6 atm. Measurements of OH and NH<sub>2</sub> were performed using narrow-linewidth laser absorption at 307 nm and 597 nm, respectively; NH<sub>3</sub> and MMH were measured using CO<sub>2</sub> laser absorption at 9.6 and 10.22 microns, respectively; and CH<sub>4</sub> was measured using DFB laser absorption at 3.4 microns. Measurements are compared to current MMH pyrolysis and oxidation kinetic mechanisms. Significant differences exist between the measurements and these models, much of which can be attributed to uncertainties in the rate constants and branching ratios for MMH decomposition.

Paper #10

**Temperature Time-History Measurements in a Shock Tube Using Diode Laser Absorption of CO<sub>2</sub> Near 2.7 $\mu$ m***Wei Ren, Sijie Li, David F Davidson and Ronald K Hanson*

Shock tubes can be used to study chemical kinetics at elevated temperatures as they provide a well-controlled pressure and temperature environment. The initial temperature (T<sub>5</sub>) and pressure (P<sub>5</sub>) behind reflected shock waves can be routinely inferred from the measured incident shock velocity by using the traditional shock equations. However, non-ideal effects such as incident shock attenuation and boundary layer growth, disturb the uniformity of flow properties and results in temperature and pressure variations with time and position behind the reflected shock wave. These changes can be predicted using Mirels boundary layer theory. When performing chemistry study in a shock tube, this variation in reaction temperature can cause large uncertainties in the measurements of rate coefficients and ignition delay times. In this work, a temperature sensor with 40 kHz bandwidth based on wavelength-modulation absorption spectroscopy of CO<sub>2</sub> was applied to investigate the temperature time-histories behind both incident and reflected shock waves. The sensor accuracy was first demonstrated by measuring the initial temperature (1100-1500 K) of CO<sub>2</sub>/Ar behind reflected shock waves at a location 2 cm from the shock tube endwall. Temperature time-histories behind incident shock waves (640-850 K) and reflected shock waves were then measured at a second location 69.3 cm from the endwall. Repeatable experimental results reveal the fact that the temperature in region 2 declines slightly and then raises again, which is not predicted by Mirels theory. However, an improved Mirels model that includes the effect of the laminar-turbulent boundary layer transition, recently developed in our laboratory, can explain this observation. We expect this gasdynamic model can be implemented in other cases to further extend our knowledge of the shock tube performance.

Paper #81

### **Auto-Ignitions of Methane at Intermediate and High Temperatures**

*D.G. Ignatenko, N. Joshi, V.V. Leschevich, V.V. Martynenko, O.G. Penyazkov, K.L. Sevrouk, S.I. Shabunya, A.V. Skilondz, V. Tangirala*

Autoignitions of CH<sub>4</sub>/Air mixtures at equivalence ratios  $f = 0.5 - 2$  and gas density of 2 and 4 kg/m<sup>3</sup> were studied in shock tube and rapid compression machine at the temperature range of 900 - 100 K. Ignition times and autoignition modes were measured by using OH, CH emission observations, pressure and ion-current measurements. Experiments show the reduction of mean activation energy of methane/air mixtures in comparison with shock-tube tests at elevated temperatures. Linear Arrhenius approximations of RCM results demonstrate reasonable coincidence with a high-temperature shock-tube induction time curves. Empirical correlations for methane ignition times have been deduced from the experiments. Database for validations of chemical kinetic mechanisms under wide temperature range has been obtained.

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#### **10:00 (R1A) DDT - I**

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Paper #74

### **Role of Transverse Shock Waves on DDT in a Very Rough-Walled Channel**

*G. Ciccarelli, C. Johansen and M. Kellenberger*

Experiments looking at flame acceleration and DDT in a channel with a rough bottom wall was performed. The channel is 7.6 cm wide and the effective height is 3.8 cm, the surface roughness is created by a layer of 1.26 cm (and 0.63 cm) diameter beads. High speed shadowgraph video was used to capture the explosion front structure. Abrupt transition to detonation occurred at initial pressures greater than 12 kPa, the detonation eventually fails because the cell size is smaller than the effective channel height. For initial pressures of 9 and 10 kPa the front accelerates continuously to a velocity well in excess of the speed of sound of the combustion products and just below the CJ detonation velocity. This demonstrates it is possible to achieve a smooth transition from diffusion driven flame propagation to shock ignition driven detonation wave. It is proposed that flame acceleration past the speed of sound of the combustion products is possible in a very rough-walled channel because lead shock interactions with the rough surface can result in vorticity generation in the reaction zone and auto-ignition at hot spots on the wall.

Paper #234

### **Experimental and Computational Study on DDT for Hydrogen-Methane-Air Mixtures in Tube with Obstacles**

*Rafal Porowski, Andrzej Teodorczyk, Knut Vaagsaether, Dag Bjerketvedt*

DDT in hydrogen-methane-air mixtures have been studied by experiments and numerical simulations. The geometry in the experiments and simulations where a 6 m long, 140 mm ID tube with repeated obstacles with blockage ratios between 0.4 and 0.7. The spacing of the obstacles where 1, 2 and 3 tube diameters. The hydrogen-methane-air mixture was stoichiometric and the fuel mixture was varied from 0 % methane to 50 %. Both simulations and experiments showed fast deflagration, quasi-detonation and DDT followed by a CJ-detonation.

Paper #313

### **Oscillating Propagation of Near-Limit Detonations of CH<sub>4</sub>/O<sub>2</sub> System in a Small Diameter Tubes**

*A. SUSA, S. Hasegawa, H. Yokoyama, T. Endo, Y. Ogawa, Y. Morii, N. Tsuboi*

We measured oscillating behavior of CH<sub>4</sub>/O<sub>2</sub> system near-limit detonations in a small diameter glass tubes. Oscillating processes were examined experimentally by changing the initial pressure and tube diameter. The failure process in the oscillating cycle strongly depending on the initial pressure and tube diameter. That is, the decoupling process of shock and flame depends on the strength of shock wave and the tube diameters.

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#### **10:00 (R1B) Heterogeneous/Multiphase Reactive System - I**

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Paper #329

### **Ignition of Aluminum Particle Clouds Behind Reflected Shock Waves**

*Kaushik Balakrishnan, Allen L. Kuhl, John B. Bell and Vincent E. Beckner*

Extending on a companion paper in this colloquium, the dispersion, ignition and combustion characteristics of aluminum particle clouds is investigated numerically behind reflected shock waves. It is observed that a higher proportion of the Al cloud by mass burns for a higher initial cloud concentration. Vorticity from the cloud wake and from that deposited by the reflected shock cause the particle cloud to convolute, and this effect is particularly very significant for higher concentration clouds. Faster ignition delay times and higher overall Al burning by mass are observed for stronger incident shock Mach numbers due to the consequent hotter gas temperatures behind the reflected shock wave. A mass-weighted ignition parameter is introduced in this study and is identified to be particularly useful to determine overall cloud ignition trends.

Paper #246

### **Effects of Addition of Energetic Nanoparticles on Fuel Droplet Combustion at Dilute and Dense Particle Loading**

*Yanan Gan and Li Qiao*

The burning characteristics of fuel droplets containing aluminum nanoparticles at dense and dilute loading rates were investigated. Physical and chemical methods to disperse particles evenly in liquids and to avoid agglomeration were

described. Droplets were suspended on the crossing point of two thin silicon carbide fibers and the burning process was recorded using two orthogonally located high-speed digital cameras with and without backlight respectively. Droplet temperature history was acquired using fine wire thermocouples with data acquisition systems. Particle concentration, surfactant concentration, type of base fluids were varied to study their effects on droplet burning characteristics and burning rate. The results show that at high particle loading rates without presence of a surfactant, nanoparticles tend to agglomerate easily. And the burning process has two distinctive stages - burning of the liquid fuel droplet as the first stage and burning of the large particle aggregate as the second stage. At low particle loading rates, however, most particles were transported to the flame zone shortly after ignition and were burned during the burning process of the liquid droplet. The results also show that addition of surfactant reduces droplet burning rate because of a surfactant layer formed around the primary droplet which inhibit diffusion. Similarly, addition of particles also reduces droplet burning rate, especially at high loading rate because of the solid agglomerate formed inside the droplet which also inhibit diffusion.

Paper #150

#### **Flame Fronts in Iron Suspensions Dominated by the Effect of Discreteness**

*Sam Goroshin, Francois-David Tang, Andrew J. Higgins*

The exact solution for a flame front propagating in a heterogeneous system of discrete, point-like heat sources is obtained without resorting to a representation of the sources by a spatially continuous function. When the flame front is influenced by discreteness, a propagation limit with non-zero flame speed appears if the sources are regularly distributed in space. The flame speed in the discrete regime of propagation is independent of the combustion time of the sources. This discrete regime of front propagation is observed experimentally in suspensions of iron particles burning in oxygen-xenon mixtures.

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### **10:00 (R1C) Pre-mixed Flames - I**

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Paper #61

#### **Outwardly Propagating Spherical Flames with Thermally Sensitive Intermediate Kinetics and Radiative Loss**

*Huangwei Zhang, Xialing Zhang, Zheng Chen*

Due to the simple flame configuration and well-defined flame stretch rate, the outwardly propagating spherical flame (OPF) method is one of the most favorable methods to measure the laminar flame speed and Markstein length. In the literature, OPF was been extensively studied by using asymptotic techniques. However, only one-step, irreversible, global reaction model was employed. In such a one-step model the fuel is converted directly into products and heat, and thus the role of energetic active radicals is not considered. Numerous elementary reactions related to fuel and reactive intermediate species appear in practical combustion of hydrocarbon fuels. As such, flame propagation is not only influenced by properties of fuel, but also by those of intermediate species (especially radicals involved in chain branching reactions). In order to achieve more essential understanding of spherical flame propagation, chain-branching kinetics of intermediate species should also be considered. The outwardly propagating spherical flames (OPF) with thermally sensitive intermediate kinetics and radiative loss are asymptotically investigated in the present study. The theoretical correlation describing flame propagating velocity and flame radius of large-flame-radius OPF is derived, which includes Lewis numbers of fuel and radical species, heat release and radiative heat loss. The effects of Lewis numbers of fuel and radical as well as radiative heat loss on OPF and the Markstein length are examined. It is found that OPF is strongly influenced by the fuel Lewis number, radical Lewis number and radiative heat loss. Besides, it is shown that the Markstein length increases with the fuel Lewis number and radiative heat loss, while decreases with the radical Lewis number.

Paper #70

#### **Characteristics of Laminar Premixed H<sub>2</sub>/CO/CH<sub>4</sub>/Air Opposed-jet Flames**

*T. S. Cheng, Y.-C. Chang, Y.-C. Chao, G.-B. Chen, Y.-H. Li, C.-Y. Wu*

Extensive fossil fuel consumptions have resulted in rapid fuel depletion as well as atmospheric and environmental pollutions. In order to reduce these impacts, two alternatives are currently considered: either to improve the combustion efficiency with considerable reductions in the pollutant emissions into the atmosphere or more significantly, to replace fossil fuel usage as much as possible with environmentally friendly, clean and renewable energy sources. Among the various renewable energy sources, the use of gasified biomass that contains a mixture of carbon monoxide, hydrogen and methane, together with carbon dioxide and nitrogen, can be more versatile and attractive. It becomes essential, therefore, to develop combustion techniques that can burn the gasified biomass or low-grade syngas effectively and to understand chemical and physical properties of flames for such kind of fuels. Since the combustion characteristics of blended fuels may differ substantially from those of single-component fuels, therefore, the detailed investigations of flame structures and chemical kinetics of blended fuels are of vital importance. Literature survey indicates that no detailed investigation on the characteristics of H<sub>2</sub>/CO/CH<sub>4</sub>/air flames has been reported. Therefore, in the present study, the premixed H<sub>2</sub>/CO/CH<sub>4</sub>/air flames are studied to delineate its burning phenomena, flame structures, and chemical kinetics. The combustion characteristics of the stoichiometric, premixed H<sub>2</sub>/CO/CH<sub>4</sub>/air opposed-jet flames are experimentally and numerically investigated. Results show that the predicted flame temperatures and their spatial distributions are in good agreement with the measured data. The calculated laminar burning velocity indicates that the maximum value occur at the condition of 90% CO - 10% CH<sub>4</sub> and 94% CO - 6% CH<sub>4</sub> for 10% and 20% of H<sub>2</sub> additions, respectively. Finally, we found that the reaction  $\text{OH} + \text{CO} \leftrightarrow \text{H} + \text{CO}_2$  plays an important role in H<sub>2</sub>/CO/CH<sub>4</sub>/air flames.



Paper #159

**Weak Flame Responses to Octane Number and Pressure in a Micro Flow Reactor with a Controlled Temperature Profile***Mikito Hori, Akira Yamamoto, Hisashi Nakamura, Takuya Tezuka, Susumu Hasegawa and Kaoru Maruta*

For developing cleaner and more efficient internal combustion devices, the understandings on ignition process of practical fuels are required. This study focused on ignition characteristics of a blended fuel of n-heptane and iso-octane, which is a Primary Reference Fuel (PRF) of gasoline. And as a well-defined, simple experimental system to investigate the ignition characteristics of the fuel, a micro flow reactor with a controlled temperature profile is employed in this study. In the micro flow reactor, a quartz glass tube with a smaller inner diameter than the ordinary quenching diameter is heated by an external heat source so as to have a stationary temperature profile (300 - 1300 K). Due to the small inner diameter, the gas phase temperature in the tube strongly depends on the temperature of the inside surface of the tube. The flow in the tube is laminar and constant pressure. In the previous study, flame responses to the inlet flow velocity were investigated using PRF100 (iso-octane 100%)/air mixture under the atmospheric pressure. In a very low flow velocity region ( $U < 8$  cm/sec), stable weak flames with multiple reaction zones (Weak flames) were observed. Observation of weak flames is expected to be efficient to investigate the ignition process of the fuel at each temperature region. Focusing on this weak flames phenomena, their responses to the various octane numbers and the pressures were investigated. In addition, one-dimensional computations were conducted using detailed reaction mechanism of PRF. Obtained computational results were compared with experimental results. First, the weak flames responses to various octane numbers were examined under the atmospheric pressure. In the case of PRF0/air, three-stage reaction zones, which consist of cool flame and two separated hot flames, were observed. The cool flame was weakened and second hot flame shifted to higher temperature region, as octane number increased. Computed HRR profiles well reproduced the experimental results. By conducting the experiments and computations to investigate the weak flames response to octane numbers, the capability of the micro flow reactor to distinguish and examine the different ignition process for various octane-rated fuels was demonstrated. Then, further experiments and computations were conducted to investigate the weak flames response to pressure. As the pressure increases, increasing cool and first hot flame and their shifts to low temperature region were confirmed. These tendencies were intensified especially for the low octane-rated fuels. Difference of ignition characteristics with various octane numbers was characterized by low and intermediate temperature oxidation especially under high pressure. By investigating oxidation characteristics in each temperature region separately for various octane-rated fuels under elevated pressure, potential of the micro flow reactor, which enable us to obtain the unique understandings on ignition characteristics of practical fuels, was confirmed. And further investigation has a possibility to show an alternative index to octane number which systematizes ignition characteristics of practical fuels. The obtained results should be useful for the diverse ways, for example, reaction path analysis, development and validation of reaction kinetics, which are supposed to be future works.

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**11:45 Session (S1) Toward a Better Understanding of Shock-Tube Flows and Ignition Behaviors - II**

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Paper #110

**Interpretation of Low-Temperature, High-Pressure Ignition Data from a Shock Tube with Significant Pre-Ignition Pressure Rise***Christopher J. Aul and Eric L. Petersen, Henry Curran, Mustapha Fikri and Christof Schulz*

Discrepancies between shock-tube data and simulation results have been observed for methane, propane, and fuel blends with up to  $C_4$  alkanes at temperatures below 1100 K. These discrepancies can in part be attributed to a significant rise in pressure (and correspondingly temperature) before main ignition behind the reflected shock wave. This early, significant increase in pressure is not predicted by chemical kinetics and is at present suspected to be due to early reactions in this facility and others alike, as evidenced by the accompanying appearance of excited intermediates such as  $OH^*$  and  $CH^*$ . While the origin of this early reaction and subsequent pressure rise is not known at this time, it appears for the cases presented herein that it is not the result of a facility-induced pressure rise due to boundary layer interactions. Nonetheless, when the measured pressure rise is taken into account, the discrepancies between the shock-tube data and the simulation results are rectified. The pre-ignition pressure (and thus temperature) increase greatly accelerates the reactions in the gas mixture behind the reflected shock wave in a shock tube, leading to the earlier-than-expected strong ignition. A previous set of methane-blend ignition experiments near 800 K and 20 atm were used to demonstrate the approach, with excellent results. A similar comparison was shown for a fuel-lean propane-air set of experiments at 30 bar. A concluding point that should be made is that for shock-tube experiments showing extreme pressure increases such as those discussed herein, documenting the ignition delay time data by using the initial temperature and pressure behind the reflected shock wave is inadequate. Some representation of (at least) the measured pressure increase should be given, whether in the form of an equation or the actual time-dependent pressure measurement.

Paper #163

**Optical Investigation of Shock Induced Ignition of Different Biofuels***K.A. Heufer, H. Olivier, S.P. Medvedev, S.V. Khomik*

In the present study shock tube ignition delay time measurements for three different biofuels, i.e. ethanol, 2-MTHF, and 2,5-DMF, are performed. Pressures have been varied from 5 to 13 bar and temperatures from 920 to 1300 K. High temperature ignition data have been correlated using Arrhenius approach. The focus of the present study lies on optical investigations of the ignition process. A rectangular shock tube in combination with a high speed Schlieren setup has

been used to perform time resolved visualizations of the ignition. At high temperatures all investigated fuels behave similar. Homogenous ignition occurs near the end wall followed by a short deflagration stage and transformation to detonation. At low temperatures local spot ignition occurs for ethanol and 2,5-DMF followed by a deflagration of the whole fuel-air-mixture. In contrast 2-MTHF does not show spot ignition but homogenous ignition at low temperatures. In this case the combustion process is significantly faster than for the deflagration process of ethanol and 2,5-DMF. These different ignition modes can have a significant influence on combustion engine performances. For SI engines fuels are preferable that do not tend to detonate like ethanol and 2,5-DMF. Homogenous auto-ignition as observed for 2-MTHF is an important aspect for diesel engines or modern engine concepts like HCCI for improving performance and reducing emissions.

Paper #231

#### **Towards Consolidation of Hydrogen-air Ignition Data from Shock Tube and Flow Reactor Experiments**

*Sergey P. Medvedev, Sergey V. Khomik, Aleksander K. Heufer, Herbert Olivier*

The investigation of self-ignition of 15% hydrogen in air mixture was performed in the shock tube operated under the over-tailored conditions. Pressure and emission recording along with high-speed photography were used for registration of ignition events. The determination of ignition delay under transient pressure/temperature conditions was performed by applying the Livengood-Wu integration technique. It was found that in the low-temperature range ( $T < 900$  K) the normalized ignition delay data are nearly two times less than that predicted by the correlation of Peschke and Spadaccini (1985). A reasonable agreement with flow reactor data shows that the proposed technique of over-tailored shock tube operation is suitable for simulating ignition of lean hydrogen-air mixtures under gas-turbine conditions.

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#### **11:45 (R2A) DDT - II**

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Paper #27

#### **Deflagration-to-Detonation Transition in Highly Reactive Combustible Mixtures**

*M. A. Liberman, M. F. Ivanov, A. D. Kiverin, M. S. Kuznetsov, A. A. Chukalovsky, T. V. Rakhimova*

High resolution numerical simulations are used to study the mechanism of deflagration-to-detonation transition (DDT). The computations solve two-dimensional, time-dependent, reactive Navier-Stokes equations including the effects of compressibility, molecular diffusion, thermal conduction, viscosity and detailed chemical kinetics for the reactive species with subsequent chain branching, production of radicals and energy release. It is shown that from the beginning the flame accelerates exponentially producing shock waves far ahead. On the next stage the flame acceleration decreases and the shocks are formed close ahead of the flame front. The final stage is the actual transition to detonation. During the second stage a compressed unreacted mixture of increased density enters the flame producing a high pressure pulse which enhances reaction rate and the heat release in the reaction zone with a positive feedback coupling between the pressure pulse and the reaction rate. As a result the peak of the pressure pulse grows exponentially, steepens into a strong shock which is coupled with the reaction zone forming the overdriven detonation. This new mechanism of DDT is different from the Zel'dovich's gradient mechanism. The temperature gradients, which appear in the form of hot spots and the like, are not suitable to initiate detonation.

Paper #76

#### **Deflagration-to-Detonation Transition in Hydrogen-Air Mixtures with Concentration Gradients**

*K.G. Vollmer, F. Ettner and T. Sattelmayer*

The hazardous potential of hydrogen-air mixtures has intensively been studied assuming a perfect mixture of fuel and oxidant. However, comprehensive risk assessment studies have shown that an inhomogeneous mixture with a vertical concentration gradient is much more likely to be generated in a real accident scenario. From a safety point of view, the open question remaining is if the established criteria to determine whether deflagration-to-detonation transition (DDT) can occur or not, like the 7-lambda criterion, can be applied to inhomogeneous mixtures as well. For this purpose, an injection mechanism is designed to produce vertical fuel concentration gradients inside a horizontal tube. The tube is equipped with obstacles to enhance flame acceleration. Photodiodes and pressure transducers record flame and shock arrival times. By varying fuel content, strength of concentration gradient, blockage ratio and spacing of the obstacles inside the tube, a large variety of configurations is examined. The maximum flame velocity observed in each experiment is compared with the velocities obtained from one-dimensional theory. DDT can be attributed to a distinct velocity rise from the sound speed of the combustion products to the Chapman-Jouguet velocity of the mixture which goes along with a considerable rise in maximum pressure. It is found out that in homogeneous mixtures, the 7-lambda criterion often predicts DDT reasonably well. However, the presence of a concentration gradient can move the point of DDT to considerably higher or lower fuel concentrations. This can clearly be attributed to the multi-dimensional effects occurring in the different configurations. It is concluded that DDT criteria for homogeneous mixtures are not sufficient to assess scenarios with fuel concentration gradients. As the latter ones represent the more realistic accident scenarios, further research is required to quantify the additional effects and to produce more general DDT criteria.

Paper #310

#### **Effects of Shock Waves, Boundary Layer and Turbulence on Flame Acceleration and DDT in Highly Reactive Mixtures**

*M. Kuznetsov, J. Grune, I. Matsukov*

The deflagration-to-detonation transition experiments with highly reactive hydrogen-oxygen mixtures have been carried out in a channel geometry with respect to investigate effects of advancing shock waves, boundary layer and turbulence

on flame acceleration and DDT. Linear rectangular channels of 50x50 mm and 5x5 mm with glass windows or transparent capillary tubes of 2-4 mm id were used for detonation experiments. Three basic stages of DDT were observed experimentally: (1) the exponentially accelerated “finger” flame producing shock waves far ahead of the flame; (2) the second stage when the flame acceleration law changes so that the advancing shock waves are generated directly on the flame front, (3) the final stage is actual transition to a detonation. During the first stage, the flame accelerates exponentially as “finger” flame due to geometry factor. Flame develops up to sonic speed in a laminar flow independent of the tube roughness because boundary layer is too small. It was shown that the smaller the tube diameter the less distance is required for the flame to reach sonic speed. During the second stage, due to the “tulip” flame formation the flame acceleration law changes in such way that shock waves are formed in the immediate proximity ahead of the flame front, formally on the flame surface. This provides the conditions for strong feedback between flame and advanced shock with formation of preheat zone. The preheat zone consisting of chemically frozen material adjusted ahead of the flame front. The role of turbulence again is not evident in smooth channels filled with highly reactive mixtures. For low pressures of  $p=0.1 - 0.2$  bar the tube was not long enough and very intensive flame acceleration and DDT were initiated due to collision of reflected shock waves and flame. Detonation can also occur after 1-5 shock wave reverberations until pressure and temperature of unreacted material will reach conditions for the flame to be accelerated fast enough for DDT. Shock-flame interaction and adiabatic compression of unreacted material play an important role for detonation preconditioning and DDT process. Boundary layer and turbulence do not play a role for DDT in relatively short smooth tubes filled with highly reactive mixtures.

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**11:45 (R2B) Heterogeneous/Multiphase Reactive System - II**

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Paper #53

**Auto-ignition Conditions of Iron Micro Powders in Heated Oxygen***Vladimir V. Leschevich, Oleg G. Penyazkov, Jean-Christophe Rostaing*

The experiments have been conducted on auto-ignitions of iron powders with particle sizes ranged from 6  $\mu\text{m}$  to 125  $\mu\text{m}$  at oxygen pressures up to 28 MPa and temperatures varied from 550 to 1100 K. The conditions that can provoke spontaneous ignition of the metal particle layers were obtained by means of rapid compression machine (RCM). Ignition times were measured by using emission observations and pressure measurements. For different particle sizes, a number of observations on ignition and combustion characteristics have been built as functions of the oxygen density and temperature. The variation of particles temperature during combustion was measured by photoemission method based on analysis of photoelectron energy distribution. Collected experimental database is useful for development and validation of mathematical models describing auto-ignition and combustion phenomena of iron particles in heated oxygen.

Paper #265

**Interfacial Instabilities in Explosive Gas-Particle Flows***David L. Frost, Yann Gregoire, Samuel Goroshin and Fan Zhang*

Experimental studies have shown that when solid particles are explosively dispersed, the particles often develop a nonuniform spatial distribution. This may take the form of clusters of particles or coherent jet-like particle structures which may persist for some distance during the dispersal process. Particle clustering influences the particle aerodynamics, particle-gas mixing and burning, and blast wave propagation and is a ubiquitous feature of enhanced blast metalized explosives. A series of exploratory experiments has been carried out to investigate the influence of particle diameter and density and explosive mass on the development of instabilities at the front of an expanding particle cloud. Both spherical and conical charge arrangements were used. In the latter, a bed of dry particles was placed above a spherical explosive charge at the apex of the cone. The experiments show that the spatial uniformity of the expanding particle cloud depends on the particle size, density and ratio of the mass of the particle layer to the mass of the explosive charge. An examination of the relative tendency for instabilities to develop on the surface of the particle bed suggests that a particle compaction Reynolds number corresponding to the ratio of inertial forces to particle viscosity forces plays an important role in the breakup of the particle bed. The number of particle jets that form during explosive dispersal increases with increasing Reynolds number.

Paper #43

**Models for Fast Combustion Waves in Nanocomposite Thermite Powders***Benjamin D. Shaw, Birce Dikici, & Michelle L. Pantoya*

The combustion of nanometric aluminum (Al) powder with an oxidizer such as molybdenum trioxide ( $\text{MoO}_3$ ) is studied analytically. The analysis was performed to identify combustion wave propagation models that are in concurrence with experimental results from flame tube experiments. Both deflagration and detonation models were investigated. In the deflagration models, individual Al particle gasification characteristics were evaluated to determine whether powder deflagrations would propagate in a fashion such that particles would evaporate before entering the primary reaction zone. Evaluation of characteristic times relevant to propagation of a deflagration reveals that particles only less than about 1.7 nm in diameter evaporate before appreciable chemical reactions occur. Because experimental studies typically use Al particles greater than 1.7 nm in diameter, it is concluded that nanocomposite powder deflagrations would typically be controlled by multiphase diffusion effects and particle interactions. Deflagration models based on particle interactions and multiphase diffusion, however, predict orders of magnitude slower propagation rates than what are experimentally observed. This study also considers detonation wave models and uses a one-dimensional Chapman-Jouget approach.

Detonation waves are analyzed assuming both frozen and equilibrium sound speeds in multiphase mixtures. Wave speeds that are in basic agreement with experimental data are obtained provided that multiphase equilibrium sound speeds are applied at the downstream edge of the detonation wave. The results indicate that the fast combustion waves observed with nanocomposite Al-MoO<sub>3</sub> powder mixtures are likely multiphase detonations and that equilibrium sound speeds of multiphase mixtures play an important role in determining speeds of fast combustion waves.

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**11:45 (R2C) Pre-mixed Flames – II**

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Paper #260

**Premature Flame Initiation in SI Engines: Modeling Studies on the Role of Residual Gas***M. Magar, R. Schießl, U. Maas.*

In this article the influence of residual gas on the occurrence of pre-ignition, a premature onset of combustion with deflagrative flame propagation in SI engines is discussed. A modeling approach is presented combining numerical simulations in a homogeneous reactor model with simple statistics. The cylinder charge is modeled as an ensemble of homogeneous reactors with a statistical distribution of residual gas. Through the simulation the required conditions (residual gas temperature and mass fraction for given initial pressure, temperature and fuel-air-ratio) for pre-ignition are determined. The varying distribution of the residual gas in the cylinder charge is modeled by a beta-pdf. Thus the pre-ignition probability for a given residual gas temperature and a mass fraction variance can be estimated. The results show that even very small overall amounts of residual gas can, if concentrated in a few regions of the combustion chamber trigger a local autoignition whereas if the residual gas mixes homogeneously with the fresh gas, no effect was observed.

Paper #328

**Effects of Hydrogen Peroxide on Methane Premixed Flames***Guan-Bang Chen, Yueh-Heng Li, Tsarng-Sheng Cheng, Hung-Wei Hsu, Yei-Chin Chao*

The effect of hydrogen peroxide on methane/air premixed flames are numerically investigated. Hydrogen peroxide is used as fuel additive or oxidizer. Results show that the laminar burning velocities are increased no matter H<sub>2</sub>O<sub>2</sub> is used as fuel additive or oxidizer. When H<sub>2</sub>O<sub>2</sub> is used as fuel additive, the adiabatic temperature is not increased obviously, especial in the fuel-lean conditions. However, when H<sub>2</sub>O<sub>2</sub> is used to replace air, the adiabatic temperature is obviously increased. OH concentration is always increased unless lower H<sub>2</sub>O<sub>2</sub> concentration is used. For CO emission, the CO emission is decreased with adding H<sub>2</sub>O<sub>2</sub> as fuel additive. Using H<sub>2</sub>O<sub>2</sub> to replace air will increase CO emission. If H<sub>2</sub>O<sub>2</sub> has a lower concentration (30% and 40% in the study), CO emission will be decreased. In respect to NO<sub>x</sub> emission, using H<sub>2</sub>O<sub>2</sub> to replace total air will never produce NO<sub>x</sub>. For the other cases, the NO<sub>x</sub> emission is always increased. Finally, the results of sensitivity analysis show that the reactions  $2OH + M \leftrightarrow H_2O_2 + M$  and  $OH + H_2O_2 \leftrightarrow HO_2 + H_2O$  play important roles in CH<sub>4</sub>/air/ H<sub>2</sub>O<sub>2</sub> flames.

Paper #127

**Effect of Elevated Pressures on Laminar Burning Velocity of Methane+Air Mixtures***M. Goswami, S. Derks, K. Coumans, M.H. de Andrade Oliveira, A.A. Konnov, R.J.M Bastiaans, C.C.M Luijten, L.P.H de Goey*

Flame speed is an important parameter required in simulating combustion systems like IGCC and designing burners. The present work aims to measure flame speed of CH<sub>4</sub>-air mixtures at conditions up to 5 bar at different equivalence ratios using heat flux method that stabilizes a flat flame. The heat flux method is based on measuring the net heat loss from the flame to the burner and tuning the unburnt gas velocity such that no net heat loss to the burner is observed. This will be an adiabatic state of the flame. This method offers convenience as no flame stretch is involved and does not require to be extrapolated. The results derived from the experiments are compared with simulations utilizing two most popular chemical reaction mechanisms. The paper also aims to analyze the importance of certain reactions in methane combustion.

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**14:30 (S2) Shock Induced Ignition - I**

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Paper #31

**Shock Tube Measurements of Ignition Delay Times for the Butanol Isomers***I. Stranic, D. P. Chase, J. T. Harmon, S. Yang, D. F. Davidson, R. K. Hanson*

Butanol is a bio-fuel candidate with several important advantages over ethanol. It has a larger energy density, is not hydroscopic, which means it can be transported in gasoline pipelines, and can be blended with gasoline in higher concentrations [1]. As a result, there is significant interest in developing a chemical kinetic mechanism in order to accurately model butanol combustion. One of the simplest methods to evaluate the global accuracy of a chemical kinetic mechanism is by measuring the ignition delay time of a fuel behind the reflected shock wave in a shock tube. Although ignition delay time measurements of the butanol isomers exist, no single study has measured delay times for all isomers over a wide range of conditions. These measurements are needed to allow direct comparisons of model simulations with a consistent set of data. Here, ignition delay time was measured for all four isomers of butanol. Conditions covered temperatures between 1100 and 1600 K, pressures between 1.5 and 43 atm, and equivalence ratios of 1.0 and 0.5 in mixtures containing 4% O<sub>2</sub> dilute in argon. Several other data sets were collected at 1.0-1.5 atm in order to replicate conditions used by previous researchers. Additional data were collected at 23 atm for stoichiometric 1-butanol mixtures in

air at temperatures as low as 800 K. To our knowledge, these are the first low temperature measurements of 1-butanol ignition delay time at near-constant volume conditions. These low-temperature measurements were performed using driver inserts and driver gas tailoring to insure near-constant-volume test conditions.

Paper #54

#### **Methyl and Ethyl Esters as Biodiesel Surrogates: Observations on Trends in Ignition Behavior**

*Benjamin Akih-Kumgeh, Jeffrey M. Bergthorson*

A sustainable energy future will likely involve increased use of biofuels such as biodiesel. On the other hand, concerns about the associated costs and environmental neutrality, prompts a closer look at biofuel production methods with the goal of improving the sustainability of the process. While biodiesel is mainly produced by methanol-based transesterification of fatty acid triglycerides in acidic or alkaline media, the possibility of using other alcohols are being explored with increasing interest. Successful system level tests of ethyl ester as biodiesel have been reported. The possibility of using mixtures of methanol and ethanol in the transesterification of soy bean oil have been explored by Joshi et al., concluding that the resulting methyl and ethyl ester mix can offer improved physical properties. Further use of various alkyl esters beside methyl esters in combustion engines can be guided by understanding their relative combustion and physico-chemical properties through systematic experimental studies. Previous studies by Metcalfe et al. explored the relative ignition of the ester isomers, ethyl propanoate (EP), and methyl butanoate (MB), concluding that the EP is more readily ignited than MB under the same conditions. In a recent study of the ignition of selected C<sub>3</sub> oxygenated hydrocarbons, the current authors showed that ethyl formate (EF) is more reactive than its ester isomer, methyl acetate (MA). In this study new experimental data for EP and ethyl acetate (EA) are reported. Together with literature data for methyl formate (MF), EF, MA, and MP, their ignition behavior is explored to reveal the effect of methyl and ethyl ester groups on the same carboxylic acid. This relative behavior is further put into perspective by considering the effect of ester isomers as exemplified by the three surrogates, MP, EP and MB. These comparisons are done for mixtures of fuel, oxygen and argon under conditions of constant equivalence ratios, phi, oxygen/argon ratios, D, and nominal pressures, p, over a range of post-reflected shock temperatures, T.

Paper #104

#### **Shock Tube Study of the Influence of NO<sub>x</sub> on the Ignition Delay Times of Natural Gas at High Pressure**

*J. Herzler, C. Naumann*

The influence of NO<sub>x</sub> on the combustion characteristics of natural gas is important for the modeling of gas turbines and HCCI engines with exhaust gas recirculation, and of gas turbines with reheat combustion. Even small amounts of nitrogen oxides lead to significantly shorter ignition delay times because NO and NO<sub>2</sub> are recycled in the hydrogen and hydrocarbon oxidation environment. This was found for a variety of systems like H<sub>2</sub>, CO, CH<sub>2</sub>O, C<sub>1</sub>, C<sub>2</sub> and higher hydrocarbons. Only few studies were performed at high pressures, mainly by the group of Dagaut in a jet-stirred reactor, by Rasmussen et al. in a laminar flow reactor and by Sivaramakrishnan et al. in a single-pulse shock tube. There are no ignition delay time studies of natural gas in the presence of NO<sub>x</sub> at high pressures despite the importance of these data for modern combustion concepts. Therefore we performed studies of natural gas reference fuel (92 vol% CH<sub>4</sub>, 8 vol% C<sub>2</sub>H<sub>6</sub>) / O<sub>2</sub> / NO<sub>2</sub> / Ar mixtures with NO<sub>2</sub> contents of 20 - 250 ppm NO<sub>2</sub> at gas turbine relevant conditions (16 bar, Φ = 0.25 - 1) in a shock tube. Even these small amounts of NO<sub>2</sub> lead to a significant reduction of the ignition delay times. The influence of NO<sub>2</sub> on ignition delay times is increasing with decreasing equivalence ratio. The experimental results are predicted very well by simulations with different mechanisms. We used combinations of the hydrocarbon subsystem of the RD mechanism, which is very well suited for simulations of natural gas at these conditions, with different NO<sub>x</sub> subsystem by Rasmussen et al., Sivaramakrishnan et al. and Hori et al. No significant differences are found between the predictions of the individual mechanisms. Sensitivity analyses at 1100 and 1300 K show that the most important reactions describing the influence of NO<sub>x</sub> at our conditions characterized by high pressure and low NO<sub>x</sub> concentrations are R1 CH<sub>3</sub> + NO<sub>2</sub> ⇌ CH<sub>3</sub>O + NO and R2 NO + HO<sub>2</sub> ⇌ NO<sub>2</sub> + OH. With increasing temperature R3 NO<sub>2</sub> + H ⇌ NO + OH gains importance. The influence of NO, which is the main NO<sub>x</sub> species formed during combustion, on the ignition can also very well be predicted by the mechanisms validated in this study because NO and NO<sub>2</sub> are closely related by the reactions above. Simulations show that its influence is about half as strong as the one of NO. Rasmussen CL, Rasmussen AE, Glarborg P. (2008). Combust. Flame 154: 529. [2] P. Dagaut P, Nicolle A. (2005). Combust. Flame 140: 161. Sivaramakrishnan R, Brezinsky K, Dayma G, Dagaut P. (2007). Phys. Chem. Chem. Phys. 9: 4230. Herzler J, Naumann C (2009). Proc. Combust. Inst. 32: 213. Hori M, Matsunaga N, Marinov NM, Pitz WJ, Westbrook CK. (1998). Proc. Combust. Inst. 27: 389.

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#### **14:30 (R3A) DDT – III**

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Paper #41

#### **Effect of Radiation Preheating on Dynamics of Wrinkled Flames**

*Vladimir Karlin*

~~In this work effect of radiation preheating of unburnt mixture by propagating deflagration front is studied from the viewpoint of its ability to form a promoting temperature gradient and trigger transition to detonation. We investigate the effect of radiation preheating of the unburnt mixtures, when they are traveling through the wrinkles on the flame surface, in order to estimate a possibility of significant temperature rise. Further, numerical simulations of a simplified mathematical model are carried out. They demonstrate plausibility of the proposed mechanism of the deflagration to detonation transition.~~

Paper #207

### **Effect of Wall Conditions on DDT in Hydrogen-Oxygen Mixture**

*Motoki Fukuda, Edyta Dzieminska, A.Koichi Hayashi, Eisuke Yamada and Nobuyuki Tsuboi*

The transition from deflagration to detonation is one of the phenomena are not elucidated enough until today passed for about 130 years from detonation is verified experimentally in 1840s. These days due to the progress of a computer, various numerical studies on DDT have been starting to perform. However there are a few performances considered the pressure dependency of reaction rate constant. In this study I reduced calculation load by placing a shock wave in the flame front and analyzed it with the details chemical reaction model for  $H_2/O_2$  mixtures that considered pressure dependence in both adiabatic and isothermal wall. As a result, the influence of the wall conditions on DDT process became clear. We could obtain the explosion on the flame tip and on the wall with accurate values of parameters such as pressure or temperature.

Paper #330

### **One-dimensional Evolution of Fast Flames**

*V. N. Gamezo, A. Y. Poludnenko and E. S. Oran*

We consider the evolution of very fast flames in a model system with an extremely high thermal conduction. One-dimensional time-dependent computations based on Navier-Stokes equations show that these flames tend to accelerate. The acceleration may eventually lead to a detonation. In particular, we observe weak detonations that appear as thick, well-resolved reactive shocks, and propagate with velocities above  $D_{c,j}$ . Implications of the results on the deflagration-to-detonation transition in real systems are discussed.

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## **14:30 (R3B) Flame Instability and Acceleration**

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Paper #288

### **Short-Term Prediction of Combustion Instability in a Lean Premixed Gas-Turbine Combustor Using Nonlinear Time Series Analysis**

*Takuya Ikawa, Masahito Amano, Hiroshi Gotoda, Takaya Miyano, Shigeru Tachibana*

Periodic and chaotic behavior in combustion dynamics that can be observed as a result of combustion instabilities in fundamental and practical combustion systems are of importance to present-day combustion physics and nonlinear science research. We have recently investigated the dynamic behavior of the combustion instability in a lean premixed gas-turbine combustor from a view point of nonlinear dynamics. On the basis of the deterministic nature of the dynamic behavior extracted by a sophisticated nonlinear time series analysis, the short-term prediction of the pressure fluctuations in combustion instability has been performed in this work. The short-term predicted pressure fluctuations obtained by updating the data library of the phase space coincide very closely with the measured pressure fluctuations. The obtained results show that the nonlinear time series analysis we applied in this work has potential use for predicting the short-term dynamic behavior of the combustion instability with high accuracy, which has not been previously reported in the fields of combustion science and physics.

Paper #119

### **3D Numerical Simulations of Spherical Flames Instability and Acceleration in Shock Accelerated Flows**

*Yuejin Zhu, Gang Dong, Baochun Fan, Yixin Liu*

In present study, the three-dimensional reactive Navier-Stokes equations coupled with one-step Arrhenius chemical reaction are employed to simulate the 3D spherical flames instability and acceleration induced by incident shock and its reflected waves for an ethylene-oxygen-nitrogen mixture. In particular, the effects of shock wave strength and spherical flame number on the shock-flame interaction are focused and investigated. The results show that the severe distortion and rapid acceleration of flames occur when the reflected shock wave has passed through the flames. The spherical flame number has no significant influence on the flame evolution. Compared with the single spherical flame case, a reactive shock bifurcation structure in the double spherical flames case more likely appears on the wall due to the larger total flame surface area. The shock wave strength has important influence on the flame instability and acceleration. The shock wave with higher strength can produce stronger reactive shock bifurcation which is related to formation of hot spot that leads to a detonation, while the shock wave with lower strength cannot lead to a detonation but only disturb and accelerate flame. For strong shock wave case, the formation of hot spot is due to the convergence and collision of the compressed waves of flame fronts from x, y and z directions in the pocket of unburned mixture. The mechanism and location of formation of hot spot are different from 3D simulation by Gamezo et al. (Proc. Combust. Inst., 2005, 30:1841). The time histories of volume, mass burning rate, total heat release rate and mean vorticity magnitude of the distorted flames are presented and compared for all of cases. The comparisons suggest that shock heating and vorticity generation during shock-flame interaction play the important roles in flame instability and acceleration, especially for incident shock and its reflected waves with high strength.

Paper #28

### **Hydrogen-Oxygen Flame Acceleration in Channels of Different Widths and Deflagration-to-Detonation Transitions for a Detailed Chemical Reaction Models**

*M. F. Ivanov, A. D. Kiverin, M. A. Liberman*

The flame acceleration in channels of different widths, shock wave formation in the upstream flow, and transition from deflagration to detonation (DDT) in hydrogen/oxygen mixture are studied using high resolution simulations with a detailed

chemical kinetic model. It is shown that in wider channels ( $D > 1\text{mm}$ ) the initial stage is the exponential increase of the flame velocity which turns into the stage of a slower acceleration, acceleration with flame speed increase determined by power law with rate less than unity. In thinner channels ( $D < 1\text{mm}$ ) the exponential growth of the flame velocity is not bounded in time and an initial deflagration wave accelerates exponentially till the transition to detonation. When the compression waves produced by the accelerating flame steepen to the shock close to the flame, the unreacted mixture of increased density enters the flame producing a high pressure pulse, which enhances reaction rate and the heat release in the reaction zone with a positive feedback coupling between the pressure pulse and the reaction rate. As a result the peak of the pressure pulse grows exponentially, steepens into a strong shock and forms overdriven detonation. Results of the high resolution simulations are fully consistent with experimental studies of DDT in hydrogen/oxygen gaseous mixtures.

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**14:30 (R3C) Pre-mixed Flames – III**

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Paper #256

**Numerical Investigation of Premixed Flames Stabilized in a Narrow Duct with a Wall Temperature Gradient***G.P. Gauthier, G.M.G. Watson and J.M. Bergthorson*

Energy production systems involving flames in narrow channels offer many advantages in terms of combustion and thermodynamic properties. The enhanced wall/fluid heat transfer taking place in small ducts provides a way to harvest and promote the heat released by a flame. When the flame thickness is of the same order as the tube diameter, the flame structure is significantly influenced by hydrodynamic effects which are in turn tightly coupled to thermo-diffusive effects. Hence, the flame profile not only varies axially along the tube length, but also varies radially. This radial dependence is typically not considered in the investigation of flames inside tubes, as one-dimensional models are generally used. These models are considered to provide an effective means of predicting qualitative flame behaviors. However, the relative importance of two-dimensional effects on these predictions is yet to be assessed. In this work, two-dimensional simulations of premixed methane flames stabilized in a 2mm diameter duct subjected to a specified wall temperature distribution are performed. The two-dimensional nature of these flames is investigated. The variation of mixture composition is used to evaluate the leading order effects influencing the flame behavior. Different mixture compositions having equal laminar flame speeds are compared to determine the relative importance of laminar flame speed on flame position. To evaluate the influence of two-dimensional effects, results obtained from a one-dimensional model that includes a constant Nusselt number assumption are compared to the two-dimensional results. It is found that flames in tubes exhibit a structure that is two-dimensional. Structure properties such as flame curvature and flame thickness are qualitatively observed to vary based on mixture composition. Laminar flame speed is shown to be of leading importance in predicting the flame position. The consideration of heat transfer with the wall further improved the prediction of trends in flame position. However, other two-dimensional effects can significantly influence the physics of the system, as demonstrated by the relative inaccuracy of the constant Nusselt Number model in the case of rich methane-air mixtures. It was also shown that the one dimensional model does not provide quantitatively accurate results, as flame positions are significantly underpredicted.

Paper #227

**High-Pressure Turbulent Burning Velocity Measurements at Constant Reynolds Numbers***C. C. Liu, S. S. Shy, M. W. Peng, C. W. Chiu, Y. C. Dong*

Turbulent combustion at elevated pressure is one of influential yet knowledge-lacking fields in combustion research, and may be one of the cornerstones of the next combustion era. Measurements of turbulent burning velocities ( $S_T$ ) may be the most general approach to the understanding of high-pressure turbulent combustion. Our previous findings indicate that increasing pressure has a promotion effect on  $S_T$ , due to the enhancement of flame instabilities via the thinner flame at elevated pressure. However, increasing pressure also increases the turbulent Reynolds number ( $Re_T$ ) due to the decrease of kinematic viscosity. The present study therefore aims to determine whether such  $S_T$  enhancement by increasing pressure is due to the effect of increasing  $Re_T$ . Using the same experimental methodology, this work presents the  $S_T$  measurements of lean  $\text{CH}_4$ -air mixtures at  $\phi = 0.8$  and different initial pressure varying from  $p = 0.1\text{ MPa}$  to  $p = 1.0\text{ MPa}$  under various turbulent conditions, in which values of  $Re_T$  are kept constant. Results show that  $S_T$  decreases with increasing  $p$  in minus exponential manners at any constant value of  $Re_T$ , having similar pressure dependence of laminar burning velocities  $S_L$ . Besides,  $S_T$  increases with increasing  $Re_T$  at any constant value of  $p$ . It is also found that the normalized turbulent burning velocities ( $S_T/S_L$ ) behave approximately independent of  $p$  at any constant value of  $Re_T$ . However, the values of  $S_T/S_L$  still increase with increasing  $Re_T$  at any constant value of  $p$ . The present result clearly shows an important message that  $Re_T$  may still be a suitable indicator for the coupling effect of turbulence-pressure interaction on turbulent burning enhancement. These results should be beneficial to our further understanding of high-pressure turbulent combustion.

Paper #269

**Variable Density Premixed Thick Flame Propagation in a Microchannel with Heat Conducting Walls***Mark Short and David A. Kessler*

The study of flame propagation in a narrow channel is an important topic in several areas related to microscale combustors. Previous work has examined the structure and dynamics of variable density thick flames (flame width larger than the channel height) in non-adiabatic narrow channels. The current work extends this analysis by considering the role played by a conductive solid wall between the channel and an outer insulation layer. The analysis is a formal

asymptotic study of thick flame behavior for small Peclet number. The influence of the thermal properties of the wall on both steady and unsteady flame dynamics are analyzed.

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**16:15 (S2) Shock Induced Ignition – II**

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Paper #188

**Oxidation of Selected Aromatics Behind Shock Waves**

*O. Mathieu, G. Pengloan, N. Chaumeix and C.-E. Paillard*

In this study, the auto ignition delay time of aromatic hydrocarbons that are found into gasoline fuels (namely benzene, toluene and ethyl-benzene) were studied in shock tubes at high temperature between 1300 and 2000K. The ignition delay time of styrene, an important combustion intermediate of these aromatic compounds was also studied. Equivalence ratios of 0.5, 1.0 and 1.5 were investigated using very diluted mixtures in argon. Most of the study was performed around atmospheric pressure, although experiments around 1.8 MPa were carried out for benzene. The results of this work present an extension of the data set available into literature for benzene, toluene and ethyl-benzene and, to our knowledge, there are no shock tube ignition delay measurements for the styrene available into literature. Arrhenius relationships between the auto ignition delay time, the temperature and the mixture components concentration were derived from experimental results in most of the cases. For each fuel and condition, it was found that the reactivity of the mixture is increased as the oxygen is added whereas an increase of the hydrocarbon concentration induces an increase of auto-ignition delay time.

Paper #203

**High-Pressure Shock Tube Experiments of the Ignition of 3-Pentanone-Doped n-Heptane and Iso-Octane/Air Mixtures**

*Mustapha Fikri, Leonel R. Cancino, Michaela Hartmann and Christof Schulz*

Ignition-delay times for 3-pentanone/iso-octane (10/90% by volume) and 3-pentanone/n-heptane mixtures (10/90% by volume) have been determined in a high-pressure shock tube under engine-relevant conditions ( $p_5 = 20 - 40$  bar) for equivalence ratios  $\Phi = 0.5$  and  $1.0$  over a wide temperature range  $690 \text{ K} < T_5 < 1270 \text{ K}$ . The results were compared to ignition delay times of pure iso-octane and n-heptane fuels and to pure 3-P/air mixtures under identical conditions. Attempting to represent the experimental results numerically, a detailed kinetics model for PRF/3-pentanone mixtures is proposed. The model overpredicts the ignition delay times especially in the low temperature range. However, it is still able to reproduce the overall trend of the experimental data. As found in simulations and already confirmed by experiments, for lean condition 3-pentanone reduces the reactivity of n-heptane. For stoichiometric conditions, however, it does not alter the ignition delay by more than 11% at 850 K and 20 bar (with 10% 3-pentanone). The chemical effect of adding 3-pentanone to iso-octane is inverse, leading to retardation of the main ignition. Further investigation of the model is needed and the model used in this work needs further development to account for the low temperature chemistry.

Paper #342

**A High Temperature Shock Tube Study of n-Butylbenzene Oxidation**

*Colin Tobin, Kenji Yasunaga, John Simmie, Judith Würmel, Henry Curran, Olivier Mathieu*

A heating system was added to our high-pressure shock tube in order to facilitate the study of n-butylbenzene in the gas phase due to its low vapor pressure. The temperature measured along both the manifold and driven section of the shock tube showed a low degree of scatter throughout the system. The n-heptane validation of the shock tube using two different fuel addition methods closely agreed with that of Stanford's data which ensured accuracy and precision was being achieved in all the data obtained. The variation of the equivalence ratio had a common impact on reactivity at the varying pressures of 1, 10, and 30 atm. The crossover from low to high temperature chemistry occurred at varying temperatures and a similar pattern of reactivity amongst the equivalence ratios was observed at each pressure. The fuel rich mixtures were most reactive in the low temperature region while the fuel lean mixtures were least reactive. The opposite was true in the high temperature region in which the fuel lean mixtures were the most reactive given that there was a higher percentage of oxygen present in the lean mixtures. The effect of pressure at particular equivalence ratios also had a common pattern amongst all equivalence ratios studied. The data taken at 1 atm was the least reactive increasing from 10 to 30 atm.

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**16:15 (R4A) DDT – IV**

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Paper #56

**Flame Acceleration and Transition to Detonation in an Array of Cylinders**

*Takanobu Ogawa, Vadim N. Gamezo, Elaine S. Oran*

We study flame acceleration and DDT in an array of cylinders. Cylinders 1cm in diameter are placed 2cm apart in a symmetric layout, and the space between cylinders is filled with a stoichiometric  $\text{H}_2$ -air mixture at 1atm and 298K. We solve the compressible reactive Navier-Stokes equations. The energy release rate is modeled by a one-step Arrhenius kinetics. For handling curvilinear geometry, we develop a solver based on an embedded boundary method. Initially, the flow is at rest, and a flame is ignited at the center of the array and spreads cylindrically. Computations show effects of the cylinders as a series of events leading to DDT. During the initial flame acceleration, the speed of the flame depends on the direction of flame propagation since some directions are more obstructed than others. This affects the macroscopic



shape of the expanding burned region, which forms concave boundaries in more obstructed directions. As the flame accelerates, shocks form ahead of the flame, reflect from cylinders, and interact with the flame. When the shocks become strong enough, their collisions with cylinders ignite the gas mixture, and detonations form. We further study the dependency of flame speed on the angle of its propagation by simulating an initially planar flame that propagates through a rotated array of cylinders. The rotation angle corresponds to the direction of flame propagation in the case of the cylindrically spreading flame. The result shows how the angle affects flame acceleration. At some angles, the flow impinges on cylinders more often than others, and this results in slow flame acceleration. The flame stretching is also affected by the angle, since the flow around cylinders varies with the angle. At some angles, the wake of a cylinder creates long funnels of the unburned material, and the resulting increase in the flame surface accelerates the flame. The flame speed depends on the combination of these effects of the angle.

Paper #270

#### **Geometry-Specific Scaling of Detonation Parameters from Front Curvature**

*Scott I. Jackson and Mark Short*

It has previously been asserted that classical detonation curvature theory predicts that the critical diameter and the diameter-effect curve of a cylindrical high-explosive (HE) charge should scale with twice the thickness of an analogous two-dimensional HE slab. The varied agreement of experimental results with this expectation have led some to question the ability of curvature-based concepts to predict detonation propagation in non-ideal HEs. This study addresses such claims by showing that the expected scaling relationship is only consistent with curvature-based Detonation Shock Dynamics (DSD) theory under special limiting circumstances.

Paper #261

#### **Numerical Simulation of Deflagration to Detonation Transition with Wall Cooling Effect in Ethylene-Air Mixture**

*Min-cheol Gwak, Ki-hong Kim and Jack J. Yoh*

The combustion phenomenon of present study concerns two modes of burning that are deflagration and detonation. DDT is an extremely complex process involving deflagrations, shocks and shock reflections, boundary layers and all of their interactions with each other. The mechanism of DDT occurrence is not clear, however a flame needs acceleration process for DDT to occur. The acceleration process includes i) development of turbulent flow condition, ii) hot spot generation, and iii) flame instabilities or Richtmyer-Meshkov (RM) instability, which arises when a shock wave interacts with interface separating the two fluids of different density, reactant and product in combustion. In this paper, we report fully resolved two-dimensional simulation of shock-flame interactions and the effect of wall cooling due to adiabatic and low temperature wall conditions.

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### **16:15 (R4B) Criticality of Diffusion Flames**

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Paper #50

#### **Study on Ignition-like Behavior Caused by Interaction of Curved Diffusion Flames**

*Ryosuke Nozaki, Yuji Nakamura & Akio Kitajima*

An abrupt increase in temperature, "ignition-like behavior" induced by the merging of two reaction zones of "curved" diffusion flames is studied experimentally. Authors firstly convinced this ignition-like behavior successfully by the numerical simulation based on one-step reaction model with large strain rate in the previous study. However, in general, such simple reaction model is questionable to be applied to the condition of ignition at which the chemical effect plays a key role. In this study, for the purpose to validate the numerical prediction, we attempt to capture the ignition-like behavior experimentally and its characteristics are investigated accordingly. A pair of curved diffusion flames, which was made by four slot burners (two combined counterflow burners) specially designed for the present purpose, is utilized. To investigate the characteristics of ignition-like behavior, a series of sound generated by the flame motion and movie with high time resolution are acquired by a microphone and high-speed camera, respectively. From the strong power spectrum of sound generated by curved diffusion flames interact each other, ignition-like behavior is confirmed to occur in the experiment. Frequency of sound induced by interaction of curved diffusion flames is proportional to the bulk velocity gradient, which is identical to the characteristic flow time. Tangent of the approximate line of the plot of the ignition-like behavior frequency against the bulk velocity gradient is 0.82., and this value coincides with the previous numerical result. From these facts, previous numerical prediction is eventually validated.

Paper #182

#### **Determination of the Transition Threshold from Laminar Flat Flames to Turbulent Flames by a CO<sub>2</sub> Laser Irradiation Method**

*June Sung Park, Osamu Fujita, Yoshikazu Taniyama*

In a classical study of the acoustic instability in a tube, Serby reported distinct regimes of unstable flame behaviors. These can be categorized into: (1) A curved shape with a large cell, just after ignition. Overall the flame speed is twice its laminar burning velocity due to the increased flame area. At this moment, the acoustic amplitude (acoustic velocity) increases significantly increasing the total flame area. (2) Primary acoustic instability with a flat flame surface. It features an almost planar flame front. After regime (1), the primary acoustic instability is formed with a relatively stable level of acoustic pressure. (3) A violent secondary acoustic instability with a sudden formation of cellular structures on the flame surface. (4) Turbulent motion. As a detailed investigation of the above observations, Serby and Rochwerger developed theoretical predictions through stability diagrams in terms of wave numbers and acoustic intensities, and have verified the

stability diagrams with experimental data. They used a loudspeaker at the bottom, producing a stable planar flame that was classified as the primary acoustic instability. Then, the threshold of the parametric instability leading to the turbulent motion of the flame front was given as a function of the frequency and flame surface's wave number of the imposed acoustic field by using the loud speaker. In a theoretic study of the acoustic instability Pelce and Rochwerger investigated the position of occurrence of the primary acoustic instability by predicting the growth rate of the acoustic pressure. The analysis was limited to small amplitudes of cellular flames. Previous researches considered only small amplitudes of the flame front waves as the interface of two different densities. In some cases, the amplitude of the flame front, however, changes very much, which could be a further factor to control the transition process in actual flames. This study attempts to establish and observe the transient process to the parametric instability with the sudden increase of flame surface area. We initially form a flat flame as a default state. Then, CO<sub>2</sub> laser light is irradiated normal to the flat flame. The laser irradiation into the unburned mixture deforms the flame shape, resulting in a sudden increase in the flame surface area. The shape of the deformed flame is strongly dependent on the laser power and beam diameter, which allows the generation of a desired flame wave number and wave amplitude of the flame structure. The object of this paper is to establish criteria for transition from the primary to the secondary instability in terms of laser power and to investigate how the flame configuration arising from the laser light absorption affects the onset of the secondary instability.

Paper #131

#### **A Multi-Mixture Fraction Closure for Dilute Turbulent Diffusion Flame**

*Avner Fartouk, Pierre Plion, Arnaud Mura*

The description of laminar and turbulent flames in the presence of a diluting stream is a subject of growing interest and may concern a large number of practical applications, as those encountered for instance in the field of fire safety such as gas pulverization systems or sprinkler systems. In this field of research, fast chemistry models based on either the Eddy Dissipation Concept (EDC) or the conserved scalar methodology still remain the most classical closures retained to describe non-premixed combustion. Indeed, under the assumptions of unit Lewis numbers and large Damköhler number values, the conserved scalar model provides a very efficient basis for calculating such diffusion flames. However, as soon as dilution or third stream effects come into play, such formalisms that rely on the mixture fraction concept should be revisited. Moreover, for large dilution levels, the fast chemistry assumption no longer remains satisfactory to describe the combustion processes. Actually, the level of dilution dramatically influences the chemical behavior. The purpose of the present study is, first, to modify the conserved scalar presumed PDF closure by considering a multi-mixture fraction model to account for the description of a three-feed system (oxidizer, fuel, diluent). Then, further efforts are focused on the delineation of two chemical-response sub-domains (infinitely fast or infinitely slow chemistry) associated with the introduction of flammability limits, the values of which will depend on the mean dilution ratio. Finally, the resulting modeling proposal is implemented in a CFD software package and it is used to simulate the behavior of a diffusion flame in the presence of diluting species. The experimental test case retained to assess the computational model corresponds to statistically steady methane-air diffusion flames with a coflow of diluted oxidizer. The obtained results confirm the relevance of the proposed closure.

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#### **16:40 (R4C) Premixed Flames and Laminar Flame Speed**

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Paper #152

#### **Premixed Flame Response to Disturbances in Pressure and Fuel Distributions**

*Nadeem A. Malik and R.P Lindstedt*

A critical issue in combustion studies, such as internal combustion engines, is the impact of pressure and equivalence ratio oscillations on flames. The need to investigate such phenomena with realistic chemistry has never been greater. The progress in numerical methods and computer technology now offers such a possibility and implicit solvers in particular have been receiving increased attention due to their greater stability. Malik has developed an 1D implicit combustion code TARDIS (Transient Advection Reaction Diffusion Implicit Simulations), featuring the coupling of the fully compressible flow to comprehensive chemical mechanism and detailed transport properties. The method can resolve all the convective and chemical length/time scales present in stiff chemically reacting systems. The response of stoichiometric H<sub>2</sub>/air flames subjected to simultaneous pressure and equivalence ratio fluctuations methane/air flames was studied previously; here we investigate methane/air flames in the context of premixed planar flames and outwardly propagating cylindrical and spherical flames in order to shed light on the underlying physics of thermoacoustic interactions and on the thermochemical flame structure under conditions of inhomogeneous fuel distribution and for different levels of stretch.

Paper #210

#### **Parameterization of Laminar Flame Speed Dependence on Pressure and Temperature in Hydrogen-air Mixtures**

*T. Szabó, J. Yáñez, A. Kotchourko, M. Kuznetsov, T. Jordan*

A new correlation describing laminar flame speed of hydrogen-air mixtures as a function of temperature and pressure is proposed. The correlation is developed for reactive hydrogen-air mixtures in a wide range of temperature and pressure. In a first stage, the laminar flame speed was calculated with the detailed reaction mechanism of Warnatz and Maas implemented in the code INSFLA. The results obtained were validated against experimental data and a new heuristic approximation based upon them was created. The correlation found consists of simple mathematical expressions and provides good approximation of laminar flame speed in the ranges from 200 to 600 K for temperature and between 0.1 and 10 bar for pressure.

Paper #298

**Laminar Burning Velocity and Markstein Length Relative to Fresh Gases Determination for Isooctane-Ethanol Air Flames**

*E. Varea, A. Vandiel, V. Modica, B. Renou*

Nowadays, massive consumption of fossil energy leads to higher and higher pollutant and greenhouse gas emissions. Both ecological and political contexts encourage scientists and engineers to find new bio solutions for sustainable development. Transport is one of the first challenges because of his quasy-total dependence on fuel. Automotive industry is working at the same time for increasing engine efficiency but mainly on bio blended fuel combustion and characterization. Unstretched laminar burning velocity ( $u_n^0$ ) is an essential value for fuel description (reactivity, ignition delay times, energy released) and it is necessary for kinetics mechanisms validation and tabulated chemistry. It also useful for turbulent combustion modeling. In this study, an equipped experimental constant volume bomb set up has been developed. It allows high temperature and high pressure, gaseous or pre vaporized liquid combustion for a large range of equivalence ratios. This set up is coupled with high speed tomography diagnostic. Spherical time resolved flames images are recorded at 5kHz. The main idea consists in determining a new way to calculate laminar burning velocities of blended isooctane-ethanol mixtures, without considering any fuels characteristics or physical hypothesis. The technique proposed in this study consists in a pure kinematic measurement. By definition, kinetic formulation leads to calculate laminar burning velocity as the difference between the laminar flame speed (extracted from flame radius information) and the fresh gases velocity calculated at the beginning of the preheat zone. It obliges to determine with a very good resolution the fresh gases velocity at a distance smaller than 1mm from the flame front. The recent work of Balusamy et al. (2010) demonstrates the interest of this approach. This paper proposes to extend this work for direct measurements of laminar burning velocity by high speed fresh gases velocity determination. An experimental study for validation has been carried out on ethanol air flame at 0.1MPa, 373K for a range of equivalence ratio from 0.7 to 1.5. It has shown its efficiency and also gives an essential key parameter on flame combustion behavior to stretch factor that is Markstein length relative to fresh gases. The first results are consistent with literature and new set of measurements on blended isooctane-ethanol mixtures are in progress for ranges of temperatures and pressures up to 573K and 2MPa.

**08:30 (S3) Dynamics of Large Scale Fire and Explosions - I**

Paper #333

**Summary of the Phoenix Series Large Scale LNG Pool Fire Experiments***Thomas Blanchat, Paul Helmick, Richard Jensen, Anay Luketa, Regina Deola, Jill Suo-Anttila, Jeffery Mercier, Timothy Miller, Allen Ricks, Richard Simpson, Byron Demosthenous, Sheldon Tieszen and Michael Hightower*

With the growing use of imported LNG to meet increasing U.S. and regional natural gas demands, damage or disruption from a spill to LNG import terminals or harbor facilities could curtail LNG deliveries and impact natural gas supplies. As LNG imports started to increase in the U.S. in the early 2000's, a number of hazard studies were conducted that resulted in widely varying consequence and hazard estimates resulting in broad public concern over the adequacy of current hazard and consequence analysis techniques. Subsequent Sandia analysis [Hightower et al. 2004] highlighted some primary knowledge gaps that were limiting the fidelity of site-specific risk assessments due primarily to the lack of large-scale LNG spill, fire, and damage data. Experimental studies used to justify current hazard analyses were 10 to 100 times smaller in scale than potential incidents. The limiting factor in conducting the needed larger-scale experiments was that they were thought to be cost prohibitive. While much progress has been made in LNG threat, consequence and vulnerability assessment; for example, a general approach to risk evaluation has been developed and used for a basis in site-specific risk assessments; there are still knowledge gaps for very large scale LNG pool fires that limit Blanchat, T. K. Phoenix LNG Pool Fire Experiments 23<sup>rd</sup> ICDERS – July 24 - 29, 2011 – Irvine 2 the fidelity of site-specific risk assessments and remain a focal point of concern. These knowledge gaps result in the need to make assumptions in hazard analysis that may or may not be warranted and could lead to over predicting or underestimating hazards and impacts to the public, property, the economy, or energy reliability. To address these concerns, the United States Congress funded the US Department of Energy (DOE) in 2008 to conduct a series of laboratory and large-scale LNG pool fire experiments at Sandia National Laboratories (SNL or Sandia herein) in Albuquerque, New Mexico. The focus of the LNG pool fire testing efforts were to improve the understanding of the physics and hazards of large LNG spills and fires by conducting laboratory experiments and fire tests of LNG spills, on water, producing pools of up to 100 m in diameter. These tests were expected to better represent the fire behavior of spills postulated from current and future LNG carriers. Due to its unique chemistry, methane fires behave differently compared to other hydrocarbon fuel fires, but are expected to follow the trend of heavy hydrocarbon fuel fires, where the surface emissive power (SEP) of a pool fire increases to reach a maximum value then decreases to reach a limiting value with increasing diameter. For LNG, the limiting SEP value is unknown and verifying the actual values required the improved laboratory and large-scale experiments funded by the US Congress. These large scale spreading LNG pool fire experimental datasets, combined with small-scale gasburner experiments, support pool fire model development and validation for extrapolation to a scale of a potential LNG spill of 200 - 400 m or larger in diameter.

Paper #221

**Computation of Large Scale Fires in Complex Geometries - a Means to Safeguard People and Structural Integrity in the Oil and Gas Industry***Bjørn F. Magnussen*

Fire safety is one of the most important issues in the oil and gas industry. Accidents happen with serious, sometimes dramatic consequences where (A) lives are lost, facilities destroyed, environments contaminated, economics in danger (B) and credibility of the industry at stake. A number of serious challenges have to be met by the industry to prevent or mitigate fire related accident. Questions may be raised like: (1) What about the strategies for accident prevention and mitigation? (2) Are the strategies understood and treated at right levels in the organizations? (3) Are the companies willing to take lessons from recent accidents or do they feel that they have sufficient knowledge? (4) Are the companies aware of and utilize the best available technologies or willing to pay for necessary technology development? (5) Is the intercommunication between different levels in the organization or between companies executed in such a way that the messages are understood and actions executed? To meet these challenges, the industry needs technologies that can be utilized to pre-design the safety measures. This means predictive computational methods that can handle fire evolution and fire mitigation in complex geometrical environments, methods that can be trusted, and methods that can depict the results in such a way that decisions can be made by people with different knowledge or experience background. This paper demonstrates and discusses the development of a coherent technology for fire safety assessment in the oil and gas industry based on the Eddy Dissipation Concept (EDC) by Magnussen. It includes a review of the concept and its physical basis and the implementation of the EDC and other models into a dedicated fire simulation code, Kameleon FireEx KFX®. KFX® is basically a general purpose code with a wide operational domain from fire relevant problems to low NO<sub>x</sub> problems in burners and furnaces. Coherent technology in this respect means similar operational platforms and no adjustable constants in the physical submodels. In industry application the problem owners and decision makers, and the scientists often have very different background of practical and theoretical understanding. A big challenge is therefore to create common understanding of the problem and the consequence of the results. This is achieved in KFX® by extensive use of graphics and video animations. Examples of validation related to the turbulence-chemistry interaction, water droplet radiation interaction, gas dispersion and fire evolution will be shown.

Paper #236

**Flame Spread Characteristics of Fire Retardant Fabrics***Andres F. Osorio, Chris Lautenberger, Carlos Fernandez-Pello, David Urban, Gary Ruff*

Flammability testing of non-fire retardant (NFR) and fire retardant (FR) fabrics is often conducted in standard temperature and pressure (STP) conditions (1 atm., 25° C, 21% O<sub>2</sub>, 79% N<sub>2</sub>)[1, 2, 3] However usage of NFR and FR fabrics is not

just limited to STP conditions, like for example cabin environments proposed for future space exploration by NASA. Recent studies on ignition and flame spread characteristics of thin materials considered by NASA have been used to develop correlations predicting flame spread rates[5] and analyze self-extinguish behavior under varied oxygen concentrations[4]. This work focuses on analyzing flame spread behavior of Nomex HT90-40, 100% Cotton and 60%/40% Cotton/Polyester fabrics under different environmental conditions. In addition a skin simulant located beneath the test sample will be used to study effects of environmental variables in heat transfer through the thin material test samples.

Paper #103

### **Mathematical Modelling of a Large-Scale Ventilated Tunnel Fire**

*Hui Ying WANG*

In ventilated tunnel fires, smoke and hot combustion products may form a layer near the ceiling. The pioneering theoretical work related to tunnel fire science is found by Thomas, on the backlayering length of hot smoke upstream the fire against a cross-stream in duct flow. In the previous works, CO and soot productions are not included, and neglecting of heat transfer inside the wall results in an over-prediction of temperature. The objective of the present study is to examine the feasibility of our numerical models for understanding the effect of crossflow velocity on the local CO and soot concentrations. Influence of heat loss inside the tunnel wall on the temperature profiles is clearly shown. Large Eddy Simulation (LES) for the fluid dynamic equations of three-dimensional elliptic, reacting flow is coupled with soot production and radiation models. Applying the filtering operation to each term in the conservation equations of mass, momentum, energy and species, and decomposing the dependent variables into resolved and subgrid components results in the filtered governing equations

Paper #132

### **Prevention of the Explosion of Acetylene Cylinders Involved in Fire: Experiments and Simulations**

*F. Ferrero, M. Beckmann-Kluge, M. Kreißig, U. Schmidtchen, K. Holtappels*

Pressurized cylinders for the storage of acetylene may explode with generation of a fireball, if they come in contact with a strong heat source, for example a fire. Since acetylene (chemical formula  $C_2H_2$ ) is capable of decomposing explosively into carbon black and hydrogen without the presence of oxygen - provided its temperature and/or pressure are sufficiently high-, such cylinders are extremely dangerous. In fact, once the decomposition reaction is initiated by the fire exposure, this reaction may still run after the heat source is removed, i.e. the flames are extinguished. This may eventually lead to the cylinder rupture, since the decomposition reaction is self-sustained by the heat it releases. One way to prevent the burst of heated acetylene cylinders involved in fire is to cool them with water. Nevertheless, as reported in Kurth (1999), this method may be ineffective if critical conditions in the cylinder are achieved, i.e. if the reaction rate of decomposition has reached a point, where the related heat production exceeds the heat removed by the water cooling. In order to assess the effectiveness of the water cooling as a safety measure to prevent the burst of acetylene cylinders involved in fire, a total of 13 fire exposure experiments (bonfire tests) have been performed with fully loaded cylinders of 8.9, 10 and 50 L in volume. During the tests, the temperature at different spots in the cylinder interior and the head pressure were recorded. In some of the experiments a cooling system was activated some seconds before the expected burst. Thus, the fire was extinguished and the cylinder was cooled, in order to observe if an explosion could be prevented. Together with the information acquired from lab-scale tests, the data recorded during the experimental campaign were used for the development and validation of a mathematical model to predict the heat transfer in acetylene cylinders during the fire exposure and the afterward cooling with water. The current paper presents a short summary of the performed work and may provide a valuable help for improving the handling of acetylene cylinders involved in fire.

Paper #68

### **The Extension of Eddy Dissipation Concept in the Framework of Large Eddy Simulation and the Subsequent Modification**

*Z.B.Chen, J.X.Wen, B.P.Xu and S.Dembele*

The RANS based eddy dissipation concept (EDC) has been modified and extended to the LES framework according to the turbulent energy cascade. This has involved modifications to most equations and derivation of new equations. The ratio of the fine structure mass to the total mass in the original EDC was linked to the characteristic velocity scales and largely responsible for the temperature under-prediction of the temperature near the fire base. This has now been modified based on previous experimental findings which linked it to the integral length scale and avoided the use of total kinetic energy which cannot be explicitly calculated in a LES. Validations have been conducted for a number of medium scale pool fires but only the results for methanol pool fires are included due to limit of space.

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## **09:10 (R5A) Detonation Limits and Engine**

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Paper #268

### **Numerical Investigation of $H_2$ - $O_2$ Layered Detonation in Narrow Channel**

*Masatsugu Okamura, Akiko Matsuo*

The previous experiments of scramjet engine with a hypermixer (HM) injector, which generates streamwise vortices for enhancing supersonic mixing and combustion, was examined in a Mach 8 simulated flight condition at High Enthalpy Shock Tunnel(HIEST) of JAXA, Japan. In the case of equivalence ratio 1.0 and 1.5, the transient combustion wave, which propagates opposite direction to the main flow, were observed. The properties of pressure were well agreed with

those of Chapman-Jouguet detonation wave, and indicate that this combustion wave was a kind of detonation wave. The mixing condition in the combustor was numerically investigated by Kodera et al. The mixture had a gradient of fuel density in the cross-section in the combustor, where  $H_2$  mole fraction was higher at the center and lower near the wall. Therefore the transient combustion wave, which observed in the examination of HM injector, was a kind of a layered detonation that is a detonation propagates to the layered mixtures. In this work, a layered detonation was numerically investigated to clarify the effect of parameters in the layered detonation, which was observed in the experiments of HM injector, using two-dimensional Euler equations with  $H_2 - O_2$  detailed reaction model. The layered mixtures had double layers in vertical direction. Equivalence ratio of the upper layer was out of detonable concentration (lower than the detonation limit) and that of the lower layer was stoichiometric. In the experiment of HM injector, the height of combustor was 12mm, and it correspond to the cell width. Therefore, this work was conducted in the narrow channel, where the one cell appears, to investigate the structures in the layered mixtures. Important parameters in this work were non-detonable layer equivalence ratio in the upper layer and its width to reveal the characteristics of the layered detonation. A series of simulations showed that the reactivity of layered detonation had a strong relationship to the non-detonable layer concentration. The propagation mechanisms in the layered mixtures were well explained by the transverse wave strength. Furthermore, the propagation velocity of the layered detonation well agreed with the CJ velocity of the average equivalence ratio of layered mixtures.

Paper #187

#### **Numerical Simulation on Two-Dimensional Detonation including Boundary Layer Effects**

*Nobuyuki Tsuboi, Youhi Morii, A. Koichi Hayashi, Mitsuo Koshi*

Two-dimensional full Navier-Stokes simulations with the detailed chemistry model were performed for  $H_2$ /air detonations in a channel in order to estimate the viscous loss effects on the detonation under the low pressure environment. The present NS code is confirmed to resolve the boundary layer by comparing with the theoretical results. The velocity deficit on the NS simulations fairly agree well with that on the modified ZND calculations. The velocity deficit on fine grid is 3.4% for  $d=10$  mm though it is 5% for  $d=7.5$  mm. The velocity deficits increase rapidly as the channel width is smaller than 10 mm. The grid resolution effects on the velocity deficits are approximately 1%. The detonation for  $d > 10$  mm stably propagates in the channel while that for  $d < 10$  mm becomes unstable. This feature coincides with the rapid increment of the velocity deficit for  $d < 10$  mm. As the channel width is lower than 10 mm, the leading shock and the flame front periodically separates and interacts, and the detonation becomes unstable.

Paper #106

#### **Fuel Effects on Rotating Detonation Engines**

*Douglas A. Schwer and Kailas Kailasanath*

Rotating detonation engines (RDE's) represent a novel approach to using the higher efficiency detonation thermal cycle without some of the drawbacks of pulse detonation engines (PDE's). The current paper extends a numerical model for hydrogen-air RDE's to represent a wide range of hydrocarbon-air and hydrocarbon-oxygen premixtures. The models use an induction time parameter model for the chemical reactions, and both 2-gamma and temperature dependent specific heat thermodynamic properties for energy. Results show that the 2-gamma model accurately represents the detonation pressure, temperature, and wave velocity for the hydrogen and hydrocarbon-air results, while the temperature dependent properties are needed for hydrocarbon-oxygen results. RDE results are shown for ethylene, ethane, and propane with both air and oxygen as the oxidizer. Specific impulses ranged from 175 s for ethylene/oxygen up to 2570 s for ethane/air.

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### **09:10 (R5B) Shock Induced Combustion and Detonation**

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Paper #13

#### **Cellular Structure in an Oblique Detonation Wave**

*Jimmy Verreault, Matei I. Radulescu, Andrew J. Higgins*

Numerical simulations of an oblique detonation wave attached to a wedge are conducted using a single-step Arrhenius equation to model the chemistry. For the chosen non-dimensional chemistry parameters ( $Q=10$  and  $E=30$ ), pressure instabilities are observed along the detonation front. By observation of the evolution of these instabilities, a cellular structure can be recognized, similar to that of normal self-propagating detonations. The cell size of the oblique detonation is compared to that of an equivalent normal detonation wave, and the agreement is good at the early stage of the evolution.

Paper #243

#### **Numerical Modelling of Shock-to-Detonation Transition in Methane-Air Mixture**

*Semenov Ilya, Utkin Pavel, Demidov Nikita, Akhmedyanov Ildar*

Detonation of natural gas-air mixture is very important and promising problem from the sense of energy plants effectiveness increasing. Besides the importance of investigation of detonation initiation critical conditions in natural gas-air mixtures is connected with explosion hazards in coal-mining industry and natural gas production. Current work is the continuation of the series of works in which the authors within multidimensional approach investigated shock-to-detonation transition (SDT) in stoichiometric propane-air mixture due to the tube walls profile. The multidimensional 2D and 3D numerical experiments on SDT in methane-air mixture under normal conditions in tubes with parabolic contraction, connecting section of narrow diameter and conical expansion are performed. The shape of parabolic contraction and divergence angle of cone expansion are found which provide SDT for the incident SW Mach number 3.0.

The results of 3D numerical investigation confirm in whole the results of 2D findings. It is important to note that the findings reported in the paper are in good agreement with the recent experimental investigation.

Paper #274

#### **Numerical Investigation of Shock-Induced Combustion around a Cylindrical Body**

*Taku Segawa and Akiko Matsuo*

In this study, shock-induced combustion around a cylindrical body was numerically investigated using two- and three-dimensional Euler equations with the simplified two-step chemical reaction model. In 1960s and 1970s, shock-induced combustion around a spherical projectile flying at hypervelocity into a combustible gas was investigated in a number of ballistic range experiments. The unsteady features of shock-induced combustion were taken by shadowgraph at the specific conditions, and the pictures clearly showed the periodic oscillations of reaction fronts. The oscillation patterns of unsteady shock-induced combustion were classified into two regimes of the regular and large-disturbance regimes, depending on the manner of the oscillations. Numerical simulations of shock-induced combustion around a spherical projectile were also conducted for the last few decades and revealed the unsteady mechanism of the two regimes. The simulated flow fields newly showed the unsteady state, which is much stronger than the previous two regimes, and its oscillation is not periodic because the transverse wave appears away from the axis and propagates toward the stagnation streamline. Based on the previous experimental and numerical works on the spherical projectile, the unsteady features around a cylindrical body are numerically investigated in this paper. In two-dimensional analysis, the regular regime, the large-disturbance regime and the unsteady state appear as observed in the visualization around a spherical body. However in three-dimensional analysis, the transverse detonation propagating in the one side of the spanwise direction appears in front of the cylinder for  $d=3\text{mm}$ , where the regular regime appears in two-dimensional analysis. In the present simulations, we used the periodic boundary condition in the spanwise direction and added the artificial disturbances at an initial condition to induce the spanwise velocity. This boundary condition implies that the spanwise length is infinite for the one-sided propagating detonation wave, and therefore the transverse detonation propagates maintaining the wave structure of detonation. A series of simulations with various spanwise lengths were carried out to see the behavior of the transverse detonation. When the length of transverse detonation is over a certain value, the number of transverse detonations increases. This threshold is equal to the cell width, which is obtained by two-dimensional channel analysis of the C-J detonation.

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#### **09:10 (R5C) Blow-off and Extinction**

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Paper #195

#### **Influences of Ultrasonic Waves on Blow-off Limits of Lifted Jet Flames**

*Mitsutomo HIROTA, Takuya TSUJI, Yuji NAKAMURA and Tsutomu SAITO*

This research investigated the effects of an ultrasonic standing wave on a lifted jet flame to improve combustion stability near lean flammability limit conditions. The authors proposed a combustion control system employing high-frequency oscillation generated by a bolt-clamped Langevin transducer with a horn and a reflector that affects local flow fields of the leading edge of the lifted jet flame. The frequency of this oscillation was 20.27kHz so that it had high directionality, since a plane wave and a standing wave were easily formed. Our research examined the flame characteristic changes in high-frequency oscillation upstream of the leading edge of a methane-air laminar lifted flame. We first found evidence that an ultrasonic wave improved blow-off limits of the lifted flame. The stability limit of the lifted jet flame was measured by controlling the airflow velocity at a constant fuel velocity. The air velocity was increased until the blow-off limit was reached. The blow-off limit with oscillation was determined by the air velocity, which increased with the oscillation until blow-off. The degree of stability improvement is related to the jet position inside a standing wave. Specifically, the flame height was reduced when the leading edge of the flame was located between a pressure node and an anti-node of the standing wave. The jet trajectory image of the acetone Planar Laser Induced Fluorescence (PLIF) method indicated that the standing wave tilted the jet flows from the jet axis. We also checked the blow-off limit when the jet axis was inclined without oscillation. When the inclined angle of the burner was set to the same value of the jet angle with oscillation, the blow-off limit was lower than that with oscillation. Namely, the flame stability with oscillation cannot be explained by only the balance of the burning velocity and the inclined inflow velocity vector at the leading edge of the flame. It indicates that sound effects increase the blow-off limit with oscillation. We also measure the variation of the preheat zone width using the acetone-OH simultaneous PLIF. In this scheme, unburned and burned zones are simultaneously visualized by acetone seeded into the fuel flow and OH generated by combustion. We then indirectly track the flame zone sandwiched between them. The visualized zone corresponds to the preheat region. The result demonstrates that the oscillation generated by the sound increases the non-luminous zone width of the acetone-OH PLIF. Therefore, we concluded that the preheat zone width of the flame at the blow-off limit was increased with oscillation and found that these two effects of ultrasonic waves contribute to the lean flammability limit.

Paper #264

#### **Experimental Study on Near Extinction Behavior of Microflame in Preheated Air**

*Kakeru Fujiwara, Yuji Nakamura*

In this study, the flame shape from stability to extinction limit (lower limit) condition and the lower fuel flow rate of a tiny methane-air jet diffusion flame is investigated in order to understand the near extinction behavior and the extinction mechanism. The near extinction behavior has been affected by adopting the high-temperature air (293K-770K) or burner material. Uniform high-temperature air is achieved by using an electric heater. Applied needle burner is made by

ceramic, stain less, brass, aluminum, whose inner/outer diameter is 0.8mm/1.2mm, respectively. The fuel flow rate is measured by soap bubble meter. Flame image is taken by digital camera through the quartz window installed on the wall of combustion chamber and flame height as well as quenching distance are obtained to be analyzed. It is found that the extinction limit theory (for micro-scale diffusion flame) developed by Kuwana and Ida could be applied to express the limiting flame behavior under high-temperature air and the lower fuel flow rate is described as the function of air temperature. The quenching distance is increasing with closing to extinction limit and this trend can be described as thermal balance between the flame and the burner. The flame height and quenching distance at near extinction condition have linearly proportion in each air temperature. This relationship quantitatively corresponds to the each burner material. As a consequence the extinction limit (lower limit) is organized by the Damköhler-number and extinction is caused that decreasing the reaction rate is attributed to heat loss to the burner wall. Besides, the smallest limit of the flame scale is predicted on the basis of the relation between the flame height and quenching distance at near extinction.

Paper #299

**Study on the Effect of Premixed Gas Addition on the Anti-Blow-Off Performance of Jet Diffusion Flame**

*Makihito NISHIOKA, Kosuke MIYAZAKI, Hiroki TAKAYAMA, Akane UEMICHI*

Jet diffusion flames have been widely used for a variety of practical applications because of their extensive range of safety and high controllability. However, when low-grade fuels such as biogas are used, they are apt to be lifted or blown off because of their weakness of reactions. So it is desirable to develop new techniques to improve the anti-blow-off performance of jet diffusion flames of such fuels, since effective utilization of them as an energy resource is now becoming more and more necessary. Recently we conceived an idea of addition of small amount of premixed gas at the flame base for enhancing the reaction kernel, and applied the idea for the stabilization of "pseudo biogas" (methane diluted with nitrogen) which cannot be stabilized on an ordinary injector at all because of the weakness of reactivity. In this study, we performed experiments of jet diffusion flame of pseudo biogas using a coaxial double-tube burner, in which small amount of rich premixed gas of equivalence ratio 4.0 is injected from a gap between the tubes, and measured the limit of blow off both by main fuel jet and by coflowing air. As a pseudo biogas we used a fuel mixture composed of 30% methane and 70% nitrogen, which is too weak to form a diffusion flame on an ordinary injector tube even for a very small injection velocity. Additionally, detailed-kinetics numerical simulations were conducted for investigating the phenomena occurring around the reaction kernel of the flame base formed on the coaxial double-tube burner. As a result, it was found that as the injection flow rate of additional premixed gas injected from the gap is increased the blow off limit is at first improved, and then turns to decrease or to be constant at a critical flow rate. In the case of blow off by main fuel jet, the flame was not blown off up to the highest jet velocity of 13 m/s. And in both cases of blow off by coflowing air and by main fuel jet, the largest blow off limit was attained when the distance between the exit planes of two coaxial tubes is 12 mm, which is the largest value used in the experiment. This means that a long flameless zone is formed between the rims of two coaxial tubes. We subsequently performed a numerical simulation to examine the phenomena occurring in the latter zone, and found that the reaction kernel at the base of the diffusion flame is extended outwardly forming a kind of "reaction zone wing". Considering the concentration gradient of methane formed by diffusion in the long flameless zone, the wing is thought to be a kind of premixed flame that is formed in the same manner as the lean side branch of a tribrachial flame. That is, as a premixed flame the wing has a considerably high local burning velocity that can balance the local flow velocity, which has the effect to promote the anti-blow-off performance of the jet diffusion flame.

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**11:45 (S3) Dynamics of Large Scale Fire and Explosions - II**

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Paper #138

**DDT in Highly-congested Environments - the Buncefield Vapour Cloud Explosion**

*J.S. Puttock and A. Pekalski*

The Buncefield incident in 2005 involved a significant vapour cloud explosion on a site that had little pipe-work congestion and it therefore required investigation to determine how significant overpressures had been generated. Numerous experiments, since about 1980, have shown that a flame burning through a thin cloud in open space does not accelerate significantly. However, the presence of obstacles (e.g. in petrochemical plant) in the path of the flame can generate turbulence and flame folding. Both enhance the burning rate and can lead to the positive feedback known as the Shchelkin mechanism. Thus, even without confinement, congestion can generate high flame speeds and therefore high pressure. This process has been quantified in hundreds of experiments performed since the 1980s. At Buncefield, the density of pipework and other obstructions was very low. However, the two lanes adjacent to the depot were bordered by wide verges containing trees and very dense undergrowth. Indeed, the branches constituted a network of flow obstructions considerably denser than that presented by pipes etc. in highly congested process plant. However, this does not explain the damage in open areas; it has been concluded [[1]] that this was caused by a detonation following deflagration to detonation transition (DDT).

Paper #250

**Deflagration-to-Detonation Transition in Unconfined Media**

*A.Y. Poludnenko, T.A. Gardiner, E.S. Oran*

Deflagration-to-detonation transition (DDT) can occur in a wide variety of environments ranging from experimental and industrial systems on Earth to astrophysical thermonuclear (type Ia) supernovae explosions. In recent years, substantial progress has been made both experimentally and theoretically in elucidating the nature of this phenomenon in confined systems with walls, obstacles, etc. Shocks in such systems can be formed both by the overall fluid expansion caused by



the energy release in the flame, as well as by the repeated interactions of the flame-generated acoustic waves with solid obstacles and with the flame itself. Once a shock of sufficient strength is formed in the system, DDT can occur through a variety of different mechanisms, such as shock collision with an obstacle or shock-flame interactions and the formation of the induction-time gradients. At the same time, it remains unclear whether a subsonic turbulent flame initially present in an unconfined, unpressurized system without pre-existing shocks can undergo DDT and, if such transition is possible, what its mechanism would be. In this work, we present results of the direct numerical simulations of the interaction of high-speed turbulence with premixed flames in a stoichiometric hydrogen-air mixture. We demonstrate that at sufficiently high, but subsonic, turbulent velocities, the turbulent flames are inherently unstable and are susceptible to the development of the detonation without assistance of any external shocks or solid boundaries.

Paper #247

**Modelling of Flame Acceleration Due to Intrinsic Instabilities in Industrial Scale Explosions**

*Helene H. Pedersen, Prankul Middha, Trygve Skjold, Kees van Wingerden, Bjørn J. Arntzen*

Modelling of explosions using Computational Fluid Dynamics (CFD) is useful for performing risk assessments in the petrochemical industries that handle flammable gases and liquids. In order to represent large-scale explosions in complex geometries, submodels for e.g. combustion and turbulence are necessary. In the CFD-tool FLACS, the accelerating effect of flame instabilities during the early phase of flame propagation is modelled by an empirical equation that controls the effective burning velocity during the transition from laminar to fully turbulent flow regimes. Recent validation work suggests that it is necessary to review and improve this model in light of the experimental and analytical efforts that have been made on the subject since its implementation. In the present work, we focus on the effect of intrinsic instabilities, i.e. the hydrodynamic instabilities due to the expansion of the gas through the flame, and thermal-diffusive effects. If the initial flame is allowed to develop freely for a while, acceleration due to intrinsic instabilities can have a significant effect on the later development. This situation is relevant especially for large-scale geometries. In order to study the flame acceleration during the initial phase of combustion in FLACS, validation against experiments addressing unconfined explosions in uncongested geometries was performed. The results indicate that the model might benefit from an approach that also takes into account the Markstein number effects.

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**11:45 (R6A) Detonation Dynamics and Structure – I**

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Paper #112

**Periodic Oscillation and Fine Structure of Wedge-Induced Oblique Detonation Waves**

*Mingyue Gui, Baochun Fan, Zhihua Chen*

Oblique detonation wave stabilized over a body has been studied due to the ongoing development of high-speed propulsion systems, such as ODW engines and ram accelerators. In this study, an oblique detonation wave induced by a wedge is numerically analyzed using a fifth-order weighted essentially non-oscillatory (WENO) scheme with one-step irreversible reaction. The results show that the front of oblique detonation wave is composed of two different parts: the oblique shock wave (OSW) and the oblique detonation wave (ODW). If the wedge is long enough, according to the flow field structures and oscillation features the ODW is also divided into three regions: ZND model-like structure, single-sided triple point structures and dual-headed triple point structures. Simultaneously the triple point traces are recorded to obtain the different cell structures.

Paper #116

**Visualization of the Initiation and Stabilization Process of an Oblique Detonation Wave around a Projectile**

*Shinichi Maeda, Jiro Kasahara, Akiko Matsuo*

Spherical projectiles were launched into stoichiometric acetylene-oxygen mixtures diluted with argon or krypton under the projectile velocities were about 1.1 times of Chapman-Jouget (C-J) velocities. An initiation and stabilization of oblique detonation waves (ODWs) around the projectiles were visualized with high time and spatial resolutions using Schlieren technique and a high-speed camera which had 1 microsecond frame speed. It was reported that unsteady wave structures called Straw Hat types consisting of a shock-induced combustion and C-J ODW were observed near the criticality to stabilize ODW, and they were divided into two propagation types whether C-J ODWs could be stabilized or not (Kasahara et al. 2001, 2002, Maeda et al. 2011). In this study, the wave structures of Straw Hat types were suggested and confirmed by dozens of continuous images. They had triple points at the intersections of the bow-shock and C-J ODW with a transverse detonation or shock wave. The shock waves existing inside the Straw Hat types made Mach intersection near the central axis of projectile. The initiation process of ODW by a projectile was visualized placing the flange to set a diaphragm in the observation region. The strong shock wave existed ahead of the projectile, and it was diffracted apart from the projectile just after the diaphragm rupture. A chemical reaction was initiated by the shock compression. The ODW establishment at far field needed a strong initiation process which was similar to a re-initiation process in a detonation diffraction. The detonation wave was initiated by the local explosion on the diffracted shock wave. It expanded almost spherically, and its upstream side establishes the ODW front at far field. The curvature radius of detonation wave around the projectile increased as the projectile travelling. And the result of this study indicates that the critical curvature radius is needed for stabilizing the ODW at far field.

Paper #136

**Coherent High Frequency Instabilities of Detonations***Leung, C., Radulescu, M.I., Sharpe, G.J.*

The nonlinear pulsating mechanism of one-dimensional detonations was studied numerically using a simple two-step chain-branching model with separate induction and reaction zones. Numerical simulations were performed for a wide range of parameters, which revealed four distinct pulsating regimes classified according to the mechanism controlling the frequency of the pulsations. The present study focuses on the high and very high frequency pulsations. The dynamics of these regimes were clarified by reconstructing the characteristics, representing the trajectory of pressure waves and particle paths. The novel very high frequency regime, with periods of oscillation less than one induction time, involves coupling between the acoustic and the reactivity disturbances propagating, respectively, along the C- and C0 characteristics. These are generated at successive lead shock pulsations and arrive at the reaction zone simultaneously. For all regimes, the dominating mechanism of the pulsating instability was found to be in good qualitative agreement with Toong's phenomenological model based on the wave dynamics in a square wave reaction zone structure.

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**11:45 (R6B) Gas Turbine Combustors**

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Paper #102

**Effects of the Recess Length of a Coaxial Injector on a Transcritical LO<sub>2</sub>/H<sub>2</sub> Jet Flame***A. Ruiz, T. Schmitt, L. Selle, B. Cuenot and T. Poinsot*

In rocket propulsion using liquid propellants, innovative injection systems, with varying recess lengths of the coaxial injectors, have a strong impact on the combustion chamber behaviour. In a LO<sub>2</sub>/H<sub>2</sub> rocket engine at nominal operating conditions, the combustion chamber pressure (typically around 10 MPa) is above the critical point of both reactants while the oxygen is injected in a liquid-like state, at a subcritical temperature (around 100 K). This particular injection mode is designated as "transcritical". Such conditions make experimental studies extremely difficult and costly. As a consequence Computational Fluid Dynamics (CFD) has been extensively used for decades in the development of rocket propulsion systems. The Reynolds Averaged Navier-Stokes (RANS) method is commonly used by aerospace manufacturers to carry out parametric studies around a given design and determine the most promising one before undertaking hot fire tests. However, the predictive capability of the RANS method for new designs is limited and Large Eddy Simulation (LES) is now preferred to study them. In the present work, the LES technique is used to analyse the effect of the recess length of the inner LO<sub>2</sub> tube from the outer H<sub>2</sub> tube, on the flame characteristics. This recess length is a critical design parameter, as it impacts directly the flow and flame stability. The unsteady turbulent reactive flow is predicted in a laboratory-scale combustion chamber, using a single-element coaxial LO<sub>2</sub>/H<sub>2</sub> injector with and without recess, at operating conditions close to a cryogenic liquid rocket engine at the nominal point. Results show that the recessed injector induces high strain due to more confinement of the flow. As a consequence, the flame shape and length is totally different from the non-recessed injector.

Paper #233

**Extension of LSI Functionality for Gas Turbine Applications***P. L. Therkelsen, D. Littlejohn, R. K. Cheng*

Low swirl injector (LSI) technology is being evaluated for use in gas turbine (GT) engines. The LSI is a lean premix (LP) combustion technology originally developed for fundamental studies of flames. It operates differently than traditional high swirl LP GT injection systems, which utilize a bluff body or an aerodynamic recirculation zone to stabilize flames. The LSI utilizes a divergent flow to stabilize a flame by exploiting the turbulent displacement flame speed of propagating LP flames. The flame burns in a region where the turbulent flame speed matches the decreasing flow velocity as it diverges from the injector exit. Modern GTs, designed to run on pipeline quality natural gas (NG), must meet strict pollutant emission limits. The formation of NO<sub>x</sub> is dependent upon flame temperature and subsequently the equivalence ratio  $\phi$ . Engines are primarily operated by burning LP fuel/air mixtures to satisfy these limits, NG fueled LSI GT engines have achieved NO<sub>x</sub> emissions levels less than 5 ppm @ 15% O<sub>2</sub>. Extending the lean blow-off (LBO) limit to a lower  $\phi$  would increase the functionality of a LSI based GT combustion system by further reducing NO<sub>x</sub> emissions. The LBO limit can be altered by operating at different operating conditions (pressure and temperature) or by stabilizing the weak LP flame by reducing flow field disturbances. One source of flow disturbance is the transition from the injector to combustor dump plate. This transition results in a corner recirculation zone with large vortex structures that can perturb the LP flame. In order to reduce the LBO limit for NG engines the impact of these vortices must be reduced. There is considerable interest in the use of syngas, derived from gasified coal, as a primary fuel for large utility-sized GT engines in Integrated Gasification Combined Cycle (IGCC) power plants. LSI combustor systems are being developed for use with HHF. Coal derived syngas is a high hydrogen fuel (HHF) with hydrogen content ranging between 80 and 90%. In this study, HHF is comprised of 90% H<sub>2</sub> and 10% CH<sub>4</sub>. HHF burns with higher flame temperatures than NG flames for a given  $\phi$ . For practical use in GT engines, thermal output levels must be on par with NG flames. However, due to the highly reactive nature of hydrogen, operation at the same thermal outputs as natural gas poses a risk of flame flashback. The use of HHF syngases in commercial GT engines necessitates the design of modified or alternative combustion systems that can burn this fuel without the potential of flashback, while producing an adequate level of thermal output. Extending the flashback limit of the LSI combustor would benefit development of a HHF GT engine. This study reports on efforts to extend the functionality of LSI based combustors to meet the operability needs of both NG and HHF fueled GT engines. A flare quarl has been designed to promote flame stability by reducing corner recirculations and to provide the naturally diverging flame a structure to align with.

Paper #314

**Effect of Fuel Nozzle Geometry on the Stability of Non-Premixed Turbulent Methane Flame***Mohsen Akbarzadeh and Madjid Birouk*

An experimental assessment of the effect of fuel nozzle geometry on the stability of turbulent, non-premixed methane flame is presented. The burner consists of a central fuel nozzle surrounded by an annulus of co-airflow. Four nozzles with different geometries having similar exit cross-sectional areas but different internal/orifice geometry (circular, rectangular, square and triangular nozzles) were tested. The main focus of the present study was on determining the flame lift-off, blowout and reattachment velocities, which are indicators of the stability of non-premixed methane flame. The flow mean velocity and turbulence profiles along the centreline plane were also measured. The experimental data revealed that both the lift-off and blowout velocities of the asymmetric nozzles' flames (i.e. rectangular and triangular nozzles) are higher than those of the square nozzle and circular nozzle (axisymmetric nozzle). In addition, these results showed that beyond a specific co-airflow rate, reducing the fuel exit velocity does not result in the flame reattachment; but instead, the lifted flame extinguishes before it settles down on the burner. The base of the lifted flame, which changes depending on the jet fuel exit velocity, stabilizes right downstream of a local minimum of the  $u/U$  profile.

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**11:45 (R6C) Electric Aspects of Combustion**

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Paper #206

**Two-dimensional Modeling of the Ignition Length Decrease in Hydrogen Mixture with Oxygen Excited in Electric Discharge***A.A.Chukalovsky, K.K.Klopovsky, M.A.Liberman, Yu.A.Mankelevich, N.A.Popov, O.V.Proshina and T.V.Rakhimova*

There is great interest in application of non-equilibrium plasma for the plasma-assisted combustion [1]. It was demonstrated both experimental and theoretically that plasma active particles, mostly radicals influence burning process leading to decrease of ignition temperature, reducing induction delay time or length of induction and increasing the flame velocity. In addition to radicals vibrationally and electronically excited molecules can also enhance the chemical reaction rates at reduced temperatures. There are very few data on the influence of non-equilibrium plasma with electron excited molecules (especially  $O_2(^1\Delta_g)$ ) on initiation and branching reaction in fuel-contained mixtures in hydrogen (hydrocarbon)-containing mixtures. The measurements of the rate constants of these reactions as a function of temperature are complicated both by the presence of active odd oxygen (radical O + ozone  $O_3$ ) in plasma itself and by the secondary reactions at elevated temperatures. The role of  $O_2(^1\Delta_g)$  generated in the discharge plasmas on the ignition was demonstrated in recent experiment [2], where atomic oxygen was removed in heterogeneous reactions on the wall covered with HgO [2]. All the same, concentration of atoms O(3P) was not measured, while our previous investigations showed, that for similar discharge conditions, some residual concentrations of odd oxygen remained in the excited oxygen flow. The objective of the present study was to reveal the main processes with singlet oxygen which stimulate the initiation and branching chain reactions of combustion in hydrogen-oxygen mixtures. For this purpose the comprehensive numerical study of all stages of the experiment [2]: DC discharge in oxygen, transport in drift tube and flow reactor were carried out. The calculations of discharge were performed using one-dimensional self-consistent model of DC-discharge with constant gas flow through the tube at constant oxygen pressure. To simulate the flow reactor and the drift tube two-dimensional (in axial symmetry) gas dynamic model of mixing reactor was used. The reaction scheme for  $H_2$ -  $O_2$  mixture used in our simulations has been tested for induction time values in a wide range of parameters: pressure, temperature and composition. It was supplemented by reactions for active particles -  $O_2(^1\Delta_g)$  and  $O_3$  including 16 reversible reactions. The modeling showed a good agreement with experimental data on the ignition length. It was shown that residual odd oxygen concentrations in excited gas from discharge are sufficient to actuate branching reactions skipping the stage of direct initiation. The influence of singlet oxygen on the initiation and branching chain reactions of combustion in hydrogen-oxygen mixtures was analyzed. The sensitivity of the induction length to the total rate constant was revealed. The probability of branching channel in the reaction  $H + O_2(^1\Delta_g) \rightarrow O + OH$  was observed depending on the value of the total rate constant. The estimated value of the reaction rate  $H + O_2(^1\Delta_g) \rightarrow O + OH$  equals  $(2.4 \pm 0.2) \cdot 10^{-13}$  at 780K.

Paper #302

**Simulated Gravity Using Electric Fields in Microgravity Combustion***S. Karnani, D. Dunn-Rankin, F. Takahashi, Z-G. Yuan, D. Stocker*

The objective of this study is to improve the understanding of flame behavior under the influence of electric fields. When applied to a flame, an electric field can produce an ion-driven body force that acts similarly to the way that gravity can direct less dense gas via buoyancy. The small concentration ( $\approx 10$  parts per billion) of charged species make chemical effects an unlikely explanation for the observed behavior. Instead, effects are generally attributed to the ion wind, an action-at-a-distance effect, which can alter a flame's behavior and can be used as a localized actuator. The following described work compares a jet flame under the influence of an electric field in 1g and  $\mu g$  using the NASA 2.2-s Drop Tower to identify the roles of two transport mechanisms, buoyancy driven convection and ion wind driven convection, in controlling flame shape.

Paper #201

**Numerical Simulation of the Effect of the Ion-Driven Wind on Flame Stability***Memdouh BELHI, Pascale Domingo, Pierre Vervisch*

The application of electric field is known to have the ability to improve significantly the flame stability. In the few numerical studies, interested in combustion interaction with an electric field, the anions are overlooked. The stabilization

mechanism is generally supposed to be ionic wind. To verify this assumption, a mathematical model, which includes anions, has been developed. The Navier-Stokes equations along with transport equations for charged species and the electric potential Poisson's equation are solved. The studied configuration is a lifted diffusion methane/air flame. The model reproduces the tendencies of experimental observations. An analysis of the effect of ionic wind on the flame propagation mechanism is proposed.

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**14:30 Session (S3) Dynamics of Large Scale Fire and Explosions - III**

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Paper #226

**Radiation Based Initiation of Vapour Cloud Explosions***M. A. Hadjipanayis, F. Beyrau and R. P. Lindstedt*

Fast flame propagation modes in large vapour cloud explosions are typically regarded as a consequence of high levels of turbulence. However, there are cases where so far no single propagation mode (detonation, high speed deflagration, deflagration to detonation transition) can fully explain the combination of an apparently episodic event with the severe over-pressures observed. In one such incident, the Buncefield explosion in the UK, the Health and Safety Laboratory (HSL) concluded that a different mode of flame acceleration may be responsible for the observed inconsistencies. The Buncefield site was covered with large quantities of dry leaves and other dead vegetation and a possible mechanism based on premixed explosions in gas clouds seeded with char-forming, porous particulates has been formulated. The proposal is based on the pioneering work of Moore and Weinberg, but differs in the sense that it assumes an episodic/unstable flame propagation mode. The basis for the suggestion arises partly from evidence obtained using CCTV footage, which suggests an episodic propagation mode with an average flame speed of 150 m/s. The observed timings are such that the radiative ignition mode of propagation is arguably only plausible if flammable pockets can be ignited within 40 ms through radiation from fireballs no further than 6 m away from the point of ignition. Moore and Weinberg studied the ignition of particles made from fibrous materials, such as cotton, packed into spheres and illuminated by a far-infrared (FIR) laser source and visible light from a tungsten-halogen lamp. Ignition times for particles illuminated with visible light were of the order 1 s compared to 0.1 s for FIR laser illuminated particles when subjected to the same level of radiation flux. The blackening of cotton particles resulted in a significant reduction in ignition times for the former case. The objective of the current study is to examine if char-forming organic particulates can serve as sufficiently swift initiators of combustion in explosive atmospheres as a result of illumination with radiation levels similar to those experienced in large vapour cloud explosions.

Paper #14

**Effect of Initial Temperature on FA and DDT in H<sub>2</sub>-air mixtures: CFD Simulations & Validation against Experimental Data***Prankul Middha*

There has been a continuous and increasing interest in studying hydrogen safety in recent years. One of the motivating factors is handling the safety concerns in the nuclear industry as the consequences from nuclear accidents are global, and it is very important to maintain confinement in case of a hydrogen explosion. It is well-known that deflagration to detonation transition (DDT) may be a significant threat for hydrogen explosions. Due to the high reactivity of hydrogen, DDT is likely in a variety of scenarios involving H<sub>2</sub>-air mixtures and result in large-scale damage. Calculations have shown that certain accident scenarios can be characterized by high local compartment temperatures. However, there are not many DDT experiments carried out at temperatures higher than the ambient. The experimental tests used in this article were carried out to generate DDT data at high temperatures, up to 650 K. This data can also be valuable for carrying out safety analyses for gas turbines where hydrogen is used as fuel. For this purpose, a well-documented experimental test series was carried out in the High-Temperature Combustion Facility (HTCF) at the Brookhaven National Laboratory (BNL) in the United States. The objective of the present set of experiments was to characterize the effect of the initial temperature of the mixture on flame acceleration and the potential for DDT. These experiments have been simulated using the Computational Fluid Dynamics (CFD) tool FLACS. FLACS is a commercial special-purpose CFD tool that is developed by GexCon and has been designed for modelling gas explosions in industrial-scale geometries. It has previously been extensively validated for hydrogen safety applications for dispersion, explosion as well as combined dispersion and explosion studies. The test geometry has been implemented in FLACS and simulations have been carried out for the entire concentration range as well as all three temperatures.

Paper #44

**Spherical Combustion Clouds in Explosions***Allen L. Kuhl, John B. Bell, Vincent E. Beckner & Kaushik Balakrishnan*

This study investigates combustion clouds embedded in unconfined spherical explosions. Two charge configurations are considered: a 0.5-g spherical PETN booster surrounded by a spherical shell of either 1-g of TNT solid or of 1-g of Aluminum (Al) powder; these provide the fuel for the combustion process. Detonation of booster disperses the fuel, whose expansion drives a blast wave into the surrounding atmosphere. The fuel-air interface is unstable and rapidly evolves into a turbulent mixing layer. The hot detonation products and the shock-heated air serve as ultra-strong ignition sources of the fuel-air mixture, which evolves into a spherical combustion cloud [1,2]. The evolution of the blast wave and ensuing combustion cloud dynamics are studied via numerical simulations with our two-phase Adaptive Mesh Refinement (AMR) combustion code [3,4]. Turbulent combustion inside the cloud is visualized by a color-bar representation of the temperature field. For the TNT case, combustion occurs along thin flame sheets, while a

distributed-combustion mode is realized for the Al-powder case due to two-phase flow effects. By performing reactive and non-reactive flow simulations, it was demonstrated that combustion caused no change in the pressure field during the positive phase of the blast wave - in other words, combustion in the fireball is isobaric. This finding was confirmed by experimental pressure measurements [5]. In these unconfined cases, fuel consumption was limited to ~ 60%, while for confined cases [3,4] fuel consumption approached 100% due to continued mixing induced by shock reverberations in the chamber. Taking advantage of the point symmetry inherent in these problems, the flow field was azimuthally-averaged to extract the mean fields: and their r.m.s. fluctuations: These were used to construct the evolution of the mean and r.m.s. profiles, the Reynolds stress profiles, and the turbulent kinetic energy spectrum of the mixing layer.

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**14:30 (R7A) Detonation Dynamics and Structure-II**

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Paper #146

**Oscillations in Shock-Induced Combustion near Conical Projectiles***Jimmy Verreault, Andrew J. Higgins*

Combustion instabilities around hypersonic conical projectiles are presented via Schlieren photographs of the flowfield induced by the bodies. The prediction of the type of combustion pulsations using the first Damköhler number is applied to the experimental results. A comparison with previous studies using spherical-nosed projectiles shows that a new model is needed to describe the combustion instabilities produced by conical projectiles.

Paper #242

**Response of Cellular Detonations of Finite Perturbations***Lee John H.S., Fortin Yannick*

The present paper reports an experimental investigation of the transient relaxation processes of a cellular detonation subsequent to a large perturbation. The perturbation is generated by passing the detonation through a perforated plate or a wire grid. Two mixtures that have different structures and regularity of the smoke foil patterns are investigated:  $C_2H_2 + 2.5O_2 + 70\% Ar$  and  $C_3H_8 + 5O_2$ . The relaxation processes are observed via schlieren photography. It is found that when the detonation structure is severely perturbed, the re-establishment of the detonation originates from local explosion centers, a process similar to the onset of detonation in DDT. However if the structure is only slightly perturbed (e.g. when a wire grid is used), the original cellular structure is re-established when the perturbations decay rapidly downstream of the wire grid. It is found that the relaxation processes are similar for both the Argon diluted "stable" mixture and the propane "unstable" mixture even though the initial cellular structures prior to the perturbation are quite different.

Paper #63

**Numerical Study of Detonation Structure in a Channel with Porous Wall***K. Mazaheri, M. Sabzpooshani, Y. Mahmoudi, M. I. Radulescu*

To study the propagation of gaseous detonations in a channel with porous wall, 2-D Euler equations with a single step Arrhenius kinetics model are integrated in the present study. Different mixtures with both high and low activation energy, characterized by their irregular and regular detonation structure, are studied. It is found that the failure mechanisms of a detonation wave, propagating in a porous channel, are attenuation of transverse wave and mass divergence into the permeable wall. However, mass divergence has major role in detonation failure. The present results reveal that, as activation energy increases, higher number of transverse waves in the channel width are required to re-generate new triple points, in order to overcome the effect of mass divergence into the porous wall and support the self-sustenance propagation of detonation waves. In the porous section there is a competition between the triple point elimination at porous section and re-amplification of new triple points across the detonation front due to the interaction of the transverse waves, which reflect from the upper and the lower walls. Hence, as the number of transverse waves increases the re-generation of new triple points at detonation front increases and the detonation is more likely to retain its self-sustained propagation. The results also depict that close to the porous wall the front curvature increases. If the curvature extends to all the channel width, the wave fails to propagate. In contrast to the previous observations, this effect is seen for both regular and irregular structures. For unstable detonations, the critical limit,  $d/\lambda$ , is found to be higher than that of stable detonations, while previous experimental investigations reported that in high activation energy mixtures the critical limit is lower. It is suggested that this significant discrepancy manifests the effect of turbulent mixing in controlling the reaction rate in highly unstable detonations, which is not considered in the present simulation due to low grid resolution.

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**14:30 (R7B) Dynamics of Ignition – I**

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Paper #32

**Acoustic Timescale Detonation Initiation in 2-D and its Relationship with the 1-D Description***Jonathan D. Regele, David R. Kassoy, Oleg V. Vasilyev*

One dimensional numerical simulations of spatially resolved thermal power deposition on the acoustic timescale have demonstrated a mechanism to achieve Deflagration-to-Detonation Transition (DDT). This mechanism is characterized by heating a localized volume of fluid on a timescale fast enough that the fluid is nearly inertially confined and the pressure rises with temperature. Compression waves generated by the subsequent relaxation of the ephemeral high pressure spot (explosion) transition to shocks and preheat an induction zone of fluid between the lead shock and the reacted fluid. Most of the previous work in this area has focused on concept development where 1-D simulations with artificially low

activation energies are used. These one-dimensional simulations use non-dimensional activation energies in the range 10-13.8, while more realistic activation energies can be as high as 100. It has been unclear whether the concepts developed in the 1-D studies are valid in multiple dimensions and at higher activation energies. More recent results demonstrate that initiation still occurs with increased activation energy, but that a more incremental set of localized explosions occur. The current work focuses on the 2-D aspects of the DDT process. Two different 2-D simulations of acoustic timescale DDT are performed by depositing energy for a finite duration in a circular region inside of a channel. In one case DDT is achieved and in the second it fails. Explanations are presented for the differences and how transverse waves generated from the initial thermal explosion play a role in the DDT process.

Paper #218

#### **Auto-ignition at Shock-Wave Collisions in Hydrogen-Air Detonation**

*Oleg G. Penyazkov, Kirill L. Sevrouk, Khaled Alhusan*

Realistic modeling of flow and energy release associated with a detonation structure is important from theoretical point of view and practical applications. Besides, three-dimensional phenomena and interactions are also extremely important under considerations of reacting flows accompanied with shock waves at complex flow and boundary conditions. In this work we have attempted to investigate the influence of 2D and 3D shock-wave collisions on auto-ignition mechanism in induction zone of hydrogen/air detonations. Different collision geometries and reactive hot spots were produced at interaction of the incident shock wave with wedge and conical walls. Induction times and auto-ignition modes of the mixtures (strong, transient and weak) were measured by means of pressure, ion current and emission observations. Particular attention has been paid in experiments to determining the critical ISW intensity required for initiation of different auto-ignition regimes. The results were compared with a reference data obtained behind normally reflected shock waves.

Paper #122

#### **Experimental Analysis of Laser-Induced Spark Ignition of Lean Turbulent Premixed Flames**

*Cardin, C., Renou, B., Cabot, G., Boukhalfa, A.*

Lean turbulent flames are encountered in many applications, such as car or aeronautical engines, and thus, their study is a fundamental subject in combustion science. When the flow becomes lean and highly turbulent, ignition is more complex and some questions are still open, because of the numerous parameters influencing the mechanisms of flame kernel initiation and propagation. In the present study, spark ignition in lean and highly turbulent premixed flows is experimentally investigated. The Minimum Ignition Energy (MIE), which is the energy that has to be deposited in the mixture in order to ignite a self-sustained flame kernel, is measured for laser-induced spark ignition in methane/air mixtures, as a function of the turbulence intensity  $u'$  the equivalence ratio and the volume of energy deposition, function of the focal length of the focusing lens. Turbulence is generated thanks to a multi-scale injector constituted by three perforated plates, allowing to create a homogeneous, isotropic and highly turbulent flow. The burner provides a 2-D stationary flow. The measurements display a clear transition on MIE values when  $u'$  increases. Before the transition, the MIE increases slowly with  $u'$  and is of the order of the laminar MIE, whereas across the transition (for  $u' \sim 1\text{m.s}^{-1}$ ,  $Ka \sim 10$  and  $Da < 1$ ), MIE increases strongly. Since MIE is proportional to the flame thickness at the power of three, this slope breakdown could be explained by the transition between two distinct modes of flame structures. From a certain threshold of turbulence intensity, the flame kernel would not develop anymore in a flamelet regime, but in a regime where it would be strongly modified by the turbulence: the flame front would undergo an intense mixing by all the eddies of the flow ( $Da < 1$ ) and a thickening by the small eddies ( $Ka \sim 10$ ), leading to an intense stretch and possibly local extinctions. This turbulent ignition phenomenon in turbulent mixtures has already been reported by Shy et al. [1], for different experimental conditions. The study of the influence of the focal length increase and the equivalence ratio decrease (leaner mixture) reveals that the MIE increases and the ignition transition happens for a less intense turbulence, meaning that the flame kernels initiated in these conditions are less resistant toward the disruptions induced by the turbulent flow. Finally, this study reveals that there is a common criterion of ignition transition: whatever the focal lens of the focusing lens and the equivalence ratio of the mixture, an ignition transition occurs when the turbulent flow reaches a turbulent Reynolds number of the order of 360. This criterion is consistent with that of Shy et al. [1], even if the values characterizing the transitions are not the same, because of differences existing between the flow conditions, the turbulence properties and the ignition systems of these two studies. [1] Shy, S.S., C.C. Liu, and W.T. Shih, Ignition transition in turbulent premixed combustion. *Combustion and Flame*, 2010. 157(2): p. 341-350.

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### **14:30 (R7C) Laser Diagnostics**

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Paper #77

#### **Laser Spark Ignition and Flame Expansion in Swirl Burners Fuelled with n-Heptane Sprays**

*C. Letty, E. Mastorakos, M. Juddoo, W. O'Loughlin, A. R. Masri*

An experimental study of laser ignition on lab-scale swirl stabilized n-heptane spray flames has been conducted, in view of the importance of this topic for gas turbine combustor ignition. The stability map of the burner was defined, including the lean blow-off curve. Fast  $\text{OH}^*$  chemiluminescence movies allowed a classification of successful and failed events. Time-scales of initiation, full flame ignition and extinction were also extracted from the movies. Concerning the ignition behaviour, it was found that small kernels emanate very often from the spark: some of them die very quickly after the end of the spark, some of them survive during some time and move inside the combustor, and finally some kernels develop into a stable flame.  $\text{OH-PLIF}$  at 5 kHz identified the motion of thin flame sheets and some localized extinctions along the flame sheet are evident. The ignition probability becomes zero at large axial distances from the nozzle and is smaller than the probability of initiating only a kernel.

Paper #90

### **High-Speed Imaging Diagnostics Applied to the Study of Auto-Ignition of Methane Jets in a Hot Coflow**

*W. Meier, C.M. Arndt, J. Gounder, I. Boxx, K. Marr*

Auto-ignition of fuel in hot oxidizing gas is of importance for various technical applications, for example in internal combustion engines, scramjets, or gas turbine combustors. In order to better understand fundamental aspects of auto-ignition and the development of flame kernels, a basic experimental configuration was investigated in the present study. A pulsed methane jet was injected with a speed of about 100 m/s into the exhaust gas of a flat, lean premixed H<sub>2</sub>/air flame. The measurements captured the beginning of the injection, the jet development, the auto-ignition events, the flame kernel development and finally the stably burning lifted flame. Several high-speed imaging techniques were applied at 5 or 10 kHz repetition rate: OH\* chemiluminescence and broadband luminescence imaging, Schlieren imaging and planar laser induced fluorescence (PLIF) of OH. To achieve better spatial resolution, OH PLIF images were recorded simultaneously with luminescence images at a different angle of detection. In this way it was possible to distinguish between ignition events which took place within the laser sheet and those flame kernels which propagated into the laser sheet. The paper presents the experimental arrangement, the measurement techniques and examples of high-speed image sequences. Auto-ignition kernels appeared quite reproducible at the periphery of the methane jet and expanded rapidly. Often, several flame kernels appeared almost simultaneously, expanded, merged and finally formed a lifted jet flame. The temperature of the exhaust gas of the H<sub>2</sub>/air flame was chosen around 1600 K leading to auto-ignition at a downstream location of approximately 33 mm. The stabilization region of the steady burning lifted flame was very close to this downstream position. The stabilization region was, however, difficult to define exactly because auto-ignited flame islands appeared frequently from below the mean lift-off height and moved downstream to merge with the main flame.

Paper #166

### **Detection of Soot Incandescence and PAHs Fluorescence at the Proximity of the Inverse Diffusion Flame by Using Laser Diagnostics**

*Noriaki Nakatsuka, Yasushi Imoto, Jun Hayashi, Miki Taniguchi, Kenichi Sasauchi, Fumiteru Akamatsu*

One of the serious problems for electric power generation by woody biomass gasification, that is an energy conversion process of the woody biomass, is tar formation. One way to reduce tar is by oxidative and thermal cracking by partial combustion of the producer gas in the gas reformer, an apparatus stage subsequent to the biomass gasifier. During the partial combustion process of the producer gas, an inverse diffusion flame is formed when oxidizer is supplied to producer gas. Cracking and polymerization of tar occur simultaneously at the proximity of the inverse diffusion flame. This polymerization of tar into soot is, however, a significant problem in the gas reformer. It is, therefore, important to clarify the mechanisms of soot formation at the proximity of the inverse diffusion flame, and to apply the findings to the reforming of containing tar by means of partial combustion of the producer gas. Here, polymerized tar grows into soot passing through polycyclic aromatic hydrocarbons (PAHs). For the past several decades, some growth mechanisms of PAHs have been proposed. These mechanisms are common to the primary PAH growth followed by abstraction of a hydrogen-atom from the reacting hydrocarbon by a gaseous hydrogen atom. We can, therefore, point to the possibility of suppression of the soot formation by controlling the hydrogen concentration at the proximity of the combustion region. As an approach to the problem of soot formation as a consequence of partial combustion of producer gas containing tar, experimental study was conducted to clarify the effect of hydrogen concentration at the proximity of the inverse diffusion flame on soot formation, and the growth of PAHs that is a precursor of soot. In the present study, laser induced incandescence (LII) and laser induced fluorescence (LIF) were used to measure soot volume fraction and PAHs concentration, respectively. Whereas the LII signal intensity was decreased by hydrogen addition, the signal intensity was maintained relatively constant with nitrogen addition to the oxidizer. Thus, soot formation was suppressed by the chemical effect of a small amount of additional hydrogen (approximately 0.5 % against the total enthalpy of the model producer gas), rather than by a slight change in oxygen concentration and the flow velocity of the oxidizer. Meanwhile, the volume concentration of PAHs was increased by the chemical effect of a small amount of additional hydrogen to the oxidizer. The above results indicate that soot formation was suppressed, whereas the concentration of PAHs (i.e. soot precursors) increased by hydrogen addition to the oxidizer of the inverse diffusion flames. This occurred because a higher concentration of molecule hydrogen in the combustion region caused a decreased in the forward reaction rate of the hydrogen abstraction reaction of PAHs, increasing PAHs without active sites. This led to the lower soot inception from PAHs with active sites formed by the hydrogen abstraction reaction. In addition, the lower soot volume fraction decreased the rate of the surface growth of soot with PAHs, which increased PAHs.

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## **16:15 (S3) Dynamics of Large Scale Fire and Explosions - IV**

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Paper #148

### **Estimating Blast Effects from an Accidental Release of High-Pressure Silane**

*J. Chao, C.R. Bauwens, S.B. Dorofeev*

Silane is a pyrophoric gas that can potentially autoignite when exposed to air under normal atmospheric conditions. In an accidental high-pressure release of silane, an explosive silane-air vapour cloud can form prior to autoignition. The resulting vapour-cloud explosion is characterized by very high flame speeds, which can result in serious blast damage, even for relatively small releases of silane. In the present study, practical estimates of credible worst-case releases are formulated by estimating the amount of silane that can be accidentally dispersed into air and the distribution of silane concentration in the vapour cloud. The corresponding blast effects (i.e., overpressure and positive impulse) is then

determined and used to specify safe-separation distances for various practical silane installations. Although thermal and projectile hazards should also be considered, only blast effects are treated in the present investigation using structural damage to buildings as a specific example.

Paper #149

**Effect of Vent Deployment Pressure and Panel Inertia on Vented Gaseous Explosions**

*C. Regis Bauwens, Sergey B. Dorofeev*

Explosion venting is a commonly used method to minimize or prevent damage to an enclosure caused by an accidental explosion. By opening part of the surface area of the enclosure, venting relieves the pressure generated by the explosion with the goal of maintaining a pressure below the design strength of the structure. The size, type and release pressure of the vent, however, can play a strong role on how pressure inside the enclosure develops. In the present study, the effect of panel release pressure and panel density is examined for the range of values typically used for room-sized enclosures and industrial occupancies. In addition to the experimental results, a simple model for the prediction of the pressure transient associated with the opening of the vent is developed. For the range of deployment pressures and panel densities used in this study, it was found that the vent deployment pressure transient depended on both the release pressure and on the panel density, increasing with both parameters. It was also found that the pressure transient associated with the opening of the vent had little or no impact on the subsequent external explosion and structure-acoustic pressure peaks. Thus, for panel densities and release pressures typical for room-sized or larger enclosures, the pressure transient caused by the deployment of the panel can be treated independently from the rest of the process. This allows for each pressure transient to be correlated individually and for the use of the peak with maximum overpressure to size the vent panel. A simple model to describe the opening of the vent and its associated pressure transient was developed. The model performed well, particularly for higher vent deployment pressures, providing reasonable estimates for the external explosion pressure transients.

Paper #283

**Numerical Simulations of Large Scale Hemispherical and Pancake Cloud Detonation**

*A. Heidari and J.X. Wen*

The present study is motivated by the need to validate modeling approaches for detonation propagation pattern, pressure, velocity and drag impulse for consequence analysis of real scale accidental scenarios. Using the same modeling approach described in Heidari et al. [1,2], numerical simulations were carried out for large scale hydrogen-air and propane-air detonations in a hemispherical geometry with 300 m<sup>3</sup> volume and a propane-air pancake cloud. The hemispherical hydrogen-air detonation was set up with the same configuration as the full scale tests of Groethe et al. [3]. The predictions were found to be in reasonably good agreement with the measurements for overpressure and impulse. Comparison of the predictions for the propane-air hemispherical and pancake cloud detonation has illustrated some salient differences that may have implications for accident investigation.

Paper #301

**Explosion Venting and Mixture Reactivity Influences in a Small Vessel**

*Fakandu, B.M., Kasmani, R.M., Andrews, G.E. and Phylaktou, H.N.*

Explosion venting is influenced by the reactivity of the gas mixture. This is normally correlated using either the laminar burning velocity, UL, or the deflagration index, KG = (dp/dt)<sub>max</sub>V<sup>1/3</sup>. This work used a small 90 litre vessel that ensured that the flame propagation during venting was laminar and enabled conventional laminar flame venting theory to predict the influence of reactivity through the UL term. It is shown that UL can be directly related to KG and hence that laminar flame venting theory can be expressed in terms of the KG reactivity parameter, which is normally used in the experimental presentation of venting data and in venting design standards. The work shows that the treatment of hydrogen in the design standards, significantly underestimates the overpressure for vented hydrogen explosions and more work is required in this area.

Paper #327

**Preliminary Large-scale DDT Experiments at NIOSH Lake Lynn Laboratory**

*R. K. Zipf, Jr., V. N. Gamezo, M. J. Sapko, W. P. Marchewka, K. M. Mohamed, E. S. Oran, D. A. Kessler, E. S. Weiss, J.D. Addis, F.A. Karnack and D.D. Sellers*

Preliminary methane-air deflagration-to-detonation transition (DDT) experiments are performed to examine whether DDT could occur in sealed areas of underground coal mines. The detonation tube used for these studies is 73 m long, with the internal diameter d=105 cm, and closed at one end. The test gas is 97.5% methane with about 1.5% ethane, and the composition of methane-air mixtures varied between about 7 to 14% methane by volume. Flame evolution was observed for a spark ignition in the tube with a limited number of baffles (orifice plates) near the closed end. In all experiments, baffles with a blockage ratio BR = 0.6 and spaced at S = d were added to the detonation tube starting from the closed end. The number of baffles was systematically increased from 0 to 20. In a test without baffles, the flame in near stoichiometric mixture accelerated very slowly and only reached a velocity of less than 100 m/s upon exiting the tube. Maximum pressure was less than about 0.5 MPa. For tests with 6 or more baffles, the flame in near stoichiometric mixture accelerated rapidly to over 600 m/s and generated strong shocks with a magnitude of 1.5 MPa or more. DDT appeared in the smooth section of the tube far outside the last baffle in tests with 9, 10, 11, and 18 baffle sets. For tests where detonations appeared, the flame speed before DDT had reached a velocity of 750 m/s or more, and the shock speed had reached a velocity of 800 m/s or more. So far, the tests were performed for up to 20 baffles, and DDT has not been observed within the obstructed section of the tube. The mechanism for the DDT in the smooth section of the tube



is not well understood, but data analysis shows that DDT is related to fast flames and possibly detonations that bypass the main detonation tube through the gas mixing and recirculation system. More studies are needed to understand this mechanism of DDT using experiments that prevent the flame bypass via the recirculation system. Additional experiments are underway with more baffles and with different BR. Experiments also show that it is possible to develop high flame speeds and high shock pressures for mixture compositions that are far from stoichiometric.

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**16:15 (R8A) Detonation Cellular Structure-I**

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Paper #162

**Influence of the Reaction-to-Induction Length Ratio on the Stability of Cellular Detonations**

*Bijan Borzou, Brian Maxwell, Matei I. Radulescu*

Using a two-step model for the reaction zone of detonations, the first step controlling the duration of the thermally neutral induction zone, while the second controlling the duration of the exothermic reactions, the present study investigates the role of the induction to reaction zone length on the cellular detonation stability. For all other parameters kept constant, it is shown that thinner exothermic main reaction zones have a destabilizing effect, yielding smaller and more irregular cells. Good agreement is found with previous results relating the dynamic behaviour of detonations to the stability parameter CHAI, given by the product of the activation energy and the ratio of the induction and reaction lengths in the steady ZND structure.

Paper #275

**On Cellular Pattern Formation in Detonation Propagation**

*Kazuhiro Ishii, Yuta Okitsu, Koji Morita, Shogo Sayama*

This paper aims to clarify the mechanism of cellular pattern formation on smoked foil records by applying other materials and to find alternative tools to visualize detonation characteristics. The experimental results show that it is possible to obtain cellular patterns in detonation propagation using CaCO<sub>3</sub> particles, fly ash, heat sensitive paper, and pressure sensitive paper instead of smoked foil. The symmetrical cellular pattern with the smoked foil is demonstrated for CaCO<sub>3</sub> particles, fly ash, and the heat sensitive paper. The asymmetry of the cellular pattern for the pressure sensitive paper is explained from its temporal response to varying temporal loading. The magnified images around the soot track by SEM and EPMA indicate local removal of soot deposit along the outline of the cell.

Paper #280

**Application of a Laser Induced Fluorescence Model to the Numerical Simulation of Detonation Waves**

*Rémy Mével, Dmitry Davidenko, Florian Pintgen, Joanna Austin, Joseph Shepherd*

Although numerical simulations have become an essential tool for detonation dynamics understanding, most of the physical constraints that exist within experiments are not accounted for which makes difficult a comparison. In the present study, a simple laser induced fluorescence model has been implemented and used to post-treat detonation wave numerical simulation results and allow a direct comparison with previous experimental visualizations of detonations in hydrogen-oxygen-diluent mixtures. The model is first applied to steady one-dimensional simulation results obtained with detailed chemistry. The effects on the fluorescence intensity of the model parameters are examined to underline the dominant processes. The model is then applied to unsteady two-dimensional simulation results obtained with reduced chemical schemes and a comparison is made with existing experimental data. The results essentially demonstrate good qualitative agreement between the experimental and calculated laser induced fluorescence intensities.

Paper #324

**Detailed Shock Configuration of Cylindrical Cellular Detonation**

*Makoto Asahara, Nobuyuki Tsuboi, A. Koichi Hayashi, Eisuke Yamada*

This study aims to investigate the detailed shock configuration of detonation wave especially the complex Mach interaction. Here, we calculate Oxy-hydrogen cylindrical detonation to get information of correlations between the cell bifurcation and the shock configuration. As a result, the following have been understood. The transverse cell appears in the area where the cell size is large. In the expanding surface of cylindrical detonation, the fine cell exists. The secondary transverse wave in transverse detonation disturbs the Mach stem.

Paper #326

**The Role of Cellular Structure on Increasing the Detonability Limits of Three-Step Chain-Branching Detonations**

*Mark Short, Charles B. Kiyanda; James J. Quirk; Gary J. Sharpe*

The role of cellular structure on increasing the detonability limits of a detonation whose kinetics are governed by a three-step chain-branching reaction is studied. In previous studies, it was demonstrated that for a sufficiently large value of the chain-branching cross-over temperature, a pulsating detonation will fail (characterized by a transition to a decoupled shock-flame complex) if the shock temperature drops below the chain-branching cross-over temperature. The purpose of the present study is to examine whether cellular detonation structure can increase the value of the chain-branching cross-over temperature at which coupled detonation solutions are observed. We demonstrate via numerical simulation that cellular solutions do extend the detonability limits, and discuss the mechanisms of self-sustained cellular detonation for values of the chain-branching cross-over temperature above those that lead to 1D pulsating wave failure.

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**16:15 (R8B) Detonation Initiation**

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Paper #147

**Direct Measurement and Relationship between Critical Tube Diameter and Critical Energy for Direct Detonation Initiation***Bo Zhang, Hoi Dick Ng and John H.S. Lee*

In this study, we investigate the direct relationship between the critical tube diameter and the critical energy for direct initiation of a detonation. Measurement of these quantities is performed respectively in a number of hydrocarbon-oxygen mixtures using a vertical circular steel tube connected to a relatively larger spherical bomb chamber. Using the new set of data, we assess the validity of a semi-empirical initiation model, namely, the surface energy model by Lee, as well as a simplified work done model. Both theoretical models provide a direct link between the two dynamic detonation parameters and comparison shows a very good agreement between the theoretical results with the experimental measurement.

Paper #279

**Near-Limit Propagation of Detonations in Annular Channels***Anne Jesuthasan, Alois Joassard, Hoi Dick Ng and John H.S. Lee*

In this study, the near-limit propagation of detonations in annular channels is investigated. Stoichiometric mixtures of methane-oxygen, acetylene-nitrous oxide diluted with 50% argon and acetylene-oxygen diluted with 70% argon are used in the experiments. Detonation velocity as well as smoke foils records of near limit detonations are obtained. It is found that by normalizing the channel length scale by the ZND reaction length, (i.e.  $L/\Delta_{ZND}$ , where L is the channel gap) the velocity variations for different channels coalesces to a single curve. Experimental results also show a strong dependence on the normalized curvature (i.e.  $1/(L/\Delta_{ZND})$ ) for detonations with high argon dilution. Detonation velocities of the order of half CJ values at failure were observed which tend to suggest instabilities provide the mechanism to maintain the propagation at such low velocities. The results obtained were compared to theory using the Fay-Dabora model. Qualitative agreement was obtained for high argon diluted mixtures, but fails to predict in undiluted mixtures.

Paper #199

**Visualization Study of Detonation Initiations Behind Reflected Shock Waves Using a High Speed Video Camera***Hiroki Yamashita, Jiro Kasahara, Akiko Matsuo*

The purpose of this study is intended as an experimental investigation of detonation initiation, using the high pressure and temperature region behind reflected shock. Then we observed transition to detonation from flame kernel behind reflected shock which has branched structure interfered with boundary layer, using a high-speed camera and schlieren method. A shock tube was employed as a experiment system. A stoichiometric acetylene-oxygen mixture was chosen as a combustible gas. When temperature and pressure behind reflected shock was 1042 K, 206 kPa respectively, combustible gas was ignited and transitioned to detonation wave. As the results of the present study, we observed that ignition points were located in the vicinity of triple point trajectory behind reflected shock which has branched structure interfered with boundary layer. Additionally, visualization results showed that a detonation wave propagated spherically with approximate CJ-velocity, setting an ignition point as a center, behind reflected shock.

Paper #96

**High Speed Stereoscopic Shadowgraph and Its Digital 3D Reconstruction***Q Wang and Y Zhang*

A stereoscopic shadowgraph system is set up based on conventional z-type schlieren apparatus. It consists of two inclined converging beams formed by two pairs of parabolic mirrors. Two synchronised high speed cameras are applied to record the shadowgraph image pairs simultaneously. A precisely etched metal mesh is used to calibrate the stereoscopic shadowgraph system. By combining the calibration parameters and coordinates of the matching points in stereo images, the depth information and the 3D view of the shadowgraph images are obtained. The developed stereoscopic technique is then applied to investigate the 3D structure of the interface between hot gas and ambient air produced by a gas turbine igniter. The time resolved 3D hot gas development has been reconstructed successfully. The stereoscopic shadowgraph technique has been shown to be an effective 3D visualization and quantitative reconstruction method.

Paper #272

**Onset of Detonation by Forced Ignition behind an Incident Shock Wave***S. Ishihara, T. Kojima, K. Ishii, H. Kataoka*

Deflagration to detonation transition (DDT) has been studied by many investigators and several explanations have been given to DDT process. Nevertheless, the knowledge on DDT is still insufficient for predicting where and when exactly onset of detonation occurs because of following two issues; one is poor reproducibility of strength of the precursor shock wave, which is responsible for variation of the position and time of a micro-explosion ahead of the accelerating flame. The other is less ability to control behavior of the flame acceleration or transition from laminar to turbulent flames. In the present work, forced ignition of an unreacted gas behind an incident shock was conducted using a shock tube so that onset of detonation occurred in the fully controlled flow field. The incident shock wave was generated whose strength was as much as that of the precursor shock in the DDT process. Ignition timing was controlled so that the distance from the incident shock wave to the ignition position could be varied to study effects of the interaction between propagating

flame and the boundary layer on detonation initiation. As for the method of ignition, spark discharge and laser ablation were used. Spark energy of less than 10 mJ was supplied to avoid direct initiation. A capacitive spark discharge whose duration was a couple of hundreds of nanoseconds was applied to the concentric planar electrodes whose gap was 1 mm. For laser ablation, Nd:YAG laser pulse whose wavelength was 532 nm and duration was 5-10 ns was used. Laser energy was varied from 5 mJ to 195 mJ. An ethylene-oxygen mixture with equivalence ratio of 1.2 was charged into the test section as a test gas at an initial pressure of 25 kPa, 35 kPa, and 100 kPa and at a room temperature. Ignition timing was controlled so that the distance from the incident shock wave to the ignition position was varied from 10 mm to 500 mm. As a result, it was found that there was a tendency that ignition whose position was located further from the incident shock wave caused prompt initiation of detonation. This tendency was independent of the initial pressure, ignition energy, and the ignition method. From differences of area of the soot record pattern which was drawn by the flame front arrival at the soot coated wall, it is considered that development of the boundary layer at the vicinity of the wall affected the propagation manner of the flame near the wall, varying the process of the detonation initiation.

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**16:15 (R8C) Diagnostics**

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Paper #83

**Measurements of the Three Dimensional Structure of Flames at Low Turbulence***M.R. Harker, M. Lawes, C.G.W. Sheppard, N. Tripathi and R. Woolley*

The development of spark ignited flame kernels in a turbulence field is strongly dependent upon the nature of three dimensional (3-D) turbulence adjacent to the ignition source. The turbulence scales vary in 3-D from shot to shot, resulting in successive flame kernels developing differently and thereby causing cyclic variations in spark ignition (SI) engines. It is necessary to quantify the scales affecting the flame at any instant for the accurate measurement of burn rate of such flame kernels, which requires visualization of the flame surface in 3-D. The experiments reported here employ multiple sheet mie-scattered light technique to successfully characterise a non-stabilised expanding turbulent flame kernel in 3-D. A novel algorithm was developed to calculate turbulent flame parameters such as flame surface density, reaction progress variable and the statistics of flame curvature from the 3-D flame structure.

Paper #179

**Investigation of the Ignition by Repetitive Streamer Discharges Using Time-resolved OH LIF Measurements***Detlef Markus, Aljoscha Hallermann, Tim Langer, Frank Lienesch, Ulrich Maas*

The ignition of hydrogen/air mixtures by repetitively pulsed nanosecond streamer discharges and subsequent flame propagation were examined. Inside a closed vessel the mixtures were ignited using high-frequency alternating voltage (up to 20 kV, 740kHz) and a rod/plane electrode configuration. Four sequential snapshots of two-dimensional OH distributions were received during one ignition event by the use of laser-induced fluorescence. Therefore, two Nd:YAG lasers are used to pump a dye laser leading to four consecutive laser pulses in the spectral range of 283 nm with a minimum delay of 50  $\mu$ s between two laser pulses. The detection system for the OH fluorescence uses a beam splitter arrangement to split the collected light after each laser pulse onto one of four independent CCD detectors. The time resolved two-dimensional OH LIF images give detailed information about the ignition volume and early flame growth.

Paper #216

**Effects of the Width of Droplet Size Distribution on Soot Formation in Spray Flame***Jun Hayashi, Junichi Fukui, Noriaki Nakatsuka, Fumiteru Akamatsu*

Spray combustion is a highly complex reactive two-phase phenomenon in which many simultaneous processes affect one another, including dispersion of fuel droplets, their evaporation, chemical reactions of the fuel vapor with the oxidizer, and combustion reaction associated with the formation of soot. Atomization is the earliest process of spray combustion. Spray characteristics, such as mean droplet size, mean spray velocity and droplet size distribution, are determined through the atomization process. Those characteristics have significant effects to the whole processes of spray combustion and spray flame structures. However, since those spray characteristics are difficult to control independently from the other physical characteristics of atomization, effects of the width of droplet size distribution on the spray combustion phenomenon and soot formation in spray flame have not been elucidated. In order to clarify the detailed spray flame structures, conducting fundamental experiments and numerical simulations is useful, particularly for simple flow fields such as laminar counterflow. The purpose of this study is, therefore, to investigate the effects of width of droplet size distribution of the fuel spray on the soot formation of spray flames stabilized in a laminar counterflow field. A frequency-tunable vibratory orifice atomizer is employed to carefully control the droplet size distribution. This atomizer is able to generate an arbitrary droplet size distribution independently from the other spray characteristics. Two-dimensional spatial distributions of soot formation area in the spray flames with different droplet size distributions are analyzed by laser induced incandescence (LII). In addition, the detailed local structures of spray combustion characteristics are examined by means of three-dimensional direct numerical simulation (3D-DNS) of spray flames. Results show that the soot formation area decreases in the poly-dispersed droplet size distribution condition. This tendency stems from the difference in flame structure. The portion of premixed-like flame increases under the poly-dispersed droplet size distribution conditions. And the spray combustion area enlarged in axis direction because evaporation rate of poly-dispersed droplet size distribution is varied.

Paper #80

**Influence of Heat Release on Swirl Flow Dynamics From High Speed Laser Measurements in a Gas Turbine Model Combustor**

*Christoph M. Arndt, Adam M. Steinberg, Isaac G. Boxx, Wolfgang Meier, Manfred Aigner*

Swirl burners are often utilized in practical combustors, such as those found in gas turbines (GT), because swirl-induced vortex breakdown presents an effective mechanism for flame anchoring and stabilization. In many cases, vortex breakdown is accompanied by coherent vortical structures termed precessing vortex cores (PVC), which spiral around the flame axis in the shear layer between the inflow and the inner recirculation zone. While PVCs are frequently identified in non-reacting swirl flows, their appearance in swirl flames has been reported to a lesser extent. Generally, the presence or absence of a PVC in a GT-like flame changes the flame shape and dynamics significantly. In the present study, an optically accessible gas turbine model combustor for lean premixed flames has been operated under both reacting and non-reacting conditions in order to investigate the behaviour of a PVC and the influence of combustion on the PVC. Simultaneous OH chemiluminescence and stereoscopic particle image velocimetry (PIV) measurements have been performed at a sustained repetition rate of 5 kHz in combination with acoustic probes. A confined swirling methane/air flame with an equivalence ratio of 0.82 and a thermal power of 30 kW, operated at atmospheric pressure, and the corresponding non-reacting flow were analyzed. The mean flow fields of the reacting and non-reacting case were compared as well as the frequency spectra of the acoustic probes. Coherent flow structures were identified by means of spatio-temporal proper orthogonal decomposition (POD) analysis and phase-averaging. The non-reacting flow exhibited a PVC structure, as determined from POD and phase averaged flow-field analysis. The dominant frequency of the PVC at 530 Hz was also visible in the acoustic measurements in the combustion chamber. In the reacting case, the burner had an acoustic mode at approximately 365 Hz. The flow field featured a periodic vortex shedding in the inner shear layer that interacted with the inflow. However, the PVC was damped out in the reacting case. The flow field structures and the influence of the periodic instabilities are discussed in the paper.

Paper #139

**Effect of Iron Pentacarbonyl on Soot Formation behind Shock Waves**

*G. L. Agafonov, V. N. Smirnov and P. A. Vlasov*

A strong influence of iron pentacarbonyl additives on soot formation during the pyrolysis of propane/Ar mixtures behind shock waves was revealed. A novel kinetic mechanism of the thermal decomposition of  $\text{Fe}(\text{CO})_5$  and the formation of free iron atoms and iron nanoparticles was tested. This mechanism correctly describes the available experimental data. A qualitative explanation of the experimentally observed effects of  $\text{Fe}(\text{CO})_5$  additives on soot formation was proposed. In our opinion, the nascent iron nanoparticles serve as soot precursors for further surface growth with the formation of soot particles. The influence of small  $\text{Fe}_n(\text{CO})_m$  fragments and small  $\text{Fe}_n$  clusters on soot formation process is less probable because of a rather short life time of these species.

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**08:30 (S4) Supercritical Combustion - I**

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Paper #213

**Progress in Transcritical Combustion : Experimentation, Modeling and Simulation***Sébastien Candel, Thomas Schmitt and Nasser Darabiha*

Transcritical conditions correspond to situations where the operating pressure exceeds the critical pressure but the injection temperature is below the critical value. Such extreme conditions, which are encountered for example in high performance rocket engines, introduce fundamental scientific challenges with many technological implications. Advances on these issues are reviewed in this article. It is shown that progress has been substantial on the experimental level and that this has provided an important data base for parametric analysis and model development. Improved real gas thermodynamics and transport models have allowed investigations of geometrically simple problems such as combustion of spherical pockets or in strained flames formed by the counterflow of transcritical and supercritical streams. Calculations of complex flames formed by transcritical injection of reactants have also been carried out using RANS models, but much of the recent effort has been focused on the adaptation of computational tools for large eddy simulation of transcritical flows. Recent calculations of typical transcritical injection configurations indicate that simulations can suitably retrieve flame structures and trends observed experimentally. It is concluded that progressively more complex configurations will become tractable with advanced transcritical LES tools and that this should help improve current understanding of fundamental processes and advance design methods.

Paper #244

**Shear Coaxial Jets Subjected to an External Acoustic Field***Ivett A. Leyva, Doug Talley, Sophonias Teshome, Juan Rodriguez, Jeffrey Graham*

What happens to the mixing processes in a shear coaxial injector as the working fluids cross into the supercritical regime is the first topic of this paper. The second topic is how the mixing reacts to external acoustics. The interest on knowing the response to acoustics arises from the ever present concern of developing combustion instabilities on a new engine design or new operating conditions. The results presented here are solely concerned with all-nitrogen shear coaxial injectors exiting into a nitrogen atmosphere. This choice allows us to have a single critical point making it easy to know exactly the thermodynamic state of the inner and outer jets and the chamber. Being non-reacting allows us to focus on the fluid mechanics instabilities of a coaxial jet and their response to external acoustics.

Paper #335

**Supercritical Fluid Flow in Rocket Motor Engines***Guillaume Ribert, Hongfa Huo and Vigor Yang*

Designing a rocket engine combustion chamber requires a particular attention to the cooling system and the propellant injection and combustion. The wall heat transfer is a key-point to increase the life cycle or prevent the failure of combustion chamber walls. Regenerative or forced convection cooling are the most common methods used: a cryogenic fluid, typically hydrogen or methane, in a supercritical state, i.e. both the pressure and temperature are above the respective critical values of the fuel, flows in small channels that are imbedded in the chamber walls and the nozzle throat portion, and absorbs heat from the hot-gas side wall. For such configurations, experiments over the past ten years have shown significant thermal-load sensitivity to the channel geometry and fluid properties. For example, the use of high aspect ratio (height/width) cooling channels (HARCC) is a promising technique to reduce the near wall temperature of the combustion chamber for a limited pressure drop. After travelling through the cooling system, the coolant fluid is injected into the combustion chamber in which a very high pressure of the order of 10 MPa and above prevails. The identification of the resulting supercritical flame stabilization mechanism is essential to provide insight into the supercritical combustion dynamics. A poor flame stabilization may lead to harmful instabilities or flame blow-off. For instance, at low (0.15 MPa) and intermediate (1.0-2.5 MPa) pressures the experimental results show that the methane flame is lifted off from the rim of the LOx post, and less stabilized compared to LOx/H<sub>2</sub> flame. However, at near- and supercritical pressures, experiments show that the flame is attached/anchored in the vicinity of the LOx post. This high pressure observation is similar to the behavior of the supercritical LOx/H<sub>2</sub> flames studied by Mayer et al. In addition, Singla et al. observed that the LOx droplets penetrated into the inner flame resulting in a secondary flame and a larger expansion angle, when both LOx and CH<sub>4</sub> were injected at trans-critical conditions, i.e. pressure is above critical but temperature is below critical. However, LOx droplet penetration was not observed when CH<sub>4</sub> was in gaseous phase, and when the LOx was injected at subcritical temperatures. From these observations, it is clear that the flame stabilization and subsequent development is still not well understood for supercritical LOx methane combustion. In the present article, both issues are studied with one numerical code which has the following characteristics.

Paper #338

**Theoretical and Numerical Investigation of Kerosene Mixing in a Swirl Injector at Supercritical Conditions***Kuk-Jin Kim, Jun-Young Heo and Hong-Gye Sung, Vigor Yang*

Advanced propulsion systems are operated at supercritical conditions exceeding the thermodynamic critical state. Hence, the study for the mixing and combustion process of the propellants is indispensable at supercritical conditions. Because of the peculiarities of substances at supercritical conditions, the conventional methods for property analysis are inappropriate so that the applicable thermodynamic relationships for a wide range of pressure and temperature must be employed. Among the propellants, kerosene fuels are quite unwieldy in theoretical and numerical analysis because of a large number of hydrocarbons, reactions, and thermophysical parameters. Therefore, kerosene surrogate models are

considered for the abbreviation of real fuel components. In this study, the surrogate models of JP-8/Jet A are applied to kerosene mixing at supercritical conditions. The results of numerical analysis at supercritical condition are compared with those at transcritical condition.

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**09:10 (R9A) Detonation Cellular Structure – II**

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**Paper #67****Large Eddy Simulation of Flame Acceleration in an Obstructed Channel***Craig Johansen and Gaby Ciccarelli*

Large eddy simulations (LES) of early-time flame propagation using a flame surface density combustion model have been undertaken and compared to experiment. From the onset of spark ignition at the closed end of a confined channel, the development of the flow field in the unburned gas ahead of the flame has a large influence on the rate of flame acceleration leading up to DDT. The presence of fence type obstacles distributed on the channel surface distorts the unburned gas flow and enhances flame acceleration. Initially, the flame interaction with small recirculation zones at low flame speeds results in a relatively smooth roll-up of the flame surface. Later, the generation of a shear layer from the obstacle tips results in the production of turbulence, which increases the total transport of mass, momentum, and energy in the flow. The flame shape becomes highly stretched in the stream-wise direction as small vortical structures form in the shear layer. The development of these small three-dimensional flow structures wrinkles the flame surface, which enhances the bulk burning rate. As a result, a feed-back loop is formed between the volumetric burning rate and the unburned gas velocity, causing flame acceleration. It was found that the main features in the flame shape continually evolve from changes in the recirculation zone structure. Predictions of the overall flame shape and large flame structures agree well with experimental schlieren images. Quantitatively, the simulations accurately predict the experimental flame-tip velocity oscillations and the increase in flame area.

**Paper #73****Mach Reflection in Detonations Propagating through a Gas with a Concentration Gradient***F. Eitner, K.G. Vollmer and T. Sattelmayer*

The instabilities occurring in a gaseous detonation front produce the well-known cellular structures which can be reproduced numerically by recording the maximum pressure history in a computational domain. Up to date, nearly all studies concerning detonation cells, no matter if experimental or numerical, have been focused on perfectly homogeneous mixtures. In the present study the investigation of detonations propagating perpendicularly to a concentration gradient is conducted analytically and numerically. First, a semi-analytic tool is presented to compute the detonation front shape, incident angle, and the way it reflects from the enclosing walls. Three possible ways of reflection are encountered. Then, more details about the instabilities of the reaction front are revealed using Euler simulations with a detailed reaction scheme. It is observed that if the concentration gradient exceeds a certain limit, the cellular soot print pattern distorts and finally vanishes to be replaced by a pattern of unidirectional lines. The explanation for this phenomenon can be found in the way the oblique detonation front is reflected from the enclosing walls. If Mach reflection occurs, it goes along with asymmetric pressure loads and influences the propagation velocity as well. The predictions made with the semi-analytic tool presented first meet the observations made with the Euler simulations.

**Paper #145****Geometrical Characterization of the Reaction Front in Gaseous Detonations using Fractal Theory***Hoi Dick Ng, Hamid Ait Abderrahmane, Kevin R. Bates and Nikos Nikiforakis*

In this work, we explore an alternative way to quantify the degree of instability of cellular detonation from geometrical consideration of the reaction front within the detonation structure using fractal theory. We analyze the two-dimensional cellular detonation waves obtained from numerical simulations using a multi-component model based on the TCFC formulation together with a one-step Arrhenius chemical kinetics for a range of activation energy. By varying the activation energy, the cellular detonation pattern becomes more irregular and chaotic. The objective here is to measure the fractal dimension and use it as a parameter to quantify geometrically the degree of corrugation of the reaction front structure in unstable gaseous detonation. Attempt is made to link the fractal dimension of the highly unstable detonation front with other fractal dimension measurement of scalar interfaces in classical shear and fully developed turbulent flow in light to elucidate the turbulent nature of highly unstable gaseous detonations.

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**09:10 (R9B) Flame Ignition and Quenching – I**

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**Paper #11****Ignition Probability of Lean Premixed Bluff-Body Flames***S. F. Ahmed and E. Mastorakos*

Turbulent lean premixed bluff-body flame ignition has been studied in terms of flame extinction, ignition visualization and ignition probability. Extinction of this flame follows the standard characteristics of premixed flames as extinction velocity increases with the increase of equivalence ratio. High speed camera images show that the behavior of the flame propagation after the ignition depends mainly on the ignition location relative to the recirculation zones similar to the non-premixed bluff-body flames. Moreover, the flame inside the side recirculation zone quenches soon after the whole flame lights-up. Failed ignition has been viewed close to the extinction flow conditions of the flame. Igniting the flame away from

the extinction conditions results in 100% ignition probability regardless of the ignition location. However, close to extinction, ignition probability decreases gradually as we move away from the center of the burner and achieving ignition is not possible at all outside the central recirculation zone.

Paper #60

#### **Spark Ignition of Kerosene-Air Mixtures**

*Sally P. M. Bane, Stephanie A. Coronel, Philipp A. Boettcher, Joseph E. Shepherd*

Quantifying the risk of accidental ignition of flammable mixtures is extremely important in industry and aviation safety. The concept of a minimum ignition energy (MIE), obtained using a capacitive spark discharge ignition source, has traditionally formed the basis for determining the hazard posed by fuels. While extensive tabulations of historical MIE data exist, there has been little work done on ignition of realistic industrial and aviation fuels, such as gasoline or kerosene. In the current work, ignition of kerosene is examined experimentally using very short duration, low energy capacitive sparks as the ignition source. As done in previous work, the results of the kerosene tests are analyzed using statistical tools to obtain probability distributions for ignition versus spark energy or energy density. The results are then compared with results from previous work on ignition of lean hydrogen-based mixtures used in aviation testing and two hexane-air mixtures, as well as previous test results for Jet A. Preliminary results show that, under certain conditions, kerosene may be ignited with much lower ignition energies than previously thought.

Paper #172

#### **A New Look at Global Quenching of Premixed Flames by Turbulence**

*C. C. Liu, S. S. Shy, M. W. Peng, Y. C. Dong*

In 2002, Yang and Shy reported a global quenching (GQ) criterion of premixed methane-air flames by intense isotropic turbulence in a fan-stirred cruciform burner characterizing by a Bradley's Karlovitz number ( $K_B = 0.157 Ka$ ) and the equivalence ratio ( $\Phi$ ), where  $Ka = (u'/S_L)^2(Re_T)^{-0.5}$  and  $u'$ ,  $S_L$  and  $Re_T$  are respectively r.m.s. turbulent fluctuating velocity, laminar burning velocity and turbulent Reynolds number. Here we ab initio scrutinize such criterion based on both previous and a few newly-obtained data using a modified  $Ka$  and a reaction zone Péclet number ( $Pe$ ) indicating the diffusivity ratio between turbulence and chemical reaction, in which the local transport diffusivities at reactant temperature are replaced by those at mean temperature of reactants and products. This modified criterion is then compared with a newly-found ignition transition representing the boundary of different modes of turbulent kernel development showing broken reaction zones (RZ) with filament structures. We found that critical values of  $Ka$  ( $Ka_c$ ) for the onset of GQ are generally, except for very rich cases, higher than the  $Ka = 100$  line that separates the thin and broken RZ regimes proposed by Peters. These  $Ka_c$  values versus  $\Phi$  form a parabolic curve with a maximum  $Ka_c = 380$  occurring near  $\Phi = 1$ , indicating that GQ by turbulence not only occurs in the broken RZ regime, but has a strong dependence on  $\Phi$ . By comparing these results among ignition transition, Peters's criterion and GQ, it is found that developed turbulent flames are much harder to be globally quenched by turbulence than developing flame kernels, because the latter, previously used by Leeds group to determine GQ criteria, changes mode at lower  $Ka_c$  as compared to the former. Finally, we show that  $Pe$  is a more physically reasonable parameter than  $Ka$  to describe the aforesaid phenomena.

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### **09:10 (R9C) Premixed Flames Structures**

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Paper #22

#### **A Stable Premixed Methane/Air Sub-Lean Flame Stabilized by Lean Sandwich Flames**

*Ho-Chuan Lin, Yueh-Heng Li and Yei-Chin Chao*

This experiment and simulation study successfully explain the structure of sub-lean and lean sandwich flame which is issued from special designed burner constructed with three parallel and equal spaced slots. This sandwich methane-air flame consists of central sub-lean flame and outboard lean flames. In other words, this sandwich flame is a combination flame of sub-lean and lean flames. The outboard flame can be treated as a pilot flame for supporting the central sub-lean flame. The purpose of this study is to reduce the equivalency ratio of the central flame as low as possible and to dismantle the sub-lean flames by ten characteristic streamlines for flame structure analysis. The simulation results are verified by the experiment results. The verified simulation program is then input with an extreme condition in order to separate the central and the outboard flames as far as possible for flame structure analysis. Ten characteristic streamlines are plotted along which relative properties are extracted for further analysis. By this characteristic streamline analysis, the path of heat conduction from the outboard post flame to central sub-lean and the routes of reactive radical OH and the propagation reaction are discovered. The consumption of  $CH_4$  is clearly illustrated. It is quite successful to explain how the reactive radical OH from the pilot post flame helps the ignition the central flame base and how the OH from the flame base helps the next adjacent flame to burn. The sub-lean flame is burning not only along but also across the streamlines. Half of the  $CH_4$  is quantitatively burning side-way instead of along its own streamline. The heat required to bring the mixture up to the ignition temperature are almost from the adjacent streamlines not from its downstream combustion. As a conclusion, the following two criteria are vital for a stable sub-lean combustion: (1) the hot postflame from the outboard pilot flames for heating up the mixture and (2) a sharp angle between the flame sheet and its streamline. In other words, the sharp angle, in this study 30 degree angle, between the central flame sheet and its streamline is a good environment for the sub-lean combustion to exchange the  $CH_4$  and OH.

Paper #93

**Burning Velocity of Premixed Flame Tips: Experimental and Numerical Study**

*G. Garcia-Soriano, F. J. Higuera, J. L. Castillo, P. L. Garcia-Ybarra*

An experimental and numerical study has been carried out of the region around the tip of a methane-air premixed flame attached to a circular laminar jet burner. On the experimental side, photographic records and PIV have been used to measure the shape of the reaction layer and the velocity of the gas around the tip of the flame. The numerical part of the study includes simulations of stationary axisymmetric flames with infinitely high activation energy reactions. The experimental and numerical results compare well with each other and allow to determine the curvature of the reaction layer at the tip and the velocity and strain rate of the fresh gas flow along the axis of the burner. These data, together with the planar flame velocity determined by extrapolating the velocity of the flame at the tip to the limit of zero stretch, are used to assess the well-known linear flame-velocity/flame-stretch relationship originally proposed by Markstein and later derived in the asymptotic limit of weakly curved and strained flames, as well as the phenomenological modification proposed later to extend the range of validity to larger stretch.

Paper #307

**Measurement of Flame and Flow Structures of Turbulent Jet Premixed Flame by Simultaneous Triple-Plane PLIF and Dual-Plane Stereoscopic PIV**

*Masayasu Shimura, Ayane Johchi, Gyung-Min Choi, Kaoru Iwamoto, Mamoru Tanahashi, Toshio Miyauchi*

Simultaneous triple-plane planar laser induced fluorescence (PLIF), which consists of dual-plane CH PLIF and single-plane OH PLIF, and dual-plane stereoscopic particle image velocimetry (PIV) has been applied to methane-air turbulent jet premixed flame at Reynolds number based on Taylor micro scale of 93.4 to investigate three-dimensional flame and flow structures and to clarify turbulent combustion mechanism. Dual-plane CH PLIF system consists of two independent conventional CH PLIF measurement systems and laser beams from each laser system are led to parallel optical pass using the difference of polarization, and CH PLIF is conducted in two parallel two-dimensional cross-sections. Dual-plane stereoscopic PIV was established by using the difference of wavelength. The dual-plane CH PLIF and stereoscopic PIV are combined with single-plane OH PLIF. The laser sheet for single-plane OH PLIF is located at the center of the other planes. The separation between each plane is set to about 300 micrometers. The spatial resolution of PIV is set to 158 micrometers (about three times Kolmogorov length scale) times 158 micrometers times 220 micrometers and is same as that of general direct numerical simulations (DNSs) of turbulence. This simultaneous measurement can provide three-dimensional flame front, three velocity components and nine-component of velocity gradients. Measurements in turbulent jet premixed flame provide various complicated three-dimensional flame structures such as engulfment of burnt gas, which increases area and curvature of flame front. The results of stereoscopic PIV show that the complicated flame structures are generated by strong vortex structures near flame front. Three-dimensional data of flame and flow structure will be used for the analyses of flame front curvature in three dimensions, which is established in the previous work, and of strain rate tangential to flame front. Results of the analyses will be compared to results obtained from DNS of turbulent premixed flames.

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**10:55 (S4) Supercritical Combustion – II**

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Paper #341

**Species Mixing under Supercritical Pressure Conditions**

*Josette Bellan*

Mixing of species under supercritical pressure conditions occurs in gas-turbine engines, liquid-rocket combustion chambers, diesel engines and Homogeneous Charge Compression Ignition engines. The multiple application of this phenomenon to automotive, aeronautics and astronautics areas makes this subject of high interest and explains why there has been substantial activity over the years on this topic. During approximately the last decade, there are several examples of experimental studies and of modeling and numerical studies that have changed the understanding we have of supercritical species mixing. Unlike in atmospheric flows, mixing in supercritical flows occurs in filamentary structures which populate the entire flow. These filamentary structures have been experimentally observed in fully turbulent situations and have been predicted numerically through Direct Numerical Simulation (DNS) that reached transitional states. These states are characterized by a smaller Reynolds number value than in the fully turbulent cases, however, the flow exhibits the characteristic smooth velocity-fluctuation spectrum of full turbulence. Since DNS is not a practical methodology for computing the fully turbulent flows in the aforementioned applications, another methodology, Large Eddy Simulation (LES), has been considered instead. In LES, the computational grid is coarser than in DNS, which means that the small-scale effects which are not computed must be filtered out, but since they cannot be neglected they are replaced by models called, for obvious reasons, subgrid-scale (SGS) models. The success of LES depends to a great extent on how faithfully the SGS models reproduce the small-scale behavior. For supercritical flow, the existence of the filamentary structures introduces a level of SGS modeling complexity not encountered in atmospheric-pressure flows where LES originated. Because filtering may remove a substantial part of the filaments' structure, which is crucial to mixing, models must be devised to reintroduce in the equations the filtered-out structure. The mathematical equivalent to this description will be presented as well as some examples of SGS modeling for terms particular to supercritical mixing.



Paper #284

**Low-Temperature Injection Dynamics and Turbulent Flame Structure in High-Pressure Supercritical Flows**

*Joseph C. Oefelein and Guilhem Lacaze*

High-pressure, low-temperature combustion using liquid fuels (and/or oxidizers in the case of liquid rockets) is a desirable mode of operation in state-of-the-art propulsion and power devices. Depending on the system, this combination of design attributes has the potential to provide both high-performance and/or minimal emissions. These potential benefits are offset by a variety of fundamental questions. Many of these questions center around the fact that combustion processes within the chamber are inherently turbulent, and in many cases operating pressures approach or exceed the thermodynamic critical pressure of the fuel and/or oxidizer. Operation at elevated pressures significantly increases the system Reynolds number(s), and thus inherently broadens the range of spatial and temporal turbulence scales over which interactions occur. In addition, at near-critical or supercritical conditions, thermodynamic nonidealities and transport anomalies can be dominant, and there are not clear guidelines on when or how to best account for these phenomena. To address this issue, this paper focuses on the structure and dynamics of multiphase flows at high pressures. Emphasis is placed on application of the Large Eddy Simulation technique and issues related to the development of predictive subgrid-scale models.

Paper #181

**Numerical Simulation of Cryogenic Flames Under High Frequency Acoustic Modulation**

*L. Hakim, T. Schmitt, S. Ducruix and S. Candel*

Liquid rocket engines (LREs) may develop high frequency combustion instabilities resulting from a complex coupling between transcritical coaxial jet dynamics, cryogenic combustion and transverse acoustic modes of the chamber. Despite decades of sustained research, the fundamental mechanisms driving this phenomenon are not well understood. This problem is difficult to investigate in full-scale configurations for many reasons and in particular because the power density is high and pressure and temperature conditions are extreme. Modern cryogenic LREs operate at pressures exceeding the critical value with an injection temperature that is well below its critical value. Under such extreme conditions referred to as "transcritical" the working fluid strongly departs from a perfect gas behaviour. Its surface tension and latent heat of vaporization vanish and the breakdown, atomization and droplet generation processes prevailing at subcritical pressures, no longer occur. This is replaced by mass transfer from the dense oxygen stream to the lighter surrounding stream. Thus, mixing and combustion take place in a flow featuring large density gradients. Promising experimental data have been obtained on a cryogenic combustor featuring five coaxial injectors and a high amplitude modulator. The objective of the present work is to complement these data with simulations in order to investigate the fundamental phenomena driving high frequency instabilities. Two complementary numerical studies are carried out using the Large-Eddy Simulation (LES) framework. A transcritical coaxial injector under acoustic perturbations is simulated in a first step. This case aims at studying the dynamics of a transcritical flame under transverse oscillations to get a precise insight into the physics of flame/acoustics interactions. The second simulation is a 2D configuration reproducing the experimental geometry and operating conditions. While it is clear that 2D simulations bring little physical insight in the complex three-dimensional processes involved in the experiment, this can be considered as a useful test to prepare future 3D calculations. These heavy simulations aim at retrieving experimental results to validate the numerical approach and complement the experimental data.

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**10:55 (R10A) Detonation with Confinement**

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Paper #37

**Computational Study of Detonation-wave Propagation in Narrow Channels**

*Ashwin Chinnayya and Abdellah Hadjadj*

Progress towards the miniaturization of increasingly advanced micro- and nano-electromechanical systems has highlighted the need for a better knowledge of the design of such devices. Knowledge of micro-nano pipe flows is still mandatory. In field of energy power generation, as the systems are scaled down, the thermal efficiency of conventional propellant devices is seriously degraded due to significant heat losses which can cause the combustion extinction. A promising approach is to use shock or detonation waves in gaseous media to enhance chemical reaction rates. A detonation is a rapid regime of burning in which a strong shock ignites the fuel and the burning proceeds to equilibrium behind the shock, while the energy released continues to drive the shock. It is also characterized by the presence of longitudinal and transverse instabilities, thereby subjecting the shock front to violent deceleration / acceleration. The objective of this work is to better understand the mean structure of the reaction zone that extends from the shock to the sonic surface. As for numerical modelling, the compressible multi-species reactive Navier-Stokes equations are solved using an in-house code "CHOCWAVE", including variable thermodynamic and transport coefficients depending on the species. The generalized Chapman-Jouguet condition was developed and compared to the numerical results in the case of stable multidimensional detonation. More specifically, it was shown that the transverse instabilities are attenuated with the scale reduction and eventually disappear. To this end, a scenario, based on the structure of the downstream subsonic pocket, which is correlated to the development of the boundary layer, has been proposed to explain the deficit of the detonation-front velocity. The present contribution enables us to shade more physical insight for the propagation of stable detonation fronts in narrow channels.

Paper #51

### **Experimental Study of Closed Volume Explosion**

*Laurent Munier*

This paper deals with combustion effects occurring in confined explosions of condensed high explosives (HE). In such a problem, turbulent mixing efficiency and thermal effects are still difficult to measure. This is the reason why CEA Gramat keeps on developing several experimental configurations to characterize the "fireball" dynamics and the turbulent combustion during the course of open air or confined explosion. Both TNT and HMX-based HE (called here HMX b) were tested, in order to vary the oxygen balance, and thus the afterburning phenomena.

Paper #59

### **Experimentally Observed Methods of Re-initiation During Detonation Diffraction into a Confined Volume**

*Nolan Polley, Miles Q. Egbert, Eric L. Petersen*

The diffraction of a planar detonation into a confined volume and its transformation into a diverging, cylindrical detonation was the subject of the current study. Three different re-initiation mechanisms which are responsible for the successful transformation of the planar detonation wave have been experimentally observed. Two of the re-initiation mechanisms, spontaneous and continuous reflected re-initiation have been previously observed in the literature, while a new method of re-initiation, discontinuous reflected re-initiation, has also been identified. The observance of discontinuous reflected re-initiation is believed to be responsible for the apparent discrepancy between the results of the current study and the studies by Murray and Lee (1986) and Sorin et al. (2006). Efforts are currently underway to more clearly define the boundary between continuous and discontinuous re-initiation over a wide range of test mixtures and gap size.

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## **10:55 (R10B) Flame Ignition and Quenching-II**

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Paper #92

### **3D Visualisation of Diffusion Flame Structure and Dynamics under Acoustic Excitation**

*Qian Wang, Yang Zhang, Hao Jie Tang, Min Zhu*

The laminar diffusion flame response to external acoustic excitation is investigated at low frequencies. Two typical responses are observed: the flame is oscillating either at the same or half the excitation frequency. The vortex and flame dynamics of the two typical cases are visualised by high speed schlieren and stereo images. A "vortex merging" phenomenon is observed and is responsible for the flame flickering frequency reduction to half. The 3D flame structures in the two cases are reconstructed based on the stereo images. The 3D flame topology shows a great variance from different view angles, which indicates the necessity of 3D visualisation. The 3D flame structures show dramatic differences in two cases. The flame in case 1 is long and narrow. In contrast, the flame in case 2 is shorter but with obvious tortuous shape in 3D space.

Paper #339

### **Flame Stabilization with Fuel Injection into a Cavity Adjacent to a Curved, Converging Air-flow Channel**

*Ben J. Colcord, Feng Liu and William A. Sirignano*

Thermal systems analyses have shown that turbine-burner augmentation can give better specific fuel consumption than afterburning jets and higher specific thrust than non-augmented turbojet or turbofan engines. For stationary gas-turbine engines with heat re-generation, both specific power and thermal efficiency can be increased. Achieving this potential presents a number of challenges, including injection, mixing and ignition of fuel in flows with a large three-dimensional acceleration. Here, we focus on the modeling of the flame holding using fuel and air injection into a cavity adjacent to a channel flow with inflowing high-temperature vitiated air. The compressible Navier-Stokes equation coupled with the energy equation and multiple species equations are solved using the OpenFOAM fluid dynamics package. Gaseous n-heptane is used as the fuel and the combustion is described as a one-step overall chemical reaction. A cavity mixedness is defined based on the mixedness of carbon and nitrogen atoms in the cavity, thereby accounting for the mixedness of reactants and products. The effects of cavity dimensions, injection locations, and channel curvature and convergence on cavity mixedness and burning efficiency are investigated. It is seen that the cavity mixedness is a good indicator of the burning efficiency. For two-dimensional straight-channel flows, injection of both fuel and air from the upstream wall of the cavity (parallel configuration) gives higher values for cavity mixedness and burning efficiency than any other injection configuration investigated. The reinforcing configuration, with fuel injection high on the upstream wall and air injection low on the downstream wall so as to reinforce the natural cavity circulation, gives the lowest burning efficiency. The disrupting configuration, with the fuel and air injection located to disrupt the natural circulation, has a burning efficiency between the two other configurations. Unsteady visualizations show that the parallel injection configuration causes significantly more vortex interaction close to the injection locations where fuel and air concentrations are highest. This causes faster mixing and a higher burning efficiency. For the parallel injection configuration in a two-dimensional curving channel with the cavity on the inside channel wall, both cavity mixedness and burning efficiency decrease as the radius of curvature decreases. The low-temperature, high-molecular weight fuel is much more dense than the vitiated channel-flow air, so decreasing the radius of curvature tends to force the unburned fuel from the cavity. Since the parallel injection configuration mixes the fuel and air efficiently in the cavity, the mixedness and burning efficiency are reduced by the increased centrifugal force.

Paper #319

### **Parametric Numerical Studies on Auto-Ignition around a Single Fuel Droplet**

*Pratyush Sharma, Robert Schießl, Ulrich Maas*

Detailed numerical simulations of the auto-ignition of single methanol droplets embedded in quiescent air have been performed in a closed volume with the assumption of spherical symmetry. The influence of various parameters, namely ambient air temperature and pressure, droplet radius and global equivalence ratio on the auto-ignition delay time of the droplet is investigated. The results are used to identify regions in parameter space where a simplified treatment of droplet ignition is possible. This is the case, e.g., if the droplet lifetime and the time required for mixing between fuel vapor and ambient air (mixing time) are much smaller than the ignition delay time. Another case is when the ignition delay time is much larger than the droplet lifetime, but much smaller than the mixing time. In general, the physical and chemical time scales involved in the ignition process can be decoupled if they are strongly different. Under these conditions, droplet ignition can be treated as the corresponding ignition of a homogeneous reactor with same global enthalpy and equivalence ratio, or as ignition in the inhomogeneous gas phase.

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## **10:55 (R10C) Flames Structures**

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Paper #194

### **Radiative Extinction Characteristics of Low-Lewis-Number Counterflow Premixed Flame in Microgravity and Its Correlation with Flame Ball**

*Koichi Takase, Hisashi Nakamura, Takuya Tezuka, Susumu Hasegawa, Xing Li, Philip Wang, Kaoru Maruta*

A consideration on radiative extinction characteristics of low-Lewis-number counterflow premixed flame in microgravity and its correlation with flame ball were conducted as preliminary examination for future space experiment. Numerical simulations of  $\text{CH}_4/\text{O}_2/\text{Xe}$  and  $\text{CH}_4/\text{O}_2/\text{Kr}$  were conducted by PREMIX-based counterflow flame and flame ball codes. Xe and Kr were selected as inert gas in the present computation to obtain low-Lewis-number mixture. The ratio of oxidizer mole fraction to inert mole fraction,  $Z$ , is fixed to 0.141. When equivalence ratio was fixed, two extinction limits of a counterflow flame at high and low stretch rates were obtained. C-shaped extinction limit curves were formed for both Xe and Kr. Maximum temperature decreased with a decrease of stretch rate at low stretch rate. Maximum temperature decreased with an increase of stretch rate at high stretch rate. Radiation fraction increased with the decrease of stretch rate in almost all stretch rates. Therefore, radiative extinction at lower stretch rate was predicted. However, radiation fraction decreased with the decrease of stretch rate close to the radiative extinction limit. Flame ball diameters decreased with a decrease of  $\text{CH}_4$  mole fraction. The extinctions of flame balls were observed. Flammable region of  $\text{CH}_4/\text{O}_2/\text{Xe}$  flame was larger than that of  $\text{CH}_4/\text{O}_2/\text{Kr}$  flame. The extension of flammable region is due to lower Lewis number of  $\text{CH}_4/\text{O}_2/\text{Xe}$  mixture. To further examine the correlations between radiative extinction characteristics of low-stretched counterflow flame and flame ball, microgravity experiments were conducted very recently using parabolic flight of airplane operated by DAS, Nagoya, Japan. Using  $\text{CH}_4/\text{O}_2/\text{Xe}$  mixture at  $Z=0.141$  and stretch rate of  $3 \text{ s}^{-1}$  while equivalence ratio decreases from 0.63 to 0.30, the formation of a ball-like flame around equivalence ratio of 0.4 was observed at the stagnation position. The transition of flame shape occurred after the counterflow flames extinction. The computation showed that the radiative extinction of  $\text{CH}_4/\text{O}_2/\text{Xe}$  counterflow premixed flame at equivalence ratio of 0.37 occurred at  $5 \text{ s}^{-1}$ . However, the flame ball solution was obtained at the same equivalence ratio. It seems that around equivalence ratio of 0.4, the radiative extinction of low-stretched counterflow flame and the formation of a ball-like flame occurred. However, the formed ball-like flame moved outward along counterflow streamline.

Paper #66

### **Flame Surface Density Measurements in Interacting Premixed Flames Using Experiment and DNS**

*T.D. Dunstan, F. T. C. Yuen, E. Mastorakos, N. Swaminathan, K. N. C. Bray*

Direct Numerical Simulations (DNS) and planar Rayleigh scattering data from experiment are analysed to assess the effects of flame interactions on Flame Surface Density (FSD) in premixed turbulent V-flames. Twin and single V-flames with statistically identical turbulent inlet conditions are used to directly compare interacting and non-interacting flames. DNS results from a twin V-flame at a higher turbulence intensity are also presented. Two methods of calculating FSD are discussed: the surface-conditioned FSD and the generalised FSD, and the results compared. The surface-conditioned FSD is analysed in terms of probabilistic and quantitative components; the first representing intermittency through the probability of finding an isosurface at a given location, and the second being the mean conditional scalar gradient magnitude. All three quantities are compared at different streamwise locations to capture the development of the flame downstream from the flame holder. Experimental results are subjected to statistical hypothesis tests to account for the underlying uncertainty in the data, and are found to be in qualitative agreement with the DNS. In all cases, higher FSD values are found in the interacting flames compared to non-interacting flames. The DNS data also suggest that FSD becomes saturated at higher values of turbulence intensity. The FSD is found to be dominated by the probabilistic component, with only a small change in the mean scalar gradient magnitude for interacting flames. The increased FSD found in interacting flames is interpreted as a prerequisite condition for interaction, while the effect of individual interactions is to reduce flame area.

Paper #178

**Numerical Study on Ultra-lean Premixed Flame in Swirl Flow with Recirculating of Burned Gas including Active Radicals**

*Akane UEMICHI, Yasuo KONDO, Makihito NISHIOKA*

To explore the possibility of ultra-lean combustion, we performed detailed-kinetics numerical simulations of a methane-air premixed flame in a swirling flow. Previously, we calculated a co-rotating counterflow twin (premixed) flame that can be treated one-dimensionally by introducing a similarity solution, and found that its flame structure is quite different from an ordinary planar one-dimensional premixed flame. In the ultra-lean case of the former flame, an additional stagnation point is formed within the flame zone and fresh reactants are transported over the stagnation point against the backward convection by diffusion. The equivalence ratio of the leanest extinction limit obtained by neglecting radiative heat loss is 0.32, and 0.42 by employing an optically thin radiation model. We expect that the true lean extinction limit exists between these two equivalence ratios, so it is desirable to check it experimentally. However, it is obviously impossible to realize a rotating counterflow twin flame of infinitely large radius experimentally, and if a burner of finite radius is used the comparison with the above numerical results will be meaningless since the backflowing gas composition must be much different. In this study, we performed 2D numerical simulations of combustion in a swirl burner whose shape is circular truncated cone with cylindrical tail, which is much more likely to be realized experimentally. As a result, it was found that a stable ultra-lean premixed flame of equivalence ratio 0.35 is successfully formed near the stagnation point between the injected premixed gas and the recirculated burned gas. In this swirl burner a complicated flow field with a number of vortices is formed by the strong swirling flow, but at least around the flame tip the flow configuration is considerably similar to that of the rotating counterflow twin flame. And the fact that the reaction zone is formed in the burned gas side of the stagnation point under the ultra-lean condition was also observed in the swirling flame. Moreover, we found that the swirling flame of equivalence ratio 0.35 can be successfully formed even when the optically thin radiation model, which may overestimate the radiative heat loss, is employed. We compared the burned gas compositions for the equivalence ratio 0.35 among the equilibrium state, the rotating counterflow twin premixed flame, and the 2D swirling flame, and found that the active radicals, O, OH and H, are largely increased from the equilibrium values in both of the rotating counterflow twin flame and the 2D swirling flame. This is thought to be one of the causes to realize ultra-lean combustion in the above two flames.

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**09:00 (S5) Detonation Analog – I**

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Paper #289

**On Detonation Analogs***Aslan Kasimov*

The paper is devoted to the analysis of detonation analogs. After a brief review of well-known "mathematical" analogs proposed by Fickett and Majda, we discuss such "physical" analogs of detonation as a hydraulic jump and a traffic jam. These two classes of analogs are distinguished by their origin, the first one ("mathematical") being an ad hoc invention while the second one ("physical") representing a real physical phenomenon that shares some similarities with detonation. The key point behind the analogy between detonation and another physical system is their description by hyperbolic balance laws that admit self-sustained traveling shock waves as their solutions.

Paper #277

**Dynamic Behaviour of Analog Detonation Systems***Kiyanda, C.B. and Ng, H.D.*

The development of reactive models analogous to the reactive Euler model is reported. Two models are formulated, based on the inviscid Burgers' and shallow-water wave equation. The linear stability analysis and numerical simulations of those two models will determine the minimal level of complexity a model requires to produce unstable, oscillatory, propagating detonation waves. The influence of varying the reaction scheme for the two models will also be investigated. Preliminary numerical results using the reactive Burgers' model with a one-step Arrhenius reaction term show that now oscillatory solutions exist for the range of "activation energy" between 0.1 and 10. These preliminary results suggest that the existence of both forward and rear-facing characteristics is necessary for the model to be unstable. Further numerical simulations along with the linear stability analysis will be able to answer this and other questions.

Paper #137

**Non-Linear Dynamics and Route to Chaos in Fickett's Detonation Analogue***Matei I. Radulescu, Justin Tang*

The present study presents a numerical analysis of Fickett's detonation toy-model, that is Burgers' equation with a deterministic forcing term mimicking a chemical reaction. The model chemical reaction consists of a thermally neutral induction layer with Arrhenius state-dependence, followed by an exothermic reaction layer with state-independent rate. Direct numerical analysis is performed on the system, where it is shown that the dynamics admit pulsating solutions, very similar to real detonations. Furthermore, it is shown that the pulsating dynamics undergo universal period doubling bifurcating dynamics, similar to many other non-linear systems, including pulsating detonations, as first shown by Ng et al. in 2005. Finally, the simplicity of the model permits us to explain the instability mechanism. Through analysis of the model written in characteristic form, the amount of amplification of the amplitude of internal waves propagating towards the front is proportional to the time spent in the reaction layer, akin to the SWACER mechanism. When the internal wave motion becomes in phase with the reaction zone path, maximum amplification is achieved. This instability is accentuated with increase sensitivity of the induction time to shock changes.

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**09:00 (R11A) Detonation Propagation**

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Paper #71

**Experimental and Numerical Study on Detonation Propagating in an Annular Cylinder***Xudong Zhang, Baochun Fan, Zhenhua Pan, Mingyue Gui, Zhihua Chen*

In this paper, the flow features of rotating detonations in the annular chamber are investigated experimentally and numerically, and the self-sustaining propagation mechanisms are examined.

Paper #98

**Planar Toroidal Detonation Propagation through Gradual Expanding Channel***Masashi Wakita, Masayoshi Tamura, Akihiro Terasaka, Kazuya Sajiki, Tsuyoshi Totani and Harunori Nagata*

Experimental investigations of the toroidal planar detonation wave propagation around the reflector, which consists of a cylinder body and a conical body, revealed the effects of the ratio of the annular gap width and cell size of the detonation wave ( $L/\lambda$ ) on the detonation transition. When the conical angle is  $30^\circ$ ,  $45^\circ$  or  $60^\circ$  the threshold value of  $L/\lambda$  between the "Go" and "Nogo" is approximately 4, which is the same as the value at conical angle =  $90^\circ$ . Accordingly, when the angle exceeds  $30^\circ$  the conical body has no effect on detonation transition enhancement. On the other hand, the promotion effect obtained by the conical body of  $15^\circ$  is extremely high and the threshold value is approximately 2. This is because transverse waves in a detonation wave can reach the sidewall of the conical body, when the conical angle is sufficiently small, and it produces a strong reflection on the wall.

Paper #193

### **Study on Detonation Waves Propagating through Curved Channels**

*H. Nakayama, T. Moriya, J. Kasahara, A. Matsuo, Y. Sasamoto and I. Funaki*

Detonation propagation phenomenon in curved channels with a rectangular cross-section is examined in the present study. A stoichiometric ethylene/oxygen mixture gas and five types of curved channels with different inner radii are used. The depth of these channels is so thin in order to make the detonation structure two-dimensional and to record the triple point trajectories of the detonation clearly. A high-speed video camera is used to visualize the detonation propagating through the curved channels. A new visualization technique is developed to observe simultaneously the wave front motions and triple point trajectories of the detonation in the curved channels. In this new visualization technique, short-time open-shutter photography (SOP) is performed for each individual frame of the high-speed camera and the SOP images are superimposed. The ratio of inner radius of curved channel ( $r_i$ ) to detonation cell width ( $w$ ) is an important factor determining the stability of the detonation propagating through the curved channels. The expansion wave from the inner wall of the curved channel attenuates and/or quenches the detonation in a small  $r_i/w$  condition. The influence of the expansion wave is weakened with increasing  $r_i/w$ . The detonation propagation becomes quite stable in a sufficiently large  $r_i/w$  condition. The cell structure and smooth wave front of the detonation can be sustained in such a stable propagation mode, and the wave front shape of the detonation becomes constant as the detonation propagates through the curved channels and the detonation propagates at a constant speed. It appears that the detonation propagation mode transitions from unstable to stable in the range  $21 < r_i/w < 32$  in the conditions of the present study.

Paper #278

### **Stability of Chain Branched Detonation Waves with Slow Initiation**

*Megumi Lopez-Aoyagi, Josue Melguizo-Gavilanes and Luc Bauwens*

Most fuels, and in particular hydrogen, are characterized by chain-branching kinetics. Typically, initiation is rather slow compared to chain-branching. In that situation, even if the von Neumann point lies inside the chain-branching region, a thin zone of intense reaction separates long initiation and completion regions. Stability will then be affected mainly by modes with a frequency that resolves the main reaction zone. The current work presents a formulation in the slow initiation limit, in the framework of the stationary solution formulated by Bedard-Tremblay et al. (2009)

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## **09:00 (R11B) Detonation Structure: General**

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Paper #108

### **Three Dimensional Simulation for the Effects of Fuel Injection Patterns in Rotating Detonation Engine**

*Liu Meng, Wang Jian-Ping*

This study shows that different fuel injection pattern may change the wave's shape and distribution. Proper utilization of combustion products may improve the detonation performance. And the multiple wave fronts comply with the experimental observation. Three dimensional simulation is proved to be a better analysis to investigate various engine concepts.

Paper #58

### **Experiments on Hydrodynamic Stability of Laser-Driven Detonations in Nitrogen and Helium Gases**

*Tomohisa Honda, Akira Kawaguchi, Yoshiki Hanta, Akio Susa, Shinichi Namba, Takuma Endo, Hiroyuki Shiraga, Keisuke Shigemori and Mayuko Koga*

Hydrodynamic stability of laser-driven detonations was experimentally examined by using a glass laser at the driving laser energy flux of  $14 \text{ GW/cm}^2$ , using nitrogen and helium gases as the propagation media in the initial pressure range of 10-100 kPa. In the experiments, an aluminum target was placed in a gas at the room temperature and irradiated by laser. A laser-driven detonation was initiated from the seed plasma created on the target surface, and propagated toward the opposite direction to the drive laser. Flat plates and sinusoidally-corrugated plates were used as targets. For uniform laser irradiation, eleven or twelve laser beams, which were bundled together, were overlapped on the same area of the target surface. For diagnostics, the detonations were observed side-on by an optical streak camera and an optical gate camera. When a flat plate was irradiated by laser in nitrogen gas, the detonation front was very smooth and planar, and no transverse-wave structure was observed. When a sinusoidally-corrugated plate was irradiated by laser in nitrogen gas, the detonation front was initially sinusoidally corrugated, but the corrugation was damped with propagation. These results showed that the laser-driven detonations in nitrogen gas were hydrodynamically stable. On the other hand, when a flat plate was irradiated by laser in helium gas, the laser-driven detonation showed the transverse-wave structure. Although this shows that the hydrodynamic stability of laser-driven detonations depends on the gas species in which the detonations propagate, the mechanism for such difference is not clear.

Paper #219

### **Detonation Characteristics in Tube Filled with the Binary Fuels $\text{H}_2/\text{C}_3\text{H}_8$ -Air Mixtures**

*Guanbing CHENG, Ratiba ZITOUN, Pascal BAUER*

An experimental investigation on detonation characteristics of the binary fuels hydrogen ( $\text{H}_2$ )/propane ( $\text{C}_3\text{H}_8$ )-Air mixtures is conducted. The experiments are performed in a stainless steel tube with 52 mm inner diameter and 8.7 m length at ambient conditions with the equivalence ratio ranging from 0.7 to 1.8 and the  $\text{H}_2$  molar fraction  $x$  varying from 0.5 to 1. The self-sustained detonation velocity  $D$ , pressure  $P$  and cell size are measured and presented as a function of the equivalence ratio and of the  $\text{H}_2$  molar fraction  $x$ . The measured detonation velocity and pressure agree well with the CJ

ones. The velocity deficit does not exceed 3% and the ratio  $P/PCJ$  varies from 0.8 to 1.2. The measured average detonation cell sizes vary from 20 to 50 mm. The minimum cell size occurs at the rich-side of the mixtures. Addition of propane to  $H_2$ /Air mixtures reduces the detonability of the studied mixture. Subsequently, evolution of the cell size with  $l_i$  is determined, where  $l_i$  is the Zel'dovich-Neumann-Doering (ZND) chemical reaction-zone length computed by software Chemkin with the detailed chemical kinetic scheme Gri-mech 3.0. The ratio  $K$  between the cell size and  $l_i$  varies from 35 to 45 and seems to be independent of  $x$  and the equivalence ratio. In addition, we carry out several experiments in the 92-mm i.d tube to validate the cell size obtained in 52-mm i.d tube. The measured detonation cell size and its evolution with  $x$  are as same as those obtained in the smaller tube.

Paper #259

### **Reynolds Number Effects on the Structure and Stability of Highly Unstable Detonation Wave**

*Deok-Rae Cho, Kiha kang, Jae-Ryul Shin, Jeong-Yeol Choi*

Regardless of many studies done previously, there are quite a many unknowns still unresolved and needs a systematic investigation. One of the issues is the numerical modeling of the highly unstable detonation. As a preliminary step toward it, the effect of Reynolds number and grid resolution is investigated in this study. A series of numerical simulations are carried out for wide range of Reynolds number using coarse and fine grid system. The role of diffusion and the effect of grid resolution are clearly understood in the aspect of detonation structures and stabilities in the present study. It is considered that the numerical damping increase the mixing and combustion leading to the completion of combustion. Therefore it is recommended to introduce some sort of mathematical modeling that can account for the physical process of turbulence mixing and combustion in the highly unstable detonation structures.

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## **09:00 (R11C) Turbulent Premixed Flames**

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Paper #184

### **Subgrid Analysis of DNS of Stratified Bunsen Flames**

*W.J.S. Ramaekers, J.A. van Oijen and L.P.H. de Goeij*

Stratified flames can be considered as a combination of premixed and non-premixed flames, for which no dedicated combustion models exist. Direct Numerical Simulations (DNS) of turbulent stratified planar Bunsen flames ( $Re=3200$ ) are performed using the Flamelet Generated Manifold (FGM) reduction method to keep computational costs acceptable. Filtering of DNS data allows the determination of LES subgrid PDF's which in turn can be modeled by Presumed PDF's (PPDF). In this study it is examined whether the Flame Surface Density (FSD) model, including a PPDF closure for subgrid fluctuations in the mass burning rate, yields comparable results as a combined PPDF closure method for chemical source terms for stratified flames. A priori analysis of DNS data will be followed by application of the obtained subgrid closure methods in LES simulations.

Paper #126

### **Algebraic Models for Turbulent Transports in Flames: Applications to Stagnating and 2D Premixed Flames**

*Vincent Robin, Arnaud Mura, Michel Champion*

The thermal expansion induced by the chemical reactions taking place in a turbulent reactive flow affects the velocity field so strongly that turbulent transports can be controlled by reactions rather than by turbulence. Moreover, thermal expansion is well-known to be responsible for counter-gradient turbulent diffusion and flame-generated turbulence phenomena. In the present paper, a splitting procedure of the velocity field is used, that allows the identification of two different effects of the thermal expansion in the specific flamelets regime of turbulent combustion: (i) the thermal expansion occurring through the local flames (direct effect) and (ii) the effect of thermal expansion on the velocity field associated to the growth of the flame surface (indirect effect). The theoretical analysis shows that the thermal expansion occurring through the local flames can be treated separately so that the turbulent transport terms of the averaged scalar and momentum equations are related to the reactive scalar field. Furthermore, a new transport equation for the turbulent kinetic energy easier to close than the usual one is derived and used. Finally, algebraic closures for the turbulent transport terms of mass and momentum are proposed and corresponding results are satisfactorily compared with experimental data in the two cases of, (i) a flame stabilized in a turbulent stagnating flow and (ii) a turbulent flame stabilized by the sudden expansion of a 2D channel. Results show the ability of the model to represent in detail the behavior of turbulent transports in premixed flames.

Paper #273

### **Effects of Mean Curvature on Flame Propagation**

*I. Ahmed and N. Swaminathan*

The initial flame kernels of spark-ignition engines and accidental or controlled explosions are some examples of where one could find outwardly propagating spherical flames. Often the studies of such spherical flames use the results obtained from statistically planar flames, where the mean curvature effects are absent. Direct Numerical Simulation (DNS) studies have shown that the curvature induces significant effects on the propagation of flame fronts and flame brushes. It is expected that any change in the local strain or curvature (collectively called as stretch) would impart due influence on the scalar gradient. Thus, a parameter related to the scalar gradient would be an appropriate choice to capture these effects on turbulent flame propagation. In this work, the Reynolds-Averaged Navier Stokes (RANS) methodology will be used to study the propagation of premixed turbulent spherical flames. The reaction rate is modelled using a recently developed strained flamelet model. The mean scalar dissipation rate of a progress variable is used to

parametrise the strained flamelet. The mean scalar dissipation rate is obtained from an algebraic model. The aim of this work is to determine the effects of mean curvature on the propagation speed of turbulent flames. This is achieved by simulating turbulent spherical flames using reaction rate models accounting for mean curvature effects through the scalar dissipation rate.

Paper #186

#### **A Filtered Tabulated Chemistry Model for LES of Partially-Premixed Flames**

*P. Auzillon, O. Gicquel, N. Darabiha, D. Veynante and B. Fiorina*

The turbulent combustion model F-TACLES (Filtered Tabulated Chemistry for LES) has recently been proposed to introduce detailed chemistry effects in Large Eddy Simulations. The method, initially developed for turbulent premixed combustion, consists first in generating a chemical look-up table from filtered 1-D laminar premixed flames computed under detailed chemistry assumptions. Closure of the filtered progress variable balance equation is then carefully addressed from this filtered database. The model accounts for turbulent combustion by including sub-grid scale wrinkling effects in flame front propagation. This approach is well adapted to turbulent premixed flames and reproduces accurately flame dynamics. The objectives of the present work are to extend the F-TACLES model to turbulent partially-premixed flames. The modeling strategy is detailed in Section 2. Section 3 is dedicated to numerical tests of the model: 1-D flames submitted to equivalence ratio fluctuations are computed. Then preliminary simulations of a 3-D partially-premixed flame stabilized in a swirled burner are shown.

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### **11:10 (S5) Detonation Analog – II**

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Paper #251

#### **Molecular Dynamics Simulations of Detonations**

*Nick Sirmas & Matei Radulescu*

Molecular dynamic simulations of a reactive hard disk model have been used to investigate the structure of fast reaction waves initiated by a moving piston. An irreversible reaction consumes two reactive species, converting them into products, with the addition of energy partitioned solely into the particles kinetic energy. A threshold kinetic energy of collision, representing the activation energy of the reaction permits to control the reaction rate. The numerical solutions show the existence of quasi-steady detonation waves propagating at a velocity approximately equal to the Chapman-Jouguet detonation velocity. Investigation of the reaction zone structure revealed that the reactions proceed through a super-diffusive regime, and the reaction zone overlaps with the shock compression transition.

Paper #320

#### **Shock-like and Detonation-like Waves in One-dimensional Lattice Chains**

*Andrew Higgins*

Shock waves and detonation waves in a one-dimensional gas with a hard-sphere potential (“beads on a wire”) are studied. A simple event-driven molecular dynamics approach is used, and the results compared to continuum-based models (Euler equations, Rankine-Hugoniot relations, etc.). While a system with particles with uniform mass exhibits trivial behavior (particles simply exchange velocity in elastic impacts), it is found that a system of two or more different masses will thermalize to Maxwell-Boltzmann statistics. The introduction of energy release via a critical collision energy followed by momentum-conserving energy addition allows chemical reactions with heat release to be simulated, and the results are shown to have exact correspondence with Arrhenius kinetics with the critical collision energy being the activation energy. Piston-driven shock waves are also found to agree with the classical Rankine-Hugoniot relations. Detonation waves agree with classical Chapman-Jouguet theory provided the reactions are sufficiently slow so as not to occur within the shock front itself. This work provides a basis for forays into regimes where traditional continuum-based concepts are shown to break down, such as lattice chains with nonlinear potentials (Toda lattice, FPU, Hertzian chains, etc.). In these systems, unique mechanisms of reactive shock-like wave propagation are possible that rely upon the highly localized nature of the front that would not otherwise be seen in continuum-based models.

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### **13:30 (S6) Verification and Validation of Detonation Simulation – I**

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#### **(Topical Review) Outstanding Issues in Verification and Validation of Compressible Reacting Flow Calculations**

*J. Powers*

Paper #156

#### **Detonation Wave Attenuation by a Cylinder and the Subsequent Re-Initiation Régimes**

*R. Bhattacharjee, G. Maines, L. Maley and M.I. Radulescu*

The following abstract describes an experimental study of detonation waves diffraction behind a half-cylinder obstacle. The experiments were carried out using a stoichiometric Methane-Oxygen mixture at varying initial pressures to yield different cases. A preliminary study of the effects surface roughness has on an attenuated detonation wave, behind a half-cylinder, was also undertaken. Schlieren pictures, which illustrate the flow field of the detonation wave downstream of the obstacle, were obtained from the experiments. Preliminary numerical analyses were also carried out, for a specific case, and a comparison between experiments and numerics was drawn.



Paper #293

#### **Verification and Direct Numerical Simulation of Irregular Hydrocarbon Detonations**

*Jack L. Ziegler; Ralf Deiterding; Joseph E. Shepherd; D. I. Pullin; G. Blanquart*

We describe direct numerical simulations of irregular hydrocarbon detonations using the multicomponent, compressible, reactive Navier-Stokes equations in two spatial dimensions. The simulations utilize a hybrid, WENO/centered-difference numerical method, with low numerical dissipation, high-order shock-capturing, and with structured adaptive mesh refinement (SAMR). This enables resolution of diffusive processes within reaction zones. A minimally reduced chemistry and transport model for a propane detonation is used to accurately capture the induction time, chemical relaxation, and the diffusive mixing within vortical structures evolving from the triple-point shear layers.

Paper #62

#### **Diffusion in Gaseous Detonations**

*K. Mazaheri, Y. Mahmoudi, M. I. Radulescu*

To clarify the role of diffusion on detonation structure a two-dimensional numerical simulation is performed by solving the Navier-Stokes equations and considering the single step Arrhenius kinetic as reaction model. The effect of diffusion on the generation of vortices produced by hydrodynamic instabilities (RM and KH instabilities) is investigated in this study. All the computations are performed with resolution of 300 cells per hrl. Mixtures with both low and high activation energies, characterized by their regular and irregular detonation structures, are considered. Results provided by very high resolution reveal that the structure obtained for irregular structure by solving the Euler equations differ from that obtained by solving the Navier-Stokes equations. However, in low resolution simulations, the irregular structure obtained by solving both the Euler and Navier-Stokes equations are very the same. The major effect of diffusion occurs at shear layers and unburned pockets boundaries. Diffusion suppresses the small-scale vortices produced by KH instabilities and decreases the mixing rate of hot and cold gases at shear layers. However, behind the shock front where less concentration of small scale vortices exist, the diffusion of heat and mass from neighboring hot regions of burned material to the un-reacted gases increases the burning rate of the un-reacted pockets. In addition, the solution of Navier-Stokes equations shows that, the diffusion increases the strength of the shock front while decreases the strength of the transverse waves. Due to the absence of hydrodynamic instabilities and un-reacted gas pockets behind the main front of regular structure detonations, the results obtained by solving the Euler equations and Navier-Stokes equations are similar for detonations with regular structure even in high resolution simulations.

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### **13:30 (R12A) Detonation Front Structure**

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Paper #134

#### **Three-Dimensional Structure of Detonations in Suspensions of Aluminum Particles**

*Khasainov B., Virof F., Veyssiere B.*

Recently we have used scarce available data on the detonation cell size in suspensions of aluminum particles in air and oxygen to adjust the kinetic parameters of our two-phase model of detonations in these mixtures. The calculated detonation cell width was found by means of two-dimensional unsteady simulations using an assumption of cylindrical symmetry of the flow in the tube. However, in reality the detonation cells are three-dimensional. In this work we apply the same detonation model which is based on the continuous mechanics of two-phase flows for 3D numerical simulations of cellular detonation structures in aluminum particle suspensions in oxygen. Reasonable agreement was obtained with the aforementioned 2D results on the detonation cell width. The range of tube diameters where detonations in Al/O<sub>2</sub> mixture at a given particle size and concentration would propagate in the spinning mode is estimated (these results make a complement to our previous analysis of spinning detonations in Al/air mixtures). Coupling these results with the formerly obtained dependences of detonation cell size on the mean particle diameter can help to better plan the experimental studies of detonations in aluminum suspensions.

Paper #214

#### **Parametric Study of Double Cellular Detonation Structure**

*Khasainov B.A., Virof F., Presles H.-N., Desbordes D.*

Parametric numerical study is performed of detonation cellular structure in the model gaseous explosive mixture whose decomposition occurs in two successive exothermic steps with markedly different characteristic times via two reactions:  $A \Rightarrow B$  and  $B \Rightarrow C$ . Kinetic and energetic parameters of both reactions were varied in a wide range and results are presented which describe one-dimensional solutions for steady detonation and unsteady two-dimensional solutions of Euler equations. The range of governing parameters of both exothermic steps within which the double cellular structure is observed is identified for the considered model example. However, because it is relatively easy to perform a standard analysis of 1D steady detonation structures calculated with a detailed chemical kinetics, our results should help to identify the mixtures and the domain of their equivalence ratio where double detonation structure could be clearly observed in laboratory conditions

Paper #267

#### **Detonation Propagation through a Gradient in Fuel Composition**

*D.A. Kessler, V.N. Gamezo, E.S. Oran*

We present numerical simulations of detonations in two-dimensional channels filled with nonuniform fuel-air mixtures where the gradient in fuel composition is perpendicular to the direction of propagation. A complex wave structure

develops that consists of fuel-lean and fuel-rich detonations at the leading edge of the reaction zone and a turbulent diffusion flame downstream that consumes excess reactants that pass through the leading detonation. Transverse instabilities develop along the detonation front that further complicate the wave structure. We track the trajectories of the triple-shock configurations that form using a numerical smoke foil technique and find the cellular structures they create depend strongly on the size of the channel relative to a characteristic detonation cell size. For the largest channels considered, cell sizes grew and were distorted in non-stoichiometric regions of the mixture in a manner similar to that observed in experiments. For smaller channels, local quenching in the lean regions of the mixture had a significant effect on the propagation speed and the size and shape of detonation cells.

Paper #240

**Experimental Implementation of a Converging Diverging Nozzle Technique to Study Shock Reflections in Reactive Gases**

*L. Maley, J. Armstrong and M.I. Radulescu*

The present study presents an experimental implementation of White's technique to study reproducibly shock reflections in reactive gases. The technique consists of using a converging-diverging nozzle in order to generate laminar reaction zones consisting in a leading shock followed by a zone of energy release. These laminar detonations can then be subjected to shock reflections at a compressive corner. The technique permitted us to isolate the anomalous ignition in methane-oxygen detonations, previously reported to ignite much more readily than predicted from detailed chemical kinetic models. Detailed visualisation permitted to monitor the structure of reactive Mach reflections with unprecedented clarity and microsecond time resolution. The well-posedness of the present experimental technique may be conducive to comparison with detailed models in the future in order to address this anomalous ignition phenomenon.

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**13:30 (R12B) Detonation Initiation and Transmission**

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Paper #65

**The Onset of Detonation in Mixtures with Regular and Irregular Detonation Cellular Structures**

*J.-S. Grondin, J.H.S. Lee*

In the present research, the onset of detonation downstream of a perforated plate subsequent to the reflection of a Chapman-Jouguet (CJ) detonation upstream was investigated. Single-frame schlieren photography was used together with pressure and velocity measurements to examine the phenomena in detail. Experiments were performed with two different mixtures:  $C_2H_2 + 2.5O_2 + 70\%Ar$  and  $C_3H_8 + 5O_2$ . The former is known to have a piecewise laminar structure with a regular cellular structure while the latter has a much more irregular transverse wave pattern. Upon reflection of the CJ detonation upstream, a turbulent reaction front propagates downstream at a quasi-steady velocity which corresponds to about the sound speed of the detonation products and half the CJ detonation velocity. There is found to be a critical value of the initial pressure in which the detonation is re-initiated downstream of the perforated plate. Below the critical initial pressure, the quasi-steady reaction front decays into a deflagration after a certain period of propagation. For the propane-oxygen mixtures at critical condition, the quasi-steady reaction front is found to propagate for relatively long distances from the plate prior to the onset of detonation. In contrast, for the high argon diluted mixtures, the onset of detonation is found to always occur in the vicinity downstream of the perforated plate, when the turbulence generated by the plate has not yet decayed. Thus it appears that high argon diluted mixtures cannot self-generate the critical conditions that are required for the transition to detonation.

Paper #99

**Effects of Nitrogen Dilution on Detonation Transmission across a Sudden Expansion in a Millimeter-scale Channel**

*Wei-Chun Kuo, Po-Yuan Chiu, Ming-Hsun Wu*

Detonation transmission of stoichiometric ethylene/oxygen-enriched-air across a 1 mm to 3 mm wide 2D sudden expansion in a 1 mm deep channel was experimentally characterized under various degree of nitrogen dilution. Three transmission modes were identified. When the dilution ratio was between 15% and 20%, the reaction wave re-accelerated back to a near C-J velocity within 40 mm downstream of the sudden expansion after stalling at the sudden expansion, and then stably propagated at the near C-J velocity until the end of the channel. For mixtures with dilution ratios between 25% to 33%, the detonation wave also stall and re-accelerate to C-J detonation like first mode, but the stall velocity is lower, and recovery distance is 4 times longer. In mixtures with higher dilution ratios (37% - 40%), C-J detonation could not be sustained in the narrow section. Instead, there existed a low-speed detonation mode with a propagation velocity of approximately 1500 m/s. As the low-speed detonation wave headed into the sudden expansion, it immediately accelerated to C-J detonation in the expanded section. Soot film visualizations revealed extinction cones in both dilution ratio = 20 % and 30 % cases. Lengths of extinction cones were longer for mixtures with higher dilution ratio. Cell size was approximately 1 mm for dilution ratio = 20% mixture ( $C_2H_4+3O_2+0.75N_2$ ).

Paper #115

**Critical Ignition in Rapidly Expanding Flows Described by a Power Law**

*Maxwell, B. M. and Radulescu, M. I.*

The generic problem of ignition of a particle undergoing an expansion given by a power law rate of decay behind a decaying shock is addressed in the present study. It is demonstrated, using a one-step Arrhenius irreversible reaction, that a sufficiently strong expansion wave can quench the reaction. The critical conditions for extinction are obtained in

closed form in terms of the time scale for the expansion process and the thermochemical properties of the gas, yielding a critical Damköhler number, i.e., the ratio of the expansion time scale to the homogeneous ignition time scale. The critical ignition criteria were found in excellent agreement with numerical results. The applicability of the results obtained are discussed for ignition in rapidly expanding flows which occur behind decaying shock waves, as encountered in problems of detonation initiation by a Taylor-Sedov blast wave, and reacting jet startup, and for reactions in steady hypersonic flows around projectiles.

Paper #128

**On Some Conditions of Detonation Initiation behind a Multi-Orifice Plate**

*S. V. Khomik, B. Veyssiere, V. Montassier, S. P. Medvedev, G. L. Agafonov*

An experimental investigation was performed to establish the influence of the detonation wave parameters and detonation products composition before a multi-orifice plate on detonation initiation behind it. The experiments were carried out in detonation tubes of 106 mm in diameter, separated by a multi-orifice plate equipped by the membrane into two sections. The tube was equipped also with pressure gauges and semi-cylindrical smoked plate. The mixtures with the different hydrogen content were used before and behind the perforated plate. It is shown by the examples of mixtures with 25% and 34% of hydrogen that possibility of detonation initiation depends on detonation conditions before the multi-orifice plate. The increase of the initial pressure in the mixture before the multi-orifice plate leads to detonation initiation in the vicinity of the plate exit. The influence of mixture composition on detonation initiation does not seem to play a significant role in the conditions of the performed experiments.

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**13:30 (R12C) Turbulent Non-Premixed and Stratified Flames**

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Paper #235

**A Turbulent Combustion Model for Jet Flames Issuing in a Vitiated Coflow**

*Ronan Vicquelin, Benoit Fiorina and Olivier Gicquel*

Auto-ignition is of great importance in new technologies like HCCI and MILD combustion where exhaust gases are mixed with fresh gases in order to reduce NO<sub>x</sub> emission. In such systems, fuel and oxidizer are usually not premixed. In order to describe auto-ignition in such a non-premixed environment, unsteady laminar flamelets are computed and stored in a look-up table. A turbulent combustion model for RANS simulations is then built by presuming Probability Density Functions (PDFs) for mixture fraction, progress variable and the mixture fraction scalar dissipation rate. The model is applied to a hydrogen/nitrogen flame in a vitiated coflow. Comparison with temperature and species experimental profiles are very good. The flame lift-off height sensitivity to the coflow temperature, a very important feature, is also retrieved.

Paper #168

**Time Dependent Based Mixing Time Modelling for Diesel Engine Combustion Simulations**

*Pasternak, M., Mauss, F., Lange, F.*

An application of a probability density function (PDF) based stochastic reactor model (SRM) is one of the possible methods to simulate combustion and emissions formation in internal combustion engines (ICE). In the PDF based SRMs turbulent mixing of the in-cylinder content requires modelling. The common feature of existing mixing models is that the turbulent time scale -mixing time, must be given. The mixing time that is seen as an inverse of the mixing intensity is a crucial parameter of the mixing model. The history of the mixing time influences the level of inhomogeneities in in-cylinder mixture composition and temperature. This in turn directly affects SRM's capabilities in predicting engine-out emissions and performances. In turbulent processes occurring in ICE the mixing time is not constant. In some applications, such as in studies of homogeneous charge compression ignition (HCCI) combustion, the SRM performs accurately enough when the mixing time is approximated by the constant value over the entire engine cycle. In the case of Diesel engines however, our preliminary studies indicate that an improvement of the SRM's performance can be achieved if time dependency to the description of the mixing process is considered. In this work a model describing the mixing time as a function of time during the engine working cycle is applied. The model by means of a combination of linear and exponential functions defines regimes of various mixing intensity respectively to the physical and chemical processes occurring during the cycle. This mixing time history has been incorporated into the Curl's mixing model and used in the stochastic reactor model for direct injected engines (SRM-DI). Simulated were in-cylinder performance and engine-out emissions of an n-heptane fuelled Diesel engine working under part load conditions. The chemical kinetics modelling within the SRM-DI was based on a reaction mechanism for n-heptane. Simulation results showed that by introducing time dependency into the mixing time description, the overall capability of the SRM-DI in predicting Diesel engine performance increased. The model simulates in-cylinder parameters such as pressure, temperature, heat release rate, etc. with high accuracy. Particularly good results were obtained for engine out-emissions. For NO<sub>x</sub> and HC the relative difference between simulated and experimental data did not exceed five percent. The presented simulation method with time dependency in the mixing process, improves the overall capabilities of the SRM-DI. The method is applicable to various engine related investigations, such as engine performance optimisation or testing fuels performance under Diesel combustion conditions.

Paper #142

**Statistical Analysis and Modelling of Turbulent Fuel Mass Fraction Flux in Turbulent Stratified Flames Using Direct Numerical Simulations***Sean P. Malkeson, Nilanjan Chakraborty*

Three-dimensional compressible Direct Numerical Simulations (DNS) using a simplified chemical mechanism that is representative of hydrocarbon combustion have been carried out for statistically planar turbulent stratified flames for globally stoichiometric (i.e.  $\langle\Phi\rangle=1.0$ ) and globally fuel-lean (i.e.  $\langle\Phi\rangle=0.7$ ) conditions at different values of root-mean-square (rms) velocity fluctuation  $u'$ . The species inhomogeneity is accounted for by a random bimodal distribution of equivalence ratio  $\Phi$  that is introduced in the unburned reactants ahead of the flame. The random bimodal distribution of equivalence ratio is initialised for specified values of global mean equivalence ratio  $\langle\Phi\rangle$ , rms fluctuations in equivalence ratio  $\Phi'$  and ratio of the integral length scale of species inhomogeneity to the integral length scale of turbulence  $l_\phi/l$ . The simulation parameters in all of the cases were chosen in such a manner that the combustion situation belongs to the thin reaction zones regime. The DNS data has been used to analyse the statistical behaviour of the turbulent flux (i.e.  $\overline{\rho u_i Y_F''}$ ) of fuel mass fraction  $Y_F$  in the context of Reynolds Averaged Navier-Stokes (RANS) simulations. In the context of turbulent stratified flame modelling, transports of both the active and passive scalars need to be addressed and often the fuel mass fraction  $Y_F$  is considered to be the characteristic active scalar. The quantity  $\overline{\rho u_i Y_F''}$  appears explicitly in the transport equation of  $\widetilde{Y_F}$ . For statistically planar flames, the only non-zero turbulent flux of fuel mass fraction can be written as  $\overline{\rho u_1 Y_F''}$ . It has been found that  $\overline{\rho u_1 Y_F''}$  exhibits positive non-zero values in the unburned gas side of the flame brush due to mixture inhomogeneity and remains predominantly positive throughout the flame brush in all cases, but some negative values have been observed in conditions where the Bray number is much larger than unity. It has been found that the gradient hypothesis can predict the qualitative behaviour of  $\overline{\rho u_1 Y_F''}$  for the majority of the flame brush for the cases here. However, it has been found that  $\overline{\rho u_1 Y_F''}$  exhibits counter-gradient behaviour where the Bray number is significantly larger than unity. Moreover, it has been found that a significant variation of the turbulent Schmidt number is required for suitable quantitative predictions even for the cases in which gradient transport is prevalent. Physical explanations for the observed behaviour of the turbulent fuel mass fraction flux have been provided. In order to account for the observed behaviour, a new model has been proposed for  $\overline{\rho u_1 Y_F''}$  in the context of turbulent stratified flames for both globally fuel-lean and globally stoichiometric conditions that accounts for both gradient and counter-gradient transport.

Paper #123

**Large-eddy Simulation of an Auto-igniting Liquid Diesel-type Spray***J. TILLOU, C. ANGELBERGER, J. B. MICHEL, A. ROBERT, L. MARTINEZ, S. RICHARD, D. VEYNANTE*

The application of Large Eddy Simulation (LES) to the study of the auto-ignition of a liquid jet under Diesel like conditions is presented. A LES formulation of the Tabulated Kinetics Ignition (TKI) model is presented, that is based on an a priori tabulation of homogeneous, auto-igniting reactors simulated with complex chemistry schemes, and which in particular allows accounting for cold flame effects. This model is combined with a FPI-type model to describe the evolution of burnt gases composition after combustion. The aim of the present work is to explore whether such a simple approach, neglecting sub-grid scale stratification and scalar dissipation effects, might be sufficient in the context of LES using fine computational meshes where sub-grid effects are comparatively small. The developed model is integrated into the AVBP code and applied to the LES of a liquid jet injected into a constant volume vessel under both reactive and non-reactive conditions, and for which experimental results are available. The liquid jet is addressed using an Euler-Euler mesoscopic formulation combined with the DiturBC approach allowing imposing injector outflow conditions at a distance downstream the injector outlet in such a way that break-up phenomena do not have to be computed in the LES. The LES of the non-reactive case shows that the proposed modelling approach allows an accurate reproduction of the global and local jet structure in terms of gas penetration, jet angle and local mean. First results obtained for the reactive case indicate that the proposed approach largely under-estimates the experimentally observed auto-ignition delay. First analysis indicates that this is related to the fact that scalar dissipation effects are not accounted for accurately. Perspectives are finally given for future work to improve this aspect.

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**15:40 (S6) Verification and Validation of Detonation Simulation – II**

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Paper #89

**Stability of Flame-Shock Coupling in Detonation Waves: 1D Dynamics***Lord K. Cole, Ann R. Karagozian, Jean-Luc Cambier*

In the present study, we utilize high-order spatially accurate methods in resolving the non-linear dynamics associated with the ignition of one-dimensional detonations with complex reaction kinetics. For a spark-induced detonation, as the detonation decays towards the self-sustaining Chapman-Jouguet mode from an over-driven mode, one obtains a sequence of physical oscillations between the flame and shock front. While prior studies exploring such issues have used highly-resolved numerical simulations with a 2nd-order shock capturing scheme, in the present study, a fifth order

accurate Monotonicity Preserving Scheme (MP5) is used for high order interpolation of the system of governing equations. A third order Total Variation Diminishing (TVD) Runge-Kutta time integration scheme is used in conjunction with MP5. Since a complex chemical reaction mechanism is simulated, operator splitting is implemented to facilitate the concurrent implementation of point-implicit backwards Euler kinetics solver with the MP scheme. Direct initiation of the detonation is obtained in a chamber filled with a stoichiometric mixture of hydrogen and air by setting a region adjacent to an end-wall of the simulated shock tube at high pressure and temperature, as a simulated spark. Requirements to achieve detonation ignition with the MP5 scheme include sufficient spatial resolution, with cell size 50 micron and a sufficiently distributed simulated spark of length 0.25 to 0.5 cm. For successful detonation, at time  $t = 0+$ , a shock propagates into the unburned medium, which is rapidly heated and ignites after an induction time delay. The flame is initially strongly coupled to the shock and the wave is over-driven. As the degree of overdrive decays and the detonation approaches the CJ limit, instabilities begin to appear. These fluctuations in key properties (e.g. species concentration, temperature, and pressure) of the fluid at the flame are found to contribute to an initial stage of the flame dynamics. The present high order schemes can properly resolve high frequency modes seen in detonations. Eventually the average induction length continues to increase and a second mode can be seen which directly couples the flame speed with the shock, resulting in fluctuations with lower frequency but much higher amplitude. It is also worth pointing out that the location and approach to the onset of the instabilities may not be exactly reproducible, i.e., it may have a very high sensitivity to the past history of the wave formation. This is characteristic of non-linear systems at the onset of chaos, which brings the interesting question of whether a truly chaotic mode can be observed computationally. The current study will attempt to map the phase space of the dynamical system to elucidate this issue.

Paper #29

### **Numerical Study of Detonation Suppression with Chemical Inhibitors**

*Miltiadis V. Papalexandris and Quentin Steisel*

This paper is my contribution to the Verification and Validation Session, following the session organizers' demand. This work is concerned with a numerical study on the suppression of gaseous detonations with chemical inhibitors. In particular, we perform direct numerical simulations of the evolution of a detonation wave in a zone that contains a flame extinguisher (inhibitor). A simplified chain-branching kinetics model is employed consisting of four reaction stages: chain initiation, chain branching, chain termination and chain inhibition. Our study shows that the minimum inhibitor concentration required for detonation suppression is inversely proportional to the pre-exponential factor of the inhibition reaction stage. It is further observed that one-dimensional simulations underestimate considerably the amounts of inhibitor that are required for detonation suppression because they do not account for the stabilizing effect of the transverse waves emanating from the leading front. Thus, multi-dimensional simulations are necessary for accurate numerical predictions. Our simulations indicate that the simplified kinetic model has the potential to be sufficiently accurate for employment in detonation simulations, provided that values for the pre-exponential factors and activation temperatures are judiciously chosen. Nonetheless, since experimental data show that the required amounts of chemical inhibitor for detonation suppression vary with pressure, the simplified model should eventually be generalized to take into account pressure dependent kinetics.

Paper #33

### **Verified Calculation of Nonlinear Dynamics of Viscous Detonation**

*Christopher M. Romick, Tariq D. Aslam and Joseph M. Powers*

The dynamics of one-dimensional detonations predicted by a one-step irreversible Arrhenius kinetic model with the inclusion of mass, momentum, and energy diffusion were investigated. A series of calculations in which activation energy is varied, holding the length scales of diffusion and reaction constant, was performed. As in the inviscid case, as the activation energy increases, the system goes through a period-doubling process and eventually undergoes a transition to chaos. Within the chaotic regime, there exist regions of low frequency limit cycles. The addition of diffusion significantly delays the onset of instability and strongly influences the dynamics in the unstable regime. Because the selected reaction and viscous length scales are representative of real physical systems, the common use of reactive Euler equations to predict detonation dynamics in the unstable and marginally stable regimes is called into question; reactive Navier-Stokes may be a more appropriate model in such regimes.

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## **15:40 (R13A) High Speed Flames**

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Paper #165

### **Experimental Study on Premixed Flame Propagation in Small Channel**

*Rafal Porowski, Andrzej Dabkowski, Andrzej Teodorczyk, Felipe Alfonso Galvis Millan*

The aim of this study was to experimentally investigate a flame propagation mechanism in premixed gaseous mixtures, including some fundamental combustion characteristics such as pressure profiles and flame speed. In the experiments the flame propagation speed of a premixed stoichiometric hydrogen-air mixture contained in a constant volume channel of 200 mm length and 20 mm height was measured. Two ignition points were provided in order to widen the range of experiments to be performed with different setups. One ignition point was located in the middle of the channel and the second ignition point was located at 10 mm from the left end of the channel. Pressure signals were measured and stored by a data acquisition system. Flame propagation images were taken using high speed camera.

Paper #167

**Effects of Hydrogen Addition on Flame Propagation and Blast Wave Generation during Explosion of Methane-Air Mixtures**

*Woo-Kyung Kim, Toshio Mogi, Ritsu Dobashi*

To understand the consequence of accidental gas explosions in an open space, the effects of flame propagation behavior on the blast wave were examined experimentally. The spherically propagating flames in the mixtures of methane and hydrogen with air were focused. The results show that the flames at equivalence ratios of 0.7, 1.0, and 1.3 were intensively wrinkled and accelerated with the increases of hydrogen addition in methane/air mixtures. The overpressure of the blast wave tends to increase acceleratingly by the flame wrinkling. The flame wrinkling is considered to be generated by diffusive-thermal instability according to the analysis of the effective Lewis number. The overpressure can be predicted by the acoustic theory which indicates that the intensity of blast wave is affected, in particular, by burning velocity, volumetric expansion ratio and the flame acceleration. In particular, the intensity of the blast wave is strongly affected by the acceleration of the burning velocity.

Paper #291

**High-Speed Camera Visualizations of Flame Acceleration in a Square Channel with Obstacles: the Case of Binary Fuels H<sub>2</sub>/C<sub>3</sub>H<sub>8</sub>-Air mixture**

*Guanbing CHENG, Ratiba ZITOUN, Yves SARRAZIN, Alain CLAVERIE, Pierre VIDAL, Bernard VEYSSIERE, Pascal BAUER*

In this paper, we have performed visualization of initial stage of flame acceleration in H<sub>2</sub>/C<sub>3</sub>H<sub>8</sub>-Air mixtures using shadow technique with high speed camera. The experiments are carried out in an obstacle-filled stainless steel channel with 40 mm x 40 mm square cross-section and 4-m length at the room temperature with two initial pressures (P<sub>i</sub>=0.5 bar and 1 bar) and H<sub>2</sub> molar fractions  $x$  ( $\phi = 1.1$ ;  $x=0.9$  and  $0.95$ ). The results show that the acceleration flame results from the contraction of unburned flow near obstacle and from delayed turbulent combustion in recirculation zone behind the flame front. The evolutions of measured flame velocities are due to the acceleration or deceleration of the unburned gas which passes through the obstacles. For different  $x$ , we obtain the nearly same variation of flame velocity ( $x=0.9$  at P<sub>i</sub>=1bar) as those in mixtures ( $x=0.95$  at P<sub>i</sub>=1bar). It should be noted that the addition of propane in such binary fuels mixtures significantly reduces the flame velocity.

Paper #229

**Influence of Diaphragm on Self-Ignition of Hydrogen at Spontaneous Release into Air**

*Sergey Golovastov, Victor Golub, Dmitry Baklanov, Vladimir Bocharnikov*

Special properties of diffusion self-ignition of hydrogen were studied experimentally at a pulse discharge into a channel filled with air. Self-ignition of hydrogen occurred at a contact surface of the jet of hydrogen. Required temperatures for self-ignition of hydrogen were reached due to heating the air by a shock wave which appears as a result of the non-stationary supersonic discharge of hydrogen from the high pressure vessel. Formation of a shock wave flow structure at the pulse discharge of compressed hydrogen into the channel with air was studied, and ignition delays of hydrogen were determined.

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**15:40 (R13B) Chemical Kinetics and Reaction Dynamics – I**

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Paper #276

**Shock-induced Ignition for Simplified Chain-branching Kinetics**

*Josue Melguizo-Gavilanes, Mingjun Tian, Luc Bauwens, Zhenhua Pan*

The scenario of shock-induced ignition is likely to play a key role in deflagration to detonation transition (DDT). Flame acceleration and reflections over obstacles may result in the presence of a shock wave. Next, after further reflections, that shock will potentially cross over a slow flame, subsequently moving into reactive mixture. Neglecting diffusion, that situation can effectively be reduced to the problem of ignition between a shock and a temperature interface separating reactive from burnt or inert mixture. Numerical simulation of shock ignition is challenging because the initial conditions are singular, thus initially the region of shocked reactive mixture does not exist. In order to overcome this difficulty and solve the problem accurately and reliably, a combination of techniques has been developed which include replacing space and time as independent variables by the ratio space over time,  $x/t$ , and time, in addition to using initial conditions obtained from short time asymptotics. The transformation alone, yields a finite domain at  $t=0$  and provides for a well-resolved problem at early times, whereas the short-time asymptotics further improves the treatment of the initial conditions as it allows for a very efficient numerical simulation. The transformed problem is solved using a Weighted-Essentially Non-Oscillatory (WENO) algorithm in space and Runge-Kutta in time, both third order accurate. Results are obtained for a three-step chain-branching kinetic scheme, and show the complete ignition evolution using realistic values of the parameters to properly mimic hydrogen chemistry.

Paper #285

**Computational Singular Perturbation with Non-Parametric Tabulation of Slow Manifolds for Time Integration of Stiff Chemical Kinetics**

*Bert Debusschere, Youssef Marzouk, Habib Najm, Dimitris Goussis, Mauro Valorani*

This paper presents recent progress on the use of Computational Singular Perturbation (CSP) techniques with tabulation for time integration of stiff chemical systems. The CSP integration approach filters fast time scales from the reaction

system, thereby enabling integration with explicit time stepping algorithms. For further efficiency improvements, relevant CSP quantities are re-used via a non-parametric tabulation of the CSP information along the slow manifolds. This paper outlines the method and shows that it is competitive with implicit solvers for the simulation of CH<sub>4</sub> - air ignition.

Paper #304

**Non-Linear Response to Periodic Forcing of Methane-Air Global and Detailed Kinetics in Perfectly Stirred Reactors**

*Francesco Saverio Marra, Emanuele Martelli*

This study focus on the behavior of the combustion kinetic under the action of perturbations of finite amplitude and frequency in a Perfectly Stirred Reactor (PSR). Two main objectives are pursued: firstly, to determine the extinction line in the equivalence ratio-residence time plane, fixed the thermodynamic state conditions. Then, to characterize the response of the chemical system to periodic forcing of the state parameters in different points of the plane. Several specific locations have been selected, some of them well inside the flammability region, while the others close to the extinction line. Transient simulations of combustion of methane with air, using both global single-step and detailed chemical kinetic mechanisms, have been conducted with imposed oscillation of inlet mixture equivalence ratio and residence time around average values. The responses of the model to perturbations of inlet flow conditions are presented that highlight the limits of the very simple PSR model in application to the study of oscillations and instabilities of combustion systems. In addition, an assessment of the ability of different simplified chemical kinetic schemes to reproduce the behavior of a reference kinetic scheme (like the well-established GRI-Mech 3.0 scheme for methane combustion), under the dynamic conditions due to the inlet perturbations, is proposed. Newly, several insight, not all here reported, about the effect of simplified chemistry models on the dynamic response of this simple combustion system in terms of amplitude damping and phase shift are obtained.

Paper #198

**An Analysis of the Attractive Properties of REDIM Manifolds for Model Reduction**

*Viatcheslav Bykov, Ulrich Maas*

The mathematical model of reacting flows of a combustion process is represented by the system of partial differential equations as the closed set of the standard conservation equations. The most complicated part of this system is the conservation equations of the species concentrations. During the last decades, chemical kinetic schemes have become extremely complex-high dimensional, non-linear and stiff. In order to treat numerically such systems methods of dimension and stiffness reduction becoming very important and have been developed intensively in the last years. Many reduction methodologies focus on the chemical source term. However, because of the strong coupling of diffusion and reaction in the combustion process, many existing operator splitting methodologies which split reaction and transport terms during the integration process turn out to be problematic. On the other hand, applying the same transport term for reduced model as for the detailed one, while replacing the source term by a reduced chemistry model, can lead to inaccurate results as well. The method of reaction-diffusion manifolds (REDIM) accounts for the coupling of molecular transport with chemical reaction. It has been shown to be a very efficient tool of model reduction for reacting flows. This method exploits the existence of differences in time scales of sub-processes in combustion process leading to a decomposition of the system dynamics and as a consequence to the manifold existence. Inputs to the method are a detailed reaction mechanism, boundary conditions of the reacting flow, and an estimate of the local gradients of the scalars in the flow. The reduced kinetic mechanism is constructed as a table of a slow manifold mesh in the composition or state space. The manifold table contains all necessary information about the reduced kinetics as well as about the projection of the original system of PDE governing equations on this low dimensional manifold. This work presents the premixed free flat flame of syngas/air mixture as a reference benchmark model for study attracting properties of the REDIM. It is relatively simple example, but nevertheless, it contains main features of combustion systems. For stoichiometric mixture composition the 2D REDIM manifold was constructed on the basis of a constant gradient estimation. The decomposition of motions and attractiveness of the REDIM is investigated and verified. The source term eigenvalues are studied on the REDIM manifold, while attractive properties are analyzed with the help of detailed system solutions. The Jacobian of the source term calculated on the 2D REDIM reveals that two positive eigenvalues only are coupled with the transport - have a comparable order of magnitude. Others eigenvalues are negative and very large such that they can be decoupled, which confirms the existence of the 2D attractive REDIM for chosen configuration.

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**15:40 (R13C) Hydrogen Combustion**

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Paper #174

**Self-ignition and Flame Propagation of Pressurized Hydrogen by Sudden Release through a Tube**

*Hyoung Jin Lee, Sei Hwan Kim, Yeong Ryeon Kim, In-Seuck Jeung*

Hydrogen is regarded as a one of future fuels which will take place of oil fuels. As the popularity on the hydrogen is increased, the crucial safety problems concerned with utilization of hydrogen are storing and transportation. Due to low energy density in gas phase, hydrogen needs to be stored under very high pressure or in liquid state. Because the latter storage system is much more complex and expensive, high-pressurized hydrogen has been used. For example, hydrogen fuel-cell vehicles may possess storage pressures as high as 70 MPa. However, high pressure hydrogen installation is endangered by a risk of sudden discharge of hydrogen leading to ignition and severe accident. It has been reported that a leak of such high-pressurized hydrogen into the air can lead to self-ignition and explosions without any apparent ignition sources. The incidents have been reported by Astbury and Hawksorth. For this reason, many studies

have been conducted to understand this phenomenon and obtain the criterion to be occurred self-ignition. The first investigations concerned with a problem of high pressure hydrogen outflow ignition were carried out nearly 40 years ago. Dryer et al. discovered that spontaneous ignition requires both a sufficiently high bursting pressure and a downstream geometry for fast mixing of the expanding hydrogen and shocked air. Additionally, they postulated that turbulent mixing and the heating of the mixture by the multi-dimensional shock-boundary and shock-shock interactions might play a significant role in the generation of an ignition. Recently, this postulation has been proven by numerical simulation and experimental observations. They showed that two reaction regions inside the tube, where one reaction region is in the boundary layer and the other is in core region of the tube due to shock-shock interactions, can be generated and self-ignition can occur when two reaction regions are completely merged. Especially, using direct images, Lee et al. showed that there can be failed-ignition cases which the flame cannot sustain when it goes out to the open air, although the spontaneous ignition occurred. In addition to these efforts, several experiments have been conducted to identify the limiting conditions of self-ignition. The previous results have shown that the hydrogen jet had an increasing tendency to ignite as the downstream tube increased in length. In spite of these valuable results which the mechanism of self-ignition can be uncovered, the investigations outside the tube have been rarely reported, such as the flame propagation, flame stabilization and extinction. In this study, the experimental apparatus comprised of commercial rupture disks to simulate actual circumstances and tubes with an inner diameter of 5~10.9 mm and lengths ranging from 35 mm to 600 mm. This paper presents values of the minimum bursting pressures for self-ignition with the tube lengths and the effect of tube diameter on the self-ignition. Additionally, using the direct and shadow images outside the tubes, we investigated the flame propagation, flame stabilization and extinction based on the experimental data.

Paper #249

#### **Influence of Lewis Number and Expansion on Jet Ignition**

*Rezaeyan, N., Bauwens, L., Radulescu, M., Fachini, F.F.*

Jet ignition was first observed by Wolanski and Wojcicki in 1973. An unsteady hydrogen jet from a high pressure vessel into air was observed to ignite early on in the process. That accidental releases of hydrogen subsequent to a rupture in a high pressure storage or distribution system could ignite is significant in the framework of hydrogen safety. This is particularly true if hydrogen were to become widely used as an automotive fuel. The physical mechanism leading to ignition remains poorly understood. Diffusion between hot, air compressed by the leading shock, and cold, expanded hydrogen is one potential mechanism resulting in ignition. Ignition between two streams was analyzed by Linan and Crespo. Here, that analysis is revisited focusing upon the jet ignition problem, taking into account that expansion takes place during the release and also, non-unity Lewis number. Results show that jet ignition will only take place in fuels with Lewis number less than a threshold close to unity, and as long as the expansion rate is lower than a critical value. These results are consistent with experimental evidence. Both thresholds are determined by the analysis.

Paper #238

#### **Extinction and Auto-Ignition of C<sub>3</sub> and C<sub>4</sub> Alcohols in Laminar Nonpremixed Flows**

*Ulrich Niemann, Kalyanasundaram Seshadri, Forman A. Williams*

Alcohols produced from biomass show significant potential to be an alternative to conventional crude oil derived transportation fuels. In this experimental and computational study, the combustion of C<sub>3</sub> alcohols (n-propanol, iso-propanol) and C<sub>4</sub> (n-butanol, iso-butanol) alcohols is investigated in nonpremixed, nonuniform flows. Experiments are performed employing the counterflow configuration with a fuel stream made up of vaporized fuel and nitrogen, and an oxidizer stream of air. The strain rate at extinction is measured as a function of the mass fraction of fuel in the fuel stream. At fixed mass fractions of fuel critical conditions of auto-ignition are measured in terms of the temperature of the oxidizer stream as a function of the strain rate. Kinetic modeling is performed using a semi-detailed mechanism. This mechanism is made up of more than 7000 reactions among 300 species. Critical conditions of extinction and ignition were calculated and compared with experimental data.

Paper #248

#### **Limiting Values for the Ignition of Hydrogen/Air Mixtures by Mechanically Generated Ignition Sources**

*F. Welzel, M. Beyer and C.-P. Klages*

Mechanical equipment for use in explosive atmospheres can feature ignition hazards through hot surfaces and, in particular due to malfunctions, through mechanically generated sparks. At present, an international standard is being developed for the safety requirements of explosion-proof mechanical equipment. In this regard, ignition tests were done in two different hydrogen/air mixtures. The friction of elements which move in opposite directions cannot be ruled out. If the contact zone reaches a sufficiently high temperature, the removed particles, combined with the oxygen contained in the air, can combust. Both the high surface temperatures and the mechanical sparks can thereby be a potential ignition source for explosive atmospheres. Therefore, in the last few decades the formation of mechanically generated ignition sources has been the subject of many research activities. In addition to improving fundamental knowledge, results were integrated into European standards. Following this, a limiting value of 1 m/s for relative velocity has often been used, below which mechanically generated ignition sources are not capable of igniting an explosive atmosphere. This standard gives a hint that experimental tests have confirmed this for many situations except for ignition-sensitive gas atmospheres with hydrogen or ethylene at high contact loads. Other investigations have reported ignitions below this limit. However, the surface-related power density maybe describes the friction process more precisely than a relative velocity of the friction partners. The aim of this research is to verify the power density as a criterion for ignition in hydrogen/air mixtures.



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**09:00 (S7) Supersonic Combustion – I**

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Paper #296

**Hypersonic Propulsion and Supersonic Combustion: Review on Current Status for the Future***Vigor Yang, Jeong-Yeol Choi*

Remarkable advances in powered hypersonic flight have been achieved during last decade. A number of successful flight tests were carried out successfully those made the dreams of last 50 years come true. The successful flight test of X-51A last year opened new era of powered hypersonic flight for practical applications. Propulsion technologies of X-51A is distinguished by dual-mode ramjet (DMR) engine which starts at ramjet mode and transit to scramjet mode accelerating from supersonic launch speed and to hypersonic cruising condition. The remarkable technical advances in the DMR engine is the sophisticated handling of endothermic liquid fuel for the regenerative cooling and adaptive combustion control for the operation condition from starting to cruising. The technology will be succeeded to the combined cycle engines including TBCC (Turbine-Based Combined Cycle) and RBCC (Turbine-Based Combined Cycle) engines for large reusable systems or more affordable small systems. The sophisticated technology levels of today is thoroughly based on the scientific achievements from the experiments and analyses carried out concurrently, and the future advances depends it. Present review will address the current status and future directions in the researches and developments in hypersonic propulsion and its scientific aspects in supersonic combustion. The first half of the review will summarize the hypersonic propulsion and supersonic combustion test programs during the past and near future. International activities on ground and flight test programs will be introduced with emphasis on supersonic combustion technologies. The second half of this review will cover the supersonic combustion technologies and physics newly understood from the recent researches. It will include the fuel issues from hydrogen to liquid hydrocarbon fuels. Handling properties of fuels, fuel injection schemes and combustion characteristics of the fuels will be discussed in this regards. Another important issue is the flame structures, combustion dynamics and stabilities. Lessons learned from the recent experimental and analytical studies will be introduced with design aspects of the supersonic combustor. Research approaches including laser diagnostics and CFD techniques with modeling issues will be also discussed with some suggestions for future directions.

Paper #318

**Injection Schemes for Improved Flameholding in Supersonic Flow***Corin Segal and Qiuya Tu*

Previous analyses have shown that mixing can be enhanced using thin pylons that have only a negligible impact on pressure losses. In this study, helium and argon have been transversely injected into a Mach 1.6 airflow simulating a light and a heavy fuel injection behind a thin triangular pylon placed upstream, in the isolator. Penetration and mixing in the test section were observed at three cross-sections including the recirculation region and beyond with planar laser-induced fluorescence (PLIF). Results were compared to the no-pylon cases. The presence of the pylon resulted in improving both penetration and spreading of the jet and, at the same time, in lowering the concentration gradients in the recirculation region, an indication of improved flameholding ability.

Paper #117

**Ignition by Plasma Jet in Supersonic Flow***Kenichi Takita*

Plasma includes many chemically active species such as radicals, NO<sub>x</sub>, fuel fragments, ions, excited molecules and electrons. Therefore, ignition and combustion enhancement by plasma has been a major topic in the field of combustion research. As for ignition and combustion enhancement in a scramjet engine, the plasma jet (PJ) torch has been studied as a forced igniter and it has been actually used as the igniter in the sub-scale scramjet combustor. One advantage of a thermal plasma such as the PJ against non-thermal plasma is that thermal effect (high temperature effect) in addition to chemical effect strongly enhances ignition and combustion reactions. Therefore, thermal plasma was more effective for ignition enhancement than non-thermal plasma at very severe flow condition such as low static temperature. The other advantage of the PJ is its selectivity of supplied species to combustion field by changing components of the feedstock gas. In this paper, the author summarizes his experimental works about the influence of components of plasma feedstock gas on the effectiveness of the PJ.

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**09:00 (R14A) Detonation and High Speed Flames: Applications**

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Paper #88

**Thermodynamic Performance Numerical Simulation of Rotating Detonation Engine***Rui Zhou, Jian-ping Wang*

A new method of analyzing RDE flow field and describing the thermodynamic performance is proposed. The trajectories of fluid particles are tracked. The impact of detonation wave, deflagration wave, oblique shock wave and contact surface on the trajectories and physical parameters at fluid particles was investigated deeply. Detonation wave, deflagration wave, oblique shock wave and contact surface only have a very small interference on the trajectories of fluid particles. Fluid particles are injected into flow field, burnt by detonation or deflagration, and then ejected rapidly almost along the axis. The fluctuation at the azimuthal direction is less than 0.25% of the circumference of the combustion chamber. When fluid particles encounter with the detonation wave or the oblique shock wave, their trajectories deflect. When fluid particles encounter with the deflagration wave or the contact surface, the trajectories don't deflect. The corresponding p-v

diagram and T-S diagram are obtained by the numerical simulation, and the results of numerical simulation and ideal detonation combustion are compared qualitatively and quantitatively. The numerical simulation results agree well with the theoretical results. The thermal efficiency of 2D numerical simulation is 35.41%. The cycle net mechanical work of 2D numerical simulation is 41.32% of the ideal detonation cycle. The superior performance of RDE is further defined.

Paper #211

### **Rotating Detonation Wave Stability**

*Piotr Wolański*

In this paper the analysis of stability of rotating detonation wave in cylindrical channel is discussed. On the bases of comparison of the time of revolution of detonation wave around the cylindrical chamber to the time of new mixture formation, stability of detonation front as well as a numbers of rotating detonation heads can be predicted. Dimensionless parameter, so called detonation wave number "W" is proposed. The evaluation of this detonation wave number can allow prediction of stability of propagating rotating detonation wave as well and the prediction of the numbers of rotating detonation heads in cylindrical chamber.

Paper #158

### **Numerical Study of the Noise Generation by a Rifle Shooting with Suppressor**

*Lo, Shi-Wei, Tai, Chang-Hsien, Teng, Jyh-Tong and Lin, Yong-Jhou*

The moving bullet out of a rifle barrel is propelled by a fired explosive charge. A disturbed muzzle blast wave is initiated which lasts several milliseconds. The supersonic bullet causes an acoustic shock wave that propagates away from the bullet's moving path. Besides, the muzzle blast is a main acoustic source to far field receivers. The noise generated by blast waves was investigated in this paper. Axial symmetry, unsteady, Large Eddy Simulation (LES), and Ffowcs-Williams and Hawkins (FW-H) equations were solved by the implicit-time formulation. For the spatial discretization, second order upwind scheme was employed. In addition, dynamic mesh model was used to where the ballistic domain changed with time due to the motion of bullet. Results obtained for muzzle flow field and for noise recorded were compared with those obtained from experimental data; these two batches of results were in agreement. In this study, three cases of gunshot including an unsuppressed rifle and two models of suppressors were simulated. Besides, serial images of species distributions and velocity vectors-pressure contours in suppressors and near muzzle field were displayed. The sound pressure levels (dB) in far field that were post-processed by the fast Fourier transform (FFT) were compared. The proposed physical model and the numerical simulations used in the present work are expected to be extended to solve other shooting weapon problems with three-dimensional and complex geometries.

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## **09:00 (R14B) Chemical Kinetics and Reaction Dynamics – II**

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Paper #16

### **Hydrogen Rich Syngas Oxidative Catalytic Activity of Nickel and Inconel**

*Kimberly N. Urness, John W. Daily and G. Barney Ellison*

There is considerable interest in developing power generation gas turbines that are fueled with hydrogen-rich syngas for the purpose of reducing fossil fuel carbon emissions. To most effectively design gas turbine systems it is necessary to understand fuel combustion behavior. At present computational models and experimental results differ by three orders of magnitude in their ignition time predictions for the low temperature (700K), high pressure (20 bar) regimes common in the combustor inlet region of the gas turbine engine. Recent studies suggest that gas-phase reactions alone are not the sole contributing factor to this observed discrepancy. As heterogeneous catalytic reactions between the reactant gas and the reactor surface offer one possible explanation, an experimental study was carried out to explore this hypothesis. The experiments were performed using small resistively heated tubular reactors with matrix isolation/IR diagnostics. Reactors were manufactured from stainless steel, nickel and inconel. Both nickel and inconel displayed catalytic activity above the detectability of the experiment.

Paper #57

### **Effects of Flame Curvature on Chemical Reactions in Rich Hydrogen-Air Premixed Flame**

*Yasuhiro Mizobuchi, Tadao Takeno, Shingo Matsuyama, Junji Shinjo, Satoru Ogawa*

The effect of flame configuration on the fuel consumption rate has been studied by means of 2-D numerical calculation with detailed chemical kinetics and accurate transport properties for a rich hydrogen-air mixture. A rich hydrogen-air 1-D premixed flame of equivalence ratio 4.5, whose burning velocity is 1.38m/s, has been reproduced and stabilized in a computational domain and then a small volume of the same mixture of diameter 1.5mm has been injected with a velocity of 20.0m/s toward the 1-D flame. The high speed small volume of mixture has deformed the shape of the premixed flame, and the changes in the flame structures in the course of the flame shape deformation have been observed and analyzed. It has been found that the local H<sub>2</sub> consumption rate increases at the portion where the flame develops curvature. The full use of the numerical data has been made to understand the cause of this increase. It has been found that the acceleration of mass diffusion of the deficient species, that is O<sub>2</sub>, nor the temperature increase does not play any important roles in this increase of H<sub>2</sub> consumption rate. On the other hand, it has been found that the curvature accelerates the supply rate of H by molecular diffusion to the reaction zone, which produces the increase in the local OH concentration providing the acceleration of local H<sub>2</sub> consumption rate.

Paper #176

### **Vibrational Nonequilibrium and Electronical Excitation in the Hydrogen-Oxygen Reaction**

*Oleg V. Skrebkov*

Suggested is a theoretical model of chemical and vibrational kinetics of hydrogen oxidation based on consistent account for the vibrational non-equilibrium of HO<sub>2</sub> radical acting as a key intermediate in the process of chain branching and in a generation of electronically excited species. In terms of the proposed model, the chain branching  $H + O_2 = O + OH$  and inhibiting  $H + O_2 + M = HO_2 + M$  reactions are considered as a general multi-channel process of forming, intramolecular energy redistribution between modes, relaxation, and monomolecular decay of the comparatively long-lived vibrationally excited HO<sub>2</sub>(v) radical which is capable moreover to react and exchange of energy with another components of the mixture. The calculated results are compared with the shock tube experimental data for strongly diluted H<sub>2</sub>-O<sub>2</sub> mixtures. Such approach has enabled us to explain an observed dependence of the apparent rate constant for  $H + O_2 = O + OH$  overall reaction on experimental conditions.

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### **09:00 (R14C) Reacting Flow Dynamics-I**

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Paper #79

### **Experimental Studies on the Dynamics of Premixed Methane-Air Flames in Various Aspect Ratio Channels**

*Mohammad Akram, Sudarshan Kumar*

The aim of the present work is to investigate the flame stabilization behavior in meso-scale rectangular diverging channels of different aspect ratios. In most of the micro combustors studied, the flame is stabilized at a location where combustible mixture flow decelerates along the flow path [6]. These configurations followed either a systematic or sudden velocity gradient which enhances the flame stability limits and controls the location of flame stabilization point. This velocity gradient also helps in avoiding the flame flashback. One of the parameters which may affect the flame dynamics inside the channel is height to length ratio and this has not been considered earlier. Flame stabilization characteristics have been studied experimentally in various aspect ratio channels. It was observed that a range of flame propagation modes have been observed to exist in the channel. The dynamics of the flames is greatly affected by the aspect ratio of the channel.

Paper #91

### **Joint Velocity-Scalar PDF Modeling of Turbulent Spray Flows**

*Hai-Wen Ge and Eva Gutheil*

The probability density function (PDF) method for turbulent flows has been studied for several decades. The transported PDF method became very popular since Pope's work in 1985. It has been proved to be a successful tool for the simulation of turbulent single-phase flows, and in particular for reactive flows. The PDF method provides a computationally tractable way of calculating the statistics of inhomogeneous turbulent flows of practical importance. The major advantage of the PDF method is, that convection, body force, mean pressure gradient, and chemical reactions can be treated without assumptions - this is also true for the evaporation source term in spray flows. PDF methods describe the turbulent flow in a more complete way than the conventional turbulent models. All the moments of the considered quantities can be evaluated from the resulting PDF. Additionally, the Lagrangian PDF method takes full account of the long memory of turbulence. The past history of all the fluid particles' properties can be completely described by the multi-time Lagrangian PDF. PDF methods were applied to simulate multi-phase flows since 1990. Research in this area includes the description of the gas phase in turbulent two-phase flows with the PDF transport equation or the formulation of a joint PDF transport equation of all liquid-phase and gas-phase dependent variables. Moreover, joint PDF transport equation of the properties of droplets and gas eddies seen by droplets were used. In present work, a joint velocity-scalar PDF is introduced for turbulent spray flows. The joint velocity-mixture fraction PDF transport equation of the gas phase in turbulent spray flows is deduced. The velocity is modeled through an extended simplified Langevin model, and molecular mixing through an extended IEM model. The PDF transport equation is solved by a Lagrangian Monte-Carlo particle method. The droplet characteristics including heating, vaporization, and motion are solved by a Lagrangian droplet parcel method. To close the PDF transport equation and droplet evolution equation, the mean conservation equations of the gas flow are solved by a SIMPLE-algorithm-based finite volume method. A steady, two-dimensional, axis-symmetric, turbulent methanol/air dilute non-reactive spray flow without swirl is simulated. The results of the gas velocity are in very good agreement with experimental data, and they improve the simulation using the extended  $k-\epsilon$  model. The extended Langevin model is a very promising approach for the modeling of turbulent spray flows.

Paper #105

### **Conditional Moment Closure for Turbulent Premixed Flames**

*S. Amzin, N. Swaminathan, J. W. Rogerson, J. H. Kent*

Conditional moment closure (CMC) is a suitable method to predict pollutants with slow time scales. Although the CMC has been developed and successfully applied to various non-premixed combustion systems, its application to premixed flames is not fully tested and validated yet. The main difficulty in applying CMC to turbulent premixed flames is associated with the conditional scalar dissipation rate of the conditioning scalar, the progress variable. A simple algebraic model for the conditional dissipation rate is validated using DNS results of V-flame. This model is used in the computations of a pilot stabilised Bunsen flame using the RANS-CMC method with a complex chemical mechanism. A first order closure is used for the conditional mean reaction rate along with a standard  $k-\epsilon$  turbulence model. The computed major and minor species mass fractions and temperature are in reasonable agreement with the experiments.

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**10:45 (S7) Supersonic Combustion – II**

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Paper #155

**Exploration on Unsteady and Transient Combustion Phenomena in High-Speed Air-Breathing Propulsion***Kuo-Cheng Lin, Vigor Yang*

Flame stabilization and combustion transients during flame ignition have been a serious concern in the development of high-speed air-breathing engines due to the difficulties to anchor stable flames in a high-speed environment. The situation becomes even more challenging during the engine start-up stage at which the low chamber pressure and unsettled fuel/air mixing tend to blow out the flame, even when a flame holding device such as a cavity is employed. At a low flight Mach number, however, combustion may take place in subsonic regions, such as boundary layers, recirculation zones in flame-holding devices, or the region behind the pre-combustion shock train at the dual mode combustion. The resultant heat release then causes the flow to accelerate to a supersonic state in the downstream section of the divergent combustor. During this process, a longitudinal mode of thermoacoustic instability may develop in a spatial domain reaching from the shock train in to the combustion zone. The present work investigates, both experimentally and analytically, thermoacoustic instabilities inside an ethylene-fueled supersonic combustor with a recessed cavity flameholder. High-speed pressure transducers, positioned at the base and downstream of the cavity flameholder, are utilized to record acoustic signals under various flow conditions and flameholder geometries. The effects of fuel/air equivalence ratio, fueling scheme, and simulated flight conditions on the stability characteristics of the combustor are examined systematically. The measured acoustic oscillation frequencies and the corresponding amplitudes are used to explore the underlying flow physics. In addition, the present measurements are compared with existing acoustic data for different combustor flowpaths to help identify the mechanisms responsible for driving and sustaining combustion oscillations. The present work also attempts to establish an integrated theoretical/numerical framework within which the influences of all known effects (including the location and operating timing of air throttling and fuel injection) on the engine ignition transient and flame development can be studied systematically. The basis of the work is an integrated three-dimensional numerical analysis capable of treating detailed combustion dynamics in realistic engine environments. The physical model simulates the experimental facility operated at the Air Force Research Laboratory. It was found that the thermoacoustic instabilities inside an ethylene-fueled scramjet combustor with a recessed cavity flameholder were investigated both experimentally and analytically. Pressure oscillations with frequencies of 100-500 Hz inside the flowpath were measured and identified. The observed phenomena may be attributed to the acoustic feedback loop between the shock and flame zone, and to the acoustic-convective feedback loop between the fuel injection and flame zone. The effects of the throttling air flow on ignition enhancement and flameholding were analyzed. Air throttling generates a pre-combustion shock train in the isolator.

Paper #45

**Interaction Phenomena in Supersonic Combustors***Sadatake Tomioka & Ryo Masumoto*

(An invited presentation to 'supersonic combustion' session) Supersonic combustion ramjet and its combination with rocket engines (so-called Rocket-Based Combined Cycle engines) are expected to be efficient propulsion system both for cruise missions and acceleration missions like launch vehicles. The supersonic flow into the combustor will be decelerated due to heat release, either through oblique shock train to moderate supersonic speed, or through pseudo shock wave system to subsonic speed, the latter called as dual-mode combustion. The oblique shock train can penetrate the injector location with boundary layer separation, so that the airflow can be compressed in prior to heat release. This drastic change in the flow field, in turn, alters the fuel-jet/airflow mixing process to make this combustion phenomena within the supersonic combustor very complicated. Still, the fuel injection is the key control factor especially for the acceleration missions with airflow condition varying from moment to moment. Thus, the interaction between the airflow condition (or combustion mode) and the fuel / airflow mixing process is very important and interesting theme. In this presentation, combustor tests relating to the above mentioned interactions are described, with emphasis on the change in airflow conditions due to pressure-rise. Combustion tests were conducted to find out the effects of the perpendicular injection configurations on the mixing process, and thus, the combustor performance. When the pure supersonic combustion was attained, the configuration was effective, a better penetration resulted in a better performance. However, when oblique shock train associated with the pressure-rise due to heat release penetrated the fuel injector location, a sudden change in mixing process was found which was governed by the jet / shock system interaction, and the injector configuration had little effects on the performance. With pseudo shock wave penetration, the injector configuration had no sizable effects on the performance. Mixing experiments were conducted to further pursue the possibility of mixing control by injection configuration in the presence of the pseudo shock wave system. With identical shock system location to the injector, plume through a swept-back injector showed clearly different mixing process from that through the perpendicular injector, showing the possibility of the mixing control even in the dual-mode combustion conditions.

Paper #161

**Scramjet Engine Research of KARI: Ground Tests of Engines and Components***Soo Seok Yang, Sang Hun Kang, Yang Ji Lee*

Since 2005, KARI (Korea Aerospace Research Institute) has been studied the core technology of the scramjet engine to prepare for the scramjet engine development and international collaboration research in the future. In spite of the short period of investigation, KARI has built the supersonic wind tunnel and performed a few tests of the engine and its components to obtain the core technology of hydrogen fuel scramjet engine. In this paper, KARI's fundamental and

applied research results about the scramjet engine are summarized. The engine and its major components design and ground test results are explained. And engine performance enhancement skills are also addressed.

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**10:45 (R15A) Explosion and Blast**

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Paper #38

**Numerical Simulation and Experimental Investigation of Blast Wave Mitigation in Dry Aqueous Foams***E. Del Prete, L. Domergue, J.-F. Haas, A. Chinnayya, A. Hadjadj*

Blast waves issued from explosions in air can cause serious damages located many charge radii from the energetic material. The objective of this paper is to characterise the underlying physics of the mitigation properties of aqueous foams. The heterogeneous two-phase media is composed of gaseous cells enclosed by the liquid phase. This liquid matrix is likely to be shattered into a dense spray by the shock impingement. Due to the contrast of impedance properties, the two fluids will be in thermo-mechanical disequilibrium, which will be decreased by relaxation processes coming from momentum and energy exchanges. An unconditionally hyperbolic Eulerian multiphase formalism is derived, where each phase obeys its own equation of state. The interactions between fluids are described with the help of constitutive relations accounting for the medium topology. The flow model ensures the correct estimation of the acoustic impedance of the two-phase medium. As for the numerical scheme, Riemann solvers are used to describe the microscopic fluid interactions, the summation of which provides the convective multiphase flux. Three sets of experiments have been done with Plastic explosive in air and in foam. Special care has been paid to the sphericity of the detonation and blast propagation. The unconfined case has enabled the determination of the TNT blast effectiveness factor. As for the confined case, in the mean field, an attenuation of more than a decade of peak overpressure is observed. Attenuation of positive impulses is however less marked. The heterogeneity of the two-phase medium has induced modification of the classical blast wave structure. The numerical results for peak overpressure, positive impulse have been compared favourably with experiments. Wave diagrams, fluid trajectories and the influence of relaxation processes have been examined.

Paper #42

**Investigating Ground Effects on Mixing and Afterburning during a TNT Explosion***Ekaterina Fedina & Christer Fureby*

In this paper the unconfined and semi-confined condensed phase explosions of TNT will be studied using Large Eddy Simulations based on the unsteady, compressible, reacting, multi-species Navier-Stokes equations with a Nobel-Abel thermal equation of state to gain further understanding of the physical processes involved in a condensed phase explosion and the effect of confinement on the physical processes involved. The analysis of the mixing and afterburning of TNT explosions in free air and near the ground indicated that the combustion region of detonation products and air is determined by the vorticity patterns, induced by the Richtmyer-Meshkov instabilities that arise during the explosion. When explosive is detonated above ground, the ground affects the shock propagation by creating complex shock systems, thereby changing the orientation of the vorticity, giving the afterburning a mushroom shape and increasing performance of an explosive charge by prolonging the existence of the mixing layer and thereby the afterburning.

Paper #305

**Planar Blast Scaling with Condensed-Phase Explosives in a Shock Tube***Scott I. Jackson*

Blast waves are strong shock waves that result from large power density deposition into a fluid. The rapid energy release of high-explosive detonation provides sufficiently high power density for blast wave generation. Often it is desirable to quantify the energy released by such an event and to determine that energy relative to other reference explosives to derive an explosive-equivalence value. In this study, we use condensed-phase explosives to drive a blast wave in a shock tube. The explosive material and quantity were varied to produce blast waves of differing strengths. Pressure transducers at varying lengths measured the post-shock pressure, shock-wave arrival time and sidewall impulse associated with each test. Blast-scaling concepts in a one-dimensional geometry were then used to both determine the energy release associated with each test and to verify the scaling of the shock position versus time, overpressure versus distance, and impulse.

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**10:45 (R15B) Chemical Kinetics and Reaction Dynamics-III**

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Paper #312

**Effect of Catalyst Segmentation with Cavities on Combustion Enhancement of Multi-Fuels in a Micro Channel***Yueh-Heng Li, Guan-Bang Chen, Tsarng-Sheng Cheng, Yei-Chin Chao*

In this paper we propose a novel design concept for enhancement of CH<sub>4</sub>/CO/H<sub>2</sub> multi-fuel combustion in a micro-channel by using the combined effects of catalyst segmentation and cavities, and their effects and combustion characteristics are evaluated by numerical simulation with detailed heterogeneous and homogeneous chemistries. The effects of multi-segment catalyst with/without cavities are examined and discussed in terms of multi-fuel mixture. In general, the chemical process of conventional catalytic combustion is a competition between heterogeneous and homogeneous reactions for fuel, oxygen and radicals. Nevertheless, the objective of using catalyst segmentation and cavity in a micro-reactor is to integrate both advantages of the heterogeneous and homogeneous reactions to enhance

fuel conversion and promote complete combustion in a short distance. In this catalyst configuration, the heterogeneous reaction in a prior catalyst segment can produce chemical radicals and catalytically induced exothermicity, and homogeneous reaction is subsequently induced and anchored in the following cavity. H and OH radicals from hydrogen and methane also change the chemical pathway of CO oxidation. In the way, full multi-fuel conversion and complete combustion can be achieved in a short distance. The existence of cavities can appreciably extend the stable operational range of the micro-reactor in a wide variety of inlet flow velocities. Moreover, cavities in a small-scale system can further stabilize the flame, and also serve as the heat source to enhance reaction. These outstanding features of this catalyst configuration facilitate wide applications in various small-scale power/heating generation systems.

Paper #26

#### **Reaction Kinetics Mechanism for Chemiluminescent Species**

*Trupti Kathrotia, Uwe Riedel*

Luminescence occurring due to chemical excitation, referred to as Chemiluminescence, is found in the visible and ultra-violet (UV) band of the flame spectrum. In hydrocarbon flames the four major emitters found are OH\*, CH\*, C<sub>2</sub>\*, and CO<sub>2</sub>\*, here star (\*) refers to electronically excited molecules. The spontaneous emissions of chemiluminescence species offer an inexpensive diagnostics of flames and combustion processes. It is non-intrusive in nature and allows to avoid expensive laser instrumentation. In early 1970s chemiluminescence has been identified as a marker for heat release, reaction zone and equivalence ratio, thereby providing a relatively easy diagnostics alternative for online measurement of these features in practical combustion applications. However, the relationship between chemiluminescence, heat release and equivalence ratio is relatively unknown except for a few correlations available in literature for a small range of conditions. The reaction kinetics mechanism that can explain the formation and consumption of these species is not well studied. Therefore it is of interest to develop a reaction mechanism which can predict the excited species measured at shock-tube and one-dimensional laminar flame experiments and that can be further used in combustion applications.

Paper #252

#### **Computer Aided Detailed Mechanism Generation for Large Hydrocarbons: n-Decane**

*Martin Hilbig, Lars Seidel, Xiaoxiao Wang, Fabian Mauss and Thomas Zeuch*

Common engine fuels consist of a mixture of hundreds of hydrocarbons which differ in chain length and structure. For engine simulations real fuels are modeled by surrogate fuels. The most known surrogate fuel for gasoline is a mixture of n-heptane and iso-octane, and for diesel a mixture of n-decane and  $\alpha$ -methyl-naphthalene. For predicting pollutant formation more comprehensive fuel models are needed. Automatic mechanism generators can be applied to limit the amount of work in developing mechanisms for complex surrogate fuel blends. Our group developed in the past detailed kinetic mechanisms for n-heptane and iso-octane. For this we followed the mechanism generation rules provided by Curran et al., with rate constants optimized such that the base chemistry from Hoyermann et al. can be applied. We kept the reaction mechanism compact by applying the generation rules for low temperature oxidation to the fuel molecules only, and by introducing a linear lumping algorithm. In this work we demonstrate that rate coefficients, resulting from the mechanism optimization for n-heptane, can be used to generate a reaction mechanism for higher hydrocarbons i.e. n-decane. The thermodynamic data for the larger species are derived by Benson rules based on the thermodynamic data for n-heptane. The final mechanism is validated by shock tube [6-9] and jet stirred reactor experiments]. The mechanism is analyzed by reaction flow and sensitivity analyses. Ignition delay times and species concentration profiles agree well with the experimental data. Our prior work was limited to the prediction of ignition delay times. Recently detailed mechanisms for n-decane have been generated by Ranzi et al, Battin Leclerc et al. and Curran et al. To provide a tool which assists in the generation process, a semi-automatic mechanism generator was developed. The generator follows the ideas of prior work, but applies the modern object oriented database system CouchDB. All species and reaction related data such as thermo data, molecule structures, names and reaction coefficients are part of the database. In addition a Haskell based software is stored, which is used to perform graph rewriting representing the classes of reactions proposed by Curran et al. The system is not limited to those classes or coefficients, and can be easily extended.

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### **10:45 (R15C) Reacting Flow Dynamics-II**

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Paper #135

#### **Large Eddy Simulation and Experimental Study of a Trapped Vortex Combustor**

*C. Merlin, P. Domingo, L. Vervisch, J. Burguburu, G. Cabot, B. Renou*

The Trapped Vortex Combustor (TVC) is a challenging configuration where flame stabilization is achieved through the presence of a cavity. The present work describes an unsteady non-reacting and reacting annular TVC flow studied with Large-Eddy Simulation and Immersed Boundaries Method. The combustion model is based on tabulated chemistry associated with a presumed PDF. The effects of local strain rate and of heat losses are included in the modelling. The simulations are compared with experimental results and the performance of the modelling closures is discussed.

Paper #164

#### **Stability of Laminar Diffusion Flames of Methane in an Oxygen-Enriched Air Co-Jet**

*P. Gillon, M. Chahine, B. Sarh, V. Gilard, J.N. Blanchard*

Oxygen rich combustion is a mean to increase the energy efficiency and to contribute to CO<sub>2</sub> capture in the flue gas. Influence of oxygen enriched air on the stability of methane flames from non premixed laminar jets has been investigated

experimentally. The burner consists of two coaxial jets; methane flowing out of the inner, oxidizer from the outer. The flame behaviour is studied according to the proportion of oxygen in the oxidizer jet, the oxidizer and methane jets velocities. The flame is either anchored to the burner, lifted with a tribrachial structure, stationary or not or blown-out. The addition of oxygen produces a decrease of the lift-height, a reduction of the length of the reaction zone and an increase in the soot emission. These results have been reported into diagrams of stability for two methane jet Reynolds numbers.

Paper #224

#### **Impact of Flame-Flame Interaction in Identical Two Non-premixed Microflames**

*Taro Hirasawa, Kunihiro Gotanda, Hiroki Masuda, Yuji Nakamura*

In order to develop "microflame-array (MFA)", uniform plane heating device, and open the way of microflame to industrial application, we have examined, in this study, the impact of flame-flame interaction on the behavior of non-premixed microflame in terms of flame shapes, flow field, and emissions of  $\text{CH}^*$  and  $\text{H}_2\text{O}$ . The examination has been carried out based on the analysis of emission images observed through optical filter of 430 nm and 945 nm, and on the numerical simulation of flow fields by one-step, finite rate reaction of methane-air system in 3-D coordinate system. There are found to be three stages in flame-flame interaction. At the first stage, the two flames are separated but the flow interaction increases the axial velocity between burners and works for the flame to incline toward another flame and slightly increases the total power of  $\text{CH}^*$  emission. At the second stage, the images of  $\text{CH}^*$  show that the flames are gradually getting combined and obviously losing reaction zone between the tops of flames. At the third stage, no flame base can be seen between burners, and practically only one flame exists. The change of total power of  $\text{CH}^*$  emission has been discussed and explained well by considering the supposed change of fuel leakage and combustion efficiency.

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### **13:30 (S7) Supersonic Combustion – III**

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Paper #34

#### **Modeling Supersonic Combustion**

*C. Fureby & V. Sabel'nikov*

Computational modeling of supersonic combustion is becoming increasingly important if we are to realize the development of aerospaceplanes and new space launchers. Compared to experimental investigations high-fidelity numerical modeling allows inspection of the whole computational domain in space and time, thereby allowing the researcher to explore different aspects of the flow. The obvious drawbacks are of course that small features, e.g. turbulence and turbulence chemistry interactions, cannot be resolved, and modeling is inevitable. Since several models usually are interacting with each other and with the numerical methods used to solve the equations care has to be taken when developing and using simulation models, and when analyzing results from numerical simulation models. Here we will discuss several aspects of modeling supersonic combustion, primarily for dual-mode ramjet and scramjet combustion. Both theoretical aspects of the modeling and validation as well as flow elucidation aspects will be discussed.

Paper #97

#### **Influence of Residence and Scalar Mixing Time Scales in Non Premixed Combustion in Supersonic Turbulent Flows**

*Laurent GOMET, Vincent ROBIN and Arnaud MURA*

The description of non-premixed combustion in supersonic turbulent flows still offers challenging issues from both the physical modelling and numerical points of view. In supersonic reactive flows, the essential influence of self-ignition phenomena is well-known, and even in the absence of any pressure discontinuity, the mechanism of viscous dissipation is likely to influence the early development of chemical processes. This phenomena is the direct consequence of the conversion of kinetic energy into enthalpy which is no longer negligible in high Mach number flows. A large amount of valuable information has been gathered to address theoretically, numerically and experimentally this specific aspect. Several experimental test rigs have been designed and studied, and in many of them hydrogen is injected into a main flow of air which can be vitiated or not. For sufficiently high preheated air flows, self-ignition conditions are reached inside the mixing layer that develops between the two supersonic streams. In previous analyses devoted to such conditions, chemical kinetics as well as associated finite rate chemistry effects have already received considerable attention. However, it seems worth recognizing that the representation of flow time scales, such as residence and mixing time scales, still requires further work. The present modelling study is devoted to this peculiar point. A transport equation for the quantity of residence time is implemented in order to evaluate the mean residence time associated with both oxidizer and fuel injection streams, while a transport equation for the mean scalar dissipation rate is considered to estimate the scalar mixing time scale. The model capabilities are evaluated through a comparison of numerical results with the data obtained from experimental studies devoted to supersonic co-flowing jets of hydrogen and vitiated air. The comparisons performed between the computational results and the experimental data suggest that, despite their complexity, the main physical processes are well-described by proposed approach.

Paper #154

#### **Numerical Study of $\text{H}_2+\text{CO}$ Turbulent Combustion with Supersonic Coflow in Confined Geometries**

*Jeong-Yeol Choi, Vigor Yang*

The successful flight test of X-51A opened new era of powered hypersonic flight for practical applications. A technology that distinguishes X-51A from previous scramjet flight test is the dual mode ramjet (DMR) engine. DMR engine starts at ramjet mode and transit to scramjet mode accelerating from supersonic launch speed and to hypersonic cruising

condition. A disadvantage of the DMR is the complexity caused by the regenerative cooling system using endothermic fuel. The complexity would be acceptable for a reusable system, but not for an expendable ones. More affordable concept of dual combustion ramjet (DCR) has been suggested by Billig [1] and applied for a flight test program HyFly. Though its flight tests were not successful yet due to non-combustion related problems, the concept seems to be still promising especially for expendable systems. However, regardless of the long time researches and development, many of the related works on DCR is classified and little has known publically. The dual combustion ramjet (DCR) has two flow paths, gas generator (GG) and supersonic combustor (SC). The schematics of DCR operation is summarized in Fig. 1. Liquid fuel is pre-burned in GG with the air compressed to subsonic speed. The pre-burned fuel mostly composed of hydrogen and carbon-monoxide is delivered to the supersonic combustor at high speed, then consumed by the combustion with supersonic main flow. It is considered that turbulent shear layer is the major mechanism of fuel-air mixing and combustion in this system. In the present study the characteristics of the supersonic turbulent reacting shear layer is investigated at elevated enthalpy condition with confinement effects to understand the the combustion dynamics and stabilities.

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**13:30 (R16A) Accidental Explosions and Energetic Materials**

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Paper #253

**Simulating Dust Explosion Venting Through Ducts***Diana Castellanos, Trygve Skjold, Kees van Wingerden, Rolf K. Eckhoff & Sam Mannan*

Vented dust explosions in an 18.5 m<sup>3</sup> vessel equipped with vent ducts of varying length and diameter have been simulated with the CFD code DESC. Most of the simulated results are in good agreement with experimental data for different ignition locations and duct sizes. The simulations over-predict the reduced explosion pressure for certain scenarios with small vent areas, and under-predict the explosion pressure for configurations involving vent ducts with significantly larger diameter than the vent opening. These discrepancies may be caused by inherent limitations in the model, such as the representation of particle-laden flow or the correlations used for describing turbulent combustion. It is likely that secondary explosions or flame quenching in the duct influence the experimental results. However, poor repeatability of the experiments and limited access to detailed experimental data complicates the analysis. Both experimental and simulated results are compared with predictions from various guidelines used for designing vent ducts in industry: EN 14491, VDI 3673, NFPA 68 and FM Global. NFPA 68 yields the most accurate predictions, which may be expected since the empirical correlations in this guideline originate from the same experiments. The FM Global method underestimates  $P_{red}$  for the largest vent diameter and rear ignition, but yields more conservative results for smaller duct diameters. Neither experiments nor simulations support the concept of a critical duct length used by EN 14491 and VDI 3673.

Paper #257

**Deformation of Coated Stainless Steel Tubes from Reflected Detonation***J. Damazo, J.E. Shepherd, K. Chow-Yee, J. Karnesky*

Gaseous detonations produce large pressures that may damage piping systems and containment vessels. The greatest pressure rise—and hence the greatest possibility of resulting damage—results when gaseous detonations undergo normal reflection. Here we present experimental and computational results investigating the elastic and plastic strain produced by reflecting detonation waves in welded 304L stainless steel tubes of inner diameter 127 mm and wall thickness 1.5 mm. This work builds on previous work performed in our laboratory on mild-steel tubes. Stainless steel is much better characterized than mild-steel and hence this change allows superior computational comparison. Detonations are formed in a driver tube via glow plug ignition of stoichiometric ethylene-oxygen and paddle-shaped obstacles to promote turbulence. The initial pressure is varied between 50 kPa, 200 kPa, and 300 kPa to investigate elastic deformation and plastic deformation of two distinct strain rates. The time-resolved material deformation is measured with strain gauges and an outside micrometer is employed to obtain the final post-shot diameter as a function of distance from the location of detonation reflection. Computational comparisons of both the time-resolved and final material deformation are performed in LS-DYNA using two-dimensional axisymmetric shell elements with a realistic material model that incorporates strain-rate effects to represent the tube wall. In addition to understanding and characterizing elastic and plastic deformation caused by gaseous detonations, it is also our goal to develop effective measures to mitigate this deformation. To this end, we have performed a preliminary investigation on the effect of a commercially available spray-applied polyurea compound to the material deformation. We discovered that the polyurea coating affects both the shape of the time-resolved strain signals and the final deformation with a peak strain reduction of 20.5% for a 7 mm thick polyurea layer.

Paper #08

**Nonclassical Thermal Runaway: The Bhopal Disaster and Liquid Hydroperoxide Explosives***R. Ball*

More than 25 years after the Bhopal disaster its horrific legacy is now well-documented, but the causes are still being debated in the international media. Was the tragedy due to neglect, parsimony, or procrastination by Union Carbide on safety and maintenance? Ignorance, corruption, sabotage and cover-up? Inadequate regulation of urban and industrial development? Possibly all of the above, but they are putative, secondary or socioeconomic contributing factors. The primary cause of the thermal runaway that led to the venting of a deadly mist of methyl isocyanate over the city of Bhopal on 02 Dec 1984 was physicochemical. In this belated work I present a stability analysis of methyl isocyanate (MIC) hydrolysis using a homogeneous flow reactor paradigm. Results indicate that the thermal runaway may have been due to



a large amplitude, hard thermal oscillation initiated at a subcritical Hopf bifurcation. Classical (Semenov) ignition theory cannot predict oscillatory ignition because it considers evolution of the temperature only, and periodic solutions are necessarily forbidden in a one-variable evolution. Consequently the application of Semenov theory to systems where the temperature evolution is coupled to reactant consumption gives results that are qualitatively wrong. It is shown that this type of thermal misbehavior may be endemic to liquid thermoreactive systems including liquid hydroperoxide explosives.

Paper #297

#### **Activation Effects on the Deflagration Speeds in Ni-Al**

*Y. Charron-Tousignant, B. Barrett, M. Yandouzi, M. Radulescu, A. Weck, J.J. Lee*

Gasless reaction waves in inter-metallic constituents, for example Ni and Al, have been studied for over three decades in the framework of self-propagating high temperature synthesis (SHS) of materials. In gasless systems, deflagration wave speeds are usually restricted to a few millimeters per second, thus making such systems unattractive for rapid burning rate applications. Recent work involving the mechanical activation of the powders via either arrested ball milling (ARM) has suggested that the ignition temperature can be lowered and the burn speed increased. The very large differences in burning speeds observed in loose powders, partly refined and consolidated mechanically activated powders by milling is currently difficult to explain and model. The present research reports on measurements of deflagration speeds in the Ni-Al system prepared by various techniques: different compactions of micron scale and ARM powders.

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### **13:30 (R16B) Multiphase Detonation**

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Paper #18

#### **An Empirical Model for the Ignition of Aluminum Particle Clouds behind Blast Waves**

*Kaushik Balakrishnan, Allen L. Kuhl, John B. Bell and Vincent E. Beckner*

An empirical model for the ignition of aluminum particle clouds is developed and applied to the study of particle ignition and combustion behavior resulting from explosive blast waves. This model incorporates both particle ignition time delay as well as cloud concentration effects on ignition. The total mass of aluminum that burns is found to depend on the model, with shorter ignition delay times resulting in increased burning of the cloud. A new mass-averaged ignition parameter is defined and is observed to serve as a useful parameter to compare cloud ignition behavior. Investigation of this variable reveals that both peak ignition as well as time required to attain peak ignition are sensitive to the model parameters. Overall, this study demonstrates that the new ignition model developed captures effects not included in other combustion models for the investigation of shock-induced ignition of aluminum particle clouds.

Paper #205

#### **Numerical Study on Ethanol/Air Two-phase Detonation**

*Takashi Shimada, Eisuke Yamada, A.Koichi Hayashi and Nobuyuki Tsuboi*

In this study, the detonation using a mixture of ethanol and air was analyzed using a numerical code in which the models in the gas and liquid were combined. We studied that detonation cell width with the liquid fuel concentration from 0.03 to 0.13kg/m<sup>3</sup> at 3 $\mu$ m size of droplet and 70% of initial evaporation ratio. In this condition the detonation cell width is bigger when the fuel concentration is richer. But detonation does not propagate at the concentration of 0.13kg/m<sup>3</sup>.

Paper #17

#### **The Burning Surface Temperature and Boiling Point of Ammonium Nitrate**

*Atsushi Ishihara, Masaya Nakahara*

Ammonium nitrate (AN) is still used as an oxidizer for solid-fuel rockets because of its chlorine-free characteristics and its relatively low cost. For the optimal design of rocket motors, the burning surface temperature and its dependence on pressure are required. However, these have not previously been studied in any detail. In this study, the surface temperature of AN was examined using a thermocouple embedded in a specimen. Thermogravimetric analysis (TGA) on AN was also performed. The boiling point of AN was approximately 300° at 0.1 MPa. The burning surface temperature of AN was found to be the same as its boiling point and was independent of the regression rate. Furthermore, a pressure-dependent factor obtained from the boiling point agreed well with that obtained by thermochemical methods such as TGA. Thermochemical methods were found to be useful for predicting the pressure dependence of the burning surface temperature.

Paper #315

#### **Effect of Aerodynamic Breakup on Combustion of Aluminum Particles from Heterogeneous Explosives**

*Robert C. Ripley and Fan Zhang*

Heterogeneous blast explosives contain a mixture of condensed-phase explosive, binders, and metal particles. Most often aluminum particles are used for their high heat of combustion when reacted with atmospheric air. Micrometric-sized particles are large enough that they do not react significantly within the detonation zone of the explosive itself, rather they are accelerated and heated by shock compression and are dispersed into the surrounding environment where their reaction may augment the air blast. Most aluminum particles feature a thin passive oxide coating, which is presumed to be cracked or removed by the detonation shock. The remaining pure aluminum particles have a relatively low melting point (933 K at 1 bar) that is easily reached by shock compression heating during detonation of the explosive and convective heating in the detonation products and shocked air. Molten and liquid particles may become unstable under conditions of high relative flow and may possibly fragment through aerodynamic breakup. The melting behavior of the

particles under high pressures and the feasibility of subsequent breakup in the initial expansion flow could be critical for the efficient reaction of particles. The purpose of this paper is to study the effect of aerodynamic breakup on the combustion of aluminum particles in the very near-field of detonation of such heterogeneous explosives. This paper presents a model for high pressure melting of aluminum particles and the subsequent aerodynamic breakup of liquid droplets in the transition region from detonation to the near field of heterogeneous explosives.

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**13:30 (R16C) Numerical Development**

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Paper #101

**A High-order AMR Algorithm for Chemically Reacting Flows***Cosmin Safta, Jaideep Ray, Habib N. Najm*

A high-order projection scheme was developed for the study of chemically reacting flows in the low-Mach number limit. The numerical approach for the momentum transport uses a combination of cell-centered/cell-averaged discretizations to achieve a fourth-order formulation for the pressure projection algorithm. This scheme is coupled with a second-order in time operator-split stiff approach for the species and energy equations. The code employs a fourth-order, block-structured, adaptive mesh refinement approach to address the challenges posed by the large spectrum of spatial scales encountered in reacting flow computations. Results for advection-diffusion-reaction configurations are used to illustrate the performance of the numerical construction.

Paper #78

**Numerical Studies of the Influence of Turbulence and Coherent Structures on Flame and Emission Characteristics in Lean Premixed Combustion***C. Schrödinger, C. O. Paschereit*

In this work we present the numerical investigation of a lean premixed methane-air flame under turbulent conditions, as it may occur in a gas turbine combustor, using the one-dimensional Linear Eddy Model (LEM). We study the influence of turbulent conditions on flame behavior and pollutant formation of CO and NO by varying the turbulent diffusivity and the integral length scale. Increasing the turbulent diffusivity leads to higher burning velocities and larger flame width. CO emissions are increasing whereas NO is decreasing which is closely related to the flame width and corresponding temperature fields. When the integral length scale is increased the flame width, the burning velocity and CO emissions slightly decrease whereas NO production slightly increases. The analysis shows that small scale eddies have a more significant effect on the flame and emission characteristics than large scale eddies. Furthermore, we compute the influence of fluctuations in equivalence ratio on flame characteristics as well as on CO and NO formation. Harmonic perturbations and harmonic perturbations with superposed stochastic fluctuations are investigated. Generally, oscillations in the fuel concentration lead to oscillations of flame temperature and emissions. Thereby, the forcing with the superposed stochastic fluctuations shows a much more distinct effect than the harmonic forcing alone. Stochastic perturbations are much stronger and last much longer without decreasing significantly downstream of the flame. The averaged concentrations of NO and CO are higher with stochastic perturbation and slightly lower with pure sinusoidal forcing.

Paper #192

**Development of a Chemical Kinetics Tabulation Method for the Prediction of Diesel Engine Pollutants***D.E. Tudorache, P. Auzillon, L. Thobois, N. Darabiha, R. Vicquelin, O. Gicquel, B. Fiorina*

Today, hydrocarbon fuel combustion covers most of the energy needs in transportation. Due to recent environmental concerns and regulations, automotive manufacturers aim to develop cleaner internal combustion engines (ICE) with significant reduction in fuel consumption and pollutant emissions such as CO, HC, NOx. In accordance with this, the present study aims to develop an efficient cost-cutting tabulation method to fit chemistry in Diesel engine turbulent combustion modeling. This method assumes that IC engine chemistry could be mapped by a collection of 0-D reactor computation data using as coordinates the progress variable, the energy and the density. In the first step, the chemical prediction capability of this technique is validated on 0-D simulations. It is demonstrated that this approach simultaneously captures the compression stroke, the reaction phase and the power stroke. Finally, the proposed tabulation method is coupled with the LES AVBP compressible solver following the TTC strategy.

Paper #197

**Graphics Processors as a Tool for Rotating Detonation Simulations***Michal Folsiak, Karol Swiderski, Arkadiusz Kobiera, Piotr Wolanski*

CFD simulations of detonation are computationally expensive. The processors have already reached their limits for cheap, commercially available technologies. The development of new computers is achieved mainly by increase of number of processor and the crucial feature of all modern scientific codes is their ability to perform parallel calculation. A new path was opened in application of PCs in science by development of graphics processing units (GPUs). They have reached the state, where a single core of the GPU has considerable computing power. GPU is specialized in graphics rendering-highly parallel floating-point operations that can be performed independently by many threads on large datasets. What is more, architecture of the GPU allows executing many threads of the same code at the same time, thus more transistors of GPU can be devoted to data processing than flow control. It accelerates number crunching problems like CFD even by order of magnitude. Thanks to GPU, the desktop computers have become personal supercomputers. In this work these features of the GPU are utilized in order to develop robust code for detonation simulations. The code

utilizes CUDA technology. The program enables simulation of compressible flows with energy source resulting from chemical reactions. In the program classical models of compressible inviscid flow is used. It is based on Euler equations for semi-ideal gas with chemical and geometrical source terms. Two versions of the code have been developed both for structured and unstructured grids. In order to quantitatively compare results of the work, numerical benchmarks of detonation problem were created. Computations of the same problem of cylindrical explosion were carried out on 4 similar domains. The calculations have shown that some procedures running on GPU can be faster even by the order of magnitude than the one running on CPU. On the other hand, the use of GPU demands very careful memory management, especially if more complicated cases and chemical mechanism are involved. The program has proven also its practical value. Some simulations of detonation wave for real geometries including rotating detonation are also performed and the results will be presented. Authors believe, that the compilers will evolve in a way to explicitly perform most critical optimizations of memory management or even into model similar to PGI Accelerator-simple, efficient and easy to implement. Summarizing, the CUDA technology available today is very promising, but programming of large parallel applications, such as CFD codes costs much effort and requires a very different approach to programming. This work was conducted in frame of project UDA-POIG.01.03.01-14-071 "Turbine engine with a detonation combustion chamber" supported by EU and Ministry of Regional Development.

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#### 15:40 (R17A) Mesoscale Combustion

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Paper #237

##### **The Effect of Mixture Composition on Stabilized Flames in a Meso-Scale Channel with a Wall Temperature Gradient**

*Graeme M. G. Watson and Jeffrey M. Bergthorson*

The characteristics of stable premixed combustion are studied in a heated tube with a fixed wall temperature gradient. These flames are examined experimentally and with a 1-D, volumetrically-averaged computational model with detailed chemistry. The heated tube concept is a simple, quasi one-dimensional burner configuration which has relevance to new burner technologies that utilize small channels to support stable combustion. In this study, mixture composition is studied to determine its effect on the system.

Paper #306

##### **Effects of Scale on Non-Adiabatic Swiss-roll Heat-Recirculating Combustors**

*Chien-Hua Chen and Paul Ronney*

Three different scales but geometrically identical 3D numerical models of Swiss-roll combustor were built to study the effects of scale numerically. It is found at low Reynolds number (Re) region, where the heat loss dominates extinction limits due to less thermal throughput, smaller scale combustors unexpectedly showed better performance (in terms of lean extinction limits). This is because, for different scale combustors, internal heat transfer coefficient (for heat exchange)  $U_E$  are inversely proportional to their length scale, while external heat transfer coefficient (for heat loss)  $U_L$  are almost independent to their length scale. Therefore, smaller scale combustors can obtain more heat recirculation due to less heat loss and sustain the reaction in leaner conditions. A dimensionless group  $\alpha = U_L A_L / U_E A_E$  ( $A_L$  and  $A_E$  are heat loss area and heat exchanger area respectively) is defined to show the heat loss effect. If the  $\alpha$  were forced fixed by artificially adjusting external heat transfer coefficient and emissivity based on the length scale, extinction limits for different scale combustors showed almost the same values at low Re region. While at high Re region, the smaller scale combustors showed worse performance. Because when the Re increases (flow velocity increases for the same combustor), the extinction limits are gradually restricted by insufficient residence time, and also, the reaction time scale is not changed when the size of combustor changes. Therefore, smaller scale combustors have less residence time at the same Re, and more fuel is needed to obtain higher temperature to accelerate the reaction rate. A convergent trend of Damköhler number (Da) at extinction limits for different scale combustors was observed as Re increases. Consequently, Re,  $\alpha$ , and Da are three dimensionless groups that characterize the extinction limits of geometrically identical Swiss-roll combustors.

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#### 15:40 (R17B) Flame Extinction

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Paper #84

##### **Experimental Investigation on Flame Extinction Process of Non-Premixed CH<sub>4</sub>/Air Flames in an Air-Diluted Coflow by CO<sub>2</sub>, N<sub>2</sub> or Ar**

*Jiesheng MIN and Françoise Baillet*

Diluted combustion systems are widely used nowadays as in exhaust gas recirculation combustion systems which are proved to be an effective way to improve combustion efficiency and to reduce pollutant emissions, NO<sub>x</sub> or in fire extinguishment. Phenomena involved in flame stabilization, like liftoff and extinction remain real key points in the control of the diluted combustion. Previous work (Min et al., 2010, Comb. Sci. Technol.) highlighted the influence of a diluent addition on flame liftoff phenomena as well as its relative effects between dilution, thermal, and chemistry. This work aims to investigate the influence of different diluents (CO<sub>2</sub>, N<sub>2</sub>, Ar and CO<sub>2</sub>+Ar) added to air-stream on the lifted flame stabilization properties, as well as the process of flame extinction within a large range of aerodynamic conditions. In the physical space ( $Q_{\text{diluent}}/Q_{\text{air}}$ ,  $U_{\text{air}}$ ,  $U_{\text{CH}_4}$ ), extinction limits are expressed as a 3D surface  $E_{\text{extinction}}$  composed of two parts intersecting at the line  $U_{\text{CH}_4} = U_{\text{CH}_4,\text{ex}}$  expressed only as a function of  $U_{\text{air}}$ . For  $U_{\text{CH}_4} > U_{\text{CH}_4,\text{ex}}$ , extinction limits are

described by a characteristic surface which linearly decreases with  $U_{air}$  increase and is independent of  $U_{CH_4}$ . It concerns lifted flames for which the burner rim is not involved in the stabilization mechanism. For  $U_{CH_4} \leq U_{CH_4,ex}$ ,  $E_{extinction}$  coincides with a part of the flame lifting surface,  $F_{lifting}(Q_{diluent}/Q_{air}, U_{air}, U_{CH_4})$  previously described by Min et al. (2010, Comb. Sci. Technol.). Indeed, flames, necessarily attached to the burner in that domain, can still exist even at a dilution level higher than the former characteristic values due to the wake structure developing behind the burner rim. But as flames lift off by dilution, extinction occurs soon afterwards. Furthermore,  $K_{diluent}$ , defined as the capability of a diluent to break flame stability by extinction phenomenon relative to that of  $CO_2$ , furnishes the relative order between extinction limits measured with diluents. Its values,  $K_{CO_2} = 1$ ,  $K_{N_2} = 1.9$  and  $K_{Ar} = 2.9$ , are the same as those obtained for lifting limits, indicating that as for liftoff  $CO_2$  has the greatest influence, followed by  $N_2$ , and then Ar. Moreover, liftoff height  $H_L$  and an apparent flame radius  $R_p$  are simultaneously quantified to follow the liftoff process which may lead to extinction. Unique curves have been found with the three diluents to describe  $H_L$ -evolution and  $R_p$ -evolution respectively when  $(Q_{diluent}/Q_{air})/K_{diluent}$  is used as the normalized abscissa. This arises from the fact that an identical burning velocity ( $S_L$ ) at the propagation leading-edge is obtained provided that oxidants are diluted by the same value of  $(Q_{diluent}/Q_{air})/K_{diluent}$  appearing as a similarity-law quantity.  $H_L$  follows an exponential-like evolution against the former abscissa for the entire measurement domain.  $R_p$  presents a similar evolution behavior, but only for lifted flames with  $H_L < 10D_i$ . A flame radius over-increase is observed on condition that lifted flames stabilize inside the complete mixing region ( $H_L > 14D_i$ ).

Paper #316

### Rate-Ratio Asymptotic Analysis of the Structure and Mechanisms of Extinction of Nonpremixed $CH_4/N_2-O_2/N_2O/N_2$ Flames

*Kalyanasundaram Seshadri, Xue-Song Bai and Forman A. Williams*

Rate-ratio asymptotic analysis is carried out to elucidate the structure and mechanisms of extinction of nonpremixed  $CH_4/N_2-O_2/N_2O/N_2$  flames. Steady, axisymmetric, laminar flow of two counterflowing streams toward a stagnation plane is considered here. One stream, called the fuel stream, is made up of a mixture of methane ( $CH_4$ ) and nitrogen ( $N_2$ ). The other stream, called the oxidizer stream is made up of a mixture of oxygen ( $O_2$ ), nitrous oxide ( $N_2O$ ), and  $N_2$ . A reduced five-step mechanism is deduced from a detailed chemical kinetic mechanism. This five-step mechanism is employed in the asymptotic analysis. Chemical reactions are presumed to take place in a thin reaction zone that is established in the vicinity of the stagnation plane. On either side of this thin reaction zone, the flow field is inert. These inert regions are called the outer structure. In the thin reaction zone chemical reactions are presumed to take place in three layers---  $CH_4$ -consumption layer, the  $O_2$ -consumption layer, and the  $N_2O$  consumption layer. Asymptotic analysis of these layers gives the value of the scalar dissipation rate, at extinction. The strain rates at extinction are calculated from the scalar dissipation rate. They are compared with experimental data and those computed using detailed mechanisms.

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### 15:40 (R17C) Numerical Simulations

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Paper #19

### 2D Direct Numerical Simulation of Intermediate Species Diffusion in Low Temperature Oxidation Process

*Atsushi Teraji, Takahiro Morikawa, Takashi Ishihara, Yukio Kaneda*

Two-dimensional direct numerical simulation (DNS) was applied to auto-ignition of n-heptane/air mixture. The diffusion of intermediate species was studied in terms of the influence on the ignition delay. The chemical reaction process. The simplified reaction mechanism was used in this study. Likewise, the influence of turbulence was investigated by comparing the results of 0 dimensional simulation and two-dimensional direct simulation of non-turbulence condition. In conclusions, the ignition delay was strongly affected by the different diffusion speeds of intermediate species. It was shown that the outflow of OH radical having larger diffusion coefficient decreases the reaction rate at the high temperature point. On the contrary, the reaction rate was enhanced by the influx of OH radical at the low temperature point.

Paper #151

### A Numerical Study of the Markstein Hypothesis in Finite Thickness Flames with Realistic Chemistry

*Nadeem A. Malik*

In this study, an implicit method, TARDIS (Transient Adevection Reaction Diffusion Implicit Simulations), featuring the coupling of the fully compressible flow to the comprehensive (realistic) chemistry and detailed transport properties, is used to investigate the Markstein hypothesis in premixed hydrogen/air and hydrocarbon/air flames at atmospheric pressure. It is widely believed that the difference between the stretched and unstretched flame speed (the velocity deficit  $S_L-S_n$ ) is given asymptotically by an expression proportional to the flame stretch. In cylindrically and spherically symmetric flames the velocity deficit is linearly proportional to the curvature of the flame.  $S_L-S_n \sim 1/r_u$ . However, of special interest is whether this hypothesis is valid under conditions of realistic chemistry in finite thickness flames. Our results from TARDIS for expanding and imploding  $H_2$ /air and  $CH_4$ /air flames show non-linear fractional power-law in the velocity deficit,  $S_L-S_n \sim (1/r_u)^p$ ,  $0 < p < 1$ . The expanding  $H_2$ /air shows a quite different anomalous non-power law behaviour.

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**10:25 Poster Session I - Detonation**

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Paper #20

**Kinetics of Drop Shattering Behind Detonation Wave**

A. G. Girin

Distribution function of quantity of torn daughter droplets by sizes is obtained at arbitrary ratio  $h$  of mass efflux rate to rate of relaxational decreasing of relative velocity of parent shattering drop and gas flow. The result is based on earlier investigation of local surface instability with due regard to changing of velocity profile across the boundary layers, as well as to changing of boundary layers thicknesses and velocity along drop surface. For weak-viscosity liquids it revealed a new type of hydrodynamic instability - "gradient instability" Mechanism of this type differs from that of Kelvin - Helmholtz type and it is caused by large enough velocity gradient inside liquid boundary layer. The theory explains the "stripping" mode of breakup as quasi-continuous dispersing from unstable part of drop surface. In speedy flows, when the criterion of gradient instability is much greater than its critical value, values of polar angle of critical point are small, so, most part of drop surface generates mist of droplets. The theory allowed to derive the differential equations of drop mass efflux (ablation) and of torn droplets quantity together with the characteristic scales for their sizes and quantity. These equations demand simultaneous solution of drop motion equation in order to determine relative velocity and equation for critical conditions of instability - to determine position of critical point. For speedy flows and spherical shape of drop we have obtained the ablation law that indicates direct influence of drop motion law on it. At approximation of experimental data for drop velocity versus time in the exponential form, we have integrated the equation of drop mass efflux and have obtained drop mass history. The distribution function was then obtained by integrating the equation of torn droplets quantity and distributions for various values of definitive parameters were calculated. The formula allows to calculate intermediate distribution of droplets torn to arbitrary time moment. The analysis showed, that values of  $h$  slightly higher than 1 are inherent to flows behind shock and detonation waves, the values greater than 4 correspond to ablation of liquid meteoroids and the case, when  $h$  less, than 1, - to incomplete shattering of viscous drops. In former case the finite moment of whole drop breakup was established. In latter case dispersing terminates before the drop is completely shattered, because of quick reducing of main reason of dispersing - relative velocity. In view of lack of empirical data about laws of drop motion for various gas-droplets systems the main relations of shattering drop kinetics were obtained on reliable ground of theoretical laws. They were found analytically as solutions of system of non-linear differential equations of drop motion, drop mass efflux and quantity of torn droplets in a speedy uniform gas stream at neglecting by drop deformation influence. The two approaches of determination of drop motion law, which are based on empirical and theoretical methods, have lead eventually to similar distribution functions, but theoretical approach has the advantage being independent from lack of empirical data, so obtained formula is applicable to any gas - droplets system.

Paper #25

**Detonation Initiation by a Temperature Gradient for a Detailed Chemical Reaction Models**

A. D. Kiverin, A. A. Chukalovsky, M. F. Ivanov, M. A. Liberman

The evolution from a temperature gradient to a detonation is investigated using high resolution numerical simulations for combustion mixture whose chemistry is governed by a detailed chemical kinetics. We employ a model representing an initial linear temperature gradient in the fuel. Emphasis is on comparing the results with previous studies that used simple one-step kinetics. It is shown that the evolution to detonation from temperature nonuniformities is considerably different for one-step kinetics models than for chain-branching kinetic models and it is different in different fuels for the same initial conditions. A detailed chemical model has a profound effect on the validity of Zel'dovich's spontaneous wave concept for detonation initiation by a gradient of reactivity. The evolution to detonation from a temperature gradient is considered for hydrogen-air and methane-air mixtures at different initial pressures. The analysis shows that for a detailed chemical kinetics the temperature gradients, which was thought to appear in the form of hot spots and the like, are not satisfy the criteria to initiate detonation, and the gradient mechanism can not be origin of the deflagration-to-detonation transition.

Paper #47

~~The Influence of Initial Temperature on Detonation Structure~~~~Lin Zhi-yong, Liu Shi-jie, Liu Wei-dong, Zhou Jin~~~~There is an abundance of data in the literature on detonation research at ambient initial temperature. However, under some conditions, the initial temperature of premixed mixtures may vary and does not equal to the ambient temperature. Most of the previous works mainly focused on the global parameters of the detonation systems by experimental research, neglecting the details of flow field. Through numerical method, this paper will pay more attention on the influence of initial temperature on the detonation structure. At high initial temperature, the difference between shocked thermodynamic property after mach stem and incident shock is small, and the strength of transverse wave decreases. Under this condition, the ability of detonation wave to resistant flow field disturbance decreases.~~

Paper #64

**Triple Points Collision in Unstable Detonations**

Y. Mahmoudi, K. Mazaheri, M. I. Radulescu

In the present work, the detonation structure in high activation energy mixture, which is characterized by its irregular structure, is investigated numerically. The process of transverse wave and triple point collision at the end of the both, first and second half of detonation cell cycle is then examined by a very high-resolution simulation of 600 cells per half reaction zone length. Consequently, the origin of large unburnt gas pockets behind the front is determined. During the

reflection in the first-half cell, as the triple point collides with the upper wall, the transverse shock interacts with the unreacted pocket and after reflection of the triple point, the transverse wave collides with the wall. In the second-half cell, the triple point and the transverse wave, collide simultaneously with the wall. In second half-cell, the detonation structure after reflection is single-Mach configuration, but the strong transverse wave switches from primary triple point before collision, to a new one after reflection. In the first half-cell, however, the structure is Double-Mach configuration and does not change before and after reflection. Upon reflection in both first- and second-half, cell due to the detachment of the jet flow and shear layer, the reaction zone decoupled from the shock. After some time a new jet, forms and the reaction zone sticks to the shock front again. The tongue-like unreacted gas pocket detaches from the front, during the reflection process at the end of the first half-cell. The simultaneous interaction of triple point and transverse wave with the wall at the end of the first half-cell produces high-pressurized region at the boundary, which results in formation of large vortices via Richtmyer-Meshkov instability. Thus, in the second half-cell, where the shock strength decreases substantially, the heat resealed via ignition of this pocket due to large vortices helps the self-sustenance propagation of detonation wave.

Paper #69

#### **A Dataset of Critical Energy for Direct Initiation of Spherical Detonations in Some Hydrocarbon-Oxygen Mixtures**

*Bo Zhang, Hoi Dick Ng and John H.S. Lee*

The critical energy for direct initiation of detonation is an important dynamic parameter to provide a quantitative measurement of the detonation sensitivity of an explosive mixture in an unconfined environment. In this study, the critical energy for direct initiation of spherical detonations in four gaseous fuels ( $C_2H_2$ ,  $C_2H_4$ ,  $C_3H_8$  and  $H_2$ ) - oxygen mixtures at different initial pressures, equivalent ratios and amount of argon dilutions are reported. Experiments are carried out in a spherical bomb and direct initiation is achieved via a high voltage capacitor discharge. The effective spark energy is estimated from the analysis of the current output. The aim of this paper is to summarize a new set of reliable experimental data which, on one hand, can provide safety hazard assessment of these fuels and use for theoretical model validation, but also serve as reference base of comparison for the equivalent hazard of explosion of different hazardous chemical substances.

Paper #86

#### **Experimental Demonstration of a Multi-Tube Pulse Detonation Engine with a Rotary Valve**

*Han Qixiang, Zhang Yadong, Zhang Qi, Wang Jiahua*

Experimental demonstration of a pulse detonation engine (PDE) prototype, which incorporated with a rotary valve and multiple tubes, and utilized a mixture of kerosene and air, was described in this paper. Six detonation tubes of the PDE prototype with 60 mm equivalent diameter and 1000 mm length were arranged in a sector-annular configuration on a 219 mm diameter circle. The PDE was operated with a rotary valve and a gasdynamic valve to distribute the air and rich-fuel gas into the tubes respectively. The histories of gas pressure were measured to verify the regularity of detonation process in tubes. It was concluded that the PDE could operate in frequency 3x20Hz coordinately. Proof of the rotary-valved, multi-tube PDE operation was successfully demonstrated.

Paper #95

#### **Experimental Study of DDT in Hydrogen-Air behind a Single Obstacle**

*Gaathaug A. V., Bjerketvedt D. and Vaagsaether K.*

This is an experimental study of detonation deflagration transition in a square channel. Hydrogen and air are ignited at one end and propagate in a 1 meter section before it reaches an obstacle. The flame burn very fast through the obstacle and in a jet behind it. High local burning rates and heating of reactants in front of the flame lead to local explosions behind the obstacle. DDT is observed along the walls of the channel. Different hydrogen concentrations and various obstacle blockage are investigated and reported in this paper. The results are recorded with high speed camera and pressure records. The experimental results are also compared with numerical simulations of similar cases.

Paper #100

#### **Numerical Simulation of Deflagration and Initiation of Detonation**

*S.N.Martyushov, T.Elperin, O.Igra*

A simplified two-stage reactive flow model was used for simulating flows of reactive oxygen-hydrogen inviscid gaseous mixtures in which detonation and combustion take place. Flows with detonation initiation and transition in different types of pipes with obstacles were numerically investigated. Detonation is an extremely efficient means of combustion. Taking advantages of nearly isochoric combustion process, detonation has higher thermodynamic efficiency than conventional isobaric combustion. This feature of detonation is used in different designs of pulse detonation engines. Optimizing size of a pulse detonation engine requires achieving a transition from deflagration to detonation

Paper #107

#### **Three Dimensional Simulation of Rotating Detonation Engine without Inner Wall**

*Shao Ye-Tao, Wang Jian-Ping*

This three dimensional simulation has analyzed the flow field, and finds out the influence from the ignition process and curvature of the chamber wall. The work proves that the overset grid is fine enough to depict the detonation waves movement without non-physical oscillation. The development of the detonation waves shows that detonation waves may ignited and extinguished repeatedly during the collisions of the initiation period. A two-head steady central symmetric detonation flow field is finally converged.

Paper #114

**Spontaneous Ignition of Hydrogen Jets in the Presence of Reflected Shock Waves**

*Maxwell, B. M., Tawagi, P., Radulescu, M. I.*

The current study addresses spontaneous ignition of hydrogen jets that are released into a confined oxidizer environment. Specifically, reflected shock wave interactions with the transient jet upon release and the associated ignition limits are under investigation. Experiments are conducted in a shock tube where hydrogen gas is initially separated from oxygen by a diaphragm and a plate containing a single pore. An acetylene-oxygen driver is used to drive a strong shock wave through the test section, causing hydrogen to flow into oxygen. A high speed camera is used to capture any resulting combustion. Results indicate that the strength of the incident shock wave and the presence of reflected shock waves from the shock tube walls dictate whether or not ignition occurs.

Paper #120

**A Study on Deflagration to Detonation Transition in Injected Hydrogen/Air Mixtures**

*Masanori Yabe, Masaki Naitoh, Teruo Yoshihashi, Tetsuro Obara and Shigeharu Ohyagi*

The problem of transition from deflagration to detonation (so called DDT) is one of the most important problems of combustion science and technology. The problem has been attacked by many combustion scientists and engineers from a long period of time. But the problem has not been solved yet because it includes many complex but fundamental physico-chemical phenomena such as an acceleration of flame, a formation of shock wave and interaction of chemical kinetics with the shock wave. Because many studies on the DDT were performed from a fundamental point of view, then they assumed a uniform mixture at rest before ignition. But in many practical situations, such as the pulse detonation engine (PDE) as well as the accidental explosion hazards in the pipelines, mixtures may not be uniform and still. In the PDE, fuel and oxidizer will be injected directly into the combustor, then they will be mixed inside the chamber and they will be ignited before they become uniform and at rest. As far as the authors know, there was no study concerning on the DDT in such non-uniform mixtures. The present study, aiming at obtaining a fundamental aspect on the DDT in a non-uniform mixture with some turbulence, was conducted by using a detonation tube equipped with high-speed solenoid valves which inject a fuel gas and an oxidizer gas. Obstacles which enhance the DDT were installed near the ignition region. Hydrogen and air were selected as a mixture and an initial pressure was atmospheric. The tube has a rectangular cross-section of 25 x 30 mm and 3000 mm in length. At the igniting end of the tube, there installed two fast action solenoid valves injecting fuel and oxidizer gases. Mass flow rates of the injection were measured before the main experiments. There are six measuring ports, P1 through P6, quipped with pressure transducers and ionization probes along the tube. A Shchelkin spiral with a pitch of 25 mm and a blockage ratio of 0.35 is inserted at the most upstream position in length of 500 mm. The results show that for the uniform mixtures, the detonation was not initiated for the equivalence ratio above 2.0 and the DIT shows a minimum value near the stoichiometric mixture, while, for the injected mixtures of the present experiments, it was not initiated for the overall equivalence ratio less than 2.0 and the DIT slightly decreased as the overall equivalence ratio increases. For the injected cases, the local equivalence ratio should not be equal to the overall equivalence ratio and the distribution of concentration is important for this DDT process.

Paper #121

**Numerical Simulation of Pulse Detonation Engine Working Process Initiated by Small Energy**

*WANG Wei, FAN Wei, Qiu Hua, YUAN Cheng, PENG Changxin, YAN Chuanjun*

The research presented in this paper focused on the simulation of the operation of pulse detonation engine with small energy ignition model. A finite-rate chemistry computational fluid dynamics model and second order upwind scheme had been used in the 2-D simulation of detonation. Spark ignition model in CFD software was used to simulate the spark plug ignition which is similar in the experiment. The results of simulation were well agreed with those of the experiment. It is demonstrated that the methods of mesh generation and calculation in this paper can be used in the simulation of working process of detonation engine initiated by small energy ignition.

Paper #125

**Simulation of Detonation Wave Passage through Cloud of Chemically Inert Solid Particles**

*Fedorov A.V., Tropin D.A.*

Investigation of the detonation attracted much attention over the years, for example, in connection with the prevention of catastrophic explosions. In this study, methods of numerical simulation of detonation suppression by finite-size clouds of inert particles was investigated. It was found that the addition of chemically inert solid particles is an effective way to control and modify the combustion and detonation in gaseous systems. This method can be used, for example, in order to reduce the detonation wave velocity and the length of the reaction zone. In a one-dimensional unsteady formulation of the mechanics of heterogeneous media the process of detonation suppression in hydrogen-oxygen mixture and sand particles distributed in the space was described by the equations of nonequilibrium gas dynamics in a two-speed, two-temperature approximation. To describe the chemical transformations in the detonation wave the model with detailed kinetics was used. In the problem of suppressing the detonation of a finite-size inert particles cloud / filter with a constant volume concentration equal to the critical value for an infinite cloud the minimum length of the particle cloud / filter was determined. This is such length that after the frozen shock wave and the wave of the ignition and combustion, resulting in the decay of a detonation wave in the cloud, exit from the filter deflagration to detonation transition was not observed. When studying the influence of volume concentration distribution in the cloud / filter on the suppression of detonation, it is revealed that the decrease in volume concentration of particles from critical to some less leads to less efficient quenching of the detonation wave compared with the case of constant concentration. Presumably this is occurs because of the influence of particles on the gas-dynamic flow pattern (geometric effect). When studying the influence of nonmonotonic

distribution of the particles volume concentration in the cloud it was shown that the determining parameter in the process of suppression of detonation is not the volume concentration of particles and their weight, but the length at which the wave of ignition and combustion quenching.

Paper #130

#### **Experimental Study of Flame Acceleration and Deflagration-To-Detonation Transition**

*Kong-Qian SUN, Yi-Ning ZHANG, Kun GUO*

Flame acceleration and deflagration-to-detonation transition (DDT) of acetylene-air mixtures were studied experimentally. The flames were accelerated by stagger obstacles. The schlieren device and high-speed camera were used to observe the external flow field. Various equivalence ratios for acetylene-air mixtures were discussed. The results show that deflagration-to-detonation transition is determined by the obstacles and equivalence ratios. For different equivalence ratios, different styles of flame can be obtained. At the equivalence ratio of 0.91, the obstacles enhance deflagration to detonation. The precursor shocks and turbulent flame waves are strengthened and coupled by complicated reflect waves in the process of DDT. The deflagration wave is discretized in external flow field, coincide well with the flame at the end of duct.

Paper #173

#### **Physics of Detonation Propagation in Rotating Detonation Engine**

*Takayuki Yamada, Yuho Uemura, Nobuyuki Tsuboi, A. Koichi Hayashi and Eisuke Yamada*

Rotating detonation engine (RDE) has a high performance for aerospace thruster, which is driven by detonation. There are several detonation engines where pulse detonation engine (PDE) is mainly studied and developed up to now and a prototype PDE was flied in 2010. However since its thrust comes out intermittently, PDE has a problem of low thrust density. On the other hand RDE provides its thrust continuously and its performance is promising. RDE research started long time ago by Voiseknovskii in 1959 and just recently an extensive research is accelerated experimentally and numerically. The experimental work on RDE is performed to get its engine performance and the numerical one to get its physical structure of detonation propagation. In the present study a three-dimensional numerical model of a RDE is simulated using Euler equations with a detailed hydrogen-oxygen chemical reaction model which has a revised high pressure mechanism to observe a detailed detonation wave and its propagation structure. The number of grids is 601x31x601 and size of each is 5micrometer. Many futures of RDE, which were obtained by 2D calculation, are confirmed using this 3D calculation such as the cell structure by transverse waves, the Kelvin-Helmholtz instabilities, and the detailed propagation mechanism of transverse waves. The transverse wave yields at the high temperature spot where the detonation front interacts with the contact surface between the fuel hydrogen flow and the burned product flow. The present 3D results as well as the previous 2D results show that the triple points and the transverse waves come out at the edge of the interaction point between the detonation front and the contact surface. This is one of the important findings in the present study. At the detonation front the detonation cell pattern appears due to the transverse wave propagating to the perpendicular direction to the detonation front propagation direction. When the transverse wave collides with the inlet wall, an ignition occurs to create the new transverse wave. At the downstream side of the detonation front, the new transverse wave yields at the high temperature region due to the interaction described previously. The detonation cell pattern is uniform near the inner tube and the centrifugal force may give the higher pressure profiles near the outer tube wall and the lower pressure profiles near the inner tube wall. Since the detonation rotates along the tube wall in the direction perpendicular to the thrust flow direction, the interaction between the detonation front and the shock wave and the previous round flow gives the Kelvin-Helmholtz instabilities and results in vortices. The present 3D results provide us to understand the complex transverse wave propagation mechanism and detonation front structure.

Paper #190

#### **Moving-Component-Free Pulse-Detonation Combustors and Their Use in Ground Applications**

*T. Endo, A. Susa, T. Akitomo, T. Okamoto, K. Kanekiyo, Y. Sakaguchi, H. Yokoyama, S. Kato, A. Mitsunobu and T. Takahashi*

For realization of compact high-power pulse-detonation combustors, we developed a technology by which high-frequency operation of a pulse-detonation combustor became possible. In this operation mode, valves for gas supply, by which the operation frequency of a pulse-detonation combustor is usually restricted, are kept opened all the time of operation. By this technology, pulse-detonation combustors become highly powerful and durable. The principle of the gas-supply method we developed is simple. When pressure in the pulse-detonation combustor near the gas-supply port is higher than the gas-supply pressure, the gas is not supplied. On the other hand, when pressure in the pulse-detonation combustor near the gas-supply port is lower than the gas-supply pressure, the gas is supplied. Therefore, by adjusting the gas-supply pressures so that the gas-supply pressures for fuel and oxidizer are lower than the gas-supply pressure for purge gas, the purge gas starts to be supplied after detonation initiation prior to the fuel and oxidizer, and then the residual hot burned gas is automatically purged before the fresh detonable gas is supplied. In order to demonstrate high-frequency pulse-detonation-combustor operation by the developed gas-supply method, we developed a compact pulse-detonation combustor and successfully operated it at 200 Hz by using ethylene as fuel, oxygen as oxidizer, and argon as purge gas. Further, in order to verify the versatility of the developed technology, we carried out experiments on thermal spraying and turbine drive, as examples of ground applications of the developed pulse-detonation combustors. As a result, the developed pulse-detonation combustors were successfully usable in these experiments.

Paper #196



**Surface Chemical Reaction of Laser Ablated Aluminum Sample for Detonation Initiation***Chang-hwan Kim, Ardian B. Gojani and Jack J. Yoh*

We explore the evolution of metal plasma generated by high laser irradiances and its effect on the surrounding air by using shadowgraph images after laser pulse termination; hence the formation of laser supported detonation and combustion processes has been investigated. The essence of the paper is in observing initiation of chemical reaction between ablated aluminum plasma and oxygen from air by inducing high power laser pulse (>1000 mJ/pulse) and conduct a quantitative comparison of chemically reactive laser initiated waves with the classical detonation of exploding aluminum (dust) cloud in air. Findings in this work may lead to a new method of initiating detonation from metal sample in its bulk form without the need of mixing nano-particles with oxygen for initiation.

Paper #217

**Comparison of Conditions of Direct Detonation Initiation by Spark with one by Pulsed Arc According to the Gradient Mechanism of Ya.B. Zeldovich***Korytchenko K.V., Poklonskiy E.V., Galak O.V.*

A method of detonation initiation by a gradient mechanism (overall ignition) where there is a pressure balance in the discharge channel with ambient pressure during the process of the energy input is of scientific interest. It is similar to the process of the detonation initiation by deflagration to detonation transition in a detonation tube where the increase in pressure due to combustion is not compensated by the gas expansion because of the large scale of combustion zone. That leads to a rise of intensity of a compression wave which transforms into a detonation wave then. In the case of detonation initiation by this mechanism, the requirements to the electric discharge, particularly in the specific power of the energy input into the discharge channel, change. It is calculated that the detonation initiation takes place in stoichiometric hydrogen-oxygen mixture of atmospheric pressure when the specific power of the energy input equals  $W = 6000 \text{ W/cm}^3$  which is three orders of magnitude lower than it is in the powerful spark discharges. The energy is deposited by the radius  $r = 1 \text{ cm}$  and the deposition time  $t_{\text{inp}} = 0.1 \text{ ms}$ . Assuming that the strength of an electric field in the positive column of the discharge channel at given discharge duration is about  $E = 10 \div 100 \text{ V/cm}$ , we get the required density of the discharge current, which is about  $j = 60 \div 600 \text{ A/cm}^2$ . It is possible by such magnitudes of the current density in certain conditions to obtain electron emission from the cathode without the origin of cathode spots. It is one of main requirements for technical realization of the discharge energy input into a large volume. A magnitude of the discharge current ranges from  $I = 180 \div 1800 \text{ A}$  in this case. Thus, evaluating the magnitudes of the strength of the electric field, the discharge current and the discharge duration, we come to the conclusion that driving of the parameters of energy input into the discharge channel is technically feasible. It is concluded that the most advanced way to solve the problem of repetitive detonation initiation by low input of electric energy is using the arc driving discharge in realization of detonation initiation by gradient mechanism.

Paper #222

**Effect of an Axial Electric Field on Detonations***Vsevolods Kamenskihs and John H.S. Lee*

We have re-visited an early study by Bone, Fraser and coworkers [2] and carried out an experimental investigation to study the effect of an axial electric field on the propagation of gaseous detonation waves. Stoichiometric  $2\text{CO} + \text{O}_2$  (saturated with water) at atmospheric pressure and stoichiometric  $\text{C}_2\text{H}_2 + \text{O}_2$  mixture, diluted with 85% argon at 28kPa were used in the experiment. Electric field ranged from 200V/cm to 7500V/cm. The upper limit for the electric field was kept below the breakdown value (depending on the initial pressure of the mixture and electrode distance). Apart from streak photography photodiodes were used for more precise velocity measurements. The voltage and current time histories were also monitored as the detonation traversed the electric field region. We did not observe a 40% velocity deficit reported by Bone and coworkers [2] when a single head spinning detonation in  $2\text{CO} + \text{O}_2$  propagated through a region of 5000V/cm electric field. The fact that we observed no discernable change in the detonation structure or velocity due to the electric field, is due to the very low ion concentration in the reaction zone. Thus, the effect of electrostatic force on the detonation wave is negligible. Moreover, in the case of  $2\text{CO} + \text{O}_2$  mixture at 1 atm neither the extraction of ions at the electrode nor the discharge ahead of the detonation had any influence on detonation structure and velocity. The effect of a discharge was more pronounced in the case of  $\text{C}_2\text{H}_2 + \text{O}_2 + 85\% \text{Ar}$  mixture at low initial pressure of 28kPa. An arc discharge which developed ahead of the detonation significantly perturbed the detonation by igniting the mixture upstream of the detonation, resulting in failure of the detonation.

Paper #228

**Effect of Transmission of Detonation from Smaller to Larger Tube on the Performance of PDE***Abhishek R. Bhat, N Harish, P. J. Paul*

The study of detonation initiation remains in the forefront of research as it is central to optimizing the performance of the Pulse detonation engine. In this paper the study of transmission of detonation from small to larger tube and its effect on specific impulse of the PDE has been studied. The method of transmission has been investigated in detail in several earlier studies. Stoichiometric mixture of  $\text{H}_2$ -Air is used as a fuel air mixture for the study. In these experiments detonation is initiated at the closed end in a smaller tube of 1m length and 5mm diameter. Pressure transducers were attached along the length of the tube for measuring the velocity of combustion wave. The flame accelerates after passing over the shelekin spiral and propagates as a galloping detonation at 900m/s. The detonation gets transmitted into larger tube of 5cm diameter at the closed end of the tube. The larger tube is attached with a shelekin spiral and a perforated plate for the enhancement of DDT. The pressure transducer readings show that the transmitted wave does not transit to the CJ (Chapman Jouguet) condition but propagates as a fast deflagration or a sub CJ detonation at approximately 850m/s. The

main results from this study is on the measurement of specific impulse for the various fill fractions. The specific impulse is calculated by integrating the pressure with respect to time, which is measured at the head end of the larger tube. The results show that the specific impulse produced by the sub CJ detonation can be higher than that due to the CJ detonation under low fill fractions. In longer tubes at larger fill fractions this sub CJ detonation will eventually fail leading to the loss in specific impulse. This study also shows that there is a critical value of fuel-air mixture fill length of of 1.2m approximately above which the sub CJ detonation fails leading to loss in specific impulse. In the cases when fill length is less than this critical value the specific impulse produced by the sub CJ detonation or fast deflagration is higher than that of the CJ detonation case. The comparison of the head end pressure profiles for these cases shows that the plateau pressure in case of sub CJ detonation maintains slightly higher average pressure. This may be due to that fact that the Taylor wave will be weaker in this case as compared to the CJ case.

Paper #232

### **On the Detonation Structure in Ozone**

*Aslan Kasimov, Vladimir Shargatov*

We investigate one-dimensional detonation in gaseous ozone using several different kinetic mechanisms for its reaction. The detailed mechanism of ozone decomposition consists of three reversible reactions among  $O_3$ ,  $O_2$ , and  $O$ . Using a high-order shock fitting method for the solution of reactive Euler equations with accurate treatment of chemical reactions as well as the mixture thermodynamics, we explore the structure of the steady state solution and its dynamics. We find that different sets of rate constants lead to significantly different structure of the reaction zone with characteristic length scales differing by orders of magnitude. Implications for detonation stability are explored.

Paper #258

### **Formation of Detonation in Confined Moving Regions**

*V.A. Levin, I.S. Manuylovich, V.V. Markov*

The attempts to actually use detonation in motors and other different energy devices posed a number of problems for the researchers. The most important among them is the task of detonation initiation in the confined space. Results of experimental and theoretical investigations of detonation initiation using rotation or deformation of combustion chambers are not known until now. The one-dimensional problem on detonation initiation by the piston is certainly referred to the issue being considered. The combustible-mixture flow inside and outside the rotating elliptic cylinder enclosed in the circular cylinder is considered to estimate feasibility of detonation initiation during rotation. Special rotating cylinders with blades are examined as detonation initiators. Critical parameters at which detonation is formed are evaluated. The analogy with detonation initiation in the combustible mixture flow in the channel having the specific spiral form is presented. The numerical method based on the S.K. Godunov scheme with the mobile computation mesh is used to perform this investigation in the framework of one-stage kinetics of stoichiometric air-propane mixture burning. The detailed flow pattern that allows us to identify features of detonation occurrence at movement of the combustible mixture-containing area boundaries was obtained. Detonation initiation using rotation of the elliptic cylinder enclosed in the circular cylinder, both filled with stoichiometric air-propane mixture, was numerically investigated. The feasibility to form detonation both inside, and outside the elliptic cylinder was stated. Two critical angle velocities of cylinder rotation, which govern the quantitative and qualitative flow pattern, were found. The method to estimate parameters of the three-dimensional spiral channels is proposed based on the plane-sections hypothesis. The comparison with 3D simulation is presented. This work was financially supported by RFBR (grants No. 11-01-00068, 11-08-00288, 10-08-90039-Bel), Federal Agency of Science and Innovations (NSh 8424.2010.1) and Basic Researches Programs of RAS Presidium and RAS Division of Power Engineering, Machine Building, Mechanics, and Control Processes.

Paper #262

### **Numerical Simulation of the Oblique Detonation Waves in Different Regimes Initiated by Conical Projectile**

*Jeong-Yeol Choi, Jimmy Verreault, Andrew J Higgins*

Oblique detonation waves (ODWs) and shock induced combustion (SIC) stabilized over a body have been considered as a promising combustion means for hypersonic propulsion systems such as ODW engines and ram accelerators. A number of studies were carried out to examine the fundamental characteristics of an ODW and its implementation for propulsion systems. An interesting point from the previous studies are there are varieties of different ODW regimes depending on the flow conditions and configuration. Recently Verreault and Higgins showed the different regimes of combustion with aeroballistic experiment and high speed visualization. They classified the different regimes of the ODW based on the energetic and kinetic limits of the detonation initiation by high speed projectiles. Presently, computational fluid dynamics simulation is carried out to understand the flow structure of the different regimes of the combustion shown experimentally.

Paper #266

### **Generation of Detonation Due to Kinetic Energy of the Supersonic Flow**

*V.A. Levin, I.S. Manuylovich, V.V. Markov*

In connection with the use of detonation in engines and other energetic facilities a number of problems arise. Among them are detonation initiation and its stabilization within the combustion chamber. Detonation initiation in layers, in stationary medium, and in unlimited space was experimentally studied by many authors. In the case of the combustion chamber, which is limited in the crosswise direction, one might expect new effects under detonation. The paper considers the problems of detonation initiation in the supersonic flow and stationary stoichiometric air-propane mixture, which partially or fully fills in the plate channel cross-section. In the flow initiation takes place at the cost of a "bench" or a wall

which fully blocks the channel, and in the medium at rest it is caused by explosion. The investigation is performed within the framework of single-stage combustion kinetics by the numerical method based on the S.K. Godunov scheme. Critical detonation conditions connected with the inflow velocity and explosion energy were determined. In all the discussed processes one can find then unknown detonation propagation mechanism, which is conditioned by formation of complicated wave flow structure, characterized by shock wave penetration in the inert gas to the layer in front of the detonation wave, with the resulting warm-up and combustion. The process is periodic in nature, and differs from standard cellular detonation in the uniform medium. The existence of critical inflow velocities was established upon which qualitative and quantitative flow pattern is dependent. In the uniform flow two different detonation modes were obtained - with stationary wave on the "bench" and with the wave propagating to inlet channel section. In the combustible mixture layer we found three detonation modes: with stationary wave on the "bench", with the wave propagating to the inlet channel section in the form of stationary wave complex or in the mode of galloping layered detonation. As the flow rate increases, the rate of wave travel in direction of the inlet section decreases and at the rate equal to the critical one the wave turns to the stationary mode. The original computing complex with user-friendly graphical interface was developed and used to perform numerical investigation. This work was financially supported by RFBR (grants No. 11-01-00068, 11-08-00288, 10-08-90039-Bel), Federal Agency of Science and Innovations (NSh 8424.2010.1) and Basic Researches Programs of RAS Presidium and RAS Division of Power Engineering, Machine Building, Mechanics, and Control Processes.

Paper #282

### **Drag Coefficients of Hypervelocity Spherical Projectile Initiating Oblique Detonation Wave**

*Jeong-Yeol Choi, Shinichi Maeda, Jiro Kasahara, Akiko Matsuo*

A purpose of present study is to estimate the drag coefficients of a spherical projectile initiating either SIC or ODW through CFD to apply the criterion for the classification of OSIC and ODW regimes. The drag coefficients of a spherical body is well known for a long time, but there is a questionnaire whether it can be apply for the present case is quite different from the hypersonic projectiles in ordinary non-reacting flow or dissociating flows. Since, the present case involves strong overdriven detonation ahead of projectile surrounded by hot burned gas. The prediction of drag coefficient of a projectiles in detonable media has another practical importance. Embedding either inert or explosive particles becomes the design strategy of modern explosive to increase lethality and to reduce collateral damage. Thus the information on the drag coefficient of a projectile in a detonable gas taken from the present study can be applied usefully in the design procedure of those systems. CFD simulation is carried out for hypersonic projectile initiating SIC or ODW based with multispecies reacting flow model and SST turbulence model. The experimental visualization results were reproduced quite well CFD and shows good agreements with observations. The drag coefficients predicted from the CFD seems to be in the reasonable range and give the explanation on the effects of the detonative combustion around the projectile. As, the detonation initiation criterion is shown to be effective for the spherical projectile with the drag coefficient estimated presently.

Paper #286

### **Deflagration-to-Detonation Transition in Narrow Channel with For-chamber**

*Golub V.V, Baclanov D.I., Ivanov K.V., Krivokoritov M.S*

Recently hydrogen is considered to be the most perspective fuel due to ecological compatibility and high specific combustion heat. Hydrogen-air mixture has major significance for practical applications as compared with the others hydrogen-oxidizer mixes because of its availability. But its application as an energy source for small devices is difficult because of comparatively large detonation cell size and less detonability of such mixture. In general there are specific problems of obtaining gas detonation in channels with diameter less than critical one. Because of great heat losses into channel walls especially in fuel-air mixtures deflagration to detonation transition is complicated in narrow channels. The for-chamber with greater diameter at the head of the narrow channel was used in order to obtain deflagration to detonation transition. In present work deflagration to detonation transition in hydrogen-oxygen and hydrogen-air mixtures in 3 mm channel was investigated. Transition to detonation in hydrogen-air mixture was obtained in channel with the diameter less than critical one (for air mixture is equal to 3.7 mm). The dependence of run-up distance on for-chamber length was considered in terms of additional energy of burning gas in for-chamber.

Paper #322

### **The Transmission Behavior of the Over-driven Detonation across the Mixture with the Abrupt Area Change**

*Yao-Chung Hsu, Kung-Ming Chung, Yei-Chin Chao*

In this study, we would like investigate the propagation behavior of the over-driven detonation transmitting through the interface of the mixture varying and area changing in a small d/d circular tubes system. For mixture varying, the donor section is filled with fuel rich propane/oxygen mixture whereas the propane/oxygen/nitrogen mixture filled in the acceptor. Further, we also find the limiting condition for successful transmission of the detonation.

Paper #331

### **Detonation Initiation by Gradient Mechanism in Propane-Oxygen and Propane-Air Mixtures**

*A.E. Rakitin, I.B. Popov, A. Yu. Starikovskiy*

An experimental study of detonation initiation by high-voltage nanosecond gas discharge has been performed in smooth detonation tubes. A gradient mechanism was used to initiate detonations in stoichiometric propane-oxygen mixtures with different nitrogen dilution and in propane-air mixtures. Initial pressures from 0.2 to 1bar have been tested. Detonation was formed within 4 transverse tube sizes at initial pressures higher than 0.2 bar for the propane-oxygen mixture and

higher than 0.8 bar for the diluted mixture with 40% of nitrogen. The discharge energy inputs were 0.2-0.3 J. Combined with the focusing effect of the converging reducer, the gradient mechanism of detonation formation similar to the one suggested by Zeldovich has been shown to be the governing process. For the mixture with air, a detonation tube with an annular discharge chamber has been designed and tested.

Paper #336

**Numerical Simulation of Detonation Propagation in Ducts with Obstacles**

*Cheng Wang, Wenhui Han, Jianguo Ning*

Two-dimensional reactive Euler equations for the stoichiometric hydrogen-air mixture are solved numerically to investigate the effects of obstacles on detonation using a fifth-order weighted essentially non-oscillatory (WENO) scheme with a third-order TVD Runge-Kutta time stepping method. The simulation results suggest that, appropriate number of obstacles can not only accelerate wave front, but will not result in quenching of detonation wave. However, although too many obstacles can accelerate detonation propagation, they tend to lead to detonation quenching. Different spacing of obstacles exerts significant effect on formation of detonation waves. If the obstacle spacing is such that transverse waves converge at the axle and collide when they reach the next obstacle, a self-sustaining detonation wave will come into being. Otherwise, a self-sustaining detonation wave will not be formed. Reduction of the hole diameter of obstacles can effectively refrain detonation wave reappearance after propagating outside the obstacles.

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**10:25 Poster I - Explosion**

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Paper #46

**Numerical Study of Interactions between Blast Wave and Moving Bodies in Ambient and Indoor Areas***Lo, Shi-Wei, Tai, Chang-Hsien, Teng, Jyh-Tong and Lai, Ching-Chung*

This paper deals with blast effects prediction numerically on the moving bodies and a building in ambient and indoors terrains. Two-dimensional, unsteady, compressible, inviscid equations were solved by the implicit-time formulation. For the spatial discretization, the second order upwind scheme was employed. To simulate the moving bodies which impacted by the blast wave, moving mesh model was applied to shift the mesh sizes and movement. An approach to predict the blast loads (1) on the moving shells of vehicle and an immobile building in an open area and (2) on the movable window and obstacles indoors was described. Besides, serial images of transitory flow phenomena were displayed and compared by the distributions of species concentration and velocity vectors. The crashed effects, pressure and sand velocity time histories, and the movement of gravity center of moving bodies were also presented to analyze and compare with different boundary conditions. The interactions among blast waves, reflected shock waves, moving body and other obstacles were described in the results. Finally, the proposed physical model and the numerical simulations developed in the present work are expected to be extended to solve shock wave interactions with other complex geometry and boundaries.

Paper #72

**Buncefield: Reconciliation of Evidence with Mechanisms of Blast***James Venart*

The area covered by the vapour cloud was estimated to be around 120,000m<sup>2</sup> with the average height of the cloud being about 2 to 3 m. This gives a volume of between 240,000 and 360,000m<sup>3</sup>. Evidence cited in [1] suggested the emergency pump house as one source of ignition. The two most commonly known explosion mechanisms are deflagration and detonation. Both possibilities were assessed by the Buncefield Major Incident Investigation Board (MIIB) for their consistency with the observed explosion characteristics [1]. Deflagration was found to be inconsistent with the significant near field damage to most objects and cars. Detonation, however, was inconsistent with damage suffered by buildings within the flammable cloud. CFD modelling of the area immediately surrounding the emergency pump house (PH) supported a suggestion that congestion of trees and undergrowth along Cherry Trees Lane and Buncefield Lane could have allowed flame acceleration to several hundred m/s. Such high velocity may have provided an opportunity for transition from deflagration to detonation, DDT, and thus the progression of a single detonation front, from this source, into the vapour cloud from the Pump House Lagoon (PHL) W and to the S-W; see also [2] and [3]. The characteristics for direct initiation to detonation vs. DDT may be found in [4]; The former mode is dependent upon an ignition source driving a blast wave of sufficient strength such that the igniter is directly responsible for initiating the detonation. The latter case begins with a deflagration initiated by some relatively weak energy source which accelerates, through interactions with its surroundings, into a coupled shock wave-reaction zone structure characteristic of a detonation. Direct initiation by a concentrated source requires an extremely large energy deposition relative to deflagrative ignition. In this paper we very briefly review our past work on this accident [5, 6]. Based upon this we conclude that the statement made in [1], and by others, that "the most likely scenario was a deflagration outside the emergency pump house that changed into a detonation due to flame acceleration in the undergrowth and trees along Three Cherry Trees Lane" is incorrect.

Paper #118

**Mitigation of Vapour Cloud Explosions - a Review***Kees van Wingerden*

The potential of devastation of industrial installations, nearby houses and businesses and sadly enough: the potential of fatalities and serious injuries due to vapour cloud explosions is unfortunately still being demonstrated on a regular basis. Recent examples of this potential include the following accidents Buncefield (2005), Texas City (2005) and Toronto (2008), whereas past experiences can be found in overviews published by both insurers and researchers. The majority of research performed in the field of vapour cloud explosions has mainly been addressing two main areas of attention: prediction of the consequences of vapour cloud explosions and trying to understand the main combustion mechanisms governing vapour cloud explosions. Examples of research into prediction methods include the development of prediction tools for blast generated by deflagrative flames such as similarity methods and 1-D numerical methods, the development of simple fuel-air blast prediction methods using such tools as a starting point: Baker-Strehlow-Tang, the Multi-Energy method, the Congestion Assessment Method and dedicated CFD-codes such as AutoReagas and FLACS. Examples of studies addressing research into governing combustion mechanisms in vapour cloud explosions include those addressing flame instabilities, combustion dominated by expansion flow generated turbulence and DDT and detonation. Very little attention has however been given to mitigation of vapour cloud explosions, i.e. methods aiming at limiting the consequences of vapour cloud explosions with the exception of siting issues which considers e.g. re-locating control rooms or strengthening these. For siting the aforementioned simple fuel-air blast prediction methods are used. The paper addresses different potential methods to mitigate vapour cloud explosions and highlights research needs to improve or develop these methods further.

Paper #189

#### **Limiting Oxygen Concentrations - Process Safety by Oxygen Monitoring**

*K. Holtappels, V. Schröder, A. Pekalski, H.-P. Schildberg*

A simple and cost-saving way to avoid explosive atmospheres in chemical processes is the monitoring of the oxygen content in the respective gas mixture. Such a monitoring is easily achieved by installing oxygen detectors also in closed systems. The determination of the amount of fuel gas, which was very often a complex procedure, is no longer necessary. The main requirement for the use of oxygen detectors is of course the knowledge of the so called limiting oxygen concentration (LOC). The LOC is defined as maximum oxygen concentration in a mixture of a flammable substance, air and an inert gas, in which an explosion will not occur, determined under specified test conditions. If the mole fraction of oxygen in a gas mixture is below the LOC value, even the arbitrary addition of fuel gas cannot lead to explosive atmospheres. The LOC does not only depend on the test substance but also on the type of inert gas and initial conditions. Literature values which have been published for pressure dependencies show a clear linear decrease on a log scale with increasing pressure. Due to great influences of the experimental set-up used for the determination of the explosion areas this linear dependency was not validated. Furthermore other data showed a mirrored "c" shaped dependence. Therefore LOC values were determined in new apparatus with different volumes in order to gain a better understanding of the LOC behaviour at elevated conditions especially with regard to the flame propagation in a closed system considering e.g. cooling effects due to heat transfer to the vessel walls. The examinations were supported by highspeed-videos recorded in a windowed vessel (operating pressure up to 15MPa at 250°C) with an inner volume of 11-l, where the whole volume could be observed.

Paper #239

#### **Analysis of Mobilisation and Explosion Problems in Gas and Dust Mixtures**

*JR García-Cascales, F Vera García, R Otón-Martínez, A Bentaib, N Meynet*

Great effort has been done on the characterisation of multiphase problems over the years. Special attention has been paid to problems involving the mobilisation and explosion of gas and particle mixtures. This work describes the dense model implemented in DUST, a code developed by the Technical University of Cartagena, Spain and the Institute for Radioprotection and Nuclear Safety of France. It has been developed in the framework of the security of the international fusion reactor ITER. This model is based on a six-equation model which considers the effect of pressure on the solid phase by means of a compaction term. This is an Eulerian approach based on a finite volume approximation. The flux evaluation at the interfaces is carried out by means of numerical schemes extended to analyse these problems. All are approximate Riemann solvers which let us evaluate the flux accurately at each interface. The code is explicit and allows second order accuracy. This is obtained by means of variable extrapolation techniques (MUSCL approach). Some tests have been studied to analyse the behaviour of the model.

Paper #281

#### **Vented Gas Explosion in Small Vessels of L/D of 2.4**

*Fakandu, B.M., Sattar, H., Phylaktou, H.N. and Andrews, G.E.*

Most current vented explosion data in relatively large explosion vessels cannot be predicted using laminar flame propagation models, without including an empirical turbulence factor to make theory and experiments match. However, part of the flame acceleration may be the self acceleration of laminar flames over the large distances involved in large explosion vessels. The generation of flame acceleration due to turbulence created in the venting process should not change significantly with vessel size. The present work uses a very small explosion vessels with flame propagation distance to the vent for self acceleration of flames to be negligible (Kasmani et al 2010). Comparison with laminar flame theory of venting is then made to show that turbulence factors are not necessary as the measured results for open vent explosions are less than those predicted by laminar flame theory, which assumes a worst case flame area equal to the vessel wall area. European and US design standards for gas venting are based on compact vessel venting where  $L/D < 2$  with additional vent area design procedures for higher  $L/D$ . However, the majority of experimental data on venting has either a sphere or a cube with an  $L/D$  of 1 and has central spark ignition. Central ignition does not give the worst case overpressure for an  $L/D$  of 2 and this is given by ignition on the end wall opposite the vent (Kasmani et al 2007). This work was carried out for an  $L/D$  close to 2 with end ignition as this is the worst case explosions for the compact vessel geometry and should give the highest overpressures for comparison with theory and with approved vent design correlations.

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**10:25 Poster Session I - Flame**

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Paper #12

**Studies on Methanol, Ethanol, and Biomethanol Flame Structure***Akimasa Tsutsumi, Makihito Nishioka and Keiichi Hori*

Experimental study for methanol, ethanol, and biomethanol coflow diffusion flame was conducted. A new vapor system for liquid bio-alcohol fuel and a coflow burner were developed. Much attention has been drawn recently to bio-fuel as alternative fuel. Bioethanol and biomethanol are well noted alternative fuel. Biomethanol is able to be produced from scrap wood or shredded paper; therefore it is more suitable to use biomethanol than to use bioethanol. Pure-ethanol was chosen to confirm stable combustion and to establish the procedure of experiments. The structure of two-dimensional ethanol flame was simulated by using a detailed chemical kinetic mechanism and compared to experimental results. The variations of the calculated flame temperature profile agreed with the experimental result. However, the maximum temperature, the position where indicates the temperature, and hydroxyl radical distribution did not agree with the experimental results. Concerning methanol and biomethanol, flame temperature was measured.

Paper #21

**Two-Phase Spray in a Wake of Shattering Fuel Drop***A. G. Girin*

The mathematical model of two-phase polydisperse spray in wake of a drop, shattering in uniform gas stream, is elaborated. System of spray dynamics equations consists of partial differential equations of torn droplets motion, evaporation and equation of density of their quantity distribution. It allows to describe quantitatively the evaporation and acceleration of stripped mass and thereby - the formation of liquid-phase jet and vapor cloud in a wake. Parent drop is regarded as a source of daughter droplets with given source distribution function and each daughter droplet - as moving point source of vapor. The dependencies of droplets drag coefficient on velocities and sizes as well as intensification of evaporation due to their streamlining are taken into account. Formulated non-stationary two-dimensional problem for system of spray dynamics equations with obtained earlier source function was solved numerically for kerosene drop in air stream and the structure of spray was investigated. Calculations showed, that times of living of finest and largest droplets are the characteristics of liquid jet formation in spray. Soon after moment of entire evaporation of droplets of minimum in spray radius, that were stripped at the beginning, the evaporation mass rate and current value of liquid-phase mass in spray exceed their maximum values because droplets vanishing begins. After moment of vanishing of droplets of maximum radius the vanishing of droplets of new radii doesn't occur, and this is the necessary condition for stabilization of length of liquid-phase jet. The proposed model allows to calculate spray mean diameters. Parameters of two kinds were considered: the first are defined in any cross section of jet and characterize its spatial structure at fixed moment, while second are calculated at any moment for whole set of droplets and describe temporal changing of jet dispersity in total. At the beginning the bunch of first set of curves is narrow that testifies to weak polydispersity of jet, but after droplets vanishing starts, the polydispersity increases. The stabilization proceeds gradually along jet from astern part to the tip. The dependencies of second set of curves confirm the conclusions. In final state jet polydispersity is much greater than that, produced by source. The process of vapor cloud formation in spray was studied too. At the beginning the intensification of evaporation due to rapid growth of liquid surface is so large, that vapor wave appears which has sharp front similar to blast wave. After losing contact with liquid phase this wave has convective drift, keeping its form invariable. Gradual weakening of droplets source capacity generates rarefied wave in vapor mass distribution, so, far from source the distribution tends to "triangle" form, which is also characteristic of blast waves. Evaluations show that fuel - air mixture in wake of shattering drop is substantially overreached in average, as vapor density several times exceeds the stoichiometric value. Vapor oversaturation leads to overcooling of the combustible mixture. Equation of heat balance for process of vapor - air mixing yields the temperature dropping almost 300°K which means that delay of ignition may jump several orders high.

Paper #30

**Polydispersed Initiation of a Dust Suspension in a Partitioned Structure***J.M. Pascaud*

The aim of this work is to study the effects of a polydispersed ignition in a wide energy range on a dust explosion and more particularly the pressure history inside a partitioned vessel. The initiation is introduced in the form of internal energy and a calculation methodology, particularly interesting in the field of the risk assessment is used to simulate the transmission of the explosion from one compartment to another adjacent compartment by the means of the hot flow through the shared orifice and finally to generalise this methodology to a complex multi-partitioned structure. The basic characteristics of the model have been developed for the ignition and the combustion of propulsive powders and adapted to dust suspensions with appropriate parameters linked to simplified kinetics. A simple representation of the combustion phenomena based on energy transfers and the action of specific molecular species is presented. The model allows the study of the influence of various parameters such as the dust concentration, the different ignition energies and their locations, the size of the inner openings or the vent areas. The theoretical results have been compared with many data available in the literature and indicate correct preliminary trends.

Paper #55

**Soot Formation from Laminar Ethylene/Air Diffusion Flames at Pressures from 1 to 8 atm**

*Hongsheng Guo, Zhongzhu Gu, Kevin A. Thomson, Gregory J. Smallwood*

This paper investigated soot formation in laminar ethylene/air diffusion flames at pressures from 1 to 8 atm by experiment and numerical simulation using complex chemistry and a relatively detailed soot model. The numerical simulation successfully captured the qualitatively trend of pressure effect on soot formation. Both experiment and simulation show that soot volume fraction increases and the radial position of the maximum soot volume fraction moves toward the centerline, as pressure increases. The peak soot volume fraction and peak integrated soot volume fractions are approximately proportional to  $p^n$ . Further analysis of details of numerical results suggests that the increase in pressure also results in the variation in the mechanism of soot formation. At atmosphere pressure, soot formation is dominated by acetylene addition, followed by PAH condensation and inception. However, the contribution of PAH condensation quickly increase with pressure and finally significantly exceeds the contribution of acetylene addition at pressures of 6 and 8 atm.

Paper #82

**The Investigation of the N<sub>2</sub>O Catalytic Decomposition for Hybrid Rocket Ignition**

*Hung-Wei Hsu, Meng-Chun Hsu, Tsung-Sheng Lee, Guan-Bang Chen, Yei-Chin Chao*

In this study, the performance and the fundamental phenomena of the self-developed catalyst for N<sub>2</sub>O catalytic decomposition were studied experimentally. The practical ignition method for hybrid rocket system was deduced from energy analysis and the performance of the self-developed catalyst tests. New concept of the integrated igniter module is proposed and verified by the 30Kgf thrust level hybrid rocket fuel grain ignition but without thrust nozzle. This new ignition concept provides the ability of multi-mode propulsion for flexible spacecraft missions. A unique, low-cost, high-performance and non-toxic propulsion system that the nitrous oxide could not only be employed as the oxidizer and the igniter for N<sub>2</sub>O hybrid rocket operation but be used as mono-thruster for satellite propulsion application will be developed.

Paper #94

**The Structure of Nonpremixed Ethanol Flames**

*Tei Newman-Lehman, Vaibhav Kumar Sahu, Vasudevan Raghavan Kalyanasundaram Seshadri and Forman A. Williams*

An experimental and kinetic modeling study is carried out to elucidate key aspects of nonpremixed combustion of ethanol. The experimental studies are performed on flames stabilized in the coflow configuration. In this configuration two reactant streams flow parallel to each other. The reactant streams are introduced into a mixing layer above two concentric segments: an inner segment and an outer segment. Fuel stream made up of a heated mixture of prevaporized ethanol and nitrogen is introduced from the inner segment into the mixing layer. Preheated air stream is introduced from the outer segment. Measurements made include flame structure and critical conditions of blow-off. The flame structure is measured by removing gas samples from the flame and analyzing the samples using a gas chromatograph. Temperature profiles are measured using coated thermocouples. Critical conditions of blow-off give the mass fraction of ethanol in the fuel stream as a function of the velocity of the fuel stream at blow-off. Kinetic modeling of the experimental data is performed using the San Diego Mechanism. The numerical simulations are carried out using the commercial CFD software FLUENT 6.3. Flame shapes, flame structure and critical conditions of blow-off are calculated and compared with experimental data.

Paper #109

**An Approach to Construction of Universal Global Kinetic Mechanisms of Hydrocarbons Combustion**

*Ivan A. Zaev, Igor V. Prokopovich*

In the paper the approach to derivation of the universal global mechanisms of hydrocarbons combustion is proposed, which is based on the requirement to reproduce all stages of hydrocarbon self-ignition supplemented by additional reactions of fuel and radicals, relevant for other types of the combustion (plasma-assisted ignition, flames). Based on the proposed approach the global mechanisms of methane self-ignition, consisting of 10 species and 9 reaction and allowing to simulate the ignition delay time with accuracy of 50% for temperature from 1100 to 2000 K and pressure from 1 to 30 atm in lean, stoichiometric and rich mixtures, is derived. Its extension to plasma-assisted ignition is also developed without any additional adjustment of the reaction rates and keeps the same accuracy as the base global mechanism. The developed mechanisms can be applied to practical simulation of detonation and explosions in methane-oxygen-air mixtures for safety and propulsion applications, as well as in preliminary theoretical studies of plasma-assisted methane combustion to estimate the potential of new combustion technologies, using non-equilibrium plasma.

Paper #111

**High-Temperature Decomposition of Nitromethane in the Shock Waves at Pressures 0.15-36 atm and Hypothesis of the Isomerisation in Its Decomposition Mechanism**

*Nikolai M. Kusnetsov, Yuri P. Petrov, Stanislav V. Turetskii*

For the first time in broad temperature interval 1190-1490K; and  $p=1.5$  atm the decomposition of nitromethane was investigated by the yield of NO<sub>2</sub> radicals. A temperature dependence of the rate constants of the NO<sub>2</sub> radicals yield was measured. It was established that rate constants of NM decomposition measured at initial stage of NM consumption and at initial stage of NO<sub>2</sub> yield, are equal to each other at equal T and p. Computational modeling of the kinetics of NO<sub>2</sub>



radicals yield and consumption in the NM decomposition gives a good agreement between experimental and calculated data. The theoretical analysis of a competition of channels of direct NM decomposition and an isomerization of NM in its thermal decomposition was provided, and made a conclusion about the priority of the direct channel of NM decomposition with C-N bond breaking.

Paper #169

**Empirical Reduction of Dynamical Reactor Models via Chaos Sampling: Comparison with Classic Reduction Methods**

*Katarzyna Bizon, Joanna Smuła and Gaetano Continillo*

An empirical model reduction technique, yielding low-dimensional approximations of the full high- or infinite-dimensional dynamical reactive systems while retaining their essential features, is presented in this work. The first step of the procedure i.e., the sampling of the representative set of simulation data to be used for the construction of the empirical basis, is considered to be crucial for generating a global basis. Here the concept of information entropy is used to optimally select the parameter range for the sampling region. The resulting POD/Galerkin technique is successfully applied to the optimal reduction of the model of an autothermal tubular reactor with recycle. The empirical basis is constructed with data sampled in the highest entropy (chaotic) regime. As expected, the higher the entropy of the sampled orbits, the closer the approximation to the original model. POD/Galerkin is shown to perform better than the yet efficient, classic approach of orthogonal collocation on finite elements, especially in the early transient.

Paper #171

**Hydrogen Peroxide Thermal Decomposition: new Features**

*Nabiha Chaumeix, Servane Pichon, Laurent Catoire, Claude Paillard*

H<sub>2</sub>O<sub>2</sub>/H<sub>2</sub>O decomposition characteristic time have been studied behind reflected shock waves in the temperature range 1260-1700 K, pressure range 150-230 kPa and highly diluted in argon. The experimental data were compared to decomposition characteristic time predicted using kinetic models available in the literature validated for H<sub>2</sub>O<sub>2</sub> system. Despite the fact that these updated mechanisms have been validated for hydrogen oxidation, a very large discrepancy was found between the models and experimental data, indicating that the H<sub>2</sub>O<sub>2</sub> submechanism needs improvements. Based on existing hydrogen detailed chemical kinetic models, addition of new reactions and reappraisal of some reaction rates were required to improve simulation of hydrogen peroxide decomposition.

Paper #183

**On the Critical Conditions of Hybrid Dusts Ignition**

*Rogulskaya O.S., Vovchuk Ya.I.*

It is known that the risk of fire and dust explosion of combustible solid materials is much higher if the air contains even a small amount of combustible gas. These conditions arise, for example, in an atmosphere of mines where the coal dust suspended in air, which contains coal and methane. Such dispersed system is named hybrid dust. Present work describes theoretical analysis of hybrid dust autoignition with taking into account simultaneous heterogeneous and homogeneous reactions in a mixture. The proposed model is based on the approach, generally accepted in classical theory of thermal explosion. It is supposed that monodisperse spherical particles of solid fuel are uniformly distributed in a mixture of oxidizing and combustible gases. Also it is assumed that solid and gaseous fuels burning out and radiative heat transfer during preignition period are negligible. Only one first order stoichiometric reaction on a particle surface occurs. Rate of homogeneous reaction (gaseous fuel with an oxidizer) has the second order. Reaction on an internal surface of particle is absent. The method of Semenov diagram is used for finding the critical conditions of hybrid dust ignition. It is shown that for a hybrid mixture maximum dimensionless temperature on the upper limit of a stationary mode depends on parameters of particles and heterogeneous reaction, and also on concentration of combustible gas, heat and rate of homogeneous reaction. The expressions for the approximation for such dependencies as well as for the main critical value of Semenov parameter dependences on parameters of the problem is suggested. It is shown that proposed approximations give the possibility to calculate analytically the values of ignition temperatures for hybrid mixture in a wide range of variation of its parameters with accuracy quite comprehensible for practice.

Paper #185 (372)

**Fast Deflagration in the Smooth Tube in Hydrogen-Oxygen Mixture**

*Dziemińska, E., Fukuda, M., Hayashi, A.K., Tsuboi, N. and Yamada, E.*

It is possible to achieve deflagration propagating with a speed higher than a speed of sound, nevertheless there is not much said about fast deflagrations (fast flame propagation) in the smooth tubes in the recent research. We proved that it was possible to simulate supersonic deflagration in case of hydrogen-oxygen mixture in the smooth tube. Moreover one of our numerical results were compared with Urtiew and Oppenheim's experiment to verify the accuracy of the code. Propagating flame reaches velocities higher than Mach 1 and additional phenomenon, like explosion in the boundary layer, can be observed. The fast propagating deflagration is acting like a piston and causes compression waves of very high pressure. Once reflect at the wall with a big impact, they are the reason for explosion in the boundary layer, which leads to DDT process in our case.

Paper #200

**Ignition by Electric Spark and by Laser-Induced Spark of Ultra-lean CH<sub>4</sub>/air and CH<sub>4</sub>/CO<sub>2</sub>/air Mixtures***Joffrey Biet, Marie Ndem, Mahmoud Idir, Nabih Chaumeix*

Biogas is mainly composed of methane and carbon dioxide. It is used in many fields, particularly in gas turbines for its ability to reduce the production of pollutants. However, with a lower calorific value than natural gas, the combustion and the ignition of biogas is more difficult to achieve. So, in order to better control all these parameters, the development of new technology is needed. Laser-Induced Spark (LIS) ignition is foreseen as a way to achieve a high-energy ignition system. This work investigates the Lower Ignition Limit (LIL) of CH<sub>4</sub>/air and CH<sub>4</sub>/CO<sub>2</sub>/air mixtures, using two different ignition devices: Electrical discharge and LIS and presents a comparison between the ignition by electric spark and by laser induced-spark of ultra-lean CH<sub>4</sub>/air and CH<sub>4</sub>/CO<sub>2</sub>/air mixtures. LIL for these 2 types of mixtures have been determined over a wide pressure range and using the 2 different ignition systems. The experimental setup used is a spherical bomb with an internal diameter of 250 mm. The ignition and the flame propagation are visualized with a high speed camera through a Schlieren setup. The mixtures are prepared at appropriate partial pressures to reach desired equivalence ratio. One Kistler pressure sensor measures the overpressure as a function of time. The ignition is initiated at the center of the combustion chamber either by LIS or by electric spark between two electrodes. The laser used is a Q-Switched DPSS Nd: YAG at 1064 nm. A variable attenuator is used to quantify the laser energy delivered to achieve ignition of the mixture. The experiments are performed for CH<sub>4</sub>/air and (0.6 CH<sub>4</sub>+0.4 CO<sub>2</sub>)/air mixtures in ultra-lean conditions ( $0.48 \leq \Phi \leq 0.65$ ) at different initial pressures ( $P = 1-7$  bars). All the observed flames are ascending. The maximum overpressure increases linearly with equivalence ratio for the leanest mixtures. The method used to determine the LIL is based on the observation of the propagation of the flame front or of this extinction. Moreover, there is an augmentation of the LIL with the initial pressure and with the introduction of CO<sub>2</sub>. This limit increases with the initial pressure reducing the flammability range. Moreover, the introduction of 40% of CO<sub>2</sub> in the fuel mixture increases substantially the LIL. Furthermore, the Minimum Pulse Energy (MPE) is determined only in the case of LIS ignition. We have shown that the flammability limits, based on the successful flame propagation criterion, are similar using either spark ignition or laser ignition.

Paper #202

**Transient Interactive Flamelets with Tabulated Chemistry***Anders Borg, Harry Lehtiniemi and Fabian Mauss*

Incorporating chemistry and accounting for turbulence-chemistry interactions in Computational Fluid Dynamics (CFD) calculations is challenging. In order to achieve industrially acceptable simulation times, while still accounting for chemistry, and effects of the turbulent flow-field on the chemistry, methods based on transient flamelets and a flamelet progress variable have been proposed. In this work we present a method that facilitates for running a high number of transient flamelets on-line with the CFD code. Our method relies on a progress variable parameterization of the chemistry, where chemical enthalpy is chosen as the progress variable. Differences between a parameterization employing homogeneous reactor calculations and a parameterization based on transient flamelet calculations are discussed. The applicability of tabulation is demonstrated for stand-alone transient flamelet calculations, and for a simple CFD problem. A constant volume spray chamber serves as CFD test case. All results with tabulated chemistry are compared to calculation with a regular transient interactive flamelet model. A skeletal mechanism for n-heptane consisting of 121 species and 973 reactions is applied for tabulation and for on-line chemistry. In prior work a normalized flamelet progress variable was defined. The formulation allowed for deriving a transport equation in physical space where the flamelet progress  $C$  was decoupled from mixture fraction  $Z$ . In this paper we focus on how a progress variable approach can be used to speed up a transient flamelet solver. Therefore, a dependency of the progress variable source term on mixture fraction is preserved. We formulate a transport equation for chemical enthalpy and apply the flamelet transformation. Two possibilities exist for pre-tabulating the required source term: a) adiabatic constant pressure reactor calculations, or b) transient flamelet calculations. Both methods are applied to generate source-term tables for the reaction progress, using the same discretization practice. The tabulation with transient flamelet calculations introduces the scalar dissipation rate as additional table parameter. The generated tables cover the conditions during the auto-ignition process for heavy duty diesel engine part load operating conditions. The proposed concept is verified for flamelet ignition at constant scalar dissipation rate, and flamelet ignition at decaying scalar dissipation rate. Temperature and species profiles obtained using the two different tables with calculations where the chemistry was solved on-line are compared. We find that the inclusion of scalar dissipation in the tabulation work is needed to correctly capture the behavior of an igniting flamelet. CFD calculations with tabulated and on-line chemistry demonstrate the high accuracy of the tabulated chemistry. The main benefit of the proposed model is the decreased computational time required for the flamelet solver. This allows for calculating a large number of transient flamelets at affordable computational cost. This is important in order to capture the lift-off length, and associated processes such as soot formation.

Paper #204

**Chemically Unstable Gases - MITD of Ethylene Oxide Mixtures***Enis Askar, Aydan Acikalin and Volkmar Schroeder*

Ethylene Oxide (EO) is one of the most important intermediates in chemical industry. Beside other hazardous characteristics it is chemically unstable, which means it can decompose explosively without any amount of an oxidizer like air. In the past industrial explosions as a result of EO decomposition causing enormous economical and personal loss has already occurred several times. Being essential for evaluating and avoiding hazards of EO decomposition safety characteristics are determined experimentally. Methods for calculation can help to reduce laborious experimental work even if they can not replace it completely. Although a considerable experimental database for safety characteristics of EO

already exists in literature, there are still some gaps, especially concerning ignition on hot surfaces in closed systems in the absence of air and at higher initial pressures. Hot surfaces are typical ignition sources in industrial processes. In this work the minimum ignition temperatures of decomposition (MITD) of EO and EO/mixtures were determined experimentally in dependence of the initial pressure, the vessel volume and the EO-fraction with an adequate experimental set-up. An ignition could be identified quite clearly by the occurrence of pressure peaks in the experiments. MITD at initial pressures between 1 bar and 10 bar were determined using vessels with inner volumes of 200 cc and 3000 cc. The usual standards for the experimental determination of ignition temperatures are not appropriate, because they can only be applied with air and at atmospheric pressure. Moreover a simplified model for calculating of MITD was developed, simulating the pressure and temperature course inside the vessel. The calculations are based on the time dependent zero dimensional heat and mass balance equations, which were solved numerically. The results for of the calculations accord very well with experimental results. Both pressure and vessel volume dependence can be calculated with good accuracy. Results of the calculation for larger vessels are plausible, but experiments for validation are still missing yet. The influence of inert gas fractions can be simulated as well in the case of nitrogen, whereas the model fails using carbon dioxide as inert gas, which has a higher heat capacity. Probably constraints for flame propagation, i.e. heating up the gas mixture to the flame temperature, must be considered additionally for a proper calculation in this case.

Paper #223

**Performance, Fuel-Flexibility and Emissions Characteristics of a 4.97cc Wankel Rotary Engine for Portable Power**

*Chris D. McCoy, Nicholas Maiden, Mario Sánchez Sanz, Juan Ramón Arias, Ángel Velázquez, Carlos Fernandez-Pello and Albert P. Pisano*

The small scale, fuel-flexible engine system presented in this paper intends to convert liquid chemical energy (in the form of liquid hydrocarbons) into electrical energy by means of a small-scale rotary engine. This system is intended to serve as generator for use during disaster relief and military efforts providing fuel flexibility and highly portable power for communication. This paper illustrates not only the fuel-flexibility of a 4.97cc O.S. Graupner Wankel engine and its performance: power output and efficiency, but also introduces fuel-flexible emissions trends. The power and emissions characteristics of this engine are obtained via a custom built dynamometer and a Lujan auto emissions data collection system, respectively. Emission trends have been collected for methanol and gasoline and will be collected for diesel, a kerosene-like heavy fuel and biofuel (ethanol, butanol, or any other available biofuel). With further testing, best and worst case emissions profiles for various fuels and blends can be determined in addition to methodologies to reduce such emissions.

Paper #290

**Experimental Investigation of Flame Propagation in Turbulent Propane-Air Mixtures and Dust-Air Suspensions**

*Trygve Skjold and Diana Castellanos*

Dust explosions pose a hazard whenever a sufficient amount of combustible material is present as fine powder, the powder can be dispersed in air to form an explosive dust-air suspension in a sufficiently confined volume, and there is an ignition source present. Detailed modelling of industrial dust and gas explosions from first principles is a formidable task, and current methods for mitigating the effects of industrial explosions therefore rely on empirical correlations for turbulent burning velocity. Recent efforts at simulating the course of dust explosions by combining computational fluid dynamics (CFD) and correlations for turbulent flame propagation with combustion parameters derived from standardized experimental tests have produced promising results. However, the results indicate that the correlations for turbulent burning velocity used by CFD codes for gaseous fuel-air mixtures are less successful in reproducing the experimental trends observed for dust explosions. The present contribution entails an experimental study of turbulent flame propagation in a 3.6 metre flame acceleration tube, and two types of combustible mixtures: propane-air mixtures and mechanical suspensions of maize starch and air. The experimental approach is similar to that of Pu et al., but the tube used here is twice the length, has a quadratic rather than circular cross section, and is oriented horizontally instead of vertically. The main focus in the current study is to explore reliable and robust methods for detecting time of flame arrival in turbulent dust flames. The experimental procedure for tests with initially turbulent flow conditions is essentially the same for dust and gas explosions, and for gaseous fuels it was also possible to investigate initially quiescent mixtures. Only constant volume experiments are included here, since such tests are simple to perform and well suited for validating the methodology. Future work will focus on improving the methodology and exploring alternative measurement principles, such as ionization gauges or optical detection. It is foreseen that experiments with ionization gauges may clarify the uncertainty associated with the apparent premature detection of rapid temperature rise obtained with the thermocouples, since the presence of ions may serve as a less ambiguous criteria of flame arrival, compared to the observation of a visible flame.

Paper #300

**Computational Model of a Biomass Cookstove**

*Jennifer L. Jones, Ashok Gadgil, Carlos Fernandez-Pello*

Over 2 billion people worldwide (1/3 of the world's population) use biomass fuels for cooking and heating. Emissions from the combustion of biomass fuels include toxic gases and particulates that pose serious health risks for families using cookstoves, especially women and children, accounting for 1.6 million deaths globally per year. Additionally, the aggregate amount of black carbon (soot) and greenhouse gases released to the environment by cookstoves use is a major concern for the global climate. Most of the work on biomass stoves has been empirical and through trial and error. Only a handful of research groups have attempted to begin numerical modeling of biomass stoves. A numerical model is

needed because there are many people and cultures worldwide that use cookstoves and one cookstove doesn't fit all. Most stoves in operation are heavy polluters and operate inefficiently. A comprehensive, computational model of a biomass cookstove would help stove designers and policy makers bring more efficient stoves to the field, leading to decreases in health risks and environmental concerns from cookstoves use. The objectives of this work were to build a simple numerical model of a biomass stove as a first step toward a comprehensive, computational model, to assess the capabilities of the Fire Dynamics Simulator CFD program for modeling a biomass stove, and to determine the direction for future stove modeling work. Model output included visualization of the fire and flow field, and predictions of the mass loss rate, the heat release rate, stove wall temperatures, and emissions. The model predicted the highest velocity flow (on the order of 1 m/s) out of the top of the stove toward the back in a symmetric crescent-like pattern, and it is anticipated that the greatest convective heat transfer to a pot is along this region. The maximum heat release rate and burn rate were increased by 100% for the adiabatic case compared to the baseline case. Maximum stove wall temperatures were 200% higher for the adiabatic case when compared to the baseline. The maximum emission rate of carbon monoxide, carbon dioxide, and soot out of the top of the stove increased by 50% for the adiabatic case. When compared to empirical data, model predictions of  $CO/(CO + CO_2)$  versus black carbon emission reproduce one of the two branches obtained empirically and predictions were an order of magnitude less than empirical data. Due to the limitations of FDS, including conformance to a rectilinear mesh and limitations of the devices used to specify output data, another CFD program with more advanced pre-processing capabilities would be more appropriate for working with the geometry of a biomass stove. Further model refinement could enable predictions of stove performance based on various stove input conditions to ultimately design more efficient, less polluting stoves. In addition to being a contribution to fundamental knowledge in combustion of biomass fuels, heat transfer, and fluid mechanics, a comprehensive, computational model of a biomass stove would be valuable to researchers, designers, engineers, and those in public policy for various stove applications.

Paper #323

**Turbulent Premixed Methane-Air Jet Flames: A Numerical Study**

*M. Chekired, M.S. Boulahlib, Z. Nemouchi*

This paper report an application of a reduced scheme for methane combustion based on a two steps reduced mechanism proposed by N. Peters and F. A. Williams (Combustion and Flame, Vol. 68, Issue 2, pp.185-207, 1987). The experimental data of the so called F flames studied by Y.C Chen and al (Combustion and Flame, Vol. 107, No.3, pp. 223-244, 1996) were considered to test the predictive ability of the adopted reduced mechanism used in the context of Reynolds Averaged Navier Stokes (RANS) approach. The obtained numerical predictions are compared to the measurements data, showing a good overall agreement. In the context of the same study, other results reporting RANS calculations of the studied flames using various combustion chemistry models are also discussed.

Paper #325

**Predictive Flame Propagation Model for Stochastic Reactor Model Based Engine Simulations**

*Simon Bjerkborn, Cathleen Perlman, Karin Fröjd and Fabian Mauss*

A stochastic reactor model (SRM) based spark-ignition engine simulation code allowing for detailed chemistry based knock prediction has been extended with a predictive flame propagation model. The previously used Wiebe function approach, has been replaced by a turbulent flame propagation model where the underlying laminar flame speeds rely on detailed chemistry calculations. This new model development allows for studying the effects of fuel chemistry on the flame propagation event, in addition to determining the knock limit. The turbulent flame propagation model is based on a formula derived by Kolla et al. from Kolmogorov-Petrovskii-Piskunov (KPP) analysis. It was simplified to better suit the application, while retaining the features allowing for general application. Parameters which could be assumed constant for a large spectrum of situations were replaced by three parameters. The laminar flame speeds were retrieved from a extensive library, by the use of an advanced correlation function. The model was qualitatively validated for different cylinder head geometries, by comparison with earlier results from Poulos and Heywood. Good agreement was found. The model was further validated for a 4-cylinder passenger car engine, achieving good agreement with experimental data. The model shows great potential in prediction of flame propagation as well as knock for SI engines. The usage of detailed kinetics makes the model well suited for emission studies.

Paper #332

**Plasma Assisted Ignition below Self-Ignition Threshold in Hydrogen-Air and Hydrocarbon-Air Mixtures**

*L. Wu, J. Lane, N.P. Cernansky, D.L. Miller, A.A. Fridman, A.Yu. Starikovskiy*

This paper presents measurements of time evolution of hydroxyl (OH) radicals in premixed HC-air flows in the afterglow of a nanosecond pulsed discharge at atmospheric pressure. The temperature ranged from 300 to 800 K (below the self-ignition point). The fuels were methane, ethane, propane and butane, at an equivalence ratio of 0.1 from 400 to 800 K. The plasma was generated by 20 kV pulses of 10 ns duration and a <1 ns rise time at repetition rate of 10 Hz. The tip electrode shape ensured a uniform streamer discharge in the gap of 8 mm. The reactant flow rate was set at ~20 cm/s so that each discharge pulse occurred in a fresh gas mixture. Laser induced fluorescence was used to measure the concentration of OH radicals after the discharge. The energy of the excitation laser was adjusted to insure that the measurements were made under saturation conditions for all experiments. The time evolution of OH radicals was tracked by adjusting the delay time between the high-voltage pulse and the concentration measurement.

Paper #334

**Solid Rocket Motor Internal Ballistics Using a Least-Distance Surface-Regression Method**

*C. H. Chiang, Y. H. Hwang*

In the present work, we have successfully developed a practical design tool to simulate the erosive volume and associate burning area which can be integrated to solve a nonlinear, pressurization-rate dependent combustion during grain regression in solid propellant. The least distance method is first proposed and verified with a two-dimensional test problem. Then the least method is implemented to solve a three-dimensional grain burn-back problem. A simple motor of two practical configurations is examined by this method with tetrahedral cells grid arrangement to predict the erosive volume and burning area. The predicted pressure curves do reasonably agree with the projected design data.

Paper #340

**Numerical Investigation of Supersonic Combustion of the Hyshot II in the Shock Tunnel**

*Chih-Peng Chen, Dun C. Liu, Guan-Bang Chen and Ruey-Hung Chen*

There has been widespread interest in air-breathing supersonic combustion and its applications in scramjets. Due to the complexity of the engine and the high cost of experimental investigations, numerical investigations have been adopted by many researchers and, once validated by the measured results, they can be used to capture the salient features of the combustion phenomenon and flows within the scramjet. This paper aims at using the commercial software, FLUENT, to investigate the thermodynamic properties in the HyShot II combustor. To assess the effect of different turbulence models in the supersonic hydrogen-air combustion process, three turbulence models, namely, the Spalart-Allmaras (SA) model, the Realizable  $k-\epsilon$  model (RKE), and the Shear Stress Transport turbulence model (SST- $k\omega$ ) have been implemented. The evaluation of chemical reaction mechanisms is done by considering both the single-step and the multi-step reaction mechanisms. It is found that the SST- $k\omega$  model shows best results and significant difference in pressure and temperature is observed between the results obtained using the single-step and the 19-step reaction mechanisms.

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**11:10 Poster II - Detonation**

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Paper #52

**Numerical Study of Shock-Flame Interaction and Deflagration-to-Detonation Transition in H<sub>2</sub>-O<sub>2</sub> Mixtures Using a Detailed Chemical Reaction Model***A. D. Kiverin, M. F. Ivanov, M. A. Liberman*

We report two-dimensional simulations of the shock interaction with wrinkled laminar flame and deflagration-to-detonation transition in tubes with smooth slip and no-slip walls. The computations solved the multidimensional, time-dependent, fully resolved reactive Navier-Stokes equations including the effects of viscosity, thermal conduction, molecular diffusion, real equation of state and detailed chemical kinetics for the reactive species H<sub>2</sub>, O<sub>2</sub>, H, O, OH, H<sub>2</sub>O, H<sub>2</sub>O<sub>2</sub>, and HO<sub>2</sub> with subsequent chain branching, production of radicals and energy release. The objectives are to examine the effects of interaction of the incident and reflected shocks of different strength with the flame, the flame acceleration and the transition to detonation. The incident shock strength was varied from M=1.2 to 2.5. The perturbation resulting from the shock-flame interaction grows due to the Richtmyer-Meshkov instability and this leads to an increase in the burning rate. Development of the instabilities is analyzed accurately and clear scenario of the increase in flame surface and burning rate is formulated. The flame accelerates due to the wrinkling of the flame front caused by the instabilities and consequently the increase of the flame surface. Depending on the strength of the incident shock there are different scenarios of the shock-flame interaction and the transition to detonation. Results of the simulations show a complex sequence of events: from the interactions of an incident shock with an initially laminar flame, development of the RM instability and wrinkled flame front and finally the emergence of a self-sustained detonation with typical detonations cells structure. However the mechanism of detonation formation remains similar in the variety of cases: the flame couples with the pressure wave and transforms into detonation due to the concurrent increase of the pressure and reaction rate.

Paper #160

**The Determination of Atmospheric Pressure Linear Burning Rates of Solid Propellants Formulations***Frederick Paquet, Hoi Dick Ng*

Accidental propellant fires usually occur at standard atmospheric conditions. As most propellant applications are designed to operate at pressures much larger than the atmospheric value, very few published linear burning rates results are available at low pressures. In this study, the measurement of the atmospheric pressure linear burning rate of a nitrocellulose based formulation has been performed. A short review of previous publications in linear burning rate measurements is first presented. The empirical results are then shown followed by a short discussion on their analysis. It is also shown that the combustion front has a shape similar to what has been observed with other materials in past studies.

Paper #208

**Experiment Research on Continuous Detonation Engine***Jianping Wang, Tianyi Shi, Yuhui Wang, Yusi Liu, Yongsheng Li*

Continuous detonation engine is a new concept engine, which with conventional engine compared, in the thermal efficiency and rushed have essentially than the advantage. To it and experimental study to primarily validate feasibility of continuous detonation is currently the focus of the work. The author independent design and combustion chamber, inlet, ignition system, preliminary experiment verified the feasibility of continuous detonation.

Paper #225

**Study of Nitrogen Dilution, Pressure and Temperature Effects on Spherical Flames Propagation of H<sub>2</sub>/O<sub>2</sub>/N<sub>2</sub> Mixtures***SABARD Jérémy, CHAUMEIX Nabihah, CATOIRE Laurent, BENTAIB Ahmed*

Accidental explosion is still a challenging issue which has to be taken into account in the design of any new industrial or research facility. The evaluation of the explosion hazard relies on the knowledge of the fundamental properties of the targeted combustible mixtures such as the laminar flame speed, the auto-ignition delay time, the detonation cell size. These parameters are determined in well-defined laboratory experiments. In the framework of the safety of the International Thermonuclear Experimental Reactor (ITER), an analysis has to be performed regarding the explosion risk of mixtures containing hydrogen and air which may contain dust. Indeed, during the normal operation of ITER, a large amount of metallic dust (tungsten and beryllium) and graphite particles are generated due to the interaction of the plasma with the Vacuum Vessel walls. Moreover, in case of a Loss Of Vacuum Accident (LOVA) scenario, oxygen is formed leading to a mixture of hydrogen / oxygen / air / dust. If for hydrogen / air mixtures many data can be found in the literature, they become scarce when oxygen and/ or dust are included. This paper reports laminar flame properties H<sub>2</sub> / O<sub>2</sub> / N<sub>2</sub> mixtures over a wide range of hydrogen molar fraction (0.1 to 0.6), nitrogen to oxygen ratio (0.66 to 9), initial temperature (303-383 K) and initial pressure (50 - 300 kPa). The combustion of these mixtures was studied using a stainless steel spherical chamber with an internal diameter of 476 mm equipped with an electric central ignition. A high speed imaging is used to visualize the outward flame propagation from which the unstretched laminar flame speed is deduced. A high speed piezo-electric pressure transducer is used to monitor the evolution of the pressure inside the vessel during the combustion. From this signal, the maximum combustion pressure and pressure rise rate are extracted. Two detailed kinetic mechanisms (Wang and Mével models) are used to calculate the laminar flame speed and to compare to with the experimental one using a 0-D code (COSILAB software). From this comparison the most suitable mechanism will be chosen and used to derive the activation energy of these mixtures as a function of initial conditions of

composition, temperature and pressure. The main difference between these two mechanisms is the presence or not of nitrogen species. Moreover, equilibrium calculations are performed and the theoretical maximum combustion pressure (PAICC for Adiabatic Isochoric Complete Combustion Pressure) is compared to the experimental one.

Paper #295

**Asymptotic Study of Pulsating Evolution of Overdriven and CJ Detonation with a Chain-Branching Kinetics Model**

*Carlos Chiquete and Mark Short*

The pulsating dynamics of gaseous detonations with a model two-step chain-branching kinetic mechanism are studied asymptotically and numerically. The model comprises a chain-initiation/branching zone with an Arrhenius temperature-sensitive rate behind the detonation shock where fuel is converted into chain-radical with no heat release. This is followed by a chain-termination zone having a temperature insensitive rate where the exothermic heat of reaction is released. Based on an assumption of small non-dimensional inverse activation energy in the chain-initiation zone, it is shown that the pulsation period for this model must be defined by the non-dimensional activation energy times the particle transit time through the chain-initiation zone, while the length of the chain-termination zone must be of the order of the non-dimensional activation energy longer than the chain-initiation zone. A set of reduced PDEs in the chain-termination zone are derived when govern the unsteady evolution. The acoustic terms in the PDE are linearized but have spatially varying coefficients, while nonlinearity enters through the motion of the interface between the chain-initiation and chain-termination zones. Solutions of the reduced PDE system are obtained. The work sheds significant light on the ratio of length and time scales and their relationship to a basic model of gas-phase chain-branching reaction kinetics that underlie pulsating detonation behavior.

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**11:10 Poster II - Flame**

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Paper #6

**Combustion and Evolution of the Polycyclic Aromatic Hydrocarbons in Diesel Engine***Ju Hongling, Cheng Xiaobei*

Three-dimension numerical simulation in cylinder combustion was carried based on a single cylinder direct inject diesel engine, while the detail chemical reaction mechanism of n-tetradecane [7] was considered (230 chemical reactions, 92 chemical species), and enthalpy calculate subroutine of chemical species was built. The formation and evolution mechanisms of aromatic (benzene) and polycyclic aromatic hydrocarbon PAHs; phenylacetylene, styrene, naphthalene, acenaphthylene, acenaphthene, phenanthrene, pyrene, which was the precursor of soot particle, was calculated on, and soot particle mass in cylinder combustion was calculated by Belardini soot model. The effect PAHs on soot formation was analyzed. Soot-NO trade-off for different inject timings was simulated, and compared with experimental value [12]. The results show that numerical simulation of pressure through this computational model is in good agreement with the experimental results. Combustion happened firstly in the piston bowl, and then happened in other positions of the combustion chamber with the developing of combustion (develope clockwise along the piston bowl). In this process, Aromatic and polycyclic aromatic rapidly go up in the start of combustion, and then go down, and later to a stable value in the end of combustion, and distribute in the top of cylinder. According to numerical simulation for different inject timings, it is found that soot and NO emissions are best in  $-20^\circ$  TDC. Emissions of benzene, phenylacetylene, acenaphthene and phenanthrene are bigger than the others, and have a greater impact to soot formation.

Paper #7

**A Study on Flame Propagation through a Narrow Channel***Shigeharu Ohyagi, Teruo Yoshihashi, Tetsuro Obara and Jifeng Du*

This study reports behaviors of premixed flames in stoichiometric methane-air and hydrogen-air mixture propagating through a narrow channel. The flame is ignited in a n upstream chamber of volume 35 to 77 cm<sup>3</sup> and it propagates through a narrow channel with 0.3 to 2.2 mm width and 20 to 40 mm in length. Finally the flames are released into a downstream chamber. Parameters are an initial pressure, the width and length of the channel. The behaviors of flames are visualized by schlieren using high-speed video camera. The phenomena are classified into to categories of quenching and propagation whether the flame survives in the downstream chamber. The results are summarized as a dependency of quenching distance defined as a width below which a flame cannot propagate to the downstream chamber. Effects of the initial pressure, the length and the upstream volume are discussed for methane-air and hydrogen-air mixtures respectively. The following conclusions are derived. The flames ignited in the upstream chamber propagate through the channel and ignite the mixture in the downstream chamber if the width of the channel is greater than a certain critical distance which is called as a quenching distance. The quenching distance defined above is decreased as the initial pressure of the chambers is increased. For hydrogen/air mixtures, it is decreased as  $p-1.15$ , while for methane/air mixtures, it is decreased as from  $p-1.1$  to  $p-1.8$  which does not follow the usual quenching theory. The quenching distance is decreased as the volume of the upstream chambers is increased. The quenching distance is increased as the length of the channel is increased. The quenching distances for methane/air mixtures are one order magnitude larger than those for hydrogen/air mixtures.

Paper #356 (was 15)

**Characteristics of Combustion of a Rich-Lean Flame Burner with Controlled Boundary Zone between Rich and Lean Flames***Katsuo Asato, Hirofumi Yasuda, Takeshi Miyasaka, Hiroshi Eguchi, Kazusa Kondo, Hiroshi Yamashita*

The effects of an air or a fuel-air mixture supplied to a boundary zone between rich and lean flames on the characteristics of the combustion and emission of NO and CO were numerically investigated in order to develop a new type of rich-lean flame burner with low emissions of NO<sub>x</sub>, CO and a high turn-down ratio (TDR) for domestic hot water generators and room heaters. When air is supplied to the boundary zone between rich and lean flames, the formation of prompt NO is reduced owing to the marked decrease in HCN concentration at the rich flame due to diluting the rich flame mixture with the air. The formation of thermal NO is also decreased by a decrease in the temperature of the burned gas due to the air supplied to the boundary zone. The oxidation reaction of CO is promoted by the air supplied to the boundary zone and the area of high CO concentration is also reduced. The characteristics of NO and CO emissions for the rich-lean flame burner with the controlled boundary zone are superior to those for the conventional rich-lean flame burner. The NO concentration exhausted from the burner is significantly affected by the amount of NO produced at the rich flame. It is important to optimize the burning ratio of rich and lean flames and the air ratio of the rich flame to reduce NO emission from the rich-lean flame burner. The calculated results for the profiles of temperature, NO and CO concentrations, flame appearance and the limits of flame stabilization accurately predict experimental results, showing that it is possible to realize a new type of rich-lean flame burner with a high TDR and low NO and CO emissions by controlling the boundary zone between rich and lean flames.



Paper #35

### **Structural Differences between the Non-Reacting and Reacting Supersonic Planar Mixing Layer**

*Huanhao Zhang, Zhihua Chen, Baochun Fan, Xiaohai Jiang*

The two dimensional supersonic no-reacting and reacting mixing layer has been simulated with the employ of large eddy simulation and fifth-order WENO scheme. The structural changes due to the combustion have been shown. Moreover, the effects of inflow pressure on the layer structure have also been investigated.

Paper #36

### **Horizontal Flame Spread Along Paper Sheet with a Backing Board**

*Takashi Tsuruda*

For the case of horizontal flame spread along paper sheet with a backing board, lower side propagation occurs during ignition when the combustible is externally heated. The minimum separation between the combustible and backing board surfaces exists for the horizontal flame spread. If the separation is smaller than this minimum separation, no flame propagation occurs with a finite heating. Once the separation is larger than this minimum separation, flame propagation occurs. As the paper is heated externally, the thermal boundary layer grows near the paper surface. As the thermal layer grows, the temperature gradient in the horizontal direction also grows and lateral convection layer will form in this temperature boundary layer. Once, this lateral convection layer formed, the heat and mass transfer rates increases and flame propagation may occur. In this study, a numerical simulation of two dimensional flow field heated from upper side is carried out to investigate the governing mechanisms of the ignition of horizontal flame spread along paper sheet with a backing board.

Paper #354 (was 39)

### **Gasdynamics in Turbulent Premixed Combustion: Conditionally Averaged Unclosed Equations and Analytical Formulation of the Problem**

*Vladimir L. Zimont*

We state an alternative paradigm for description of the Bray-Moss-Libby (BML) turbulent premixed combustion mechanism where instantaneous chemical transformation takes place in strongly wrinkled laminar flame. The standard approach is based on Favre averaged equations and it yields a challenge of prediction of the scalar flux, which is controlled by turbulence and gasdynamics, and can be gradient, counter-gradient and neutral. Our approach is based on a special form of conditionally averaged continuity and impulse equations, which contains minimal number of requiring modeling unknowns. We state a set of unclosed equations, which describes both combustion and hydrodynamics sub-problems where the mean scalar flux and stress tensor in the premixed flame do not need special modeling. We state unclosed equations in terms of requiring modeling conditionally averaged turbulent stresses and mean chemical source and give the analytical formulation of the turbulent combustion problem, which including infinite number is unclosed equation is asymptotically closed, while every finite sub-system is unclosed and need modeling. This more general viewpoint on the problem permit, in particular, to state conceptually correct form of unclosed conditional averaged equations. A conclusion: The Favre averaged hydrodynamics equations in the context of the BML combustion mechanism is not adequate tool for description of the gasdynamic impact on the transfer in the turbulent premixed flame and this inadequacy yields a challenge of modeling the counter-gradient scalar flux phenomenon. An adequate tool is conditionally averaged hydrodynamics equation where the problem of modeling of the scalar flux (as well as the stress tensor) in the flame does not arise. Keywords: BML model, alternative approach, conditionally averaged equations

Paper #40

### **Determination of $\alpha$ -Pinene/Air Premixed Flame Speeds Involved in Accelerating Forest Fires and Real Accidents**

*Courty, L., Chetehoua, K, Halter, F., Foucher, F., Garo, J.P. and M. Rousselle, C.*

Forest fires are responsible for important damages every year, in economical and ecological terms as well as in human lives losses. They can cause important disturbance to ecosystems and, due to global warming, they are becoming an increasing threat for countries at the North of the Mediterranean Sea but also for other regions in the world. The average surfaces destroyed by forest fires every year all over the world and in Europe are respectively 28 and 1.6 billion ha. Several researches have reported that under certain conditions wildland fires behave in a surprising way, changing suddenly from an ordinary behavior (moderate rate of spread) to an explosive propagation (rate of spread and energy released much more important). This phenomenon is called forest fire blowup or accelerating forest fire for its explosive nature, or eruptive fire for its rate of spread continuous increase. Fires propagating in canyons can lead to such fire explosions and are responsible for many fatalities in the past. Indeed, the Guadalajara accident in Spain in 2005 caused the death of eleven persons. More recently, this phenomenon happened in Artemida (Greece, 2007), killing 24 persons. The mechanisms which explain this type of forest fires are not totally well known yet. There are nowadays two hydrodynamic approaches to explain this phenomenon. The first one is based on the feedback effect of the convection induced by the fire which can happen naturally in steep terrains. The second explanation is that this phenomenon is the result of an increase of the rate of spread caused by flow attachment in the direction of the fire spread. A thermochemical approach, based on the ignition of a Volatile Organic Compounds (VOCs) cloud, has been proposed in a previous work. This hypothesis suggests that the acceleration of the rate of spread is the consequence of the ignition of the VOCs emitted by fire heated vegetation and accumulated in canyons. It has been shown that monoterpene hydrocarbon ( $C_{10}H_{16}$ )  $\alpha$ -pinene is the major component emitted by a *Rosmarinus Officinalis* plant when heated by a radiant panel simulating the fire front. Very recently, it has been demonstrated using empirical correlations that the VOCs mixture is in the flammability domain in canyons where real accidents occurred. Forest fires propagation models do not take yet into account this possible VOCs cloud ignition. An accurate modeling of such a phenomenon requires measurements of the

laminar burning speed of these VOCs. Knowing this fundamental parameter, it will be possible to predict these accidents with the existing propagation models. The spherical expanding flame method has been chosen to determine the laminar combustion fundamental parameters of alpha-pinene. This is the aim of this study. The experimental setup and conditions are presented, followed by the methodology used to determine the stretch influence on the flame speed. The flame speeds of alpha-pinene/air mixtures as functions of equivalence ratio for different temperatures are then presented, discussed and compared to those obtained with real accidents.

Paper #48

#### **Local Quenching Recovery Mechanisms and Flamelet Structures in a Heterogeneous Combustion**

*Yuji Yahagi, Takayuki Kawanami, Hirokazu Takeda*

This paper discusses about local quenching and its recovery mechanisms for a heterogeneous combustion based on the turbulent flamelet structures. A heterogeneous combustion can observe in various practical combustors. Especially the gasoline direct injection spark ignition engine and the direct injection compression injection engine operating in the multi mode injections are typical examples. In order to create a heterogeneous combustion in the lab scale we proposed a turbulent opposed burner. A lean premixed CH<sub>4</sub> air impinges with a CH<sub>4</sub> diluted with N<sub>2</sub> having different turbulence conditions and creates two flames within the local quenching condition. The local quenching phenomena and two dimensional instantaneous flow structures have been measured by using a particle image velocimetry movie. The local quenching phenomena can be observed frequently near the global extinction condition. The local quenching may trigger to induce the global extinction. However, in many cases, the flame can recover from the local quenching phenomena. Four distinct local quenching recovery mechanisms namely passive mode (P mode), active mode (A mode), eddy transportation mode (E mode) and Global extinction induced mode (G mode) are observed. Those modes depend with the local quenching scale and its starting location, the local flame propagation mechanism, the bulk flow motion, and the eddy motion by turbulence. Especially, the structure of the flamelets and incoming reactive flows are very important issues to concluding the local quenching recovery mechanisms. Especially, immediately after the local quenching even, the mixing zone creates in the quenching zone. The fuel concentration of lean premixed gas may increase from the original condition and the local propagation speed increases in the zone. This increased propagation speed may become driving force to the local quenching recovery mechanisms. In addition, the flamelets transported by the eddy motion also helps to recover from the local quenching event.

Paper #75

#### **Heat Transfer Parameters During Limit Flame Propagation in Small Tubes**

*Artur Gutkowski*

Zeldovich and Spalding were the first to propose the thermal theory of flame propagation limits in gas mixtures. They shown that flame propagation in narrow channels/tubes is impossible if the characteristic dimension is smaller than the critical value. The combustion limit in channels/tubes is usually characterized by the quenching (critical) value of the Peclet number. Aly and Hermance presented thorough two-dimensional numerical simulations of laminar flame quenching, and a quenching Peclet number value of 60 for stoichiometric mixture was obtained. Their results have also shown that  $Pe_q$  increases with decreasing mixture concentration. Numerical exploration of flame propagation in tubes and in parallel plate channels, by Hackert et al., has obtained Peclet number varying from 15 to 60 according to heat loss. Experimental works of Jarosinski et al., which have been conducted in the vertical wedge-shaped channel, showed that  $Pe_q$  in a broad range of mixture composition is constant and equals to 42. For rich mixtures it gradually decreases. In this article, the downward propagation and quenching of lean premixed propane-air flames in small tubes, which are opened at the ignition end and closed at the other, are simulated using a numerical procedure for reacting flow. Mixture concentration is recognized as a limit concentration if all heat generated in the reaction is transferred to the wall and it does not cause a flame quenching. If the mixture concentration is below this limit flame is quenched just at the entrance to the tube or after propagating some distance in it. Limit flame propagation velocity for 3 mm tube diameter is equal to 17.4 cm/s. Laminar burning velocity taken from literature and corresponding to  $\Phi = 0.799$  is about 29.2 cm/s. The ratio of these two values gives 0.596 which is close to 0.61 theoretically predicted by Zeldovich. This relation is not constant for all tubes, but increases with tube diameters. Heat loss to the wall influences flame behavior in the tube. This parameter was found using a heat flux between isothermal wall and adjacent fluid. Heat transfer coefficient increases with decreasing of the tube diameters. It rises almost linearly from 42 W/m<sup>2</sup>/K for the widest tube to 178 W/m<sup>2</sup>/K for 3 mm tube diameter. Nusselt numbers for these tubes are equal to 13.4 and 18.7 respectively. It suggests that heat loss to the wall is the most intensive during flame propagation in 3 mm tube. Two quenching Peclet numbers related to limit flames were determined. The first one is based on limit flame propagation velocity instead of the adiabatic laminar burning velocity. It is equal to 21.7÷22.1. The second  $Pe_q$  was modified by taking into account thermal conditions between hot combustion products and cold wall for calculating thermal diffusivity. Using this definition calculated  $Pe_q$  is lower and is equal to 17.3÷17.8.

Paper #87

#### **Experimental Investigations on Pressure Swirl Atomized Lifted Flames in a Co-flow Field**

*V Mahendra Reddy, Darshan Trivedi and Sudarshan Kumar*

In this paper, an attempt has been made to understand the effect of the coflow velocity on the flame stabilization behavior of lifted spray flames. A spray is created using a pressure atomized swirl injector. The mean droplet size varies from 40 to 65 micro meter with a change in the injection pressure. It was observed that the flame lift-off height increases linearly

with the coflow velocity for normal air case. However when air is diluted with nitrogen, the lifted spray flame behaves differently. The flame blow off occurs at much lower coflow velocities and the fluctuations in the lifted flame are relatively much higher.

Paper #170

#### Numerical Study on Combustion Stability of n-Heptane /Air in a Micro Tube Combustor

LI Junwei, WEI Zhijun, WANG Ningfei

To understand effect of heat recover and heat loss on flame stability in a micro tube, two tube burners with and without an outer tube are designed and numerically studied, using commercial CFD software Fluent. Dimensions of the inner tube are 4 mm in inner diameter and 49.5 mm in length. The outer tube in Model 2 is 10 mm in inner diameter. Navier-Stokes equations coupled with one step reaction mechanism of heptane and air are employed and gas radiation is also considered. A pressure atomizer is used to inject liquid n-heptane droplets. n-heptane flow rate of 1mg/s is fixed, and the droplet diameter is 1 $\mu$ m. The Discrete Phase model of FLUENT has been exploited to model the droplet phase. The results show that first, for a tube burner without heat recovery, the location and temperature of diffusion flame change with the air velocity and heat loss coefficient. With increase of equivalence ratio, reaction zone is moving from the entrance to the exit. When air flow velocity is low, the flame is mainly located in the vicinity of the fuel injector and its length is very short. With the increase of air flow, the flame is stretched and its length increases. If there is a large air flow rate or heat loss coefficient, the flame would be blown out of the tube. Second, for a tube burner with heat recovery, it can stably work at a wider range of equivalence ratios and higher heat loss coefficients. But the flame position and its shape may be varied. Since the outside wall of the burner with heat recirculation is not adiabatic and the exhausts would take away heat from it. Its fuel-rich limit is smaller than that of the burner without adiabatic wall. Finally, with the increase of heat loss coefficient, the flammable limits of the latter are much wider than that of the former. This is due to the fact that hot exhausts preheat the unburned gas through the inner tube wall and the flame stability is enhanced.

Paper #175

#### Ignition Transition in Turbulent Premixed Combustion at Elevated Pressure

C. C. Liu, S. S. Shy, M. W. Peng, H. J. Chung, Y. W. Hsiu

Just recently, Shy and his coworkers conducted a series of turbulent premixed combustion experiments at atmospheric pressure condition to measure the minimum ignition energy (MIE), a probabilistic variable of 50% ignitability, of methane-air mixtures over a wide range of the equivalence ratio  $\phi$  varying from 0.6 to 1.3. They found a turbulent MIE transition, across which both values of MIE and ignition flame kernels change drastically. From their complete turbulent MIE dataset, a physical model based on a reaction zone Péclet number ( $P_{RZ}$ ) defined as the ratio of turbulent to molecular diffusivities was then proposed to explain such turbulent MIE transition. Using the same ignition methodology, this work presents a complete data set of lean CH<sub>4</sub>-air mixtures at  $\phi = 0.7$  and an initial pressure  $p = 0.3$  MPa under both quiescent and turbulent conditions, in which the normalized turbulent intensity  $u'/S_L$  are varied from 0 to about 80, where  $S_L$  is the laminar burning velocity. These high-pressure turbulent ignition experiments are conducted in a recently-established high-pressure double-chamber explosion facility, in which an inner chamber, similar to the previous fan-stirred cruciform burner used in the atmospheric condition, is resided in a very large high-pressure absorbing vessel (the outer chamber). It is found that values of MIE required for the same flammable mixtures at  $p = 0.3$  MPa are lower than those measured at atmospheric pressure under either laminar or turbulent conditions. More importantly, a MIE transition is also found to exist in the present high-pressure turbulent ignition case, showing two different regimes. In the first regime, values of MIE are found to increase modestly with increasing  $u'/S_L$  up to 60. When values of  $u'/S_L$  are increased further, a very steep increase of MIE values can be found in the second regime right after the transition. Comparison of the present high-pressure MIE data with the previous atmospheric MIE data is presented in terms of  $P_{RZ}$ . It is shown that the critical value of  $P_{RZ}$  at which the MIE transition occurs is larger for the present high-pressure MIE measurement ( $P_{RZ} \approx 6.3$ ) than that for the previous atmospheric case ( $P_{RZ} \approx 4.5$ ). This implies that the threshold of turbulence level relative to the molecular transport for the mode transition from flamelet-like turbulent wrinkled kernel to distributed-like broken kernels needs to be raised at elevated pressure due to the increase of the associated reaction intensity within the smaller flame kernel volume  $\delta_v$  where  $\delta_v \sim \delta_F^3$  and  $\delta_F$ , the laminar flame thickness, decreases with increasing pressure.

Paper #191

#### Stability of Premixed Flames in Narrow Channels

Diego Alonso and Mario Sánchez-Sanz

This paper studies the stability of premixed flames in a narrow channel with a step-wise, prescribed wall temperature, a simple model of a "Swiss-roll" reactor, straight section. We focus on the influence of the equivalence ratio ( $\Phi$ , fuel/oxydizer ratio), the reduced Damköhler number ( $Da$ , hydraulic diameter/flame thickness ratio), and the fuel (through the Lewis number,  $Le = \alpha/D$ ) on the flame dynamics, where  $\alpha$  and  $D$  are the thermal conductivity and the diffusivity, respectively. We consider a gaseous, low-Mach, premixed mixture of air and a fuel flowing in a bidimensional channel. The wall temperature is maintained at the inlet value,  $\theta = 0$ , for  $x' < 0$  and for  $x' > 0$  it jumps to a higher value,  $\theta_w$ , until the outlet section of the duct. The non-dimensional temperature is defined as  $\theta = (T - T_0)/(T_s - T_0)$ , where  $T_0$  is the inlet temperature and  $T_s$  is the adiabatic temperature.  $x'$  and  $y'$  are the non-dimensional co-ordinates along the longitudinal and transverse directions, respectively; they are referred to the channel height. The governing equations are the continuity, momentum, and energy equations for the mixture plus the reaction-diffusion-convection equations for the fuel and oxydizer mass fractions. Viscosity and the thermal conductivity follow a presumed power-law dependence with temperature. The chemical model is a single-step reaction on the form  $F + O \Rightarrow P$ , where  $F$  denotes the fuel,  $O$  the oxydizer and  $P$  the products. The combustion rate is assumed to follow an Arrhenius law. Representative values of the

Zel'dovich number and heat release parameter have been chosen and are kept fixed. Relevant previous studies are those by Kurdyumov and Pizza. Unlike the former, which analyzes the instabilities in a similar problem applying a thermal-diffusive model to a very fuel-lean mixture, we study mixtures with higher equivalence ratios and temperature-dependent properties. The latter uses a detailed mechanism to study the instabilities of a lean hydrogen/air mixture and do not consider several fuels or equivalence ratios.

Paper #212

### **Experimental Study about Instability in Global Lean Combustion**

*Marcel Martins Alves, Rogério Corá, Pedro Teixeira Lacava*

It's already known that lean equivalence ratio systems are susceptible to combustion instabilities because flame velocity is low in these systems, thereby turning more difficult for the flame to recover its structure when non-uniform energy release happens due to failures in reactant mixing process. The main objective of the present paper is to study experimentally acoustic instabilities in extremely global lean combustion situations. It is a fundamental work, but the main motivation is that some new combustor concepts for low NO<sub>x</sub> emissions in gas turbine are based on this combustion conditions in the reaction zone. The combustion chamber that was used for the experiments was built of 304 stainless steel and it is divided into 6 non-refrigerated modules. The length of the six modules are respectively 0.10 m, 0.40 m, 0.25 m, 0.25 m, 0.20 m, and 0.10 m; and the inner diameter of the chamber is 0.15 m. The feeding system of the combustion chamber consists of a device that is responsible for burning natural gas. Natural gas is supplied by a central duct and air is supplied by an annular region concentric to the central fuel. The reactants are not premixed before their injection into the chamber; however air and fuel injections are carried out in a way that a mixture is formed before the flame region. The fuel is injected radially through ten holes at the end of the duct. A disk is positioned slightly below the fuel injection holes in order to create a recirculation zone by the passage of air through the holes. On the disc, there are two rows, of ten holes each, for axial injection of air over the radial fuel flow, thereby creating a mixture between air and natural gas, which is involved by the recirculation zone, and finally ignited. In this work, instability mechanisms were experimentally studied in global lean combustion conditions. It was observed that energy, released by combustion, and flame velocity are related to each other depending on global equivalence ratio. It was also determined how the flame suffers when energy release fluctuations occur. Besides, the results showed that it is possible to obtain combustion operations in extremely lean global equivalence ratios conditions either without or with low combustion oscillation presence.

Paper #215

### **Laminar Flame Velocities and Fundamental Properties for Two Methane Based Mixtures: G27 and G222**

*Kodjo Coudoro, Nabih Chaumeix, Bentaib Ahmed, C-E Paillard*

The occurrence of an accidental explosion as a result of the ignition of flammable gases and reactive mixtures that may be released in process industries is a major concern. In most of the accidental situations, the ignition source is either an electrical spark or a hot surface, resulting in slow laminar flames which can accelerate under certain conditions and undergo transition to detonation generating overpressures high enough to cause severe material damages. Predicting and understanding the process of flame acceleration therefore became key subjects in preventing industrial hazards. However a lot of work has been done on hydrogen/air mixtures, a little less has been done on natural gas/air mixtures. The aim of the present work is to determine the fundamental properties of natural gas - air by studying two methane based mixtures (G27 and G222) and evaluate their potential for flame acceleration in a highly instrumented acceleration tube. The laminar flame velocities and Markstein lengths were determined experimentally by studying the expanding spherical flames in a combustion bomb using high speed imaging coupled to a schlieren optical setup. The experimental laminar flames speed data were used in order to validate a detailed kinetic mechanism for natural gas combustion based on published mechanisms using COSILAB - 1D freely propagating flame. The transport properties as well as the flame temperature, the maximum theoretical pressure and the expansion ratio were estimated using CHEMKIN II equilibrium calculations. Using the chosen detailed chemical kinetic mechanism aforementioned, the activation energies were derived from the evolution of laminar flame velocities as a function of the flame temperature (COSILAB - 1D freely propagating flame).

Paper #241

### **Multi-physics Modeling of Coal Gasification Processes in a Well-Stirred Reactor with Detailed Chemistry**

*Jian Xu, Li Qiao and Jay Gore*

Fuel synthesis through coal and biomass gasification can potentially provide a solution to the increasing demand of energy and transportation fuels. To theoretically understand the complex chemical processes in a gasifier and to identify the most influential parameters on syngas production, a multi-physics model with detailed chemistry was developed for the first time to simulate the gasification processes in a well-stirred reactor. The model considers gas-phase and particle-phase reactions as well as coupling between the two phases at various scales (mass and energy exchange). The gas-phase reactions use the detailed chemistry GRI-Mech 1.2 including 177 elementary reactions and 31 species as well as multi-component transport properties and variable thermodynamic properties. For the particle-phase, four surface reactions were considered ( $C+O_2=CO_2$ ,  $C+H_2O=CO+H_2$ ,  $C+CO_2=2CO$ ,  $C+2H_2=CH_4$ ). And the reaction rates were simulated by the diffusion-kinetic model with consideration of boundary layer diffusion. The coupling between the two phases including exchange of mass and energy were modeled. A code was developed to solve gas-phase and particle-phase governing equations. Numerical simulations were conducted to understand the gasification process and the effects of pressure, O<sub>2</sub> concentration and H<sub>2</sub> addition on gasification performance.

Paper #263

#### **Hydrogen Explosion Suppression in Experiments of Different Scale**

*Gavrikov A.I., Chernenko E.V., Efimenko A.A., Mayorov A.S., Privezentsev S.S., Schepetov N.G., Zaretskiy N.P.*

The problem of hydrogen safety is very important for development of hydrogen power and nuclear power plant safety. There are different ways to suppress hydrogen combustion in a closed volume: creation of inert atmosphere, usage of different types of recombiners, and injection of phlegmatizator substances. The paper presents results of experimental investigations of different phlegmatizator additives and its binary compounds used for full hydrogen combustion suppression. The work was performed in experimental facilities of three different scales (small, medium and large) for normal initial pressure. Small scale experiments were carried out in a tube 1m length, 66mm diameter. Medium scale experiments were carried out in a tube 8m length, 121mm diameter. Large scale experiments were conducted in a polyethelen film cube, total volume of the cube was 10m<sup>3</sup>. Temperature was varied from 20 to 120°C; in experiments of all scale. Twelve individual substances and six binary compounds were tested in a small scale experiments. In a series of small scale experiments three individual halogen containing substances capable of full suppression of hydrogen combustion were found. The minimum concentration of the most effective substance was 11% at 20°C; and 14% at 120°C;. In a series of medium scale experiments it was found that 12% of the same substance fully suppresses hydrogen combustion at initial temperature of 20°C; and 14% at 120°C;. Large scale unconfined experiments confirmed the possibility of full combustion suppression at 20°C; with 14% of phlegmatizator substance. The minimum concentration of the best binary mixture was found to be 12 % at 20°C; in a large scale experiments.

Paper #294

#### **Analysis of Combustion Problems in Highly Dilute Dust and Gas Mixtures**

*R.A. Otón Martínez, J.R. García Cascales, F. Vera García, A. Bentaib, N. Meynet*

In this paper the combustion of a highly dilute mixture of gases and particles is studied. By considering the volume fraction of particles is nearly zero, and neglecting the pressure on the particles, we obtain a decoupled system of equations easier to solve numerically. A computational finite volume code has been developed to deal with such kind of problems involving multiphase flow and detonation phenomena. Two different experimental works existing in the literature have been used to check the reliability of the code. The first test, based on the Chen's paper (1984) involves combustion of aluminium particles in atmospheric air. On the other hand, the second one includes the hydrogen-oxygen reaction.

Paper #311

#### **Characteristics of Propagation of CH<sub>4</sub>/CO Flames in a Confined Quartz Tube**

*C.-Y. Wu, T. -W. Chang, Y.-H. Li, Y.-C. Chao*

The propagation characteristics of blended methane/carbon monoxide diffusion flame in a confined quartz tube are investigated by using numerical method and experimental observation in the present work. The fuel is ignited downstream, and the flame base propagates toward the jet exit. In order to delineate the modification of triple flame theory for the hydrocarbon mixed with carbon monoxide, the experimental measurements were performed for verification. The results show that the triple point is not along the lines of stoichiometric mixture fraction in mixture. As the concentration of CO in fuel stream is increased, the propagation velocity of triple point is increased and moves toward rich zone.

Paper #321

#### **Combustion of Methane Hydrate**

*Melika Roshandell, Jordan Glassman, Matt Khalil,*

*Peter Taborek and Derek Dunn-Rankin*

This paper examines the combustion behavior of methane as it is released from clathrate cages in a methane hydrate. Gas hydrates (clathrates) are ice-like crystalline solids that encapsulate guest gas molecules. It has become known that a significant methane storehouse is in the form of methane hydrates on the sea floor and in the arctic permafrost. While this methane represents a potential mega-resource of energy it also represents a potential source of strong greenhouse gas. To better understand the important implications of direct utilization of fuel clathrates, we describe the structure and the combustion behavior of methane hydrate samples. The combustion studies involve determining the rate of ice melt and water evaporation during the hydrate burn. Different geometries are studied, including powder and spherical shapes.

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**11:10 WIP - Detonation**

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Paper #353

**Experimental and Numerical Investigation Into the Dynamics of Dust Dispersion From the Layer Behind the Propagating Shock Wave***Rudolf Klemens, Pawel Oleszczak, Przemyslaw Zydak*

In a number of industrial facilities and factory buildings dust layers cover floors, walls, ceilings and various installations. The dust can be easily dispersed by pressure waves generated by weak explosions or as a result of damage of a compressed gas systems. If the obtained explosive dust-air mixture is ignited, a devastating explosion may occur. The aim of the work was to study the dust lifting process from the layer behind the propagating shock wave and to determine some important parameters which later could be used for development and validation of numerical model of the process. The experiments were conducted with the use of a shock tube. For measuring the dust concentration in the mixture with air, a special five-channel optical device was constructed, enabling measurements at five positions located in one vertical plane along the height of the tube. The delay in lifting of the dust from the layer and the vertical velocity of the dust cloud were calculated from the dust concentration measurements. The research was carried out for various initial conditions and for three selected dusts: black coal, potato starch and flax. Three shock wave velocities: 450, 490 and 518 m/s and three dust layer thicknesses, equal to 1.0, 1.5 and 2.0 mm, were taken into consideration. Measurements results of the mean vertical component of the dust cloud velocity between the layer and the first laser beam were used in a new model, where the dust dispersing process is modeled as an injection of the dust from the layer. The numerical simulations were based on the Eulerian model of the dust phase. The velocity of the injected dust was obtained experimentally for various dusts, shock wave velocities and layer thicknesses described above. On the grounds of the obtained experimental results it was assumed that the vertical component of the lifted dust velocity is a function of the dust particle diameter, the velocity of the air flow in the channel, layer thickness and the dust bulk density. The calculations were performed for two models of the investigated process. In the first model, correlation was worked out for all tested dusts and in the new model, the individual correlations for every tested dust were prepared. The results obtained with use of the second model proved to be closer to the experimental results. It appeared, however, that lifting up of the dust from the thick layers, thicker than 1 mm, is a more complex process than that from a thin layers and still requires more research. Probably the problem is, that the shock wave action upon the thick layer causes its aggregation in the first stage of the dispersing process, what makes the dust lifting process more difficult.

Paper #360

**Detonation Properties of Ethylene/ Hydrogen Blended Fuels***Hidefumi Kataoka, Yutaka Asai, Atsuhiko Kawamura, Koji Fumoto, Kazuhiro Ishii*

One of the methods for deriving energy from biomass gas in high efficiency is using detonation engines. The biomass gas is mainly composed methane, hydrogen and carbon monoxide so that it needs to be treated as a blended fuel. In the present study, detonation properties of blended ethylene/hydrogen blended fuels were experimentally studied as the first step to make good use of biomass gas. The detonation tube had a total length of 4913 mm and an inner diameter of 50 mm. For measurement of detonation velocity four ion probes were placed at the wall of the detonation tube and soot foil made by aluminum was inserted into the detonation tube to record cellular structure. A Shchelkin spiral (pitch = 45 mm; blockage ratio = 0.44) with length of 1500 mm was inserted into the detonation tube for enhancement of transition from laminar to turbulent flame. In the present study ethylene-hydrogen-oxygen-argon mixtures were used as test gases. Volumetric percentage of ethylene in the blended fuel ranged from 0 % to 100 % under the condition that a total equivalence ratio is kept constant of 1.0. The fuel-oxygen mixture was diluted with argon in 75% in volume and then charged into the detonation tube at an initial pressure of 30 kPa and an initial temperature of 293 K. The experimental results show that the detonation velocities of ethylene/ hydrogen blended fuels are in good agreement with CJ velocities calculated by AISTJAN. The measured cell width monotonically increases with decrease in volumetric percentage of ethylene in the blended fuel although no linear relationship is observed between the cell width and the volumetric percentage of ethylene.

Paper #363

**Effect of Piping Shape on Self-ignition of High-pressure Hydrogen during Sudden Discharge***Toshio Mogi, Takayuki Tomizuka, Ritsu Dobashi, Yuji Wada*

When high-pressure hydrogen is suddenly discharged into air, a shock wave compresses the air which mixes with hydrogen at the contact surface, and this result in a temperature rise of hydrogen-air mixture, with the possibility of ignition. We investigated the phenomenon of ignition and flame propagation during discharge of high-pressure hydrogen. Especially, we investigated the effect of piping shape in self-ignition of high-pressure hydrogen during sudden discharge. Results showed that the ignition easily occurred when the pipe had an orifice or spiral.

Paper #366

**Pulse Detonation Engines in the Choked Flame Regime***Jim Karnesky, John Hoke, Fred Schauer*

Pulse detonation engine (PDE) operation relies on flame acceleration and deflagration to detonation transition (DDT). After a tube has been filled with a combustible mixture, it is ignited by a spark, and a flame travels toward the exit of this tube. Instabilities and obstacles cause this flame to accelerate to supersonic velocities and eventually transition to detonation. For efficient operation, the transition distance must be minimized. This has the effect of reducing the time

needed for an engine cycle, allowing increased frequency. It also increases the fraction of the reaction which takes place in the detonation regime. If DDT fails to occur in the tube, the flame will often accelerate to a steady supersonic velocity roughly half of the Chapman-Jouguet (CJ) detonation velocity. This is known as the choked flame regime. Unlike the CJ detonation, which is largely determined by the equilibrium chemistry, the choking condition is heavily dependent on the friction and heat transfer in the tube, presenting a greater difficulty to deterministic prediction of the pressure and velocity in the choking regime, and ultimately the thrust developed by the combustion. We have begun to investigate the operation of PDEs in the choked flame regime. Using hydrogen air mixtures in the AFRL research PDE, the equivalence ratio is reduced until DDT no longer occurs. The parameters varied were tube length, fill fraction, and the presence of obstacles. Stoichiometric mixtures in each of the choked geometries were found to DDT readily. Below a certain equivalence ratio, DDT would be intermittent, with successive ignition events sometimes resulting in detonations and sometimes in choked flames. Still leaner mixtures resulted in choked flames for all ignition events. In each case, velocity was measured using ionization gauges, and the resulting thrust was measured on a thrust stand. The deficit in specific impulse between the detonation and deflagration cases is reported and compared with the model of Wintenberger, et al.

Paper #368

### **Measurement of Detonation Cell Size in Ammonia Based Mixtures**

*Remy Mével, Nabih Chaumeix, Joseph Shepherd*

Ammonia is mainly used as raw material by industries producing compounds containing nitrogen, such as fertilizers. Its thermodynamic properties also make ammonia attractive for the industrial production of cold. The possibility of using ammonia as a fuel is being studied for its combustion does not produce CO<sub>2</sub> or unburned hydrocarbons. Although some detonation cell size measurements have been performed, the number of available data is very limited. The purpose of the present study is to obtain detonation cell sizes for undiluted NH<sub>3</sub>-O<sub>2</sub> and NH<sub>3</sub>-N<sub>2</sub>O mixtures over a wide range of equivalence ratios and initial pressures. Mixtures were prepared in a 50 L stainless steel cylinder from NH<sub>3</sub>, O<sub>2</sub> and N<sub>2</sub>O cylinders using the partial pressure method. The gases are then allowed to mix through diffusion for at least 4 hours. The detonation tube used is a 4.6 m long stainless steel tube with 78 mm inner diameter. Prior to each experiment, the tube is evacuated to a pressure below 15 Pa. In order to measure the detonation velocity, the other end of the tube is equipped with up to 7 pressure transducers. A high voltage electric spark is used to initiate a flame in the mixture and a 1 m long Schelkin spiral with a blockage ratio around 0.5 allows the transition to detonation of the flame. For each experiment, a soot foil is placed at the end of the tube. Detonation velocity was measured at T<sub>1</sub>=295 K, for NH<sub>3</sub>-O<sub>2</sub> and NH<sub>3</sub>-N<sub>2</sub>O mixtures in the ranges:  $\Phi=0.6-1.5$  and P<sub>1</sub>=40-100 kPa and  $\Phi=0.6-2.5$  and P<sub>1</sub>=40-100 kPa, respectively. The NH<sub>3</sub>-O<sub>2</sub> mixtures demonstrate much higher velocities than NH<sub>3</sub>-N<sub>2</sub>O mixtures. The experimental values agree well with the Chapman-Jouguet velocities. The mean velocity deficit observed was around 3 %. For leaner mixtures and at lower initial pressures, either accelerated deflagrations or overdriven detonations were observed indicating either that the detonation tube used was too short or that the mixtures were not sensitive enough to obtain self-sustained detonations. Detonation cell size measurements were performed on the same interval of conditions. The NH<sub>3</sub>-N<sub>2</sub>O mixtures are much more sensitive to detonation than NH<sub>3</sub>-O<sub>2</sub> mixtures: almost two times smaller cell size at  $\Phi=1$  and P<sub>1</sub>=71.5 kPa. Moreover, the evolutions of the cell size as a function of  $\Phi$ ; at P<sub>1</sub>=71.5 kPa appear very different for the two mixtures. The smaller cell size is observed  $\Phi=1$  in the case of NH<sub>3</sub>-O<sub>2</sub> mixtures whereas it is observed for the mixture with  $\Phi=2$  in the case of NH<sub>3</sub>-N<sub>2</sub>O mixtures. An empirical correlation of the evolution of the cell size as a function of equivalence ratio, initial pressure and the number of oxygen atoms in the oxidant molecule as been established and allows to predict the cell size within 15 % in average. Whatever the initial conditions were, the experimental soot foils appeared very irregular. Calculations of the reduced activation energy and Ng stability parameter allowed to classify the studied ammonia based mixtures as highly unstables.

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**11:10 WIP - Explosion**

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Paper #347

**Mine Explosion Simulation at ULMIS Large-Scale Facility***Victor S. Shalaev, Alexander V. Gerasimov, Sergey V. Khomik, Sergey P. Medvedev*

Experimental data on an explosion development in mines and industry are important for the safety strategy. The ULMIS is an abbreviation of the United Laboratory of Mines and Industrial Safety. This research and development organization is a result of collaboration between the Heterogeneous Combustion Laboratory of the N.N. Semenov Institute of Chemical Physics, RAS and "Shachtpozhservis" Research and Production Enterprise. This scientific organization develops and manufactures the facility for simulation of mine explosions and the first results of this activity are presented in the paper. The ULMIS large-scale facility is a duct with total length of about 67 m. The inner size of the square cross-section is 1 x 1 m<sup>2</sup>. Physically the facility consists of shorter sections that can be mounted in the different sequence. The typical configuration corresponds to the 7 m length ignition section divided from the rest part of the tube by plastic film membrane. The length of the test section is 12 m and two sections with the length of 24 m are before and behind this section. The preliminary tests with methane-air and methane-coal dust - air mixtures demonstrate a possibility to simulate explosion processes in mines when the main combustible substances are methane and coal dust. The ULMIS facility is suitable for the testing of explosion suppression devices.

Paper #349

**Pool Fire Suppression by Blankets***Fumiaki Takahashi, Jason P. Williams, Clay B. Criss, Sandra L. Olson, James S. T'ien*

A fire blanket can extinguish small incipient fires by placing over and sealing closely to a burning object to cut off the supply of oxygen. Although some products are used for kitchen (cooking oil) fires, the performance of fire blankets for large-scale liquid fires is unknown. For example, multiple deployment of fire blankets may be used (with or without fire-extinguishing foam currently used) to suppress a pool fire on the airport ground as a result of aviation fuel leakage due to accidental (e.g., mechanical failure, overruns, ground collisions) or manmade (e.g., maintenance error, terrorism) causes to avoid a subsequent catastrophic fuel-tank explosion. To gain basic knowledge of pool fire suppression processes by fire blankets, several fabric materials (aramid, fiberglass, amorphous silica, and wool/manmade fiber) were tested using three different pans (18 cm-diameter, 35 cm-diameter, and 61 cm x 122 cm) for vegetable oil (heated) and kerosene fuel. A manually operated and radio-controlled fire blanket deployment systems were fabricated for safe and precise deployment. The fire suppression performance depended on the material physical properties (fabric type, thickness, vapor permeability, and stiffness, etc.) and the type of fuels. Although kerosene fires could readily be extinguished, the heated vegetable oil was particularly difficult to extinguish due to persistent auto-ignition after suppression. Acknowledgments This work was supported by the U.S. Department of Homeland Security, the Federal Emergency Management Agency, Assistance to Firefighters Grant Program, Fire Prevention and Safety Grant (No. EMW-2007-FP-02677). Assistance in conducting the experiment by Timothy Murray, Amber Abbott (CWRU), and Mark Smith (NASA) is acknowledged.



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**11:10 WIP - Flame**

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Paper #343

**Group Combustion Characteristics inside a Motorcycle Gasoline Direct Injection Engine***Hsin-Luen Tsai, J.-Y. Chen and Gregory T. Chin*

The present study is to update the physical models in KIVA3V and simulate the spray combustion characteristics inside the motorcycle gasoline direct injection engines. The time histories of the spray injection, fuel vaporization, and flame kernel formation and development are obtained to elucidate the in-cylinder spray combustion phenomena. Spray injection timing plays a fatal role in mixture preparation, and the subsequent turbulent combustion processes within the limited time per cycle in GDI engines. Group Combustion theory is adopted to describe the group vaporization and combustion among the interacting droplets and surrounding gas. The global Chiu number is proposed and calculated to elucidate global group combustion modal change inside the motorcycle GDI engine. The effect of fuel injection timing on the global Chiu number is to demonstrate the transient Group combustion characteristics. Two major scenarios, characterized by the characteristic point: pre-ignition ( $\theta_{ig}$ ) (the largest G-value) includes the pre-vaporization, and post-vaporization regions, which exhibit the overall spray vaporization complexities inside the GDI engines. The ignition transience featured by sudden G-valued transition after pre-ignition point ( $\theta_{ig}$ ) is regarded as the unique group combustion phenomena in the GDI engine. Before the start of ignition (300CA), the group combustion mode changed from external mode to internal mode and finally single droplet mode. The fuel injection timing at 110 CA results in the best thermodynamic efficiency and its the critical value  $G^*=1.0$  for transition between external and internal group combustion modes is located at about 200 CAD. The further simulations with different operating parameters will be performed to aid the investigation of transient group combustion behaviors inside the motorcycle GDI engine.

Paper #344

**A Study of the Influence by Diluting Carbon Dioxide to Methane Counterflow Flame***Yung-Sheng Lien, Yueh-Heng Li, Guan-Bung Chen, Yei-Chin Chao*

The purpose of this paper is to observe the influence of diluting methane counterflow flame in oxy-fuel condition by carbon dioxide. In this experiment, oxidizer side(upper) is air( $O_2:21\%$ ,  $N_2:79\%$ ) and fuel side is methane first. Then add carbon dioxide( $CO_2$ ) to oxidizer side only( replace the  $N_2$ ) and both sides eventually. Strain rate is kept at 50 1/s and changing the concentration of carbon dioxide in oxidizer and fuel sides gradually. By visual observation, diluting carbon dioxide( $CO_2$ ) to oxidizer side will effect the flames to more brighter and wider. When adding to both sides, the flames will become thinner. It is obviously by adding carbon dioxide( $CO_2$ ) to the flames and the characteristics of flames changed.

Paper #345

**Enhancement of Hydrogen Reaction in A Meso-Scale Burner Using Innovative Catalyst Segmentation and Cavity***Fang-Hsien Wu, Yueh-Heng Li, Guan-Bang Chen, Yei-Chin Chao*

A novel design concept for enhancement of hydrogen combustion in a meso-scale burner by using the combined effects of catalyst segmentation and cavities was proposed, and their effects and combustion characteristics are evaluated by experiment with detailed heterogeneous and homogeneous chemistries. In general, the chemical process of conventional catalytic combustion is a competition between hetero- and homo-geneous reaction by striving for fuel, oxygen and radicals. Nevertheless, the objective of using catalyst segmentation and cavity in a meso-scale burner is to integrate both advantages of the hetero- and homo-geneous reactions to enhance fuel conversion and promote complete combustion in a confined distance. With a fixed total catalyst length (1.6 cm), multi-segment catalyst reveals better performance than single catalyst. The cavity between catalyst segments reduces the inhibition of homogeneous reactions by catalyst and promotes homogeneous reactions in this region since then neighboring catalysts help to maintain a high wall temperature. The existence of the cavity can appreciably extend the stable operational range of the meso-scale burner in a wide variety of inlet flows, as shown in Fig.1, and cavity can also serve as the heat source to provide the heat energy to enhance reaction. The results of different channel dispositions show that catalyst segments and cavity has better performance. For different flow conditions, the results indicate multi-segment catalyst and cavity disposition has extensive operation range, as shown in Fig 2. However, it can extend the blowout velocity. Although heterogeneous reactions strengthen in small channel, multi-segment catalyst still has obvious benefit. These outcomes and benefits of this catalyst configuration can be applied in the design of a small-scale power/heating generator.

Paper #346

**An Experimental Study on Influence of Markstein Number on Local Burning Velocity of Two-component Fuel Premixed Turbulent Flames***Masaya Nakahara, Fumiaki Abe, Jun Hashimoto, Atsushi Ishihara*

As combustion in most practical systems occurs in the flamelet regime and the performance of combustion devices is governed largely by burning velocity, knowledge of the burning velocity of premixed turbulent flames in the flamelet regime is important. Recent measurements and theories have suggested that the interactions between the preferential diffusion and flame stretch of laminar premixed flames affect strongly the properties of turbulent premixed flames such as the burning velocity in the flamelet regime. Therefore, the Markstein number  $Ma$ , which is a crucial parameter that should describe the sensitivity of flame stretch or curvature on the burning velocity of laminar premixed flames, has been studied widely to aim to elucidate and model the properties of laminar and turbulent premixed flames. In this study, the influence of positive stretch on the local flame properties of turbulent propagating flames in the flamelet regime was investigated experimentally for two-component fuel mixtures, whose fuels are hydrogen, methane and propane, having nearly the

same laminar burning velocity ( $S_{L0}=25\text{cm/s}$ ) and different equivalence ratios ( $F=0.8$  and  $1.2$ ). The ratio of the turbulence intensity  $u'$  to  $S_{L0}$  was set to 1.4. A 2D laser tomography technique was used to obtain the temporal local flame configuration and movement in a constant-volume vessel, and then the local flame displacement velocity  $S_F$ , curvature  $1/r$  and stretch  $K$  of turbulent flames were quantitatively measured as the key parameters on turbulent combustion. Additionally, the Markstein number  $Ma$  was obtained from outwardly propagating spherical laminar flames, in order to examine the effect of positive stretch on burning velocity. It was found that the trends of the mean values of measured  $S_F$  with respect to the additional rate of hydrocarbon, the total equivalence ratio and fuel types corresponded well its turbulent burning velocity. The trend of the obtained  $Ma$  could explain the  $S_F$  of turbulent flames only qualitatively. The local burning velocity at the part of turbulent flames with positive stretch and curvature using this  $Ma$ ,  $S_{L0}$ , attempted to be estimated quantitatively.

Paper #348

**Extinguishment of Cup Burner Flames of Propane and the FAA Aerosol Can Simulator Fuel by  $\text{CF}_3\text{Br}$  and  $\text{C}_2\text{HF}_5$**   
*Fumiaki Takahashi, Viswanath R. Katta, Gregory T. Linteris, Harsha Chelliah, Oliver C. Meier*

The fire suppressant  $\text{CF}_3\text{Br}$  has been banned for most applications except critical applications such as the suppression of cargo-bay fires in aircraft. Recently, the halon replacement agents, including  $\text{C}_2\text{HF}_5$  (pentafluoroethane, HFC-125), have been evaluated in a mandated Federal Aviation Administration (FAA) test, in which a simulated explosion of an aerosol can, caused by a fire, must be suppressed by the agent. Unfortunately, unlike  $\text{CF}_3\text{Br}$ , the other agents, when added at approximately one half their inerting concentrations, created a higher over-pressure in the test chamber and thus failed the test. Similar combustion enhancement has been described in other experiments for certain conditions; however, explanation of the phenomena is lacking. In this work, calculations have been performed for co-flow diffusion flames of propane and the FAA Aerosol Can Simulator fuel mixture (mole fractions: propane, 0.159; ethanol, 0.454; and water, 0.387), in the cup-burner configuration, with added  $\text{CF}_3\text{Br}$  or  $\text{C}_2\text{HF}_5$ . The time-dependent, two-dimensional numerical code, which includes a detailed kinetic model (177 species and 2986 reactions) and diffusive transport, has predicted the minimum extinguishing concentration of each agent in normal earth and zero gravity. Acknowledgments This work was supported by The Boeing Company.

Paper #355

**High Pressure and Temperature Lean Premixed Combustor Studies of Alternative Gas Fuels**

*David Beerer, Joe Velasco, Merna Ibrahim, Guillermo Gomez, Rich Hack, Adrian Narvaez, Prof. G. S. Samuelsen and Dr. V. G. McDonell*

Recently, alternative fuels to that of domestic natural gas have gained interest for use in the stationary gas turbine industry. This is a result of increasing costs, limited supplies of natural gas, along with increasing regulations on pollutant emissions. Examples of such alternative fuels include syngas with high concentrations of  $\text{CO}$  and  $\text{H}_2$ , exported or liquefied natural gas (LNG) which typically contains considerable concentrations of higher hydrocarbons ( $\text{C}_{2+}$ ), and refinery or digester gases with large amounts of diluents like  $\text{CO}_2$  and  $\text{N}_2$ . The combustion characteristics of these fuels at elevated pressures and inlet temperatures must be well understood before these fuels can be utilized in gas turbines. A high pressure lean premixed gas fired combustor rig has been developed in order to study these fuels at gas turbine representative conditions. Currently a low swirl injector with a flare quarl has been used for the burner geometry. The present research effort aims to quantify flashback, blow off, pollutant emissions, and flame stability as a function of pressure, inlet temperature, fuel composition, and burner geometry. Up to now, mixtures of natural gas (98%  $\text{CH}_4$ ) and  $\text{H}_2$  have been studied at pressures up to 5 atm, inlet temperatures up to 500K, velocities up to 50 m/s and firing temperatures up to 2000K. The majority of this data so far has been collected with natural gas in order to develop baseline data to compare to alternative fuels. Mixtures of methane with up to 90%  $\text{H}_2$  addition (by volume) have shown that stable flames are possible at these conditions, but flashback is still prevalent. Initial attempts to light off on high  $\text{H}_2$  fuels were not possible because the sparked induced ignition event created a pressure rise in the combustor which momentarily reversed the flow through the premixer. During this time of reversed flow (of around 10 ms), the flame propagated into the premixer and anchored on the fuel injector spokes, which damaged the swirler hardware. In order to avoid this in later attempts, light off was only conducted with natural gas and  $\text{H}_2$  was slowly added to the fuel over a time of about 1 minute until a fully stabilized high  $\text{H}_2$  flame was achieved.  $\text{NO}_x$  emissions correlate well with adiabatic flame temperature and are insensitive to flow velocity and pressure for both fuels. However,  $\text{H}_2$  flames appear to have considerably higher  $\text{NO}_x$  emissions. Ongoing work is underway to quantify this over wider range of conditions. Additionally, efforts to map the stability limits of flashback and blow off for high  $\text{H}_2$  fuels with the LSI are currently being carried out.

Paper #358

**Study on Micromix Concept Based Combustors for Higher Flame Stability Limits and Low Emission**

*Bhupendra Khandelwal, Priyadarshini Murthy, Vishal Sethi*

Problem of discharging green house gases and particulates into the atmosphere has an impact on global climate. Environmental concerns and depletion of fossil fuel resources have become the driving force for research and development for getting hydrogen as a fuel in air transport. When hydrogen is burnt the emissions consist of only water vapour and oxides of nitrogen. All emissions containing carbon and sulphur are eliminated. A subsonic hydrogen fuels passenger aircraft will on an average need 16 % less fuel than similar conventional aircraft and the advantage is 28 % in case of supersonic aircraft. Using hydrogen has an additional advantage of being safer as compared to presently used jet fuel. Liquid hydrogen can also be used as a heat sink for combustor and other parts. Due to risk of auto-ignition for premixed systems and the problems of large scale hydrogen diffusion flames, the lean non-premixing concept of

micromix combustion, which is based on miniaturised diffusive combustion, is suggested as a promising hydrogen combustor configuration. Substantial amount of work have not been done on micromix concept based combustor and combustion properties, and there is a need of doing some more study for the same. In combustors recirculation and mixing plays a vital role in stabilizing and increasing the flame stability limits. This allows the combustion chamber to operate at an equivalence ratio much lower than that used in the conventional combustors. All the previous work that has been done on micromix combustors has involved this basic concept where fuel and air is injected through several micro injectors opening up in a common combustion zone. In this principal air is introduced axially and hydrogen is injected radially to the air jet before entering the combustion zone. A new design concept of micromix concept based combustor has been proposed in this study and its feasibility has been checked by use of computational fluid dynamics. The proposed micromix concept type combustor will help in more rapid mixing of hydrogen with air and will lead to wider flammability range for the hydrogen-air flames as compared to kerosene and other micromix concept based combustors. The design considered here is aimed at improving the mixing of fuel and air in a better manner by exploring different geometry for the injection section. A method is proposed which should enable us to use hydrogen at reasonable equivalence ratio to get high thermal energy and simultaneously protecting the combustor. As the micro injectors are radially designed in concentric rings at the entry of the primary zone, it is suggested here to vary the FAR radially too. It can be designed to have higher equivalence ratio at the centre zone (inner rings) of the combustor and gradually decreasing ratio as we move radially outward. Thus the combustor liner is not exposed to maximum temperature of the primary zone. The inner skin of the combustor now experiences the relatively less temperature combustion gases which help in increasing its life without compromising the energy extraction.

Paper #361

#### **Comparison of Axial Forcing Effect on a Strongly Swirling Jet and Lifted Propane-Air Flame**

*S.V. Alekseenko, V.M. Dulin, Yu.S. Kozorezov, D.M. Markovich*

The flow structure of a strongly swirling lifted propane-air turbulent flame under periodical forcing was studied experimentally. Ensembles of the instantaneous velocity fields were measured by means of stereo PIV, and the spatial distributions of the mean velocity and intensity of turbulent fluctuations were calculated. In order to visualise the domains of intensive turbulent combustion, CH\* chemiluminescence images were captured by ICCD camera.

Paper #362

#### **Ignition Delay in Hydrogen-Air Mixtures: Low-Temperature Data Interpretation via Reaction Mechanism with Quantum Corrections**

*Andrey N. Starostin, Mikhail D. Taran, Yuri V. Petrushevich*

*Sergey P. Medvedev, Gennady L. Agafonov, Sergey V. Khomik*

A theory of quantum corrections to the constants of the rates of exothermal processes was applied to the interpretation of the ignition delay data in hydrogen-air mixtures. The performed analysis shows that the developed approach can be attractive for the explanation of anomalous temperature dependencies of exothermic reactions rates at the relatively low temperature and elevated pressure. In spite of the crude assumptions a satisfactory agreement between experimental data and theoretical estimations was achieved.

Paper #364

#### **The Effect of Heating Rates on Low Temperature Hexane Air Combustion**

*P.A. Boettcher, R. Mével, V. Thomas and J.E. Shepherd*

Autoignition of the fuel in the fuel tank or surrounding flammable leakage zones is one of the main safety concerns for the commercial aviation industry. Safety requirements are in place from standard tests for the autoignition temperature such as the ASTM E659. However, this test exhibits major deficiencies such as a limited control of the fuel-air composition and an inhomogeneity of the mixture within the vessel. It can be expected that numerous parameters, such as the pressure, the composition, and the rate at which the mixture is heated, will also influence the limiting temperature and the type the combustion. Prior laboratory research has focused on analysis techniques with low sampling rates. The objective of the present study is to investigate the effects of these parameters on the thermal ignition processes of hydrocarbon fuels, using an experimental setup that allows for precise control of the gas composition and temperature and a fast measurement rate of the fuel content. Hexane was selected as a surrogate for kerosene. Results are also interpreted using a detailed reaction model on the basis of an extension of Semenov's classical autoignition theory. A closed 400 mL Pyrex cell was used to conduct the experiments. Hexane is injected as a liquid through a septum at a partial pressure below its vapor pressure to ensure complete vaporization. The glass vessel has 2 sapphire windows, which allow monitoring of the fuel concentration as a function of time using absorption of a He-Ne laser light at 3.39 micron. The temperature inside the vessel is measured by a silica coated K-type thermocouple while the pressure is monitored using a fast-response static pressure gage. The vessel is suspended inside an aluminum shell with an air gap of approximately 3 mm. The aluminum shell is heated by two band heaters rated at a total of 800 W. Experiments were performed at three total pressures: 26, 67, and 101 kPa, at three equivalence ratios: 0.6, 1, and 1.2, and at heating rates between 5 K/min and 18 K/min. Experimental results demonstrate that, at a given mixture composition and initial pressure, two very distinct combustion events can occur according to the heating rates applied to the vessel. At sufficiently low heating rate, a slow decrease of the fuel concentration is observed with little or no increase of the pressure and temperature in the vessel. At sufficiently high heating rate, an ignition event is observed with a sharp decrease of the fuel content and an appreciable increase of the temperature and pressure. The increase of the initial pressure and of the equivalence ratio (from  $\phi=1$  to  $\phi=1.2$ ) appears to favor ignition events with lower heating rate. The modeling of the experiments was achieved using Cantera and a constant volume reactor model. The heat transfer is modeled with Newton's law to

approximate free convection inside the vessel. The wall temperature is progressively increased using the experimental heating rate. Using this model, the general trends observed experimentally were reproduced. Future work will focus on the interpretation of the kinetic aspects occurring during the slow reactions and ignition events.

Paper #365

#### **Forming Stability of Biodiesel/Water, /Water+Alcohol Emulsions, and the Burning Behavior of Droplets**

*C.H. Wang, G.J. Ueng, K.L. Pan, H.S. Su-Chen, J.Y. Yang*

In the study, biodiesel/water emulsions, with 20 to 50% water content, was successfully formed by a fairly simple device. In which, diesel and water solutions were prepared by adding 3% of span80 into biodiesel and 3% of tween80 into water, respectively, and the two solutions with desired amounts were put into a container and coarsely mixed. The coarsely mixed biodiesel/water mixture was then pressed through a fine filter and formed the stable emulsions. The results show that the emulsion can be stabilized for more than half an hour, the time needed to have stable generation of droplet for burning test, and the initial water cells with size of 1 to 5 are uniformly generated and distributed within the continuous phase of biodiesel. Inevitably, sedimentation and coalescence of water cell occurred gradually and eventually broke the emulsion after some times. The associated burning characteristics of the stabilized emulsions were tested thereafter. The stable emulsion droplets stream was formed by using the piezoelectric plate and then ignited and burned in the high temperature environment. The burning results gave a longer ignition delay time, shorter flame length, and faster burning rate as the increasing of water content in the emulsions. Be noticed that violent explosions occurred for all those stabilized emulsions. The low superheated temperature of methanol is expected to easily have droplet explosion as it added into diesel fuel. However, it was known that diesel/methanol do not mix and their emulsions cannot be stabilized even added with a large amount of surfactant. Mixing methanol and water should lower its boiling and superheated temperature as well. As for biodiesel, methanol can mix with it well at any proportion without any surfactant, but not for ethanol. Water and alcohol solution do mix well at any cases. Preparing water/alcohol solutions with 3% tween80, and followed the same mixing procedures as stated above, we then obtained the stabilized emulsion of biodiesel/ (25%water (W)+75% methanol(M)) for 5 to 50, /(50W+50M) 20 to 50, and /(75(W)+25(E)) 30 to 50% (W+M) content; and biodiesel/(25%water(W)+75%ethanol(E)) for 5 to 10, /(50W+50E) 30 to 50, and /(75(W)+25(E)) 30 to 50% (W+E) content. The results show that adding methanol extended the stable emulsions range, but not for ethanol. And the burning results show that there is no deteriorated effect by replacing parts of water with alcohol. Similarly, we had a longer ignition delay time, shorter flame length, and faster burning rate as the increasing of additives content in the emulsions. However, with the same amount of additives in biodiesel, it is hard to tell it is better to have pure water, or with some amount of alcohol instead. Parts of alcohol solve into biodiesel affect the surface property of droplet during the burning period, so as those burning characteristics. Energy content in alcohol and the fast burning should lead the proper selection of using biodiesel/(alcohol+water) emulsions.

Paper #367

#### **Prediction of Markstein Lengths for Hydrogen-Air and Hydrogen-Nitrous Oxide Mixtures**

*Remy Mével, Jonathan Regele, Sally Bane, Guillaume Blanquart, Joseph Shepherd*

The study of hydrogen combustion properties is relevant to nuclear activities risk assessment. Past and recent accidental events, respectively in USA, at Three Mile Island, and in Japan, at Fukushima nuclear complex, have demonstrated the issues associated with hydrogen-air mixtures accidental combustion. In addition, hydrogen safety is strongly related to nuclear waste storage, notably at the Hanford site, since these wastes release gaseous mixtures containing hydrogen and nitrous oxide together with other combustible products such as methane and ammonia. Flames propagating in mixtures with negative Markstein number, such as lean hydrogen-air mixtures, are well known to develop cellular instability at an early stage of the propagation. As a cellular flame front appears, the flame area increases and the flame accelerates. The energy release rate is not only linked to the flame speed but also to its instability which can be characterized by the Markstein number. Consequently, estimating this fundamental parameter is important in order to obtain a better characterization of accidental combustion events. The purpose of the present study is to estimate the capability of theoretical relationship and numerical simulations in predicting reliable Markstein numbers for hydrogen-air and hydrogen-nitrous oxide mixtures. Two methods to predict the Markstein number have been used: (i) a theoretical expression derived from the asymptotic theory by Matalon and (ii) spherical flame numerical simulations. Two detailed reaction models have been used for each mixture: the models of Li and of Wang, for H<sub>2</sub>-Air mixtures, and the models of Mueller and of Mével for H<sub>2</sub>-N<sub>2</sub>O (-Ar) mixtures. The experimental laminar burning speed measurements of Egolfopoulos et al., Vagelopoulos et al., Lamoureux et al., Verhelst et al., Taylor et al., Kwon et al. and Tse et al., for H<sub>2</sub>-Air mixtures, and of Mével et al., Bane et al., Brown and Smith, and Gray et al., for H<sub>2</sub>-N<sub>2</sub>O (-Ar) mixtures, have been selected to check the predictive capabilities of the reaction models. Accurate predictions with the models were obtained over a wide range of experimental conditions. Experimental Markstein numbers from Lamoureux et al., Verhelst et al., Taylor et al., Dowdy et al. and Aung et al., for H<sub>2</sub>-Air mixtures and from Mével et al. and Bane et al., for H<sub>2</sub>-N<sub>2</sub>O(-Ar) mixtures, have been selected as a validation data-set. Although the theoretical expression of Matalon is able to predict the trend of the Markstein number evolution as a function of equivalence ratio, the predicted values remain rather from the experimental measurements. In particular, no negative Markstein numbers were obtained. On the hand, the numerical simulations give both the trends and reasonably accurate values of the Markstein numbers over a wide range of equivalence ratios. Future work will focus on the determination of the dominant parameters that control the evolution of the Markstein number.

Paper #369

### **Microgravity Combustion of Blended Fuels with Alcohol and Biodiesel/Diesel**

*Kuo-Long Pan and Ming-Chun Chiu*

Biodiesel, which is a non-fossil fuel and can be obtained from vegetable oil or animal fats, has recently been suggested as an alternative fuel for immediate utilization as a surrogate for petroleum-based fuels. Compared to conventional hydrocarbon-based diesels that are used in diesel engines, biodiesel is appealing for several reasons, including lower emissions of greenhouse gases and pollutants such as sulfur (virtually none) and soot, as well as polycyclic aromatic hydrocarbon (PAH) and nitrated PAH (regarded as carcinogens), reduction of deforestation, increased lubricity for long-life utilization, and a higher flash point for safer storage and management. Its somewhat lower heating value, on the other hand, could be compensated for by mixing it with petroleum diesel. In doing so, performance would not be greatly affected and combustion may still be carried out within the existing burners. In spite of these observed features, few reports have been given in the literature in terms of a systematic investigation for the burning characteristics of diesel/biodiesel mixtures, as those frequently performed for droplet combustion with spherical flame geometry in the absence of natural convection. Also, most studies were performed directly in the practical burning devices, which could involve complex factors whose roles and effects cannot be clearly identified. In this study, we have systematically investigated the burning of biodiesel fuel based on the fundamental structure of a spherical droplet in a microgravity condition, which hence reduced the influence of external convection particularly from buoyancy. Furthermore, the fuel was mixed with diesel and/or alcohol (methanol, ethanol and propanol), which was another source of biological energy, for investigation of the possibility for making a better blend according to the desired properties. In particular, as compared to pure diesel and alkanes, biodiesel was found to yield much less tendency to a soot layer that could be formed in a spherical symmetry of droplet flame under the reduced gravity condition. Its mixture with the other fuels also exhibited reduction of such soot accumulation. The harmful products were further mitigated by addition of alcohol, which however needed biodiesel to serve as a connector if it was to be blended with diesel. Thereby the fundamental work revealed plausibility of using such a blend of biodiesel and/or alcohol for mitigation of pollutant production specifically of soot. The microgravity environment was made by a 0.68 second drop tower built in our lab. Measurements included the burning rate, formation of soot, and flame structure were conducted. These experiments demonstrated significant enhancement with increasing mass fraction of alcohol. Micro-explosion was observed for binary-component fuels if mixed with sufficient alcohol because its superheat limit was more easily attained regarding the lower boiling point while the fibers or internal impurities might provide heterogeneous sites to initiate nucleation. Such conditions however were excluded in the recording of data so as to perform a systematic study. The results indicated that increasing the mass fraction of alcohol would increase the burning rate, delay the formation of a soot shell, and reduce the production of soot.

Paper #374

### **Explicit Analytic Prediction for Hydrogen-Oxygen Ignition Time at Temperatures Below Crossover**

*P. Boivin, A. L. Sánchez, F.A. Williams*

This study addresses ignition of hydrogen-oxygen mixtures when the initial conditions of temperature and pressure place the system below the crossover temperature associated with the second explosion limit. The analysis begins by identifying the minimum set of elementary steps required to describe the ignition history. The resulting short mechanism of eight reactions is further simplified by noting that all chemical intermediates except HO<sub>2</sub> can be assumed to be in steady state during most of the ignition process. A further simplification is obtained by assuming HO<sub>2</sub> to be also in steady state, a very good approximation at atmospheric pressure, yielding the two global steps  $2\text{H}_2 + \text{O}_2 \Rightarrow 2\text{H}_2\text{O}$  and  $2\text{H}_2\text{O} \Rightarrow \text{H}_2\text{O}_2 + \text{H}_2$ . The numerical integrations indicate that, after a short initiation period, ignition occurs as a thermal runaway that can be described by activation energy asymptotics, yielding an explicit expression that predicts accurately the ignition time for different conditions of initial temperature and composition and atmospheric and moderately large pressures.

Paper #380

### **Probing Dense Sprays with Gated, Picosecond, Digital Particle Field Holography**

*James Trolinger, Ivan Tomov, Wytze Van der Veer, Dunn-Rankin Derek and John Garman*

There has been a demand for many years for diagnostic tools in combustion research directed to improving combustion stability and efficiency in turbine engines. These critically depend upon fuel and oxidizer mixing processes, which involve breakup and atomization in dense sprays. This poster shows work-in-progress to develop a unique, robust, fieldable, gated, picosecond, digital holography system for characterizing dense fuel particle and droplet fields under harsh conditions, including combustion. Many powerful imaging methods have failed to fulfill this requirement because noise from multiple scattering buries the signal needed to acquire a useful image. The described innovation applies digital holography and picosecond gating to limit the amount of noise, effectively generalizing existing pseudo-ballistic imaging systems that have been demonstrated in optically dense fields. Digital holography of this form can provide a detailed look at the structure of all of the particles in an essentially unlimited three-dimensional sample volume, which is of critical importance in spray combustion. Since the late 1960's, particle field holography has been used in hundreds of combustion and spray diagnostics problems where details of small, dispersed objects in large volumes are required. The methods have been applied broadly to study physical and optical characteristics of aerosols including size and shape in a large range from a fraction of a mm to several mm, including spherical and non-spherical features. Analogue holography was plagued, however, by problems mostly associated with recording on photographic media. In recent years, thanks to advances in electronic imaging systems, computers and memory, digital holocameras now offer many of the advantages associated with digital media. For example, holograms can now be recorded on small, lightweight, CCD or CMOS arrays at very high rates and can be processed in almost real time. The poster demonstrates the feasibility of a gated digital holography system that combines the methods of picosecond, particle holography with pseudo-ballistic imaging to: (a)

measure optical diameter of aerosol particles; b) locate particles and structures in 3D; (c) distinguish non-spherical from spherical particles; (e) provide sufficient sample volume; (f) possess sufficient sensitivity and dynamic range to measure the aerosol and coarse spray features (~0.1-10 mm); (g) eliminate a large percentage of optical noise arising from multiple, wide-angle, scattering, and (h) use in combustion environments. Pseudo-ballistic imaging is the critical part of the noise reduction because photons that are not scattered stay close to the optical axis and take less time to traverse the spray, allowing both temporal and spatial filtering. This improves information from deep within the spray, but does not sufficiently resolve the features. Adding phase filtering through the digital hologram further improves the image information. Details of the experimental apparatus and demonstrations of 3-D image reconstruction are provided on the poster. The results demonstrate that digital particle holography records particle and filament images in the desired size range even in highly scattering environments. They show that digital particle holography improves imaging of particles through image gain, coherence filtering, and spatial filtering. These results provide a clear path to improved imaging in dense sprays.