26th International Colloquium on the Dynamics of Explosions and Reactive Systems July 30 - August 4, 2017 - Boston, USA







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July 30 - August 4, 2017 - Boston, USA

ORGANIZER

Institute for the Dynamics of Explosions and Reactive Systems (IDERS), Seattle, USA.

RECOGNIZED BY

The colloquium is the premier international forum for the presentation of scientific contributions in the fields of explosions and unsteady combustion, where there is strong coupling between reaction and fluid mechanics. It is held on alternate years from The International Symposium on Combustion and is recognized by The Combustion Institute as a Specialists Meeting on the fluid dynamics of combustion.

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Welcome from the President

Dear participant to the 26th ICDERS,

On behalf of the board of directors of the Institute for the Dynamics of Explosions and Reactive Systems (IDERS), it is my pleasure to welcome you to the 26th International Colloquium on the Dynamics of Explosions and Reactive Systems. The 26th ICDERS marks an important milestone. Indeed, this is our 50th anniversary, and we have come a long way since the first International Colloquium on the Gasdynamics of Explosions and Reactive Systems and Reactive Systems was held in 1967 in Brussels, at the initiative of Numa Manson, Antoni K. Oppenheim and Rem Soloukhin.

I also take this opportunity to thank the host committee in Boston, chaired by Jenny Chao and Regis Bauwens, and the program committee, chaired by Ulrich Maas, Mark Short, and Steven Shy, for their wonderful work organizing a conference that you will find enjoyable and fruitful. I also expect that you will find the program to be of top quality.

Finally, I also wish you all a good time in Boston. Surely, as we plan to do, you will be able to spend a few extra days exploring Boston and the nice surrounding areas.

Welcome to the 26th ICDERS.

Luc Bauwens President, IDERS

Message from the Program Committee Chairs

ICDERS-2017 is the 26th specialist meeting on the dynamical aspects of explosions and reactive systems. Submissions were invited on technical areas of relevance to the ICDERS colloquium, ranging from detonation to chemical kinetics, from diagnostics to numerical methods, and from fundamentals to industrial safety applications. The program committee was chaired by three researchers representing varying technical areas and geographical locations – Asia, Europe, and America. The work of the program chairs was expertly supported by 21 members of the program committee, namely, J. Austin, Y.C. Chao, N. Chaumeix, A. Chinnayya, C. Chiquete, T. Echekki, M. Fikri, B. Fiorina, V. Gubernov, I.-S. Jeung, A. Kasimov, D. Kessler, D. Markus, K. Maruta, A. Matsuo, H.D. Ng, J. Regele, P. Ronney, N. Whitworth, M.-H. Wu, R. Zitoun.

This lead to submissions of more than 320 extended abstracts and 39 abstracts for work in progress posters. All papers were peer reviewed by the program committee. Due to the large number of papers that were recommended for oral presentation as a result of the review process, it was decided to organize 5 parallel sessions for oral presentations. Additionally, extended time slots around coffee breaks were reserved for poster presentations with no other parallel sessions. Unfortunately, in recent weeks we have heard from several of our colleagues who wished to attend ICDERS-2017 but were unable to obtain visas, and consequently several papers had to be withdrawn.

Three plenary lectures were invited, again reflecting the broad areas of interest to the ICDERS colloquium:

- Scott Jackson, Los Alamos National Laboratory, USA: "Condensed phase detonation: Are mesoscale effects needed to predict performance?"
- Katharina Kohse-Hoeinghaus, Universität Bielefeld, Germany: "Combustion chemistry developments between experiments, modeling, and theory"
- Hideaki Kobayashi, Tohoku University, Japan: "Dynamics of ammonia combustion"

We sincerely express our gratitude to the members of the program committee for their enormous help in selecting reviewers and guiding the review process. Furthermore, we thank all the reviewers who spent their valuable time to ensure a high quality program. We especially appreciate the enormous help of Nabiha Chaumeix. Without her help we would have been lost with the new version of the Confmaster system. In addition, we would like to thank the local committee, especially Regis Bauwens, for help with the program planning and booklet. Note that all extended abstracts will be published on the Web as Proceedings of the 26th ICDERS.

Authors of papers presented at this meeting are also encouraged to submit full-length versions to one of these journals: *Combustion Science and Technology, Combustion Theory and Modeling, and Shock Waves.* Submitted manuscripts will be peer reviewed according to individual journal standards but will be identified as ICDERS individually or as part of a special issue.

Special sessions on "The current status and future outlook on gaseous detonation research" have been organized by Profs. Andrew Higgins and Hoi Dick Ng. This includes presentations by Prof. John Lee and several leading young researchers in the field of detonation science.

While preparing the program we also learned with great sadness of the passing of Prof. Toshi Fujiwara and Prof. Paul Roth, two close colleagues who had been active in the IDERS

community over a long period. In memory of them, we have organized two special sessions with oral presentations related to their fields of research and with tributes.

Finally, if you have any comments on the current program, or suggestions for future conferences, please contact us.

The program chairs of the 26th ICDERS Ulrich Maas, Mark Short, Steven Shy

Message from the Host Committee Chairs

On behalf of the host committee and FM Global, we would like to welcome you to the 26th International Colloquium on the Dynamics of Explosions and Reactive Systems and to Boston! This year marks the 50th anniversary of ICDERS, and we are honored to be hosting this milestone meeting on the campus of Boston University, situated on the picturesque Charles River.

First and foremost, we are pleased to present a high quality technical program that was put together by the Program Committee. Highlights of the program include three invited plenary lectures on select topics that span a wide range of research interests, as well as a special session on the current state and outlook of gaseous detonations. We were saddened to hear of the passing of Toshi Fujiwara and Paul Roth. Their contributions to the ICDERS community will always be remembered and two special sessions have been organized in their memory.

In addition to the technical program, we are excited to offer a selection of social events that highlights the Boston area. Please join us on Sunday evening to start things off at the Welcome Reception, which will be held in the Ziskind Lounge of the George Sherman Union Building at Boston University (GSU). Attendees will have an opportunity to catch up with old friends and colleagues, as well as meet new ones. On Tuesday, Exponent will be sponsoring the Young Researchers Night at the Beacon Street Locale for a casual get together for young researchers to network. The Wednesday excursion will be held on Thompson Island, a 240-acre nature preserve on Boston Harbor's only private island, which boasts some of the most dramatic views of the Boston skyline. Attendees will be able to enjoy lawn games, nature walks, and a New England clam bake. All proceeds from the excursion benefit urban youth in Boston. The ICDERS Banquet will be held on Thursday at the Harvard Club of Boston, a historic club with private membership open only to Harvard alumni, where guests will enjoy a menu based on fresh, regional ingredients to delight their palates. Finally, we will close the conference on Friday afternoon with farewell cocktails and hors d'oeuvres at the Back Court on the first floor of the GSU.

We would like to extend our thanks to all of the sponsors for their generous contributions. Without these contributions, it would have been impossible to host this event. We would also like to express our appreciation to Sarah Bondar of The Charles Group for bringing together all the detailed logistics of the meeting. Her dedication and hard work has been invaluable.

Within these pages, you will also find additional information on activities in and around Boston. We hope that you will find some time to explore this wonderful city that we call home.

The host committee chairs of the 26th ICDERS Jenny Chao, Regis Bauwens FM Global

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Sponsor of the Young Researcher's Night



General Information and Maps

The colloquium is held on the campus of Boston University in the George Sherman Union. The address is 775 Commonwealth Avenue, Boston, MA 02215. The main entrance faces Commonwealth Avenue.

Layout of the George Sherman Union

From the main entrance to the George Sherman Union take the stairs up to reach the registration and information desk on the second floor. From here you will have access to all of the presentation rooms as well as the function rooms such as the Speaker-Ready room and the Board Meeting Room.





Registration and Information Desk

The registration and information desk is located on the second floor of the George Sherman Union. The hours are

Sunday	16:00-20:00
Monday	8:00-17:30
Tuesday	9:00-18:00
Wednesday	9:00-12:30
Thursday	9:00-18:00
Friday	9:00-16:00

Name Badges and Tickets

Please wear your name badges at all times. Badges are required for security purposes and must be worn for admission to plenary lectures, technical sessions, refreshment breaks and social events. Tickets are required for admission to the Excursion and Banquet.

Plenary Lectures

Plenary lectures are given on the second floor of George Sherman Union in Metcalf Hall Monday-Wednesday 9:00-10:00 before the technical sessions.

Technical Sessions

Five parallel sessions are held on the second and third floors of George Sherman Union. In the event of excessive construction noise, sessions may be moved from Ballroom A and B to the Academy Room and the Back Court and announcements would be made accordingly.

Wifi Access at George Sherman Union

Wifi name:	GSU guest
User name:	ICDERS
Password:	icders2017!

Refreshment Breaks

Coffee and refreshments are served in the Ziskind Lounge daily during the breaks between technical sessions.

Mother's Room

A mother's room is available on the third floor, room 312. Please request the keys at the reception desk.

No Smoking

Please observe the no smoking policy inside the George Sherman Union as well as on the terrace.

Drinking Age and Identification

Please be reminded that the drinking age in the US is 21 years and that outdoor drinking outside of designated areas such as bar patios is strictly forbidden. Be aware that an identification document is often needed for entering places that sell alcohol, such as bars and clubs, especially

in the evening. Foreign (non-US) ID cards may not be accepted, so please carry your passport with you if you do not have a US ID.

Transportation Exceptions

It has come to our attention that the City of Boston will be conducting construction work near the George Sherman Union at the time of the colloquium. This affects transportation on Commonwealth Avenue as follows:

- Personal vehicles cannot access Commonwealth Avenue between Buick Street and St. Mary Street. Only buses will operate in this area.
- Shuttles are provided by Boston University between 10 Buick street (on-campus housing) and the colloquium venue. These operate Sunday 17:30-21:30 and Monday-Friday 6:30-10:30 and 15:30-19:30.
- MBTA bus No. 57 can be used for travel between the colloquium venue and Blandford Street (closest inbound metro station).
- The MBTA (T) Green Line B does not operate in front of George Sherman Union, between Barbock Street and Blandford Street. MBTA Green Line B operates between Blandford Street and downtown Boston.
- Pedestrian and bike access is fully maintained on Commonwealth Avenue.



Parking near George Sherman Union

Note that parking in the city is generally expensive. Leaving the car at your accommodation and using public transport may be the best option. Daily parking rates near the George Sherman Union can reach up to 40 USD, especially since the Boston Red Sox will play at Fenway Park every night during the colloquium. The public lot closest to George Sherman Union is the Granby Lot next to 635 Commonwealth Avenue, Boston, MA 02215. Overnight parking is not available here. Parking lots offering overnight parking can be found around Fenway Park.

Taxi

The drop-off and pick-up location for taxis and other ride services (Uber, Lyft, etc.) closest to George Sherman Union is Marsh Plaza, 735 Commonwealth Avenue, Boston, MA 02215. Due to construction drop-off and pick-up directly in front of George Sherman Union is not possible. Please advise your driver accordingly.



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Lunch is not provided by the colloquium. The following lunch suggestions are marked with numbers in blue circles on the area map. All of these locations are within a 1 mi radius around the colloquium venue. Additional lunch restaurants can be found on Commonwealth Avenue, marked with a dashed blue line.

#	Name	Address	Type	Hours	Distance
-	George Sherman Union Food	775 Commonwealth Ave,	>10 different fast-	All open during	colloquium venue,
	Court	Boston, MA 02215	restaurants	lunch hours	ground floor
7	Mei Mei Restaurant	506 Park Dr,	Asian Fusion,	11:00-	0.3 mi
		Boston, MA 02215	Chinese	21:00	(7 min)
e	Jimmy John's	512 Park Dr,	Sandwiches	11:00-	0.3 mi
		Boston, MA 02215		23:00	(7 min)
4	Gyu-Kaku Japanese BBQ	1002 Beacon St,	Japanese, Barbeque	11:30-	0.4 mi
		Brookline, MA 02446		22:30	(9 min)
S	Tatte Bakery & Cafe	1003 Beacon St,	Bakery, Coffee and	7:00-	0.6 mi
		Brookline, MA 02446	Tea	20:00	(13 min)
9	Audubon Boston	838 Beacon St,	American	11:00-	0.4 mi
		Boston, MA 02215		1:00	(9 min)
٢	Saloniki Greek	4 Kilmarnock St,	Greek, Salad, Soup	11:00-	0.7 mi
		Boston, MA 02215		22:00	(15 min)
×	Sweetgreen	132 Brookline Ave,	Salad, Vegetarian	10:30-	0.7 mi
		Boston, MA 02215		22:00	(15 min)
6	Yard House	126 Brookline Ave,	American	11:00-	0.7 mi
		Boston, MA 02215		0:30	(15 min)
10	Eastern Standard Kitchen and	528 Commonwealth Ave,	American	7:00-	0.7 mi
	Drinks	Boston, MA 02215		2:00	(15 min)
11	Bertucci's	533 Commonwealth Ave,	Italian	11:00-	0.7 mi
		Boston, MA 02215		23:00	(15 min)
12	Thornton's Fenway Grille	100 Peterborough St,	American	11:00-	0.8 mi
		Boston, MA 02215		24:00	(18 min)
13	El Pelón Taquería	92 Peterborough St,	Mexican	11:00-	0.8 mi
		Boston, MA 02215		23:00	(18 min)

Thompson Island is a private 240-acre nature preserve just 30 minutes by boat from Boston Harbor's Long Wharf. It is one of the largest islands within the Boston Harbor Islands National Recreation Area and offers dramatic views of the Boston skyline. Once a Native American Trading Post, the island is now the site of an outward bound educational center. All proceeds from this non-profit outfit benefit urban youth of Boston.

Bring your conference badge and your US ID card or passport for age verification. Participants under the age of 21 are invited but alcohol is served to 21+ only.

Excursion to Thompson Island

Buses will take you from Boston University to the Long Wharf for a Boston Harbor ferry ride to the island. Once on the island, we will have an afternoon of fun activities and enjoy an authentic New England Clam Bake before returning to Boston University, and the colloquium accommodations, by boat and bus in the evening.

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Social	Program	Informatio	n

Welcome Reception

Sunday, July 30

Ziskind Lounge, George Sherman Union

Please join us for drinks and hors d'oeuvres to celebrate the beginning of the 26th ICDERS.

Young Researcher's Night

Monday, July 31

Wednesday, August 2

Beacon Street Locale, 495 Beacon St, Boston, MA 02215

The venue for the Young Researcher's Night, sponsored by Exponent, is within walking distance of the George Sherman Union and is marked on the area map. Students receive drink tickets for beer, wine or soda with their registration package. Bar food will be served. We encourage all students, postdocs and young professionals to attend this casual get-together!

18:00-20:00

19:00-22:00

14:00-21:00

Excursion Itinerary:

Bus pick-up (location marked on area map)	14:00
Arrival on Thompson Island	15:30
An afternoon of fun activities on Thompson Island –	15:30-20:00
New England Clam Bake, music and bar, lawn games,	
nature walks and bonfire with s'mores	
Departure from Thompson Island	20:00
Return to Boston University, 10 Buick Street, Holiday Inn	20:30-21:00
Brookline and Midtown Hotel	

Requires Excursion Ticket

Banquet

Thursday, August 3	
Reception	18:30-19:30
Banquet Dinner	19:30-22:00

Harvard Club of Boston, 374 Commonwealth Ave, Boston, MA 02215

The Harvard club of Boston is a historic club open for private membership only to Harvard graduates and their immediate families. The club opens its doors for our banquet dinner in its beautiful classic ballroom with wood paneling, historic paintings and glowing fireplaces.

This venue has a strict business casual dress code. Business casual would include collared shirts and casual slacks. A jacket is not required. Jeans, flip flops and athletic shoes are not permitted within the Harvard Club.

Requires Banquet Ticket

Farewell Reception

Friday, August 4

Back Court, George Sherman Union

The Farewell Reception is held in the Back Court room on the first floor of the George Sherman Union. Drinks and hors d'oeuvres are served.

16:00-18:00

Activities in Boston and Cambridge

The following list of activities gives some recommendations and is by no means exhaustive. Please find more suggestions in your Official Visitors Guide or online at *bostonusa.com*.

From the colloquium venue

Boston is known as a walking city. From George Sherman Union at Boston University, this year's ICDERS venue, walk east on Commonwealth Avenue. At the end of Commonwealth Avenue, you will hit Boston Public Garden and Boston Common. This is a great place to start your tour of Boston. For example, cross Boston Public Garden and Boston Common to find The Freedom Trail or walk further to get to the Boston Harbor.

For public transport, please note the current transportation exceptions due to construction. The green line of the "T", Boston's metro, operates from Blandford Street towards downtown Boston (inbound). Exit at Copley for shopping, at Arlington for Boston Public Garden, at Boylston Street for the Boston Common, at Park Street for the Freedom Trail or change to the red line or blue line for further destinations. On the way back, make sure you take the green line B since branches C, D and E of the green line do not serve Blandford Street. Alternatively, branches C and D go to Kenmore, just one stop from Blandford street.

Walking trails

The Freedom Trail is a must-see for every Boston visitor. It starts at the Boston Common Visitor Information Center (139 Tremont St, Boston, MA 02111) and is clearly marked by a line of red brick on the ground. On your walking map it is marked with red dots. Following the 2.5-mile trail, you learn about Colonial Boston and visit 16 historical sites such as the Old State House, the Park Street Church and the Old South Meeting House. Along the way you will cross the Boston Common, the oldest city park in the Unites States established in 1634. Schedules for guided walking tours are available at *thefreedomtrail.org*.

The Harbor Walk is a continuous walkway with an overall length of 38 miles, including the Boston Harbor waterfront. Take a stroll along the water and explore parks, public art, cafes and-most importantly–enjoy the views. A good starting point is the Christopher Columbus Waterfront Park. Find more information at *summeronthewater.org*.

Museums

Museum of Science. (*mos.org*, 1 Science Park, Boston, MA 02114). Besides permanent and temporary science exhibits, the museum also includes an indoor zoo, an IMAX theater and the Charles Hayden Planetarium.

Museum of Fine Arts, Boston. (*mfa.org*, 465 Huntington Ave, Boston, MA 02115). At the time of the colloquium, the MFA will present, amongst other exhibits, its holdings of photographs by Charles Sheeler (1883-1965) and Alfred Stieglitz (1864-1946), and will let you experience the conservation treatment of a 12-foot high portrait of Marshal Xin, dating back to China's Ming dynasty.

Isabella Stewart Gardner Museum. (*gardnermuseum.org*, 25 Evans Way, Boston, MA 02115). The museum is housed in a building resembling a 15th-century Venetian palace, with a central garden courtyard and three floors of galleries showing Gardner's collection of more than 2500 objects. Among the artists represented in the collection are Titan, Rembrandt, Michelangelo, and Raphael. Paintings are displayed alongside photographs, sculptures, textiles, silver, ceramics, rare books and architectural elements.

Attractions, Sightseeing, Universities, Sports and Shopping

New England Aquarium. (*neaq.org*, 1 Central Wharf, Boston, MA 02110). This aquarium is one of the big tourist attractions in Boston, and a major public education resource. The principal feature is the Giant Ocean Tank which simulates a Caribbean coral reef and its inhabitants. Further attractions include the Simons IMAX theater and the New England Aquarium Whale Watch (departs at Long Wharf, in front of the New England Aquarium) which takes visitors to the Stellwagen Bank National Marine Sanctuary, a feeding ground for a range of large whales 30 miles east of Boston.

Boston Duck Tours. (*bostonducktours.com*, departing daily from Museum of Science, Prudential Center, New England Aquarium). This 80-minute sightseeing tour in an amphibious landing vehicle gives you a good overview of Boston's major attractions and even takes you on a short boat ride on the Charles River.

Massachusetts Institute of Technology. The MIT campus is only a 10 minute walk from the colloquium venue. Cross the Boston University Bridge and walk east along the Charles River and you will see the MIT buildings along the river.

Harvard University. The campus is located about 2 miles north-west of the colloquium venue in Cambridge. If you are up for a 40 minute walk you can cross Boston University Bridge and follow the Charles River north-west until you reach John F. Kennedy Street. Take a right and walk towards Harvard Square where you can start exploring the area.

Boston Red Sox at Fenway Park. (*boston.redsox.mlb.com*, 4 Yawkey Way, Boston, MA 02215). The Red Sox will play at Fenway Park every night during the colloquium. Get a ticket or explore the bars and restaurants around the historical Fenway Park, which has been home for the Boston Red Sox since 1912 and is the oldest ballpark in the MLB.

Shopping. Visit Newbury Street (between Harvard Club of Boston and Boston Public Garden), Copley Place (100 Huntington Ave, Boston, MA 02116) and Prudential Center (800 Boylston St, Boston, MA 02199) for a wide range of stores and restaurants.

Technical Program Information

Oral Presentations

Presentations should last no longer than 20 minutes to allow 5 minutes for questions and changeover to the next speaker.

A Speaker-Ready room is available on the 3rd floor to prepare your talk.

Audio-Visual Equipment

Presentation rooms are equipped with projectors for computer-based presentations. Laptops running Windows 7 Enterprise with Powerpoint 2013 and Adobe Acrobat Reader are provided, along with slide presenters with integrated laser pointers.

Speakers are strongly encouraged to bring their presentation on a USB drive and to transfer their files onto the computers provided prior to the start of their sessions. Speakers may also connect their own laptops but must bring their own video adapters to HDMI.

A laptop is available in the Speaker-Ready room on the 3^{rd} floor where speakers can ensure in advance that their presentation displays properly.

Poster Sessions

Posters are presented in the Ziskind Lounge on the 2^{nd} floor of George Sherman Union. Posters must fit within the 36 in (w) x 42 in (h) space provided. Pins for attaching the posters are made available. Posters should be hung up by the authors by 9:00 and removed by 18:00 at the day of presentation.

Paper download

Extended abstracts are available for download at icders2017.com and icders.org.

Program at a Glance

Aug. 4)		Sessions		e Break		Sessions	Inch			Sessions			Friday Farewell			
Fri. (21.01 00:6	CTINT	Coffe	10.45	12:25	P		14:15	15:55			16:00 18:00			
Aug. 3)		Sessions		Break		Sessions	nch		Sessions	Break	Poster	Session	Sessions		Banquet	
Thu. (/		00:6	10:40	Coffee	11.10	12:25	Lu	02-64	15:05	Coffee	15:05	16:20	16:20	00.01	18:30 18:30	00.22
Aug. 2)		Plenary III	Break	WiD Doctars	WILL LUSICIS	Sessions	ıch					Excursion				
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Tue. (/		9:00 10:00	Coffee	10.30	12:10		Lui		13:50 15:30		Coffee	15:30 16:45	16:45	18:00		
lul. 31)	Welcome	Plenary I	Break		Sessions		ıch		Sessions		Break		Sessions		Young R. Nicht	ามสาง
Mon. (J	8:30	9:00 10:00	Coffee	10.30	12:10		Lur		13:50 15:30		Coffee	12.00	17:40		19:00 22:00	00.22

					Terrace Lounge	Flames in Narrow Tubes and Microchannels 1 Chairs: G. Dayma, K. Maruta	Large-Activation-Energy Analysis of Gaseous Reacting Flow in Pipes (808) D.M. Boza, I. Iglesias, A.L. Sánchez	Effects of Stoichiometry on Premixed Flames Propagating in Planar Microchamoles (771) D. Fernandez-Galisteo, C. Jiménez, M. Sánchez-Sánz, V.N. Kurdyumov	Numerical Study on Asymmetric Flame Spread in A Narrow Combustibe Channel (1029) T. Matsuoka, S. Murakami, T. Yamazaki, Y. Nakamura
am		ident of IDERS ssearch, FM Global	ational Laboratory, USA <i>teeded to predict performance?</i>		East Balcony	Detonation Boundary Interactions 1 Chairs: C.B. Kiyanda, M. Radulescu	Interactions of a Detonation Wave Confined by a High- Temperature Compressible M. Reynaud, F. Tirot, A. Chinnarya	Oblique Detonation Interaction with a Wall for Large Angles of Attack (1105) M. Short, C. Chiquete, J.B. Bdzil, M. Short, C.D. Meyer	Effects of Lateral Relief of Detonation in a Thin Channel (815) K.Y. Cho, J.R. Codoni, B.A. Rankin, J.L. Hoke, F.R. Schauer
lecnnical Progra	Monday	Ceremony: Luc Bauwens, Pres uis Gritzo, Vice President, Re	Scott Jackson, Los Alamos Ni <i>tion: Are mesoscale effects n</i> <i>Metcalf Hall, Chair: U. Maa</i>	Coffee Break	Ballroom B	Detonation Engines 1 Chairs: J. Yoh, R. Zitoun	Mid-Infrared Imaging of a Non-Premixed Rotating Detonation Engine (833) B.A. Rankin, J.R. Codoni, K.Y. Cho, J.L. Hoke, F.R. Schauer	Performance Evaluation of a Rotating Detonation Engine (1098) J. Nishimura, K. Ishihara, K. Goto, S. Nakagami, K. Matsuoka, J. Kasahara, A. Matsuoka, J. Funaki, H. Mukae, K. Yasuda, D. Nakata, K. Higashino, H. Moriai	Orderly Wave Initiation in a Rotating Detonation Engine (1088) C. Knowlen, M. Kurosaka
		Opening C Welcome: Lo	Plenary Lecture 1: Condensed Phase Detono		Ballroom A	Laminar Flames 1 Chairs: N. Chaumeix, Y. Ju	Effects of Pressure and Temperature on Laminar Burning Velocity of a Kerosene Surrogate (1069) R. le Dorzz, M. Bellenue, J. Sotton, C. Strozzi	Observation of Double Flame Structures in Near-Limit Premixed Flames (1083) C.B. Reuter, Y. Ju	Distinct Dependence of Flame Speed to Stretch and Curvature (1040) F. Thiesset, F. Halter, C. Bariki, C. Chanveau, L. Gokalp
					Auditorium	Chemical Kinetics and Reaction Dynamics 1 Chairs: P. Dagaut, M.H. Wu	A Rapid Compression Expansion Machine (RCEM) for Measuring Species Histories (859) <i>M. Werler, R. Schießl,</i> U. Maas	Validation of Hierarchical REDIM Based Reduced Models (1061) V. Bykov, A. Neagos, U. Maas	Predicting Large-Scale Effects During Cookoff of PBXs and Melt-Castable Explosives (852) M.I. Hobbs, M.J. Kaneshige, W.W. Erikson
		8:30	00:6	10:00	Room	Topic	10:30	10:55	11:20

Constr Reaction C3H8 C3H8 Combusti Y. Sasa	uction of Simple A Mechanisms for VAL Mixtures sidering Five on Properties (919) on Properties (918) K. Maruta	A Numerical Study on the Effect of Hydrogen Mole Fraction on NO Formation in H2/CO Syngas/Air Laminar Diffusion Flames (801) Y. Ye, Z. Gu, J.Xi, A. Haiyang, Z. Xianpeng	Pulse Detonation Operation at Kilohertz Frequency (1065) H. Taki, N. Hirota, K. Matsuoka, K. Akira, J. Kasahara, H. Watanabe, A. Matsuo, T. Endo	Effect of Boundary Streamline Deflection Angle on Detonation Propagation (1077) C. Chiquete, M. Short, C.D. Meyer, J.J. Quirk	Flame Behaviour During Propagation in Small Tubes Characterized by Different Degrees of the End Opening (869) A.N. Gutkowski, P. Jacinski, M. Lecki, B. Jedrowiak
Chemical Kinetics and Reaction Dynamics 2 Chairs: P. Dagaut, M.H. N	n	Laminar Flames 2 Chairs: N. Chaumeix, Y. Ju	The Current Status and Future Outlook on Gaseous Detonation Research 1 <i>Chairs: A. Higgins, H.D. Ng</i>	Dust Explosions 1 Chairs: R. Houim, A. Kuhl	Flames in Narrow Tubes and Microchannels 2 Chairs: G. Dayma, K. Maruta
Kinetic Effects of n- Propylbenzene on n- Dodecane Cool Flame Extinction (1101) O.R. Yehia, C.B. Reuter, Y.	hu	Influence of Monodispersed Mist of Inert Liquid on Gas Flame Propagation (1053) N.S. Belyakov, V.I. Babushok, S.S. Minaev	The Current Status and Future Outlook on Gaseous Detonation Research J.H.S. Lee	Explosion-Induced Ignition and Combustion of Acetylene Clouds (938) A.L. Kuhl, H. Reichenbach, J.B. Bell, V.E. Beckner	Stationary Premixed Flames in Narrow Tubes with External Heat Transfer (1082) A.O. Velázquez, L. Bauwens, F. Fachini
Utilization of Transport o Species and Heat Release 1 a DRG-Method-Based Reduction (996) K. Yamasaki, S. Honya, A. Uemichi, M. Nishioka	f 0	Laminar Flame Speed of Diluted DME-Air Mixtures (1019) A. Mohammad, A.N. Mohammed, K.A. Juhany, S. Kumar, R.K. Velmati	The Usefulness of a 1D Hydrodynamic Model for the Detonation Structure for Predicting Detonation Dynamic Parameters (1140) <i>M.I. Radulescu</i>	Effect of Particle Size on the Dispersion of Dust Produced by a Shock Wave (1113) O.J. Ugarte, R.W. Houim, E.S. Oran	Experiments on Flame Propagation Regimes in a Thin Layer Geometry (1132) M. Kuznetsov, J. Grune
Modeling Real Gas Equations of State in High Density Combustion (1127) C. Zheng. D. Coombs, B. Akih-Kumgeh	-	Pressure and Radiation Effects on the Dynamics of Hot and Cool Diffusion Flames (1073) C.B. Reuter, E. Lin, Y. Ju	Computation of the Mean Hydrodynamic Structure of Detonation with Losses (961) A. Chinngyya	Promotion and Mitigation of Premixed Flame Acceleration in Dusty-Gaseous Environment with Various Combustible Dust Distributions: A Computational Study (1138) S. Demir, H. Sezer, T. Bush, V. Akkerman	Pulsating Combustion of Ethylene in Micro-Channels with Controlled Temperature Gradient (755) A. di Stazio, C. Chanweau, G. Dayma, P. Dagaut
Validation of Detailed Chemical Kinetics Mechanisms for Reproduction of Ignition Delay Times of C2-C5 Alkenes (927) A. Jach, W. Rudy, A.A. Pękalski, A. Teodorczyl	د.	Laminar Flame Speed Determination for H2/N2/02/Steam Mixtures Using the Spherical Bomb Method (594) R. Grossenvres, A. Bentaïb, N. Chaumeix	Discussion Period	Turbulent Clustering of Particles and Radiation- Induced Mechanism of Dust Explosions (798) M. Liberman, N. Kleeorin, I. Rogachevskii, N. Haugen	Experimental and Numerical Study of Premixed Flame Penetration in a Set of Microchannels (845) R. Fursenchannels, E. Serschchenko, G. Urinpin, E. Odinkov, T. Tezuka, S. Minaev, K. Maruta

15:30			Coffee Break		
Topic	Ignition 1 Chairs: S. Coronel, J. Melguizo-Gavilanes	Explosion Safety 1 Chairs: S. Dorofeev, I.S. Jeung	The Current Status and Future Outlook on Gaseous Detonation Research 2 <i>Chairs: A. Higgins, H.D. Ng</i>	Flame-Wall Interaction Chairs: A. Comandini, U. Maas	Turbulent Reacting Flows 1 Chairs: A. Poludnenko, L. Vervisch
16:00	Hot Spot Dynamics: Quenching, Ignition, Flame Propagation and Extinction (1115) J. Santner, S.S. Goldsborough	Flame Arrester Performance at Increased Oxygen Concentrations (1060) S. Zakel, S. Henkel, F. Stolpe, M. Beyer, U. Krause	Critical Condition for Detonation Diffraction with Stable and Unstable Mixtures (963) J. Kasahara, A. Kawasaki	REDIM Reduced Modeling of Quenching at a Cold Inert Wall with Detailed Transport and Different Mechanisms (811) C. Strassocker, P. Bykov, U. Maas	On the Supersonic Flame Structure in the Hyshot II Scranjet Combustor (985) C. Fureby
16:25	Effect of Orientation on the Ignition of Stoichiometric Ethylene Mixtures by Stationary Hot Surfaces (981) J. Melguizo-Gavilanes, J.E. Shepherd	Effects of Open Area of a Rupture Disk on the Self- Ignition of High Pressurized Hydrogen Released Through a Tube (1023) H.J. Lee, S.Y. Lee, B.J. Lee, I.S. Jeung	Planar Blast Initiation of Detonations Using a Simplified Model (1116) S.M. Lau-Chapdelaine, L.M. Faria, R. Rosales, M.I. Radulescu	Flame-Wall Interaction in Premixed Reactive Turbulence (775) P. Zhao, L. Wang, N. Chakrabory	Extinction in Non-Premixed Ethanol Spray Flames Using Direct Numerical Simulation (1002) J.C. Tang, H. Wang, E.R. Hawkes, M. Bolda
16:50	Effect of Initial Laser Beam Diameter on Breakdown and Iguition Properties of n- Decane/Air (741) S. Rudz. P. Gillard	Modeling the Growth and Formation of Instabilities During Spherical Flame Propagation (4301) C.R.L. Bauwens, J.M. Berghorson, S.B. Dorofeev	Comparison of Models Predicting the Mode of Ignition Behind Reflected Shock Waves in the Context of DDT (990) L.R. Boeck	3-D Flame Patterns in a Backward Facing Step Mesoscale Combustor for Non- Adiabatic Wall Conditions (857) M. Malushte, S. Kumar	Dynamic Pressure Characterization of a Dual-Mode Scramjet (1157) C. Aguilera, A. Ghosh, K.H. Shin, K.H. Yu
17:15	Free	Numerical Modelling of Vented Lean Hydrogen-Air Deflagration Using Hyfoam V.C.M. Rao, J.X. Wen	Discussion Period	Heat Flux and Flow Topology Statistics in Oblique Quenching of Turbulent Premixed Flames by Isothermal Inert Walls (939) J. Lai, N. Chakraborry	Development of a Multiscale Adaptive Reduced Chemistry Solver (MARCS) for Computationally Efficient Combustion Simulations (1081) W. Sun, L. Wang, T. Grenga, Y. Ju
17:40			Adjourn		
19:00 22:00			Young Researcher's Night Beacon Street Locale		

			Tuesday		
00:6		Plenary Lecture 2: Kath Combustion Chemistry D	harina Kohse-Hoeinghaus, Uni Developments Between Experi Metcalf Hall, Chair: S. Shy	versität Bielefeld, Germany ments, Modeling, and Theory	
10:00			Coffee Break		
Room	Auditorium	Ballroom A	Ballroom B	East Balcony	Terrace Lounge
Topic	Chemical Kinetics and Reaction Dynamics 3 Chairs: U. Riedel, A. Teodorczyk	Turbulent Flames 1 Chairs: J. Driscoll, H. Kobayashi	DDT 1 Chairs: L. Boeck, G. Ciccarelli	Detonation Structure Chairs: C. Chiquete, J. Kasahara	Combustion Stability, Instabilities 1 Chairs: E. Petersen, F. Williams
10:30	Effect of CO2 Dilution on the Burning Velocity of Equinolar Syngas Mixtures at Elevated Temperatures <i>R.J. Varghese, S. Kumar,</i> <i>H. Kolekar</i>	A New Measured Regime Diagram of Turbulent Premixed Combustion, Based on Images of Flame Structure (949) A.W. Skiba, T.M. Wabel, J.F. Driscoll, C.D. Carter, S. Hammack	Flame Acceleration and Deflagration-to-Detonation Transition Through an Array of Obstacles (1109) H. Xiao, R.W. Houim, E.S. Oran	On the Averaging Analysis for Unstable Detonations (1085/1134) X. Mi, H.D. Ng, C.B. Kiyanda, A.J. Higgins, N. Nikiforakis	The Origin and Evolution of Mechanical and Thermodynamic Disturbances Caused by Localized Energy Deposition in Gaseous Volumes (816) D.R. Kassoy
10:55	Influence of Microscopic Stochastic Properties on the Auto-Ignition of Hydrogen / Oxygen Mixture (1052) C. Yang, Q. Sun	Influence of Turbulence on the Propagation of C7H8/Air Flames at Atmospheric Pressure and Temperature (1058) A. Lefebvre, M. Nair-Daoud, N. Chaumeix	Flame - Shock Wave Dynamic Studies at DDT in Djluted Stoichiometric Acetylene-Oxygen Mixtures (959) Y.A. Baranyshyn, P.N. Krivosheyev, O.G. Penyazkov, K.L. Sevrouk	Structure of Detonation Propagating in Lean and Rich Dimethyl Ether-Oxygen Mixtures (870) R. Mével	Subcritical Thermoacoustic Bifurcation in Turbulent Combustors: Effects of Inertia (828) G. Bonciolini, D. Ebi, E. Boujo, M. Noiray
11:20	Reduced Order Models for Shock-Induced Combustion of Fuel Mixtures (982) D.A. Schwer, K. Kailasanath	Combustion and Emission Characteristics of Premixed and Non-Premixed Ammonia/Air Turbulent Swirl Flames at the High Pressure and Temperature (997) <i>K.D.K.A. Somarathue</i> <i>A. Hayakawa, H. Kobayashi</i>	Stages of Flame Acceleration and Detonation Transition in a Thin Channel Filled with Stoichiometric Ethylene/Oxygen Mixture (1017) H.P. Chan, M.H. Wu	Influence of Water Sprays on a Muli-Cellular Regular Detonation (1041) G. Jarsalé, F. Virot, A. Chinnayya	The Effects of Lewis Number on the Combustion Limit, Near- Limit Extinction Boundary, and Flame Regimes of Low-Lewis- Number Counterflow Flames Under Microgravity (904) T. Okuno, H. Nakamura, T. Tezuka, S. Hasegawa, M. Kikuchi, K. Maruta

n sed n		su	ad- yee	TH - I	nal	le on le <i>r</i>
On the Effect of Pressure or Intrinsic Flame Instabilities Lean Hydrogen-Air Mixtures Part I: Detailed Chemistry Ba Direct Numerical Simulation J. Hasslberger, P. Katzy, T. Sattelmayer		Combustion Stability, Instabilities 2 Chairs: E. Pertersen, F. Willia	Experimental Study of the He. on Interaction of a Shock Wa with a Cellular Flame (1131 <i>M. la Flèche, Q. Xiao, Y. Wan,</i> <i>M.I. Radulescu</i>	On the Effect of Pressure on Intrinsic Flame Instabilities Lean Hydrogen-Air Mixtures Part II: Experimental Investigation Based on OH-PI Technique (764) P. Karzy, J. Hassberger, T. Santelmayer	Combustion Instability Prediction Using Minimal Experimental or Computation Data (1130) S. Park, A. Ghosh, K. Yu	Application of Dynamic Moc Decomposition for Stabilizati of Reactive Flow in a Subsca Combustor with an Injecton (754) Y.J. Kim, G. Jourdain, C.H. So
Free		Detonation Limits <i>Chairs: C. Chiquete, J. Kasahara</i>	Nonlinear Dynamics of Gaseous Detonations with Losses (1042) A. Sow, A. Kasimov, R. Semenko	A Study on Suppression of Detonation Propagation by Inert Gas Injection (1031) K. Ishii, K. Seki	Effect of Spatial Inhomogeneities on the Propagation Limit of Gaseous Detonations (1129) X. Mi, A.J. Higgins, H.D. Ng, C.B. Kiyanda, N. Nikijorakis	Free
Cylindrical Flame Acceleration and Deflagration-to-Detonation Transition in Confinement Space (792) W. Han, N. Du, Z. Liu, W. Kong	Lunch	Detonation Initiation Chairs: M. Ihme, P. Vidal	Numerical Simulation of Detonation Initiation by Shock-Multiple Discrete Flames Interaction (1059) A.L. Gunter, H.D. Ng, C.B. Kiyanda, K.C.T. Yuk, X.C. Mi, N. Nikfjorakis	Growth to Detonation in Hexanitrostilbene (HNS) (983) J.D. Olles, R.R. Wixom, R. Knepper, A.S. Tappan, C.D. Yarrington	Effects of Disturbance on Direct Detonation Initiation in H2/02/Ar Mixture (956) Y. Wang, C. Qi, R. Deiterding, Z. Chen	Free
Fuel Similarity and Turbulent Burning Velocities of Stoichiometric Iso-Octane, Lean Hydrogen, and Lean Propane at High Pressure (1176) M. Nguyen, L. Jiang, S. Shy		Turbulent Flames 2 Chairs: H. Kobayashi, S. Shy	Large Eddy Simulation of Supersonic H2-O2 Combustion (915) U. Guven, G. Ribert	Dependence of Limiting Oxygen Index of Buoyant Turbulent Diffusion Flame on Fuel (1074) D. Zeng, Y. Wang	The Reattachment Process of Turbulent Lifted Diffusion Jet Flames Induced by Repetitive D.C. Electric Pulse Discharges (1125) T.W. Chang, H.Y. Li, T.S. Cheng, Y.C. Chao, M.H. Shen	Combustion Characteristics of Transverse Hydrogen Jet in a Supersonic Compact Inlet/Combustor Model (858) Z.W. Huang, G.Q. He, F. Qin, X.G. Wei, S. Wang
Laminar Burning Velocities of Spherically Expanding Hydrogen/Air Mixtures for Temperatures Up to 423K at Ambient Pressure (1175) J. Beeckmann, H. Pitsch		Fire Dynamics Chairs: C.R. Bauwens, C. Proust	Smoldering Spread Velocity Along a Thin Solid in a Narrow Channel (1005) K. Kuwana, K. Suzuki, Y. Tada, G. Kushida	The Critical Conditions for the Onset of Pool-Fire Puffing (993) W. Coenen, D. Moreno-Boza, A.L. Sánchez	Horizontal Flame Spread Along a Thin Paper-Disk in a Narrow Space (1047) T. Daitoku, T. Takahashi, T. Tsuruda	Traveling Vortex in a Natural Convection Field (1011) T. Tsuruda
11:45	12:10	Topic	13:50	14:15	14:40	15:05

		Reactive Systems 1 Chairs: K. Ishii, J. Yao	The Inability of Heterogeneously Reacting Particles to Ignite Below a Critical Size (818) M. Soo, S. Goroshin, J. Lightstone, D.L. Frost, J.M. Bergthorson	The Vaporization-Controlled Inertial Regime in Nonpremixed Counterflow Spray Combustion J. Carpio, A. Linna, D. Martinez- Ruz, A.L. Sänchez, F.A. Williams	Propagation Limits of Flames in Binary-Fuel Mixtures (876) J. Palecka, S. Goroshin, J.M. Bergthorson, A.J. Higgins J.M. Bergthorson, A.J. Higgins	
	45)	Dust Explosions 2 Chairs: A. Kuhl, M. Liberman	Potential Accelerating Effect of Thermal Radiation in Dust Flame Propagation : Some Experimental Evidence (1096) C. Proust, R.B. Moussa, M. Guessasma, K. Saleh, J. Fortin	Flame Propagation in Nano- Metal Dust Explosions (768) W. Gao, M. Bi, T. Mogi, R. Dobashi	Investigation on the Diffraction of a Medium Scale Gaseous Deflagarion Pressure Wave Behind a Protective Wall (1049) <i>L. Heudler, G. Lecocq,</i> <i>Y. Grégoire, C. Proust</i>	
Coffee Break	Poster Session I (15:30 - 16: Ziskind Lounge	The Current Status and Future Outlook on Gaseous Detonation Research 3 <i>Chairs: A. Higgins, H.D. Ng</i>	Autoignition and Detonation Development From a Hot Spot in Hydrogen/Air Mixture (193) Y. Gao, Z. Chen	An Evaluation of Ignition Criteria Through State Classification and Detailed Simulation (1072) K.P. Grogan, M. Ihme	The Role of Flame- Generated Turbulence in the Deflagration-to- Detonation Transition (1247) A.Y. Poludnenko	Adjourn
		Explosion Safety 2 Chairs: S. Dorofeev, I.S. Jeung	Understanding the Effect of Multiple Adjacent Vent Panels on Explosion Overpressures (4300) C.R.L. Bauwens, S.B. Dorofeev	Re-Ignition by Hot Free Gas Jets - A Parameter Study (1026) F. Seitz, R. Schießl, D. Markus	Influence of Congestion on Vented Hydrogen Deflagrations in 20-Foot ISO Containers: Homogeneous Fuel-Air Mixtures (1120) T. Skjold, H. Hisken, S. Lakimpadiy, G. Atanga, M. van Wingerden, K.L. Olsen, M.N. Holme, N.M. Turoy, M. Mykleby, K. van Wingerden	
		Minimum Ignition Energies, Flammability Limits Chairs: M. Beyer, F. Marra	Evaluation of Flammability Limits of H2/O2 Mixtures in Conditions Relevant to Nuclear Waste Transportation: Pressure and Nitrogen Addition Effects. (1032) N. Kourne, A. Comandini, M. div, P. Jean, C. Thomas, N. Chaumeix	Effects of Composition Fluctuations on the Structure and Development of Laminar and Turbulent Flame Kernels (1043) A. Er-raiy, Z. Bouali, A. Mura	Effects of Fuel Stratification on Ignition Kernel Development and Minimum Ignition Energy (807) Y. Wang, W. Han, Z. Chen	
15:30	15:30	Topic	16:45	17:10	17:35	18:00

		0:00 - 13:00)		:00 - 13:00)	Terrace Lounge	Turbulent Reacting Flows 2 in Chairs: A. Poludnenko, L. Vervisch i Image: A. Poludnenko, L. Vervisch	 td- Two-Dimensional Numerical on Analysis on Shock Flame iry Interaction in Premixed Gas of Hydrocarbon(Oxygen with Multi-Step Reaction Model M. Iwai, K. Yoshida, Y. Morii, N. Tsuboi, A.K. Hayashi 	n a Experimental Investigation on tete the Flame Wrinkle Fluctuation Under External A coustic Excitation (978) L. Zheng, S. Ji, Y. Zhang	n Sub-Grid Scale Modeling of the Equation of State for Fully Compressible Combustion LES (931) G. Ribert, P. Domingo, L. Vervisch												
	ku University, Japan <i>ustion</i> 't				Coffee Break n Progress Poster Session (10:00 - 13:00) Ziskind Lounge	COITCE BFEAK n Progress Poster Session (10:00 - 13:00) Ziskind Lounge	Coffee Break in Progress Poster Session (10:00 - 13:00) Ziskind Lounge	(10:00 - 13:00)	(10:00 - 13:00)	(10:00 - 13:00)	10:00 - 13:00)	10:00 - 13:00)	(0:00 - 13:00)	10:00 - 13:00)	10:00 - 13:00)	(10:00 - 13:00)	(10:00 - 13:00)	ו (10:00 - 13:00)	East Balcony	Detonation Boundary Interactions 2/ Detonation Narrow Channels Chairs: A. Matsuo, X. Mi	Interaction of a Condense Phase Explosive Detonati with a Compliant Bounda (988) J.B. Bdzil, M. Short, C. Chiq
Wednesday Plenary Lecture 3: Hideaki Kobayashi, Tohc <i>Dynamics of Ammonia Comb</i> <i>Metcalf Hall, Chair: M. Sho</i>	re 3: Hideaki Kobayashi, Tohc Dynamics of Ammonia Comb Metcalf Hall, Chair: M. Sho	re 3: Hideaki Kobayashi, Toho Dynamics of Ammonia Comb Metcalf Hall, Chair: M. Sho Coffee Break	ure 3: Hideaki Kobayashi, Tol Dynamics of Ammonia Com Metcalf Hall, Chair: M. Sh Coffee Break Coffee Break Ziskind Lounge Ballroom B Detonation Engines 2 Chairs: A. Chinneyya, R. Zitoun Rectaing Detonation Wave Mechanics Through Ftylene-Air Mixtures in Hollow Combustors, and Instabilities (992) V. Anand, A.S. George,	Coffee Break				Rotating Detonation Wave Mechanics Through Ethylene-Air Mixtures in Hollow Combustors, and Implications to High Frequency Combustion Instabilities (992) <i>V. Anand. A.S. George.</i> <i>C.F. de Luzan, E. Gutmark</i>	Experimental Observations of Semi-Confined Steadily- Rotating Detomation (1084) V. Rodriguez, P. Vidal, R. Zitoun	3D Numerical Study on Continuous Detonation Engine Using Reactive Navier-Stokes Equations (1066) L. Zhang, J. Wang											
	D) Work in	Ballroom A	Chemical Kinetics in Shock Tubes, in memory of Paul Roth Chairs: L. Bauwens	The Contributions of Paul Roth in the Field of Dynamics of Explosions and Reactive Systems	Ignition Delay Time Study of Aromatic LIF Tracers in a Wide Temperature and Pressure Range (795) J. Herzler, M. Fikri, C. Schulz	High Speed Imaging of Inhomogeneous Ignition in a Shoef Tube (1004) A.M. Tulgestke, S.E. Johnson, D.F. Davidson, R.K. Hanson															
							Explosions and Combustion in IC Engines Chairs: D. Dunn-Rankine, O. Penyazkov	Direct Numerical Simulation of Two-Stage Combustion and Flame Stabilisation in Diesel Engine-Relevant Conditions (1143) D. Dalakoti, E.R. Hawkes, M.S. Day, J.B. Bell	Shock Wave and Flame Front Induced Detonation in Rapid Compression Machine (995) Y. Wang, S. Xiang, Y. Qi, R. Mével, Z. Wang	Effects of Fuel/Air Mixture Distribution on End-Gas Autoignition and Pressure Wave Generations in Knocking Combustion (1008) T. Satoh, H. Terashima, M. Ochiwa											
	9:00	10:00	10:00	Room	Topic	10:30	10:55	11:20													

Reaction Front Characterization in Turbulent Combustion Based on Entropy Production Field Curvature (1187) R. Schießl, V. Bykov	Effect of Asymmetric Fuel Injection on the Combustion Characteristics of Liquid Fuel Fired Flameless Combustor (924) <i>S. Sharma, H. Pingulkar,</i> <i>A. Chowdhury, S. Kumar</i>		
Experimental Study on Behavior of Methane/Oxygen Gas Detonation Near Propagation Limit in Small Diameter Tube: Effects of Equivalent Ratio (822) K. Yoshida, T. Inoue, Y. Morti, K. Murakami, N. Tsuboi, A.K. Hayashi	Detonation Limits in Highly Argon Diluted Acetylene- Oxygen Mixtures (802) B. Zhang		n at 14:00)
Detonation Regimes in a Small-Scale RDE (1037) S. Hansmerzger, R. Zitoun, P. Vidal	Baffled Tube Ram Accelerator Combustion (1117) C. Knowlen, T. Byrd, J. Dumas, N. Daneshvaran, A.P. Bruckner, A.J. Higgins	Adjourn	Wednesday Excursion Thompson Island rt from George Sherman Union
Experimental Study of Nitromethane Oxidation: CO and H2O Time-Histories Behind Reflected Shock Waves (911) O. Mathieu, C. Mulvihill, E. Petersen	Combustion Properties of n- Heptane/Hydrogen Mixtures (1045) A. Comandini, K. Brialix, N. Chaumeix, J. MacLean, G. Ciccarelli		(depa
Autoignition of End Gas in a Rapid Compression Machine Under Super Knock Conditions (929) Y. Qi, Y. Wang, H. Liu, J. Wang, Z. Wang	Measurement of the Carcinogenic Polyaromatic Compounds in the Exhaust Gases of a Gasoline Internal Combustion Engine (909) M.S. Assoud, O.G. Penyuzkov, I.N. Tarasenko		
11:45	12:10	13:00	14:00 21:00

			Thursday		
Room	Auditorium	Ballroom A	Ballroom B	East Balcony	Terrace Lounge
Topic	Memories of Toshi Fujiwara: Kindness, Splendor, and Physics Chairs: A.K. Hayashi, A. Matsuo	Laminar Flames 3 Chairs: F. Halter, H. Im	DDT 2 Chairs: L. Boeck, G. Ciccarelli	Diagnostics, Sensoring 1 Chairs: R. Schießl, S.Y. Yang	Reactive Systems 2 Chairs: D. Dunn-Rankin, K. Ishii
00:6	Numerical Analysis on Liquid JP10 Rotating Detonation Engine (1003) A.K. Hayashi, W. Yoshida, M. Asahara, N. Tsuboi''	Effect of Multi-Component Transport Model on Soot Prediction in Opposed-Jet Ethylene Diffusion Flames (1044) A. Borg, H. Lehtiniemi, F. Mauss	Effect of Surface Roughness on Deflagration-to- Detonation Transition in Submilimeter Channels (1067) <i>R.W. Houim, E. Oran</i>	High Speed PIV of Flame Propagation in Obstructed Channels (1070) T. Li, R.P. Lindstedt	Near-Structure Air Blast Simulations Using Zapotec, A Coupling of CTH and Sierra/SM A. Gullerud A. Gullerud
9:25	Memories of Toshi Fujiwara: E. Oran, J.H.S. Lee, J.P. Wang	Impact of Acoustic Excitation Frequency on Laminar Premixed Flame (979) L. Zheng, S. Ji, Y. Zhang	Deflagration-To-Detonation Transition in an Unconfined Space (759) A. Koksharov, V. Bykov, L. Kagan, G. Sivashinsky	Experimental Assessment of the Displacement and Consumption Speeds in Flame/Vortex Interactions (1038) F. Thiesset, F. Haller, C. Bariki, C. Lapeyre, C. Chauveau, L. Gokalp, L. Selle, T. Poinsot	Raman Study of Structural Change in 1,3,5-Triamino-2,4,6- Trinitrobenzene Under Non- Hydrostatic Pressure (903) X. Sun, C. Gao, Z. Sui, R. Dai, Z. Wang, X. Zheng, Z. Zhang
9:50	Modelling Mixing Near HE- Air Interfaces in Explosions 937) A.L. Kuhl, D. Grote, J.B. Bell, V.E. Beckner	Elevated Temperature Effects on Laminar Burning Velocity Temperature Exponent of Liquid Fuels (1012) A. Katoch, R. Kumar, S. Kumar	Propagation Mechanism of Detonations in Rough Walled Tube (1000) J. Li, J. Ning	Extinction Measurements of Soot Particles in a Diffusion Flame When Submitted to a DC Electric Field (1015) P. Gillon, V. Gilard, M. Idir, B. Sarh	Porous Wall Fed Liquid Fuel Nonpremixed Swirl-Type Tubular Flames (1114) V.M. Sauer, D. Dunn-Rankin
10:15	Memories of Toshi Fujiwara: P. Wolanski, A. Matsuo	Effects of Applied Electric Fields on Liftoff Height in Laminar Liftof Coflow-Jet Flames (976) B.H. Seo, K.H. Van, G.T. Kim, N.P. Sapkal, O. Kwon, J. Park, S.H. Chung	Free	High Speed PIV Analysis of the Combustion Regimes During Autoignition of Homogeneous Fuel - Air Mixtures in a RCM (1124) C. Strozzi, A. Delicourt, M. Bellenoue, J. Sotton	Behavior of Explosive Bubbles Behind an Underwater Shock Wave (1024) N. Watanabe, K. Ishii
10:40			Coffee Break		

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Turbulent Reacting Flows 3 Chairs: U. Maas, G. Ribert	Direct Numerical Simulations of Shock-Scalar Mixing Interaction (883) R. Boukharfane, Z. Bouali, A. Mura	High-Order Numerics for Simulating Turbulent Deflagration Fronts Over Coarse Meshes (980) E. Bossennec, G. Lodato, L. Vervisch	Fully-Implicit Density-Based Algorithms for Simulations of Arbitrary Gas Mixtures (1090) L. di Mare, F. Wang, F. Ferraro, F. di Mare	
Detonation Propagation Chairs: A. Kasimov, M. Radulescu	Visualization of Detonation Propagation in a Round Tube Equipped with Orifice Plates (1091) G. Raingford, G. Ciccarelli	Single-Head Detonation Propagation in a Partially Obstructed Square Channel (1135) M. Kellenberger, G. Ciccarelli	Detonation Propagation in Rough Tube (991) Y. Liu, J.H. Lee, H. Tan	
Detonation Engines 3 Chairs: S. Jackson, J. Yoh	Small Size Rotating Detonation Engine: Scaling and Minimum Mass Flow Rate (1133) C.B. Kyanda, S. Connolly- Boutin, V. Joseph, X. Mi, H.D. Ng, A.J. Higgins	Experimental Study on a Rotating Detonation Turbine Engine with an Axial Turbine (1080) H. Rhee, C. Ishiyama, J. Higashi, K. Akira, K. Matsuoka, J. Kasadiara, A. Matsuok, J. Funaki	Spectra Signals of Gas Pressure Pulsations in Nozzles (769) V.A. Levin, N.E. Afonina, V.G. Gromov, I.S. Manuelevsky, A.N. Khmelevsky, V.V. Markov	Lunch
Turbulent Flames 3 Chairs: P. Domingo, F. Halter	Combustion in a High-Swirl Turbulent Jet Undergoing Vortex Breakdown. Investigation by PIV and HCHO PLIK (1159) L.M. Chikishev, V.M. Dulin, A.S. Lobasov, D.M. Markovich	Experimental Measurements of Turbulent Burning Velocity in Gas Explosions with Two Obstacles of Variable Spacing: Implication to Gas Explosion Scaling (1156) A. Na'inna, H. Phylaktou, G. Andrews	Disturbance Energy Analysis of Turbulent Swirling Premixed Flame in a Cuboid Combustor (1001) K. Aoki, M. Shimura, Y. Minamoto, M. Tanahashi	
Chemical Kinetics and Reaction Dynamics 4 <i>Chairs: M. Fikri,</i> <i>A. Teodorczyk</i>	Reduction of Detailed Chemical Mechanisms by Entropy Production Analysis in the Presence of Irreversible Reactions (1055) L. Acampora, M. Kooshkbaghi, C.E. Frouzakis, F.S. Marra	On the Dynamics of Ignition Process Behind Reflected Shock Waves Under the Influence of Bifurcation (774) O. Pryor, S. Barak, E. Nimemann, S. Vasu	Effects of Variation in Sample Mass, Gas Flow and Lid on Chemical Reactions During STA Measurements (1068) D. Lázaro, M. Lázaro, A. Alonso, D. Alvear	
Topic	11:10	11:35	12:00	12:25

Combustion Stability, Instabilities 3 Chairs: V. Bykov, G. Ribert	Effects of External Heating on Flame Stability in A Micro Porous Combustor Fueled with Heptane (944) J. Li, X. Chen, M. Feng, R. Yao, N. Wang	Tomographic Visualization of Thermo-Diffusive Instabilities of Lean Hydrogen/Air Mixtures J. Goulier, N. Kouame, M. Idir, N. Chaumeix	Edge Flame Dynamics - Assisting the Stabilization of Diffusion Flames in Mixing Layers (887) Z. Lu, M. Matalon Z. Lu, M. Matalon		Reactive Systems 3 Chairs: F. Marra, J. Yao	Calculation of Thermo-Chemical Equilibrium Using Phase Diagram Methods (1102) A.E. Gheribi, J.J. Lee
Detonation Diffraction 1 Chairs: A. Matsuo, X. Mi	Propagation Characteristics of 2H2/O2/2Ar Detonations in Channels with Constant Area Divergence (1110) Q. Xiao, J. Chang, M. la Fleche, Y. Wang, M.I. Radulescu	Propagation of a Detonation in a Converging Conical Channel (984) I.H. Hung, J.H. Lee	Mechanism for Dynamical Stabilization of Detonation in Expanding Channels (791) X. Cai, J. Liang, R. Deiterding, X. Cai, Z. Lin, S. Liu	:20)	Detonation Failure and Propagation Chairs: K. Hayashi, R. Mével	Detonation Failure in Stratified Layers - the Influence of Detonation Regularity (908) A.V. Gaathaug, K. Vaagsaether, D. Bjerkervedt
DDT 3 Chairs: M. Ihme, A. Kasimov	Deflagration-To-Detomation Transition for Hydrogen- Enriched Air Mixtures Through Presure Wave Focusing in Pipes (968) S. Bengoechea, J. Gray, J. Reiss, J. Moeck, C. Paschereit, J. Sesterhenn	Numerical Study on Effects of Obstacle Shape on Detonation Transition Mechanism (1027) A. Ago. T. Nitbo., N. Tsuboi, A.K. Hayashi	Quasi-Detonation in Matrix of Cylinders (1022) P.N. Krivosheyer, A.O. Novitski, O.G. Penyazkov, K.L. Servouk	Coffee Break Poster Session II (15:05 - 16 Tickind Lounce	Detonation Engines 4 Chairs: R. Houim, C. Kiyanda	Numerical Investigation on the Behavior of Detonation Waves in a Disk-Shaped Rotating Combustor (1046) Y. Sato, A. Matsuo, J. Higashi, C. Ishiyama, K. Matsuoka, J. Kasahara
Explosion Safety 3 Chairs: C. Proust, J. Wen	Evaluation of Engineering Models for Vented Lean Hydrogen Deflagrations (1111) A. Sinha, V.C.M. Rao, J.X. Wen	The Essential Role of Science in Explosives Safety (1099) C.B. Skidmore, K.A. Fleming	A Model to Account for the Effects of Friction During Explosive Pinch (1020) R. Timms, R. Purvis, J.P. Curtis		Shock Tubes, Ignition Delay Times, Kinetics 1 Chairs: U. Maas, E. Petersen	Ignition Delay Times of Methane/Diethyl Ether Blends Measured in a Rapid Compression Machine (RCM) (812) S. Drost, M. Werler, R. Schießl, U. Maas
Ignition 2 Chairs: S. Coronel, J. Melguizo-Gavilanes	Effect of Low Initial Pressures on Ignition Properties of Lean n- Decane/Air Mixtures for Laser Induced Breakdown (332) S. Rudz. P. Tadini, F. Berthet, P. Gillard	Thermomechanics of Laser- Induced Shock Waves in Combustible Mixtures (1108) N.D. Peters, D.M. Combs, B. Akih-Kumgeh	Direct Numerical Simulation of Ignition by Hot Moving Particles (1121) T. Zirwes, F. Zhang, T. Häber, D. Roth, H. Bockhorn		Energetic Materials 1 Chairs: D. Frost, M. Hobbs	Burning Characteristics of Aluminum-Air Flames (1054) R. Lomba, F. Lespinasse, Y. Lago, C. Chanveau, F. Halter
Topic	13:50	14:15	14:40	15:05 15:05	Topic	16:20

Turbulent Fuel Droplet Vaporization and the Initial Size Effect: Experimental Data at Elevated Temperature and Pressure (1076) C. Verwey, M. Birouk	Numerical Investigation on the Initial Development of Layered Coal Dust Combustion (958) K. Shimura, A. Matsuo	Impact of Water Mist on Chemical Reaction of Methane/Air/Water-Mist Premixed Flames (1035) S. Nakanishi, Y. Ogami, M. Ho, T. Tsuruda		
Effect of Vertical Concentration Gradient on Detonation Behavior with Detailed Reaction Mechanism (776) W. Han, W. Kong, N. Du, Z. Liu	Experimental Investigation of Detonation Failure and Re- Initiation in Non-Uniform Compositions (1013) S. Boulal, P. Vidal, R. Zitoun, T. Matsumoto, A. Matsuo	Numerical Investigation of Detonation Failure in Non- Uniform Compositions and Comparison to Experiments (1030) T. Matsumoto, S. Boulal, A. Matsuo, P. Vidal, R. Zitoun		
Numerical Investigation on Detonation Behavior in a Disk-Shaped Rotating Detonation Combustor (1103) Y. Kumazawa, A. Matsuo, S. Nakagami, K. Matsuoka, J. Kasahara	A Numerical Study of H2- Air Rotating Detonation Combustor (1097) S. Yellapantula, V. Tangirala, K. Singh, J. Haynes	Generation of Detomation in a Supersonic Flow of Combustible Mixture with Use of Bended Channel (1106) V.A. Levin, J.S. Manuylovich, V.P. Markov	Adjourn	Thursday Banquet <i>Harvard Club</i> (see dress code)
Experimental and Numerical Study of the Ignition Delay Times of Primary Reference Fuels Containing Diethyl Ether (957) M. Fikri, Y. Sakai, J. Herzler, C. Schulz	Ignition Delay Time Measurements of Sarin Surrogate (TE), DMMP)- Based Mixtures in a Heated Shock Tube (1149) O. Mathieu, W.D. Kulatilaka, E.L. Petersen	Ethene / Dinitrogen Oxide - A Green Propellant to Substitute Hydrazine: Investigation on Its Ignition Delay Time and Laminar Flame Speed (1075) C. Naumann, T. Kick, T. Mething, M. Braun-Unkhoff, U. Riedel		
Spherically-Expanding Flames in Hybrid Aluminum-Methane- Oxidizer Mixtures at Atmospheric Pressure (799) J. Vickery, P. Julien, S. Goroshin, J.M. Bergthorson, D.L. Frost	Experimental Study on Effect of Large-Sized Granules in Powdery Explosives Under Drop- Weight Impact (948) Y. Wu, H. Guo, F. Huang, X. Bao	Free		
16:45	17:10	17:35	18:00	18:30 22:00

			Friday		
Room	Auditorium	Ballroom A	Ballroom B	East Balcony	Terrace Lounge
Topic	Ignition 3 Chairs: D. Markus, S. Shy	Explosion Safety 4 Chairs: T. Tsuruda, J. Wen	Detonation Modeling Chairs: C. Chiquete, M. Short	Detonation Diffraction 2 Chairs: K. Hayashi, R. Mével	Spherical Explosions Chairs: V. Bykov, R. Schießl
00:6	Flame Speed Measurements in Turbulent Dispersions of Liquid Fuels (1064) <i>P.M. de Oliveira, T. Higuchi,</i> <i>P.M. Allison, E. Mastorakos</i>	Electrochemical Reaction Kinetics for CO-CO2 Electrochemical Conversion in the Nickel-Patterned Electrode (88) Y. Luo, Y. Shi, W. Li, N. Cai	Numerical Computation of Linear Stability of Detonations (914) D.I. Kabanov, A.R. Kasimov	Propagation Behavior of Diverging Cylindrical Detonation in Mixture with Reactivity Change (962) T. Okada, A. Matsuo, J.H. Lee	Effects of Endothermic Chain- Branching Reaction on Spherical Flame Initiation and Propagation H. Li, H. Zhang, Z. Chen
9:25	A Simulation of Ignition Thresholds for Low Voltage Electrical Contact Ares in a Hydrogen-Air Mixture (910) <i>R. Shekhar, C. Uber,</i> <i>U. Gerlach</i>	Blast From Pressurized CO2 Released Into a Vented Chamber (826) <i>P.M. Hansen, A.V. Gaathaug,</i> <i>D. Bjerketvedt, K. Vaagsaether</i>	A Full Scale Hydrodynamic Simulation of Detonation and Deflagration in an Energetic Component System (892) B. Kim, J.J. Yoh	Prediction of the Critical Curvature for LX-17 with the Time of Arrival Data From DNS (1112) J. Yao, L.E. Fried, W.C. Moss	Dynamic Behavior of Spherically Expanding Flame of H2/Air/CO2 Mixture in a Closed Chamber (867) T. Katsumi, K. Aidon, Y. Itakura, S. Kadowaki
9:50	A Computational Study of the End Gas Autoignition and Shock Development by Flame Front and Local Hot Spot (1021) A. Sow, B.J. Lee, H.G. Im	Flame Spread Over Electrical Wires with Various Diameters Under Applied AC Electric Fields (943) S.H. Park, S.J. Lim, J. Park, O.B. Kvon, O. Fujita, S.H. Chung	Free	The Methods of Control of Stabilized Detonation Location in a Supersonic Gas Flow in a Plane Channel (781) V.A. Levin, T.A. Zhuravskoya	Free
10:15			Coffee Break		
Topic	Ignition 4 Chairs: D. Markus, S. Shy	Shock Tubes, Ignition Delay Times, Kinetics 2 Chairs: J. Herzler, U. Maas	DDT 4 Chairs: R. Houim, P. Vidal	Detonation in Non-Uniform Mixtures Chairs: S. Jackson, M. Short	Reactive Systems 4 Chairs: H. Im, W. Sirignano
10:45	Experimental Investigation of the Electrical Characteristics of Low- Voltage Contact-Arcs in Hydrogen-Air Mixture (907) C. Uber, R. Shekhar, U. Gerlach	Experimental Measurement of Ignition Delay Times of Thermally Cracked n-Decane in Shock Tube (788) S. Pei, H. Wang, X. Zhang, S. Xu, L. Wang, G. Liu	Exploration of Turbulence Driven Deflagration to Detonation of Fast Flames J. Chambers, K. Ahmed, A. Poludnenko	Self-Sustained Oblique Detonation in a Non-Uniform Mixture (1009) K. Iwata, S. Nakaya, M. Tsue	Measurements of Laminar Flame Speeds of Alternative Liquid Fuel Blends (825) S.F. Samim, S. Ahmed

Diffusion Flame at High Pressure with Air and Water-Laden Methane (945) A. Jorda, W.A. Sirignano	Free	Free		Reactive Systems 5 Chairs: V. Bykov, U. Maas	A Computational Analysis of Autoignition of H2/Air Mixture with Temperature Fluctuations Using Computational Singular W. Song, E.A. Tingas, S.R. Lee, H.G. Im
Numerical Study of a Gaseous Detonation Propagation Across a Density Interface (987) K.C.T. Yuk, X.C. Mi, J.H. Lee, H. Teng, H.D. Ng	Numerical Investigation on Characteristics of a Planar Detonation Wave Across Layers of Burned Gas (994) N. Ohira, A. Matsuo, J. Kasahara, K. Matsuoka	Physical and Mathematical Modeling of Interaction of Detonation Waves in Mixtures of Hydrogen, Methane, Silane and Oxidizer with Clouds of Inert Micro- and Nanoparticles (750) D.A. Tropin, A.V. Fedorov		Diagnostics, Sensoring 2 Chairs: R. Schießl, S.Y. Yang	Embedded Fiber Optic Sensors for Measuring Transient Detonation/Shock Behavior: Time-of-Arrival Detection and Waveform Determination (766) M.A. Chavez, M.D. Willis, T.T. Covert
The Influence of Turbulent Mixing on Deflagration to Detonation Transition (1078) B. Maxwell, M.I. Radulescu, A.A. Pękalski	Numerical Study of Deflagration-to-Detonation Transition in Homogenous and Inhomogeneous Hydrogen-Air Mixtures (834) <i>R.K. Azadboni, A. Heidari,</i> <i>L.R. Boeck, J.X. Wen</i>	Free	Lunch	Detonation Engines 5 Chairs: A. Chinnayya, C. Kiyanda	Experimental Investigation on Delay Time of Continuously Detonation Engine (796) X. Han, S. Zhang, Z. Ma, J. Wang
Numerical Investigations of the Impact of Tailored Driver Gases and Driver Inserts on Shock Tube Flows (1118) D.M. Coombs, B. Akih-Kumgeh	Chemical Reaction Mechanisms Validation Based on Ignition Delay Time of C1- C5 Hydrocarbons (928) <i>W. Rudy. A. Jach, A.A. Pękalski</i> , <i>A. Teodorczyk</i>	Free		Dust Explosions 3 Chairs: G. Ciccarelli, E. Oran	Analysis of Dust Cloud Combustion Using High-Speed Infrared Imaging (913) F. Marcotte, S. Savary, M.A. Gagnon, V. Morton
A Rapid Compression Machine Study of n-Decane Ignition at Intermediate Tenperatures (926) V.V. Leschevich, O.G. Penyazkov, S.Y. Shimchenko	Investigation of the Flame Kernel Propagation After Ignition by a Low Energy Electrical Discharge (1006) S. Essmann, D. Markus, U. Maas	Hot Surface Ignition Dynamics in Hydrogen-Air Mixtures Near the Flammability Limits (1100) L.R. Boeck, J. Melguizo- Gavilanes, J.E. Shepherd		Energetic Materials 2 Chairs: D. Frost, C. Proust	On Minimum Flash Ignition Energy of Energetic Igniter Using Aluminuum Nanoparticles: Effects of 2D Interparticle Distances (1139) J.Y. Yu, Y.P. Chan, Y.C. Hsu, Y.C. Chao
11:10	11:35	12:00	12:25	Topic	14:15

IR Absorption Measurements of the Velocity of a Premixed Hydrogen/Air Flame Propagating in an Obstacle- Laden Tube (1057) R. Scarpa, E. Studer, B. Cariteau, S. Kudriakov, N. Chaumeix	Study on Low Temperature Oxidation with a Separated Cool Flame of n-Heptane in a Micro Flow Reactor with a Controlled Temperature Profile (920) <i>R. Tatsumi, H. Nakamura,</i> <i>S. Hasegawa, T. Tezuka, K. Maruta</i>	Free		
Possibility of Applying Flame Chemiluminescence and Ionization Current to the Combustion Status Monitoring (933) Y. Ding, D. Durox, N. Darabiha, T. Schuller	Infrared Radiation Measurements at Failure of Mobile Gas Vessels (1034) D. Krentel, M. Rudolph, R. Tschirschwitz, M. Kluge, E. Askar, K. Habib, H. Kohlhoff, G. Mair, P. P. Neumann, B. Schalau, A. Schoppa, S.U. Storm, M. Szczepaniak	Free		
The Effect of Combustor Width on Continuous Rotating Detonation Wave Fueled by Ethylene (947) H. Peng. W. Liu, S. Liu	Numerical Study of Reinitiation Phenomenon in Continuous Detonation Engine (898) S. Yao, J. Wang	Effects of Pre-Ignition Conditions on Continuous Detonation Engine (886) S. Yao, S. Zhang, J. Wang	Friday Farewell Back Court	Adjourn
Dimensional Scaling for Propagation in Particulate Clouds with Lateral and Volumetric Losses (1126) F. Lam, X. Mi, A.J. Higgins	Monitoring of a Dust Explosion in a 10 m ³ Vessel (891) Y. Grégoire, C. Proust, E. Leprette, D. Jamois	Free		
Experimental Investigations of Combustion Enhancement of HAN-Based Green Propellant with K2CO3-Activated Carbon M.K. Atamanov, K. Hori, E. Aliyev, K. Amrousse, Z.A. Mansurov	Development of Protection Recommendations for Warehouse Storage of Li- Ion Batteries (817) B. Ditch	Free		
14:40	15:05	15:30	16:00	18:00

Poster Session I		
Tuesday, 15:30 - 16:45		
	Ignition Delay Times of Dual-Fuel Mixtures of Silane/Hydrogen at High and Low Temperatures	
PI-1	(751)	
	D. Iropin, A. Fedorov Study of the Thermal Effects of Microwaya Induced Places on Dramined Mathema Air Flames	
PI-2	Study of the Thermai Effects of Microwave Induced Plasma on Premixed Methane-Air Flames (800)	
	H.Y. Li, Y.C. Chao	
PI-3	Outwardly Propagating Spherical Flame with Cellular Instabilities and Laminar Burning	
	Velocities in Methane/Ethylene/Air Premixed Flames. (813)	
	K.H. Van, H.J. Kim, J. Park, O.B. Kwon, D.K. Lee, S.G. Kim, Y.T. Guahk, D.S. Noh, S.H. Chung	
DI 4	Combustion Characteristics of Pyrolytic Oil Droplet From Sewage Sludge (831)	
PI-4	G.B. Chen, J.W. Li, H.T. Lin, F.H. Wu, Y.C. Chao	
PI-5	On the Characteristics of Liftoff Heights in Laminar Lifted Flames of Methane in Coflow Jets	
	(836)	
	N.P. Sapkal, K.H. Van, J. Park, O.B. Kwon, B.J. Lee, S.H. Chung	
PI-6	A Detailed Numerical Simulation of an Impulsively Started N-Dodecane Lifted Jet Flame at 40	
	Bar (639) Y Minamoto IH Chen	
	Mixed Gaseous Detonation Fabrication of CNTs and CNTs doning with Fe Based Composites	
PI-7	(875)	
	N. Luo, J. Xiang, T. Shen	
	Hybrid RANS/LES Investigation of Precessing Vortex Core (PVC) in a Swirl Premixed	
PI-8	Combustor (882)	
	Z. Mansouri, 1. Boushaki Numerical Simulations of Machanachemical Degenerase for Confined DDVs Under Law Velocity	
PI-9	Numerical Simulations of Mechanochemical Responses for Confined FBAS Under Low-velocity Impact (889)	
	K. Yang, Y. Wu, F. Huang, Z. Zhang	
DI 10	Phase Transition of RDX Under High Pressure up to 50 GPa (902)	
PI-10	C. Gao, C. Zhang, Z. Sui, Y. Qu, R. Dai, Z. Wang, X. Zheng5, Z. Zhang	
	Temperature Distribution Along a Pulse Detonation Combustor in a Wide Range of Ratios	
PI-11	Between the Oxygen-Enriched Heptane-Air Mixture Components (905)	
	M. Assad, I. Chernukha, O. Penyazkov	
DI 12	Shock Induced Phase Transition of HMX Considering Initial Temperature Effects (921)	
11-12	W. Hu, Y. Wu, F. Huang	
DX 4.0	Study of Downward Flame Spread and Fire Risk Evaluation of the Thermoplastic Materials	
PI-13	(925) D. Zang, W. Zhao, C. Liu, Y. Liu,	
	R. Zong, W. Zhuo, C. Liu, A. Liu	
PI-14	<i>L Li Y Wang N Wang</i>	
DI 15	Effects of Ignition Location on Sect and Species Formation Through Treading Flows Light	
	Effects of registion Elocation on Soot and Species Formation Through Tracking Frame Light Emission and Temperature (946)	
11 15	Y. Wang, Z. Ma, Y. Zhang	
	Structure Evolution of Energetic Material LLM-105 Under High Pressure (952)	
PI-16	Z. Xu, H. Su, X. Zhou, R. Dai, Z. Wang, H. Li, Z. Zhang	
	Rise and Fall of Vortex on a Rotating Paner (953)	
PI-17	T. Tsuruda, T. Daitoku, K. Kobayashi	
	Flame Spread Along a Combustible Slope (954)	
PI-18	T. Tsuruda, K. Hiyama, T. Daitoku	
PI-19	Research of the Rocket Engine with Detonation Chamber (955)	
	M. Kawalec, P. Wolanski	
PI-20	Investigation of Co-Combustion Characteristics of Pulverized Coal with Miscanthus Floridulus	
	Biochar (960)	
	H.T. Lin, G.B. Chen, Y.H. Li, Y.C. Chao	
PI-21	Modelling Analysis of Wave Interactions During the Ignition Process of Rotating Detonation	
	W. Wei, R Wang	
	Numerical Simulation of a Single-Mode Sinusoidal Flame Interacting with a Shockwave (967)	
PI-22	W. Wei, B. Wang	
	5	

PI-23	Physical and Electrical Measurements of Different Metals Used in EBW Detonators (977) C. Valancius, J. Bainbridge, C. Love, D.R. Richardson	
PI-24	Detonation in 3D Annular Chamber with Obstacles and Water Surface on one End (1018) K. Sato, E. Dzieminska, A.K. Hayashi, Y. Tamauchi	
PI-25	A Numerical Investigation on Double-Front Detonation in Solid Explosive Mixture with Varying Aluminum Concentration (1039) W. Kim, M. Gwak, J. Yoh	
PI-26	Numerical Simulation of Rotating Detonation Under Variable Conditions (1104) V. Levin, I. Manuylovich, V. Markov	
PI-27	A Study of Interaction Between Pressure Waves and Reaction Regions in HCCI Combustion Accompanied by Strong Knocking Based on High-Speed in-Cylinder Visualization and Observation (1136) A. Iijima, K. Takeda, Y. Yoshida, Z. Lin, H. Shoji	
PI-28	Simulation Study on Detonation Propagation Driven by Piston (1137) Z. Lin, J.H. Lee, X. Mi	
PI-29	Sensitivity Study of Solid Fuel Properties and Dynamic Behavior of Pyrolysis in Non-Charring Materials (1142) S. Sabarilal, A. Syed, A. Kumar	
PI-30	Experimental Study on Laser Ignition of Low Vulnerability Propellant Based on Nitrocellulose (1071) L. Courty, J.F. Lagrange, P. Gillard, C. Boulnois	
Poster Session II		
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Thursday, 15:05 - 16:20		
	Ziskind Lounge	
PII-1	Influence of Methane Additions on Self-Ignition of Pulsed Jet of Hydrogen (777) S. Golovastov, V. Bocharnikov, O. Terekhova	
PII-2	Double Shock Experiments on PBX Explosive JOB-9003 (783) <i>X. Zhang</i>	
PII-3	Shock Initiation of Wedge-Shaped Explosive Measured with Smear Camera and Photon Doppler Velocimetry (784) <i>Y. Gu</i>	
PII-4	Analysis of the Canonical Turbulent Shock Front (809) H. Cao, T. Jin, L. Wang, K. Luo, J. Fan	
PII-5	Experimental Rotating Detonation Engine Behavior Dependence on Detonation Channel Width (819) M. Fotia, J. Hoke, F. Schauer	
PII-6	Effects of Flame Instabilities in Hydrogen-Air Explosions (820) W. Kim, T. Imamura, T. Mogi, R. Dobashi	
PII-7	3D Flame Reconstruction Using Single Camera and Fibers (824) K. Wang, F. Li, X. Yu	
PII-8	Effect of Ambient Oxygen and Temperature on Gaschromic Properties of Pt/WO3 Thin Film Exposed by Hydrogen (829) K. Yashiki, T. Matsuoka, Y. Nakamura	
PII-9	Adjoint-Based Variational Data Assimilation for the Analysis of an Experimental Pulsed Detonation Combustor with a Compact Shock-Focusing Geometry (847) <i>M. Lemke, J. Gray, J. Reiβ, J. Moeck, J. Sesterhenn</i>	
PII-10	Numerical Modeling on the Flow Characteristic of Catalytic Combustion Over a 2D Cylindrical Bluff Body (849) C.Y. Wu, C.C. Cheng, Y.S. Lien	
PII-11	The Model of Detonation Combustion in Liquid Aerosols (862) O. Girin	
PII-12	Three-Dimensional Supersonic Boundary Layer Separation Induced by Curved Sidewall (878) G. He, J. Zhou, Y.X. Zhao, Y.L. Zhao	
PII-13	Breakdown Ignition of Nonsolvent Ionic Liquid with Double Pulse Laser (897) N. Itouyama, H. Habu	
PII-14	Numerical Investigation of the Instability of Continuous Detonation Engine (934) S. Zhang, S. Yao, M. Luan, L. Zhang, J. Wang	
PII-15	Experimental Study on the Explosion Characteristics of Methane-Hydrogen/Air Mixtures (951) X. Shen, G. Xiu	
PII-16	A Study on Burning Velocity Characteristics of Meso-Scale Spherical Laminar Flames for Lean- Hydrogen-Propane Mixtures (964) M. Nakahara, Y. Maruyama, A. Ishihara, F. Abe, K. Tokunaga	
PII-17	The Finite Heat Conduction Model of Single Droplet Combustion and its Verification (972) S. Fei, Y. Qi, Y. Li, M. Wei, G. Guo, Z. Wang	
PII-18	Effect of Additional Diluents on Laminar Burning Velocities and Cellular Instability in Outwardly Propagating Methane/Ethylene-Air Premixed Spherical Flame (973) H.J. Kim, K.H. Van, J. Park, O.B. Kwon, D.K. Lee, S.G.K.Y.T. Ghauk, D.S. Noh	
PII-19	Safety Problems of Commercial Cap-Sensitive Emulsion Explosives Turnover in the Territory of the Republic of Kazakhstan (1010) I. Pustovalov, S. Aleshkova, M. Atamanov, E. Aliyev, Z. Mansurov	
PII-20	Effects of Discharge Frequency on Ignition Behaviors of DBD for Lean Methane/Air Mixtures (1014) S. Nakova, X. Gu, T. Kobavashi, S. Jeski, M. Tsue, M. Kono, K. Nakamura	
PII-21	Flame Propagation and Initiation of Detonation in a Two-Dimensional Annular Channel with Cylindrical Obstacles (1016) H. Sakai, E. Dzieminska, A.K. Hayashi, Y. Tamauchi	
PII-22	Comparison of Detailed Mechanisms for the Numerical Simulation of Unsteady Shock-Induced Combustion (1051) P.K. Pavalavanni, J.Y. Choi	

PII-23	Roughness Influence on Flame and Detonation Propagation (1056) E. Dzieminska, Y. Hara, M. Morishita
PII-24	Effect of Swirl Intensity on the Flow and Combustion Characteristics of Pulverized Biomass Flame (1086) A. Elorf, B. Sarh, S.Bostyn, V. Belandria, S. Bonnamy, M. Asbik, F. Tabet, J. Chaoufi, I. Gokalp
PII-25	Impulse Measurement of Small Scale Detonation Tubes Under Direct and Indirect Detonation Initiations (1092) J. He, W. Fan, J. Zheng, Y. Chi
PII-26	Study on Non-Ideal Detonation Behaviour Based on Analog System (1123) Y. Sun, H. Yang, C. Wang
PII-27	High Resolution Numerical Simulation of Multi-Phase Hybrid Detonation (1128) C. Wang, Y. Zhao
PII-28	Study of Hypergolic Hybrid Rocket Using Hydrogen Peroxide As Oxidizer (1141) C. Lu, Y. Chou, Y.C. Chao
PII-29	An Overview of PERWAVES: A Sounding Rocket Experiment to Examine Flame Propagation in the Discrete Regime (1146) J. Palecka, S. Goroshin, J. Bergthorson, A. Higgins
PII-30	The Study of Turbulence Effects in Highly Unstable Detonation Mode (1153) D.R. Cho, J.Y. Choi

Work-in-Progress Posters		
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	W. Xiaodong, C. Losier, V. Robin, A. Mura	
WIP-2	Modeling Expansion of Particle Clouds (986)	
	A. Kuhl, D. Grote	
WIP-3	Study of Hypergolic Hybrid Rocket Using Hydrogen Peroxide As Oxidizer (1141) C. Lu, Y.C. Hsu, Y. Chou, Y.C. Chao	
WIP_4	Combustion Characteristics of a Pinewood Pyrolysis Bio-Oil Droplet at High Ambient Temperatures (4302)	
W 11 -4	S.I. Yang, M.S. Wu, E. Lin	
WIP-5	Testing Methods for Continuous Monitoring of SO3 and H2SO4 at Flue Gas Conditions (4305) Y.C. Chien, A. Biasioli, D. Dunn-Rankin	
WIP-6	Propagation of Hydrogen-Air-Vapor Flame in Presence of Water Droplets (4306) Robertoruso, N. Chaumeix, A. Bentaïb	
WIP-7	A Review of Flame Propagation and Quenching in Pipes and Ducts Handling Combustible Dusts (4308)	
	A. Ing	
WIP-8	Sulfur Chemistry in Combustion Processes (4309)	
	M. Alzuela, M. Aolan, J.M. Colom-Diaz, A. Millera, R. Biloao An Experimental Ignition Delay Time and Chemical Kinetic Modelling Study of 1-Heyene	
WIP-9	(4311) I.I. Rodríguez-Henriguez, A. Nawdival, C. Banyon, H. Curran, F. Mauss	
	Investigation on Coal Dust Explosion Characteristics and Its Influcing Factors Using 20L	
WIP-10	Spherical Vessel (4313) Q. Li, Q. Tao, C. Yuan, Y. Zheng	
	The Influence of the Boundary Conditions on the Urea-Water Solution Decomposition in Case	
WIP-11	of Closed Coupled Selective Catalytic Reduction Systems Performance (4315)	
	K. KOgoz, F. Jaworski, A. Teodorczyk	
WIP-12	A Study of Pyrolytic Oil From Sewage Sludge Using the Taguchi Method and Its Combustion Characteristics (4316)	
	G.B. Chen, J.W. Li, H.T. Lin, F.H. Wu, Y.C. Chao	
	Development of a TDLAS Sensor for Temperature and Concentration Measurements of H2O	
WIP-13	in High Speed and High Temperature Reacting Flows (4317)	
	S. Sheehe, S. O'Byrne	
WIP-14	Stability of Premixed Gaseous Flames Propagating in Hele-Shaw Cells (4320) D. Fernandez-Galisteo, V. Kurdyumov	
	Evaluation of Increase in Maximum Pressure Caused by Flame Propagation in Semi-Closed	
WIP-15	Ducts (4322)	
	L. Murakami, N. Ito, T. Mogi, R. Dobashi	
WIP-16	Burner (4323)	
	H. Shibagaki, Y. Yahagi, I. Makino	
WIP-17	Kinetics of Combustion of Synthetic Jet Fuels (4324)	
	P. Dagaut, G. Dayma, P. Dievart, F. Karsenty	
WIP-18	Validation of FLACS-Fire for Large Scale Fires of Natural Gas/Hydrogen Mixtures (4326) D. Muthusamy	
WID 10	Effect of Pressure on the Flame Transfer Function of a Swirled Methane-Air Premixed Flame	
WIP-19	(4327) T.F. Guiberti, A. di Sabatino, W.R. Bovette, W.L. Roberts, J. Moeck, A. Lacoste	
	Decreasing the Run-Up Length to DDT Through the Application of Nanosecond Repetitively	
WIP-20	Pulsed Discharges in Place of Obstacles (4328)	
	J. Gray, A. Lacoste	
WIP-21	Simulations of Underwater Explosion Phenomena (4329)	
	A. Gavrikov, IV. Zaretskiy, A. Aleksandrov, A. Efimenko, S. Privezentsev, V. Alekseev, K. Makarov	
WIP-22	гторапе and Air Mixture – Based Short-Barrei Detonation Gun (4332) K. Korytchenko, Y. Kysternyy, O. Sakun	

WIP-23	Acoustic Response of Strained Methane-Oxygen Diffusion Flames (4334) A. Weiss, W. Coenen, A.L. Sánchez, F.A. Williams
WIP-24	Numerical Modeling on the Flow Characteristic of Catalytic Combustion Over a 2D Cylindrical Bluff Body (4336) C.Y. Wu, C.C. Cheng, Y.S. Lien
WIP-25	Effects of Stoichiometric Mixture Fraction on Triple-Flame Propagation in Strained Mixing Layers (4339) P. Rajamanickam, W. Coenen, A.L. Sánchez, F.A. Williams
WIP-26	Propagation of a Shock-Flame Complex Around a Cylinder (4341) W. Rakotoarison, M.I. Radulescu
WIP-27	Flame Propagation Behavior in Semi-Closed Pipes with Bend (4342) T. Mogi, N. Ito, L.M. J.P., R. Dobashi
WIP-28	A Statistical Representation of Pyrotechnic Igniter Output (4343) S. Guo, M. Cooper
WIP-29	Micro-Explosion and Burning Characteristics of a Single Droplet of Petrochemical Heavy Oils (4344) K. Ahuia, Y.H. Li, G.B. Chen, Y.C. Chao, Y.T. Yang
WIP-30	Modeling of Mist Explosions in the CFD Simulator FLACS (4346) L. Bernard, T. Skjold
WIP-31	Towards Analytical Predictive Scenario of a Coalmine Burning Accident (4347) S. Demir, V. Akkerman
WIP-32	Effects of Ignition Delay by Nitrogen Film Cooling on Ignition Transition of Gaseous Oxygen/Kerosene Spray Combustor (4349) W. Song, D. Shin, M. Son, J. Koo
WIP-33	On the Emission of Pollutants After Blending Conventional Fuels with Renewable Fuels. (4350) P.Dagaut, G.Dayma, F.Foucher, A. R.Shah la
WIP-34	Experimental Estimation of Laminar Burning Velocities in Hydrogen-Air Mixtures, with and Without Water Mist (4351) B.J. Arntzen, W. Puorury
WIP-35	Numerical Prediction of Shock Induced Ignition in the Presence of Fluctuations (4352) W. Wang, J. McDonald, A.A. Pękalski, M. Radulescu
WIP-36	Development and Testing of Novel LED-Based, Robust, High-Speed, Fire Detection Sensor (4353) S. Vasu
WIP-37	Small-Scale Rotating Detonation Engine Development and Testing (4354) C.B. Kiyanda, S. Ahmed, M.A. Allard, S. Connolly-Boutin, S. Fahmy, V. Joseph, M. Nashen, H.D. Ng, A. Higgins
WIP-38	Thermal Ignition Revisited with Three-Dimensional Molecular Dynamics: Role of Fluctuations in Activated Collisions (4356) N. Sirmas, R. Murugesan, M. Radulescu
WIP-39	Ethanol Deflagration to Detonation Transition (4381) A.Z. Mendiburu, J.A. de Carvalho, G. Ciccarelli, F.S. Carvalho
WIP-40	A Novel Utilization Direction for Ventilation Air Methane: Explosion Power Generation (4388) B. Nie, C. Peng, L. Yang

9:00 Plenary Lecture 1

PL1 - Condensed phase detonation: Are mesoscale effects needed to predict performance?

Scott I. Jackson, Los Alamos National Laboratory, USA

Condensed-phase explosives provide one of the most high-power and energy-dense storage materials available. They are commonly detonated to perform work on adjacent materials for engineering applications in the defense and mining industries, with several billion kilograms used in the United States alone per year. Despite their engineering utility and high level of use, very little is known about the reaction-zone physics and high-pressure product states generated during detonation of high explosives due to the extreme conditions that are generated. Condensed-phase explosives will detonate when processed by a sufficiently strong shock wave, producing product energy densities approaching 14 MJ/L and energy release rates exceeding 1 TW/sq. m, which is higher than the radiative flux at the solar surface. Conditions in the detonation reaction zone are at the upper limit of the condensed matter regime and reach pressures as high as 40 GPa, temperatures of approximately 4000 K, and detonation shock velocities above 9 km/s. These extreme conditions are sufficient to plastically deform any adjacent manmade material and this yielding can induce significant local variations in flow field of the detonation reaction zone, which is on the order 10-100 micron in thickness. Additional localized chemical and thermodynamic variations also result from the shock passage though the heterogenous microstructure of the explosive itself, which generally consists of a composite matrix of chemically complex energetic crystals and inert binding materials with variations on the order of the reaction zone thickness. In this talk, we review the chemistry and microstructure of high explosives, discuss the mesoscale effects present at scales on the order of the reaction zone thickness during detonation, and consider if resolving these mesoscale effects is critical to the prediction of detonation performance for these materials. Potential future research directions relevant to these issues are also suggested.

10:30 Chemical Kinetics and Reaction Dynamics 1

859 - A Rapid Compression Expansion Machine (RCEM) for Measuring Species Histories

M. Werler, R. Schießl, U. Maas

A rapid compression/expansion machine (RCEM), which is an extension of the conventional RCM concept, is introduced. First, the mechanical setup and operation principle of the RCEM are outlined. A RCEM-based measurement method for chemical reactions is proposed, which first stimulates reaction in the cylinder by rapid compression, and then quenches the ongoing reaction after a controlled, pre-defined time (hold time) by rapid expansion. Probe sampling of the expanded, cold gas can then be used to track the evolution of chemical species as a function of the hold time. An efficient numerical model for describing important in-cylinder processes (chemical reactions. To characterize the experiment, pressure histories from multiple compression/expansion sequences are discussed. It is shown that the compression/expansion process in our machine can be reproduced very well. First examples of quasi-time resolved species measurements conducted with the RCEM are presented.

1061 - Validation of Hierarchical REDIM Based Reduced Models

V. Bykov, A. Neagos, U. Maas

The problem of reduced model accuracy and its validation is in the focus of the study. The approach to quantify the accuracy of reduced models in a combustion system state space is suggested. It is based on an appropriate distance definition and can be implemented for pointwise discrete representation.

A slightly lean free premixed syngas-air flame is considered for illustration and verification of the suggested approach. A 3D REDIM manifold is constructed by using hierarchical approach and results of 1D, 2D and 3D reduced models are presented and compared. The study shows the suggested approach can be used efficiently to verify the accuracy of the reduced model. It is demonstrated that the 3D REDIM for the considered combustion system describes completely the transient behaviour of

the combustion system. In particular, this means that the constructed 3D REDIM manifold can be used efficiently to study premixed turbulent flames.

852 - Predicting Large-Scale Effects During Cookoff of PBXs and Melt-Castable Explosives *M.L. Hobbs, M.J. Kaneshige, W.W. Erikson*

We have made reasonable predictions of the cookoff response of large-scale systems containing plastic bonded explosives (PBXs) and a melt-castable explosive using kinetics determined from small-scale experiments. The key to scaling is to include relevant physics for the systems of interest. In the current work, we discuss cookoff of PBX 9502, PBX 9501, LX-14, and Comp-B. PBX 9502 is composed of 95 wt% triaminotrinitrobenzene (TATB) and 5 wt% chlorotrifluoroethylene/vinylidine fluoride (Kel-F). PBX 9501 is composed of 95 wt% octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) and 2.5 wt% Estane® 5703 (a polyurethane thermoplastic), and 2.5 wt% of anitroplasticizer (NP): BDNPAF, a 50/50 wt% eutectic mixture of bis(2,2-dinitropropyl)-acetal (BDNPA) and bis(2,2-dinitropropyl)-formal (BDNPF). LX-14 is composed of 95.5 wt% HMX and 4.5 wt% Estane® 5702-F1. Comp-B is nominally composed of 63 wt% hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX), 36 wt% 2-methyl-1,3,5-trinitrobenzene (TNT), and 1 wt% wax. Figure 1 shows various stages of damage for each of these explosives in Sandia's Instrumented Thermal Ignition (SITI) half-shell configuration [1].

919 - Construction of Simple Reaction Mechanisms for C3H8/Air Mixtures Considering Five Combustion Properties

Y. Sasaki, H. Nakamura, K. Maruta

Simple reaction mechanisms for propane/air mixture were constructed based on detailed reaction mechanisms by building up several steps of reactions to reproduce five combustion properties: dependences of the laminar burning velocity on the initial gas temperature, equivalence ratio and pressure (SLT, SLE and SLP); dependence of the ignition delay time on the initial gas temperature (IGT); and the intermediate profile in a laminar flame represented by CO (I-CO). To individually express flame propagation and autoignition phenomena, two fuel decomposition paths were introduced. To express laminar burning velocities in fuel-lean and fuel-rich conditions, oxygen and fuel were employed for two decomposition paths of an intermediate (CH₂O) as the third-body species. To reproduce CO profile in a laminar flame, reverse reaction from CO₂ to CO was introduced. To reduce reaction rate of the chain branching cycle at higher pressures, reaction of H₂O₂ production and its reverse reaction were introduced. As a result, all the employed combustion properties were successfully reproduced by a 10-step mechanism.

10:30 Laminar Flames 1

1069 - Effects of Pressure and Temperature on Laminar Burning Velocity of a Kerosene Surrogate

R. le Dortz, M. Bellenoue, J. Sotton, C. Strozzi

Environmental international bodies as ACARE for Europe (Advisory Council for Aviation Research and Innovation in Europe) are more and more drastic concerning turbo-engines pollution and consumption reduction. To reach the objectives of pollutant emission and consumption reductions, innovative solutions are in development as for example, constant-volume combustion. Characterizing the propagation of a kerosene-air flame in this kind of combustion is necessary. Particularly, the laminar burning velocity and the Markstein length in laminar adiabatic conditions are both key parameters to improve the efficiency of innovated turbo-engines.

In this study, a new spherical combustion chamber developed in Institut PPRIME is first validated with a *n*-decane/air premixed flame for an initial pressure $P_0 = 0.1$ MPa and an initial temperature $T_0 = 400$ K, comparing with literature data and numerical simulations. This combustion chamber is then employed to perform measurements of kerosene/air premixed flames at various temperatures ($T_0 = 400$ K to 470 K), pressures ($P_0 = 0.1$ MPa to 0.5 MPa) and equivalence ratios ($\phi = 0.6$ to 1.5). The kerosene is represented with a 3-components surrogate: the Dagaut surrogate constituted with a mixture of *n*-decane/*n*-propylbenzene/*n*-propylcyclohexane. Finally, the Luche reduced chemical kinetic mechanism is validated in terms of laminar burning velocity comparing to the measurements and using

CANTERA chemical kinetic software. This mechanism was validated for molar fractions and ignition delays during a combustion process, but never for laminar burning velocities.

1083 - Observation of Double Flame Structures in Near-Limit Premixed Flames

C.B. Reuter, Y. Ju

While the existence of cool flames has been known for centuries, new and unexpected cool flame phenomena are still being discovered today. This study investigates that extinction of a near-limit premixed hot flame into a stable cool flame for DME/O₂/O₃ mixtures in a counterflow burner. Experimental and numerical results show that the hot flame gradually transitions into a double flame as the flame speed of the low-temperature preheat zone exceeds that of the high-temperature reaction zone. The preheat zone eventually becomes an independent cool flame when the hot flame extinction limit is surpassed and the main reaction zone disappears.

1040 - Distinct Dependence of Flame Speed to Stretch and Curvature

F. Thiesset, F. Halter, C. Bariki, C. Chauveau, I. Gokalp

Focus is shed on the dependence of the flame kinematic properties (flame displacement and consumption speed) to stretch, curvature and strain. The main target is to address whether or not flame stretch is the only geometrical scalar affecting the flame speed. Our experimental configuration is a flame interacting with a vortex which contrary to spherically expanding or counter flow flames allow stretch and curvature effects to be independently studied. Our data provides strong support for the asymptotic theory developed by e.g. Bechtold and Matalon 2001, which reveals a distinct dependence of flame speed to curvature and stretch.

801 - A Numerical Study on the Effect of Hydrogen Mole Fraction on NO Formation in H2/CO Syngas/Air Laminar Diffusion Flames

Y. Ye, Z. Gu, J. Xi, A. Haiyang, Z. Xianpeng

This paper reports a numerical investigation of H_2/CO syngas NO emission in opposed-flow diffusion flame by using Chemkin. An analysis of how hydrogen fraction influence the NO emission by changing mole fraction of hydrogen is provided. Optical thin model is applied to consider the influence of radiation heat to the flame, using GRI-Mech 3.0 as reaction mechanism.

The computational predictions showed that the flame temperature increases monotonously with H_2 fraction increasing. However, the flame temperature under adiabatic condition decreases with hydrogen fraction increasing. Meanwhile, with hydrogen fraction increasing, the NO emission of syngas flame increases obviously, and the thermal route contributes the largest part of NO emission increasing, leading the variation of NO emission.

10:30 Detonation Engines 1

833 - Mid-Infrared Imaging of a Non-Premixed Rotating Detonation Engine

B.A. Rankin, J.R. Codoni, K.Y. Cho, J.L. Hoke, F.R. Schauer

The detonations propagating through the annular channel of an optically accessible rotating detonation engine (RDE) are visualized using mid-infrared imaging. The RDE is operated on hydrogen-air mixtures for a range of air mass flow rates and equivalence ratios. Images of the radiation intensity from water vapor are acquired using a high-speed mid-infrared camera and a band-pass filter. The mid-infrared images are useful for observing detonation products that indicate the instantaneous size and shape of the detonation structures, position and angle of the oblique and reflected shock waves, and possible presence of deflagration between the fuel-fill zone and expansion region. The detonations increase in height as the air mass flow rate is increased for low flow rates, experiences subtle changes for intermediate flow rates, and transitions from one to two waves for higher flow rates. Minimal radiation emission is observed directly in front of the detonation waves indicating that there is not significant mixing between the reactants and burned gases from the previous cycle. The measured mid-infrared images are similar to computed static pressure distributions reported in past work with qualitative agreement between measured and computed detonation wave heights and oblique shock angles. The mid-infrared images provide benchmark data that are useful for evaluating RDE models

and simulations, improving fundamental understanding of the detonation structure in RDEs, and identifying critical design parameters that influence RDE operation and performance.

1098 - Performance Evaluation of a Rotating Detonation Engine

J. Nishimura, K. Ishihara, K. Goto, S. Nakagami, K. Matsuoka, J. Kasahara, A. Matsuo, I. Funaki,

H. Mukae, K. Yasuda, D. Nakata, K. Higashino, H. Moriai

Detonation engines have higher thermal efficiency than conventional engines have. Therefore, many researches on detonation engines have been conducted around the world. An RDE can be used as a kick rocket motor for deep-space exploration. However, there are some problems to be solved prior to the practical use of an RDE. One of the most critical problem is heat-transfer problem. And it is necessary to evaluate the performance of an RDE in a vacuum. For the sake of thermal design and space use of an RDE, we conducted long-duration combustion test and vacuum tests. We succeed in 6-second and 10-second operations of an RDE using C/C composites. And we also achieved 250 s of specific impulse under the low back pressure of 0.4 atm.

1088 - Orderly Wave Initiation in a Rotating Detonation Engine

C. Knowlen, M. Kurosaka

The rotating detonation engine (RDE) is a promising propulsion technology for its potential to increase operating pressure in the combustor while mitigating the entropy increase penalty associated with heat addition at finite Mach. Its application is proposed for both air-breathing engines and liquid propellant rockets. At the University of Washington, we demonstrated success in initiating detonation waves in a RDE by applying a wave generator (WG), a device which sequentially fires radially mounted spark plugs to generate one or more spinning shock waves. In this paper, we present data accrued from the use of the WG in an RDE using H2+O2 propellant, with particular emphasis placed on the importance of digital signal processing in characterizing the detonation waves.

1065 - Pulse Detonation Operation at Kilohertz Frequency

H. Taki, N. Hirota, K. Matsuoka, K. Akira, J. Kasahara, H. Watanabe, A. Matsuo, T. Endo

Pulse detonation (PD) operation at the gasdynamics upper limit of operating frequency governed by the length of a PD combustor and the composition of detonable mixture is important to get the higher thrust density. Many novel PD operation methods are proposed to demonstrate PD operation at higher frequency. The PD combustor used in this experiment has a valveless oxidizer-feeding line and a piezoelectric fuel injector. The length and inner diameter of the combustor was 100 mm and 10 mm, respectively. Supercritical ethylene and gas oxygen were used as fuel and oxidizer, respectively and visualization of injection and combustion tests were carried out. In visualization experiment, the responsiveness of the piezoelectric fuel injector during the operation at 1000 Hz was evaluated using schlieren method and a high-speed camera. The duty ratio (*DR*, injection duration/duration for one PD cycle) of the actual injection was $DR_{real} = 37 \pm 1\%$ against the set duty ratio $DR_{set} = 30\%$ and the response delay of the piezoelectric fuel injector was about 25% of that of the conventional solenoid fuel injector. As the result of combustor were 2500 ± 100 m/s, namely, 128 $\pm 8\%$ of the estimated Chapman–Jouguet detonation speed and 96 % of the PD operation cycles at 1000 Hz was demonstrated.

10:30 Detonation Boundary Interactions 1

970 - Interactions of a Detonation Wave Confined by a High-Temperature Compressible Layer

M. Reynaud, F. Virot, A. Chinnayya

The very rapid energy conversion leads to consider the detonation as an alternative to the classical constant pressure combustion in the engines. However, many issues arise from its potential use for aeronautical propulsion applications because of the strongly non-ideal conditions of propagation endured by the detonation wave. Particularly in the rotating detonation engines (RDE), the detonation chamber is curved, the fresh mixture exhibits composition as well as temperature inhomogeneities and is confined by the burnt gases. The present work focuses on effects induced by a high-temperature gaseous layer on the detonation propagation.

The presence of a yielding confinement affects the dynamics of the detonation [1-3]. The divergence

of the streamlines downstream of the front results in a velocity deficit and to its curvature. The ratio of acoustic impedance between the reactive and the inert layers influences the structure of the combined wave formed by the detonation and the oblique shock. Adams [4] experimentally showed that this parameter may lead to the appearance of a new topology characterized by the presence of a detached shock. This was also addressed in the calculations of Fievishon [5]. To assess whether this parameter may affect the detonation dynamics, we performed numerical simulations of a detonation confined by an inert layer at different temperatures and for mixtures of various stability. The simulations show qualitative agreement with the experimental literature. The losses endured by the detonation affect the mean profiles and the hydrodynamic thickness. The temperature of the inert layer acts in a non-negligible way on the detonation dynamics and affects its limits of propagation.

References [1] Dabora, E. K., Nicholls, J. A., and Morrison, R. B. "The influence of a compressible boundary on the propagation of gaseous detonations". Vol. 10. 1. Combustion Institute, Pittsburgh, 1965, pp. 817–830. [2] Vasil'ev, A. A. and Zak, D. V. "Detonation of gas jets". Combustion, Explosion and Shock Waves 22.4 (1986), pp. 463–468. [3] Reynaud, M., Virot, F., and Chinnayya, A. "A computational study of the interaction of gaseous detonations with a compressible layer". submitted (2016). [4] Adams, T. G. "Do Weak Detonation Waves Exist?" AIAA Journal 16.10 (1978), pp. 1035–1040. [5] Fievisohn, R. and Yu, K. "Method of characteristic analysis of gaseous detonations bounded by an inert gas". 200. ICDERS 2015.

1105 - Oblique Detonation Interaction with a Wall for Large Angles of Attack

M. Short, C. Chiquete, J.B. Bdzil, C.D. Meyer

Much remains to be understood about the reflection and interaction patterns that can develop due to a condensed-phase detonation interaction with a confiner. In a recent study, Bdzil and Short (JFM, 2017) have examined asymptotically the flow structures that can develop when either a Chapman-Jouguet (CJ) instantaneous energy release detonation or a small-resolved heat release (SRHR) detonation impact obliquely on a rigid wall at small angles of incident. For the CJ detonation, traditional Mach stem structures are found behind the lead CJ wave. For the SRHR model, more complex patterns emerge. The purpose of the current work is to study oblique detonation interaction with a rigid wall for large angles of attack both for a CJ detonation wave and for a fully spatially distributed reaction zone detonation.

815 - Effects of Lateral Relief of Detonation in a Thin Channel

K.Y. Cho, J.R. Codoni, B.A. Rankin, J.L. Hoke, F.R. Schauer

The most obvious discrepancy between experimental studies and CFD studies of rotating detonation engines, or RDEs, is the detonation wave speed deficit in experimental systems. This experiment investigates one of the possible causes, lateral relief of the detonation wave, which is a lack of solid confinement. The effects of lateral relief on detonation wave speeds were studied in a linear channel with a rectangular cross section for hydrogen/air mixture. The 'control' section is a confined channel 5.08 cm in height, 0.76 cm in width, and 45.7 cm in length. Unperturbed wave speeds are measured near Chapman-Jouguet detonation wave speeds in this section. The detonation then transitions to the 'experiment' section, which has the same dimensions as the control section, but with lateral relief. A top boundary in the experiment section is removed prior to detonation initiation and exposes the fuel/air mixture to a 6.35 cm tall section of air in a thin channel, then to atmosphere. High-repetition rate OH chemiluminescence imaging was used to visualize the detonation wave and ion probes were used to measure the detonation wave speed. The results showed that for hydrogen/air, detonation with lateral relief was 72.3, 84.8, 88.3, 87.1, and 81.5% of the Chapman-Jouguet detonation wave speeds, for equivalence ratio of 1.07, 1.23, 1.34, 1.54, and 1.71, respectively. The detonation wave speed deficit is larger for stoichiometric and rich conditions, which is qualitatively similar to detonation speed deficit in porous media. The results explain part of the detonation wave speed deficit in RDEs, but does not fully explain it since the speeds are higher than most measured speeds in RDEs. The results indicate that lateral relief has effects on detonations propagating through unconfined rectangular channels and on the low detonation wave speeds observed in RDEs.

1077 - Effect of Boundary Streamline Deflection Angle on Detonation Propagation

C. Chiquete, M. Short, C.D. Meyer, J.J. Quirk

We systematically investigate the effect of boundary streamline deflection on detonation propagation. To this end, we perform reactive flow simulations using a simple HE model and simplified computational geometries where we enforce a straight boundary streamline in the flow at a prescribed deflection angle. The steady-state phase velocity and detonation driving zone bounds are extracted from the calculations as a function of the imposed deflection angle. We compare the unconfined steady-state phase velocity variation with sonic shock-normal angle from these simulations to the corresponding shock polar analysis predictions.

10:30 Flames in Narrow Tubes and Microchannels 1

808 - Large-Activation-Energy Analysis of Gaseous Reacting Flow in Pipes

D.M. Boza, I. Iglesias, A.L. Sánchez

The safe storage and transportation of reactant gas mixtures requires conditions that ensure a negligibly small reaction rate, achieved in storage vessels and transport pipes by lowering sufficiently the wall temperature. The seminal investigation of this problem is due to Frank-Kamenetskii (FK) (1939), who employed an overall irreversible reaction with large activation energy to study a reacting mixture undergoing an exothermic chemical reaction in a centrally symmetric closed vessel with constant wall temperature. The resulting gas-temperature distribution was seen to depend on the competition of the heat released by the chemical reaction and the heat losses to the wall, characterized by the Damköhler number δ , defined as the ratio of the conduction time across the vessel to the relevant characteristic time evaluated at the wall temperature (Zel'dovich, 1985). A slowly reacting flameless mode of combustion is found for values of below a critical value, when the heat losses to the wall are able to limit the temperature rise, in such a way that the reaction rate does not change in order of magnitude from its near-wall value. Since the overall heat-release rate is proportional to the volume of reacting gas while the heat-loss rate to the wall is proportional to the wall surface, for a given wall temperature there exists a limiting size, corresponding to a critical value of δ , above which a slow reaction cannot be maintained, and is replaced by a localized temperature runaway that leads to the formation of a flame. These classical results find direct application in connection with the safety storage of reactant mixtures, defining critical sizes for thermal explosions in chemically reacting systems. A related problem addressed here is that of reactant transportation in pipes, with specific consideration given to the entrance region adjacent to the storage container.

771 - Effects of Stoichiometry on Premixed Flames Propagating in Planar Microchannels

D. Fernandez-Galisteo, C. Jiménez, M. Sánchez-Sánz, V.N. Kurdyumov

Recent studies have shown that for premixed flames freely propagating in narrow adiabatic channels differential diffusion induced instabilities may result in non-symmetric solutions and/or oscillating and rotating propagation modes. This has been shown in the context of lean mixtures for which a single species transport equation with a single Lewis number of the deficient reactant can be used to represent the propagation problem. Here the effect of the stoichiometry is investigated within the framework of a two-reactant model and with the diffusive-thermal (constant-density) approximation. Steady-state computations and linear stability analysis show that lean mixtures of very diffusive fuels result in flames with non-symmetric shapes for positive incoming flow rates, but the symmetric shape is re-stabilized when we reach near-stoichiometric conditions.

1029 - Numerical Study on Asymmetric Flame Spread in A Narrow Combustible Channel

T. Matsuoka, S. Murakami, T. Yamazaki, Y. Nakamura

Numerical simulations are performed in order to investigate the detail process to appear the asymmetrically spreading flames in narrow channel of combustibles. 2-D, time-dependent mass and energy transport process as well as one-step chemical process in gas-phase is considered. Thick solid combustible plates (PMMA) are pyrolized via one-step reaction to evolve the fuel gas into the narrow channel. Combustibles are placed at both sides of the calculation domain, and pure oxygen with flat velocity profile is fed into the channel at the fixed rate. Oxidizer velocity and channel height are varied

from 5 to 50 mm and from 0.1 to 5 m/s, respectively. Forced ignition is made by hot spots at downstream, and subsequent flaming and opposed-mode flame spreading over the combustibles is established numerically. The transition initiates with the flame on one side moving downwardly or being delayed possibly due to the local extinction or weakening. The distribution of the heat release rate indicates that the anterior flame enhances the reaction in the downstream and it enables the posterior flame to reignite at a certain distance from the anterior flame. The result suggests that the asymmetrical configuration gives temporary stable condition to burn. Based on the transient process and subsequent flame spreading behavior, various flame spreading modes are identified; two kinds of symmetric flame spreading mode is observed are finally summarized on the velocity-channel width diagram. These modes are temporary distinguished based on qualitative observation. Thus, further study is needed to investigate the separation behavior in detail, which enables updating the classification.

869 - Flame Behaviour During Propagation in Small Tubes Characterized by Different Degrees of the End Opening

A.N. Gutkowski, P. Jasinski, M. Lecki, B. Jedrowiak

In the present work, we study numerically freely propagating flame in the stoichiometric propane-air mixture. The isothermal small tubes with one end fully open and the second one characterized by different degrees of opening are examined. The degree of opening of the tubes was equal to: 0% (completely closed), 25%, 50%, 75% and 100% (fully opened) of the tube cross-sectional area. For the smallest tube, which corresponds to a quenching diameter, opening of the right end of the tube causes an increase in the flame propagation velocity (but this velocity is almost constant) and a slight change in the flame length with respect to the propagate with higher velocities, which change with the flame position. These velocities depend on the degree of opening of the tube end as well. The larger opening, the higher velocity and flame acceleration.

13:50 Chemical Kinetics and Reaction Dynamics 2

1101 - Kinetic Effects of n-Propylbenzene on n-Dodecane Cool Flame Extinction

O.R. Yehia, C.B. Reuter, Y. Ju

Experimental and numerical investigations on the kinetic influence of *n*-propylbenzene on the extinction limit of *n*-dodecane/oxygen diffusion cool flames in a counterflow configuration have been conducted. Diffusion flame extinction limits were measured using planar laser-induced fluorescence of formaldehyde in nitrogen-diluted flames. At a fixed mass fraction of *n*-dodecane, introducing *n*-propylbenzene increases the overall reactivity of the hot flame but dramatically decreases the reactivity of its cool flame counterpart. At high temperatures (above 1500 K), oxidation of *n*-propylbenzene and its fragments contribute to the increase of the net heat release and the net production of the hydroxyl radical, thereby inhibiting major heat release and radical pool formation. The primary low-temperature chain initiation process, and a main heat release pathway, is the H-abstraction from the parent alkane by the hydroxyl radicals (RH + OH = R + H₂O), which allows alkyl oxidation to form peroxy radical isomerization and cyclization mechanisms.

996 - Utilization of Transport of Species and Heat Release to a DRG-Method-Based Reduction

K. Yamasaki, S. Honya, A. Uemichi, M. Nishioka

We propose a new DRG method for mechanism reduction, which includes the consideration of heat release rate (HRR) of each reaction step and transport of species in addition to reaction rates. In the original DRG method developed by T. Lu and C. K. Law, importance of a species is evaluated only by the reaction rates of the elementary steps related to it, and PSR is used for sampling. However, since realistic combustion phenomena are also affected by transports of species and energy, it may be

desirable to adopt some kind of flames as a sampling target in addition to PSR, and to implement the effects of transports in DRG method. Furthermore, heat release by elementary reactions is thought to be very important since it changes the local temperature that significantly affects the reactions. In our transport and heat release DRG method, 1-D premixed flame is used for sampling, and importance of species is evaluated by rates of related reactions, transport flux, and HRR's of the related reactions. In this study, validation of the new method was conducted for the 1-D premixed flames of ethylene/air and n-butane/air. Comparisons of the obtained laminar flame speed and the flame structure were made among the skeletal mechanisms created by three DRG methods; i.e. the original DRG method, the transport DRG method, and the transport and heat release DRG method. As a result, in the case of ethylene/air premixed flame, the transport and heat release DRG method produced smaller skeletal mechanism. In the case of n-butane/air premix flame, it also produced smaller skeletal mechanisms in the region of relative error on laminar flame speed of 0.1 to 1.0%.

1127 - Modeling Real Gas Equations of State in High Density Combustion

C. Zheng, D. Coombs, B. Akih-Kumgeh

In this paper, the problem of real gas equations of state for high density flow simulations is considered. The importance of such equations of state is underlined by comparing the large eddy simulation results of a propane jet into an air vessel realized using large eddy simulations with ideal and real gas equations of state. It is then suggested that parameters of a cubic equation of state, namely, the critical state variables, can be determined from the transport data of chemical kinetic models. It is further observed that the transport data of various chemical kinetic models are not necessarily consistent, suggesting further attention to this modeling problem.

927 - Validation of Detailed Chemical Kinetics Mechanisms for Reproduction of Ignition Delay Times of C2-C5 Alkenes

A. Jach, W. Rudy, A.A. Pękalski, A. Teodorczyk

The goal of the paper is to assess a performance of 15 detailed chemical kinetics mechanisms for combustion of C2-C5 alkenes based on ignition delay times. The paper provides an indication which mechanism ought to be used and under what conditions. Mechanisms being assessed are: Aramco 2.0, Blanquart 2009, Davis Law Wang C3, GRI-mech 3.0, Konnov 0.5, JetSurF 2.0, NUIG Butane, NUIG Pentane Isomers, NUIG n-Hexane, NUIG n-Heptane, Polimi C1C3 LT HT - Version 1412, Polimi C1C3 HT NOx - Version 1412, Polimi PRF PAH LT - Version 1412, San Diego 2014, Wang High T. A large data set of ignition delay times (IDTs) from shock tube experiments was collected (1020 points in total). Taking into account the whole range of experimental conditions and defined in the paper averaged error function, the best mechanism for combustion of C2H4 is NUIG Butane, for C3H6 - Aramco 2.0, iso-C4H8 - NUIG Pentane Isomers, 1-C4H8 - POLIMI PRF PAH LT 1412, 2-C4H8 - NUIG Pentane Isomers, for which a mechanism is going to be used.

13:50 Laminar Flames 2

1053 - Influence of Monodispersed Mist of Inert Liquid on Gas Flame Propagation

N.S. Belyakov, V.I. Babushok, S.S. Minaev

The combustion of premixed gas mixtures containing inert liquid microdroplets was studied using the one-dimensional approximation. The dependencies of the burning velocity and flammability limits on the initial conditions and on the properties of liquid droplets were analyzed. Effects of droplet size and concentration of added liquid were studied. For droplets evaporating in the reaction zone, the burning velocity is independent of droplet size, depending only on the concentration of the added liquid. With the increase of the droplet diameter, the droplets pass through the flame reaction zone with a further vaporization in the combustion products. It was demonstrated that for droplets above a certain size there are two stationary modes of flame propagation with a transition of hysteresis type. The transition is the result of the appearance of the super-adiabatic maximum temperature in the flame reaction zone and the temperature gradient with heat losses to the combustion products due to the vaporization of

droplets as they pass through the flame reaction zone. The critical conditions are similar to the flammability limits of laminar flame with thermal mode. The maximum decrease in burning velocity and in the combustion temperature at the turning point (critical conditions) correspond to the predictions of classical theory of flammability limits.

1019 - Laminar Flame Speed of Diluted DME-Air Mixtures

A. Mohammad, A.N. Mohammed, K.A. Juhany, S. Kumar, R.K. Velmati

The laminar flame speed of CO_2/N_2 diluted dimethyl ether (DME)air mixtures is determined experimentally at atmospheric pressure and elevated mixture temperatures over a range of mixture equivalence ratio ($0.8 \le \Phi \le 1.3$) using a mesoscale high aspect-ratio diverging channel. In this method, planar flames at different initial temperatures were stabilized inside the channel using an external electric heater. The magnitude of burning velocities was acquired by measuring the flame position and initial temperature. The mass conservation of the mixture entering the inlet and the stationary planar flame front is applied to obtain the flame speed. The laminar flame speed at different initial mixture temperatures is plotted with temperature ratio for the diluted mixtures where a reference temperature of 300 K is used. Enhancement in the laminar flame speed is observed with mixture temperature for DME-air mixtures with CO₂ and N₂ dilutions. A significant decrement in the flame speed is observed with dilution. The addition of CO₂ has profound influence when compared to N₂ addition on both flame speed and temperature exponent.

1073 - Pressure and Radiation Effects on the Dynamics of Hot and Cool Diffusion Flames

C.B. Reuter, E. Lin, Y. Ju

Due to the importance of low-temperature chemistry in the ignition of many hydrocarbons, cool flames continue to be studied in great detail. However, despite the growing number of cool diffusion flames studies performed at atmospheric pressures, very few investigations have taken place at elevated pressures closer to engine-relevant conditions. In this study, the effects of elevated pressure and radiation on dimethyl ether diffusion flames are examined numerically. It is seen that the similarities in hot diffusion flames at constant pressure-weighted strain rate do not extend to cool flames due to changes in the nature of low-temperature chemistry across different pressures. At elevated pressures, N₂ diluent addition to the oxidizer is shown to shift the extinction limits of the hot flame dramatically and enables the formation of a steady "mild flame" branch sustained by intermediate-temperature chemistry. Computing these high-pressure diffusion flames with radiative losses included further increases the stability of the "mild flame" branch due to the presence of a hot flame radiative extinction limit.

594 - Laminar Flame Speed Determination for H2/N2/O2/Steam Mixtures Using the Spherical Bomb Method

R. Grosseuvres, A. Bentaïb, N. Chaumeix

During severe accident in Pressurized Water Reactor (PWR), the interaction between the fuel rod and steam leads to the build-up of an explosive atmosphere inside the containment building. This atmosphere is mainly composed of hydrogen, oxygen, nitrogen and water. In case of an ignition by an energy source (electrical discharge spark, hot surface, etc.), a flame occurs and is capable to threaten the containment building. To assess this capability, a criterion of flame acceleration permits to distinguish fast flames from slow flames. The criterion of flame acceleration is based on properties of the mixture and geometry. The present study focuses then on the evaluation of fundamental combustion parameters: laminar flame speed, Markstein length, activation energy and Zeldovich number. The experimental work is conducted over conditions relevant to severe accident in PWR: equivalence ratio ($0.8 \le \phi \le 4$), initial temperature (296, 333, 363, 413 K), dilution ($N_2/O_2 = 3.76, 5.67, 9$), and steam (%mol.). Laminar flame speeds S_L^0 are simulated using COSILAB code in order to verify their validity in the conditions of the present work. They are then used to obtain other fundamental combustion parameters as the laminar flame thickness δ , the Effective Lewis number Le_{eff}, the activation energy Ea and the Zeldovich number β .

13:50 The Current Status and Future Outlook on Gaseous Detonation Research 1

1140 - The Usefulness of a 1D Hydrodynamic Model for the Detonation Structure for Predicting Detonation Dynamic Parameters

M.I. Radulescu

The present study provides a method to determine experimentally the global reaction rate law in a 1D hydrodynamic model for the detonation structure. The experiments consist of determining the velocity deficit dependence on lateral flow divergence in our recently suggested exponential horn geometry. This geometry provides the ability to maintain attenuated detonations at a constant mean speed, while simultaneously controlling the lateral flow divergence in each mean streamtube. The calibration uses the well-established theory of 1D detonations with lateral flow divergence. We demonstrate that the empirical rate law derived from experiment can be subsequently used to predict the dynamic detonation parameters, such as the critical direct initiation energy. Excellent agreement is found with experimental data. Alternative methods to obtain the mean exothermic rate in cellular detonations from the underlying cellular structure are discussed.

961 - Computation of the Mean Hydrodynamic Structure of Detonation with Losses

A. Chinnayya

In the ideal ZND model, the reaction zone length matches the distance from the leading shock to the sonic plane. When losses are taken into account, this is no longer the case and the chemical reaction is not fully completed at the sonic plane location. The thermicity condition thus incorporates the losses which balances the heat release. Detonations are also known to develop a multidimensional cellular structure, of which the regularity can be related to the activation energy, all other thermodynamic parameters being fixed. There is thus a need of include these dynamics aspects of the detonation propagation into a dedicated length scale.

This then lead to the definition of the hydrodynamic thickness, which can be seen as the generalization of the length of the ZND subsonic reaction zone. It corresponds to the distance between the mean location of the leading shock and that of the mean sonic plane.

From the computational point of view, we can rely on Favre-averaging flow-fields, obtained by computations of the reactive compressible flows [1]. We can then analyze the influence of the hydrodynamic instabilities and irregularity of the detonation process, which change according to the value of the activation energy on the hydrodynamic thickness and the corresponding average structure. From 1D unsteady computations [2,3], we can see that the activation energy threshold leading to the onset of longitudinal instabilities is lowered by the losses. Moreover, they increase the fluctuations, which act as a further source of losses and thus lead to a higher velocity deficit. As the mixture is more unstable, a clear departure from the laminar structure can be observed and the length of the hydrodynamic thickness becomes several times the laminar counterpart. The analysis could be performed in the instantaneous shock-attached frame. Indeed, averaging an oscillatory moving shock in the coordinates attached to mean shock velocity can result in a smooth profile for the mean shock spike, which is then rather difficult to analyze as a shock. This analysis focuses on what sees the leading shock, consequently could be considered as "biased". In addition, it can be inferred from a hyperbolic analysis of the mean equations that the mean sound speed is augmented with a turbulent sound speed. However, the generalization of the latter formalism to a 2D context is not straightforward. In Ref. 1, the authors compute the hydrodynamic mean structure in the ideal case, without losses. The hydrodynamic thickness is consistent with experimental findings, of the order of some cell sizes. Ref. 4 deals with 2D detonations with losses, induced by a yielding confinement. The analysis was performed on one line of the flow field and then compared to the Wood-Kirkwood model. There is an increase of the chemical length and the hydrodynamic thickness as a function of the activation energy. The mean sonic location is delayed by the mechanical and thermal fluctuations far from the end of the main heat-release reaction zone. The end of the mean subsonic reaction zone thus corresponds to the stabilization of the production of these fluctuations and the presence of a small heat-release zone.

When losses are involved in the case of mildly unstable detonations, on contrast to what is featured by the generalized ZND model, the hydrodynamic thickness slightly increases, certainly because of the

increase of the fluctuations. Moreover, the scaling of the detonation velocity deficit as function of the mean curvature breaks down, even if the half-reaction length and corresponding cell size remain roughly identical.

In addition, there is a need to obtain the whole multidimensional mean structure, which would be the mean analog of the multidimensional laminar detonation structure [5], based on the equations written in the instantaneous shock-attached frame [6].

We also found that the aforementioned evaluation is quite different from that of experiments. In the latter case, the hydrodynamic thickness is inferred from the decay of the pressure fluctuations downstream of the leading shock [7,8]. How these two approaches bring about coherent results remain an issue.

Numerical simulations show that averaging the chemical source term leads to a lower effective activation energy [2,9], suggesting that the fluctuations remove part of the thermal sensitivity of the mixture. A question thus arises of what would be the transients, i.e. the dynamics of failure if we were to simulate the mean equations, along with the different closure terms to be modelled.

References

[1] Radulescu M. I., Sharpe G. J., Law C. K., Lee J. H. S. (2007). The hydrodynamic structure of unstable cellular detonations. Journal of Fluid Mechanics, 580, 31-81.

[2] Sow A., Chinnayya A., Hadjadj A. (2014). Mean structure of one-dimensional unstable detonations with friction. Journal of Fluid Mechanics, 743, 503-533.

[3] Ng H. D., Zhang F. (2012). Detonation instability. In Shock Waves Science and Technology Library, Vol. 6 (pp. 107-212). Springer Berlin Heidelberg.

[4] Reynaud M., Virot F., Chinnayya A. (2017), Interactions of a Detonation Wave Confined by a High-Temperature Compressible Layer, 26th ICDERS, Boston

[5] Bdzil J. B. (1981). Steady-state two-dimensional detonation. Journal of Fluid Mechanics, 108, 195-226.

[6] Taylor B. D., Kasimov A. R., Stewart D. S. (2009). Mode selection in weakly unstable twodimensional detonations. Combustion Theory and Modelling, 13(6), 973-992.

[7] Jarsalé G., Virot F., Chinnayya A. (2016). Ethylene–air detonation in water spray. Shock Waves, 26(5), 561-572.

[8] Lee J. H. S., Radulescu, M. I. (2005). On the hydrodynamic thickness of cellular detonations. Combustion, Explosion and Shock Waves, 41(6), 745-765.

[9] Borzou, B., & Radulescu, M. I. (2016). Dynamics of detonations with a constant mean flow divergence. arXiv preprint arXiv:1606.05323

13:50 Dust Explosions 1

938 - Explosion-Induced Ignition and Combustion of Acetylene Clouds

A.L. Kuhl, H. Reichenbach, J.B. Bell, V.E. Beckner

We investigate the explosion-induced ignition and combustion of acetylene clouds in a rectangular chamber ($10 \times 10 \times 39$ cm). In the experiments, a 0.2 g PETN charge was located at x = 9.7 cm, and a soap bubble (d = 5 cm) filled with pure acetylene was located at x = 27 cm. Detonation of the charge created a blast wave that crushed the soap bubble, inducing mixing with air; after 27 ms, the cloud ignited forming a turbulent combustion cloud. This problem was simulated with our compressible AMR code. The flow was modeled by the compressible Navier-Stokes equations under the unity Lewis number assumption. Arrhenius-based kinetics were used to model ignition. Adaptive mesh refinement was used to capture turbulent mixing on the grid (*iLES* approach). Computed pressures were found to be in agreement with measured pressure histories.

1113 - Effect of Particle Size on the Dispersion of Dust Produced by a Shock Wave

O.J. Ugarte, R.W. Houim, E.S. Oran

The effect that the particle size produces on the interaction between a shock wave and a thin layer of dust is studied by solving two sets of coupled, unsteady, multidimensional Navier-Stokes equations, one for the compressible gas and one for the incompressible particles. The computational system

includes a layer of limestone dust, made of uniform-size particles, which interacts with a shock of strength M_s = 1.4. Two cases are investigated; one where the dust is made of 20 micro-meter particles and another where the dust is made of 80 micro-meter particles. Particle dispersion is investigated by comparing vertical accelerations due to Archimedes, gravitational, intergranular, drag and lift forces. The simulations show that the shock produces both the compaction and dispersion of the dust layer for the two particle sizes. The dust compaction evolves to a compaction wave that later reflect off of the channel. Reflection of the compaction wave occurs nearer to the shock for 20 micro-meter particles than for 80 micro-meter than for 80 micro-meter particles. The drag force opposing the particle lifting, however, is also larger for 20 micro-meter particles, resulting in the higher dispersion of 80 micro-meter particles.

1138 - Promotion and Mitigation of Premixed Flame Acceleration in Dusty-Gaseous Environment with Various Combustible Dust Distributions: A Computational Study

S. Demir, H. Sezer, T. Bush, V. Akkerman

While combustion of dust and of gaseous fuels has been studied quite well, flame propagation in a combined dusty-gaseous environment, especially with a non-uniform dust distribution in the gas, still remains an enigma, which commands both the fundamental interests and practical relevance, such as the critical need to reduce the risk of disastrous explosions in coal mines. In this study, computational simulations of the compressible hydrodynamic and combustion equations are performed, with the combustible coal dust particles incorporated into the original CFD platform by means of the classical Seshadri formulation. Specifically, a real dusty-gaseous environment is replaced by an "effective" gaseous fluid with locally-modified, dust-induced flow and flame parameters. Keeping in mind a mining passage configuration, flame propagation in pipes is considered, with various pipe radii and four coal dust distributions: (a) homogenous, (b) linear, (c) cubic and (d) parabolic. In each case, we have identified the similarities and differences in the evolution of the flame shape morphology and its propagation velocity. It is shown that a non-uniform dust distribution may result in extra distortion or local stabilization of the flame front, which promotes or reduces the total flame front surface area, thereby facilitating or moderating the flame acceleration scenario. Overall, the effect of non-uniform dust distribution becomes substantial when the pipe radius exceeds a certain critical value proportional to the flame thickness.

798 - Turbulent Clustering of Particles and Radiation-Induced Mechanism of Dust Explosions

M. Liberman, N. Kleeorin, I. Rogachevskii, N. Haugen

We show that clustering of dust particles in a turbulent flow ahead of the primary flame gives rise to a significant increase of the radiation absorption length. This ensures that clusters of dust particles even far ahead of the flame are sufficiently exposed and heated by the radiation from the primary flame to make them multiple ignition kernels capable to ignite the secondary explosion in a large volume of fuel-air mixtures. The multiple radiation-induced ignitions of fuel-air mixtures by ignition kernels in a large volume ahead of the primary flame increase efficiently the total flame area, resulting in a strong increase of the effective combustion speed, defined as the rate of reactant consumption of a given volume. The extent, to which the rate of combustion and overpressures increase, depends on the parameters of the turbulent flow ahead of the flame. It is shown that the radiation-induced multi-point ignitions of the oscerved level of damages in unconfined dust explosions, e.g. such as the 2005 Buncefield vapor-cloud explosion.

13:50 Flames in Narrow Tubes and Microchannels 2

1082 - Stationary Premixed Flames in Narrow Tubes with External Heat Transfer

A.O. Velázquez, L. Bauwens, F. Fachini

Because of their ability to burn very lean mixtures, there has been a significant interest in superadiabatic flames in recent years. This has led to significant work, experimental, numerical and analytical, as reviewed in Fachini & Bauwens (2017). Here, we consider a steady flame in a long narrow tube

exposed to a known temperature on its outside wall. The formulation is similar to the literature (e.g. Lee & Maruta 2012, Zamashchikov 2000, Zamashchikov & Minaev 2001, Ju & Xu 2005, Pereira et al. 2011), but the focus is on exact analytical solutions to the one-dimensional problem, using a convection model for heat transfer on the tube walls. The solution technique is largely similar to that of MacIntosh and Protero (1991). However here, as in Fachini and Bauwens (2017), it is applied to the full tube instead of half, and the boundary conditions allow for superadiabaticity. The work differs from Lee and Maruta (2011), Zamashchikov (2000), Zamashchikov and Minaev (2001) and Ju and Xu (2005) in that a closed form solution is obtained; it also is restricted to a fixed flame location.

1132 - Experiments on Flame Propagation Regimes in a Thin Layer Geometry

M. Kuznetsov, J. Grune

A series of experiments on different combustion regimes in a thin layer geometry were performed for stoichiometric H2/air mixture in a rectangular chamber with dimensions of 20 x 90 x h cm³, where *h* is the thickness of the layer (h = 1, 2, 4, 6, 8, 10 mm). Three different layer geometries were investigated: (1) a smooth channel without obstructions; (2) the channel with a metal grid filled 25% of space and (3) filled 100% of space. Five categories of flame propagation regimes were classified. Special attention was paid to the analysis of critical condition for different flame propagation regimes as function of the layer thickness and roughness. It was found that thinner layer suppresses the detonation onset and even with a roughness, the flame is available to accelerate only to sonic velocity. Only in a channel thicker than 4 mm the detonation may occur. A global extinction in a channel of 1-mm gap was observed for stoichiometric hydrogen-air mixture due to heat losses and steam condensation at the walls.

755 - Pulsating Combustion of Ethylene in Micro-Channels with Controlled Temperature Gradient

A. di Stazio, C. Chauveau, G. Dayma, P. Dagaut

Nowadays with the demand for high efficiency systems, there is growing development and application of micro electro-mechanical systems (MEMS devices) which may generate more energy than the modern batteries. In this context, a new experimental device has been developed. It consists of a micro tubular reactor with a controlled external temperature profile. The high gas temperature allows autoignition of the mixture and the flame stabilization in reactors with inner diameter smaller than the ordinary quenching diameter. The temperature profile along the tube is measured continuously using an infrared camera while an EMCCD camera is used to collect the CH emission from the flame. The present experimental study on fuel/air mixtures reacting in narrow channels has been undertaken to provide detailed information on flame combustion at micro-scale. Three kinds of flame behavior were observed: (i) bright and stable flames under high flow velocity, (ii) flames with repetitive extinction and ignition (FREI) in the middle flow rate range, and (iii) weak flames at low flow rates. The presence of oscillating transitional regimes was also investigated and a detailed analysis of the unstable regimes (determination of frequencies and characteristic times) was carried out. Three fuels were used, namely methane, ethylene, and acetylene. The effect of different parameters was investigated: inlet velocity, equivalence ratio, and reactor size. Numerical simulations were also conducted to study the ignition characteristics of unstable flames.

845 - Experimental and Numerical Study of Premixed Flame Penetration in a Set of Microchannels

R. Fursenko, E. Sereshchenko, G. Uriupin, E. Odintsov, T. Tezuka, S. Minaev, K. Maruta

Results of experimental and numerical study of flame penetration in the set of planar quartz ducts with non-uniform channel sizes are presented. The regions of existence of different combustion regimes in equivalence ratio / mixture flow rate plane are obtained. These regimes include burner stabilized flames, upstream propagating flames and flames stabilized under the burner external surface. The effect of channels sizes and their mutual arrangement on dynamical flame behavior and combustion regimes are studied. Numerical results obtained in the frame of thermal-diffusion model are compared with experimental data and the results of such comparison are discussed.

16:00 Ignition 1

1115 - Hot Spot Dynamics: Quenching, Ignition, Flame Propagation and Extinction

J. Santner, S.S. Goldsborough

In the elevated pressure and temperature environment in rapid compression machines (RCMs) and engines, flame kernel formation and growth is a complex process. In fundamental RCM experiments, this is thought to affect mild ignition, thus complicating modeling efforts. In engines, this process can cause pre-ignition heat release, altering combustion timing, reducing efficiency, and in some cases leading to knock. Flame kernels in these geometries can form due to heterogeneous temperature and mixture fields. The present work parametrically investigates flame kernel formation and extinction behavior over a range of temperature inhomogeneities that might be present within an RCM. We find that flame formation is primarily governed by competition between hot-spot dissipation and ignition, while flame extinction is governed by flame structure and Lewis number (Le) effects.

981 - Effect of Orientation on the Ignition of Stoichiometric Ethylene Mixtures by Stationary Hot Surfaces

J. Melguizo-Gavilanes, J.E. Shepherd

The risk of accidental ignition of flammable mixtures by a hot surface is of particular importance for industry. Accurate measurements and modeling of the minimum surface temperature for ignition to occur are needed to estimate the risk of hot surface ignition. Previous work for stationary hot surfaces have determined critical conditions for ignition in terms of surface size, material and heating rate. However, less attention has been paid to studying the effect that the orientation of the hot surface has on the reported ignition thresholds. The present study examined this question by numerically determining the minimum surface temperature required to ignite a stoichiometric ethylene-air mixture using a stationary vertical and horizontal hot cylinder. Results showed that for the mixture considered, simply changing the orientation of the heated surface, while keeping the remaining parameters of the problem fixed, yielded an ignition threshold that is 128 K lower for the horizontal cylinder than the threshold obtained when the vertical cylinder was used. This outcome provided further evidence that numerical determination of hot surface ignition thresholds requires a detailed simulation that includes appropriate initial and boundary conditions, and that is capable of capturing the interaction of the hot surface with the buoyancy flow induced by the heating of the gas. It is precisely this interaction that results in regions where the thermal boundary layer is thicker favoring the establishment of the critical conditions for ignition to occur.

741 - Effect of Initial Laser Beam Diameter on Breakdown and Ignition Properties of n-Decane/Air

S. Rudz, P. Gillard

Traditional spark plug igniters are widely used in engine applications. This technology is better known among others and some limitations appear in its control in term of space and location of the deposited energy. An alternative laser igniter device to overcome this problem is more and more studied. The principle of this technology is to focalize a Gaussian laser beam in the center of a combustion chamber. However optics used to focalize the laser beam are a crucial point to achieve ignition. The focal length and the beam diameter of the laser are two parameters that one can control. Some experimental works have been done about the effect of the focal length but few have investigated the beam diameter. This last parameter is of interest because due to the size of the combustion chamber used in this work this parameter can be adjusted on a larger range than the focal length. As a consequence it allows to achieve a higher intensity at the focal point.

The presented experimental work highlights the role of the beam diameter for the same laser source in the ignition process of a reactive mixture. In this paper 5 beam diameters have been investigated for 5 equivalent ratios of n-decane/air mixture at 1 bar and 347 K with the Langlie method. Results yield that ignition needs less and less energy sent from the laser source when the beam diameter is more and more expanded. Moreover a way to compare those results to the ones of the literature with different optics is shortly discussed.

16:00 Explosion Safety 1

1060 - Flame Arrester Performance at Increased Oxygen Concentrations

S. Zakel, S. Henkel, F. Stolpe, M. Beyer, U. Krause

Flame arresters prevent the propagation of a gas- or vapor explosion from one section of a plant to another. Choosing the appropriate flame arrester from a broad variety of types for different scenarios requires knowledge about the specific properties of the combustible that may be present. The standard testing conditions are the so called atmospheric conditions, which describe the temperature and pressure range usually supposed to be human working conditions with air as the oxidizing gas. As most of the chemical processes are driven beyond this conditions, the maximum experimental safe gap (MESG) as the criterion for choosing the proper flame arrester is critically reviewed. In this study the focus is on the extend, to which the addition of oxygen influences the performance and safety margins of a flame arrester at elevated pressure and whether the changes in performance are comparable to the properties of the MESG. It was found that a small increase of the oxygen content in an explosive ethylene/oxygen/air-mixture leads to severe restrictions on the use of flame arresters. The safety margins from higher test pressures are quickly depleted at the operational pressures. The maximum safe gap at the pressure which is only just safe in the arrester tests does not seem to be constant for different oxygen concentrations. This means, that the reliability of arresters in oxygen enriched atmosphere cannot simply be deduced from MESG at atmospheric conditions.

1023 - Effects of Open Area of a Rupture Disk on the Self-Ignition of High Pressurized Hydrogen Released Through a Tube

H.J. Lee, S.Y. Lee, B.J. Lee, I.S. Jeung

Experiments are conducted to investigate the self-ignition of a high pressurized hydrogen, which is released suddenly into the air by failure of the rupture disk. This study is aimed to investigate an initial flow, which is formed immediately after failure of rupture disk, and to observe different ignition patterns with various open area of a disk. To analyze the self-ignition characteristics, visualization image is acquired, and pressure and light signals is measured along the tube. The visualization images showed that the initial ignition region exists near the rupture disk, but it doesn't affects the whole process of the self-ignition. It seems that the ignition is always started from the boundary layer. When open area ratio is reduced sufficiently, the self-ignition does not occur. When the area ratio is higher than 0.25 it seems that the mechanism of self-ignition initiated from the heating and mixing induced by the shock and flow interactions is preserved from the pressure that the self-ignition can be initiated and it seems that the mechanism might be different.

4301 - Modeling the Growth and Formation of Instabilities During Spherical Flame Propagation

C.R.L. Bauwens, J.M. Bergthorson, S.B. Dorofeev

When evaluating the consequences of accidental explosions, accurate prediction and modeling of the rate of flame propagation is crucial for hazard assessment. In a freely expanding spherical configuration, however, the growth of the Darrieus-Landau instability results in significant flame acceleration. Characterization of this flame acceleration is needed to properly capture the behavior of large scale flames.

In this study, a simple model describing the growth of multiple generations of cells on a flame surface is developed and compared with experiments from a previous study. In future work, this approach may be used to quantify the parameters responsible for spherical flame acceleration.

1093 - Numerical Modelling of Vented Lean Hydrogen–Air Deflagration Using Hyfoam *V.C.M. Rao, J.X. Wen*

With the aim to develop and validate an open source computational fluid dynamics (CFD) solver for vented hydrogen explosions in realistic geometric configurations and presence of obstacles, HyFOAM, has been developed on the basis of the open source CFD code OpenFOAM. In comparison with the original OpenFOAM code, HyFOAM includes improved combustion treatment with turbulent flame speed correlation, which accounts for the Lewis number effect and Darrieus-landau instabilities. The

unstretched laminar flame speed correlation valid between equivalence ratios of 0.33 and 0.47 has also been incorporated. An older version of the code before the modification to include the Lewis number effect has been previously validated with published data of Bauwens et al. (2011) and reported in the previous ICDERS by Rao and Wen (2015). As the first step of validation for the updated solver in the present study, predictions have been conducted for a recent hydrogen-air vented deflagration test in an ISO container without obstacles. The hydrogen concentration is 15% by volume. The predicted pressure trace curve at the peak pressure location is found to be in reasonably good agreement with the measurements. The results have demonstrated the potential of the present numerical modelling for simulating lean hydrogen-air mixtures deflagrations in vented explosions scenarios.

16:00 The Current Status and Future Outlook on Gaseous Detonation Research 2

963 - Critical Condition for Detonation Diffraction with Stable and Unstable Mixtures

J. Kasahara, A. Kawasaki

We visualized the detonation diffraction with a high-speed video camera by using the two optical techniques of shadowgraph and multi-frame, short-time, open-shutter photography (MSOP). MSOP is the method that enables us to visualize the wave front and the cellular structure by detecting the detonation self-emission over a relatively long time period. The reinitiation events and propagation of detonation in a bent tube were examined by Nakayama et al. under a variety of conditions. In our previous work, using a high-speed video camera made it possible to track the transformation of the wave shape at 2 µs resolution and to observe the reinitiation process, in particular the movement of the transverse detonation wave, directly. However, the dependence on mixture stability was not clearly visualized in our prior studies. In the present experimental study, the positions of the local explosion in reinitiation angles varying from 30° to 150° in a stoichiometric ethylene-oxygen mixture and more stable mixtures (the more stable mixture experiments will be performed by the final manuscript deadline).

1116 - Planar Blast Initiation of Detonations Using a Simplified Model

S.M. Lau-Chapdelaine, L.M. Faria, R. Rosales, M.I. Radulescu

The prediction of critical blast energy for detonation initiation remains an open problem, with order of magnitude agreement between theory and experiment in the best of cases. While previous work points to the importance of unsteady terms, stability, and choice of chemical model, the problem remains difficult to probe due to the complexity of the Euler equations. This study proposes to simplify the direct initiation problem through the use of a toy model, in order to gain further understanding on the direct initiation of detonations. Fickett's detonation analogue with a two-step induction-reaction model and Arrhenius sensitivity is used as an example of how simplified models may help understand direct initiation. The simplified model recreates many features of one-dimensional Arrhenius blast initiations, such as the super-, sub- and critical initiation regimes, especially a low activation energy.

990 - Comparison of Models Predicting the Mode of Ignition Behind Reflected Shock Waves in the Context of DDT

L.R. Boeck

The phenomenon of deflagration-to-detonation transition (DDT) has been widely studied experimentally, numerically and analytically. A central interest is to predict the critical conditions for onset of detonation. In obstructed tubes, the most common mechanism leading to the onset of detonation is the reflection of precursor shock waves at obstacles and channel walls, causing local strong ignition. This mechanism can be isolated and studied scientifically in shock tubes.

The present discussion concerns detonation initiation by shock reflection (strong ignition) as the final stage of deflagration-to-detonation transition. Detonation initiation is treated in isolation from the flame acceleration process. Normal shock reflection at a flat wall is considered.

The discussion focuses on the question of which fluid-mechanic, gas-dynamic and chemical-kinetic effects govern the mode of ignition upon shock reflection and eventually determine whether detonation is initiated directly. For this purpose, theoretical models from the literature are evaluated. These models

by (i) Voevodsky and Soloukhin, (ii) Meyer and Oppenheim, (iii) Grogan and Ihme and (iv) Thomas et al. consider different phenomena to determine the ignition mode: (i) the dominating chemical pathway, i.e., branched-chain vs. straight-chain reaction; (ii) sensitivity of ignition delay time on temperature; (iii) time-scale comparison between shock bifurcation and ignition delay; and (iv) time-scale comparison of expansion and ignition delay for shock reflection at flat-plate obstacles.

Critical incident shock Mach numbers leading to strong ignition based on these models are determined for a stoichiometric hydrogen-air mixture at initial pressures between 5 and 101.3 kPa and an initial temperature of 298.15 K. Initial pressure affects the results in all models, but only models (iii) and (iv) take into account the effect of geometric scale. A clear validation of any model requires the variation of initial pressure and geometric scale. Future work may target a validation of models for strong ignition as part of an effort to better understand deflagration-to-detonation transition. Eventually, a main question is which physical effect provides a lower bound for strong ignition by shock reflection, independent of geometric scale.

16:00 Flame-Wall Interaction

811 - REDIM Reduced Modeling of Quenching at a Cold Inert Wall with Detailed Transport and Different Mechanisms

C. Strassacker, V. Bykov, U. Maas

In this work, the Reaction-Diffusion manifold (REDIM) method is further developed for flame-wallinteractions and demonstrated for the problem of a methane/air flame head-on quenching at a cold inert wall. A detailed transport mechanism of the molecular transport is now accounted for and it is based on the mixture averaged approximation of Curtiss-Hirschfelder including thermal diffusion. Moreover, the influence of different detailed chemical reaction mechanisms is studied. The problem of flame quenching at cold wall and the model configuration is briefly discussed. Then, the key stages of the construction of the REDIM manifold for this configuration and for transient regimes are presented. Finally, the results of detailed and reduced computations are compared and discussed. It is shown that the difference between different mechanisms is larger than the model reduction error. The results of computations with the detailed transport model are in a better agreement with experimental results than computations with unity Lewis-number.

775 - Flame-Wall Interaction in Premixed Reactive Turbulence

P. Zhao, L. Wang, N. Chakraborty

Flame-wall interaction (FWI) is of special importance to understand turbulent combustion in the confined space. In the present work the interaction between the turbulent premixed flame and the solid wall with different boundary conditions has been numerically investigated in a newly proposed counter flow like model. The premixed flame front are convected downstream by the fresh reactants at the turbulent state fed from the inlet boundary and finally anchored with the presence of a solid wall boundary. The four lateral boundaries are open for the outflow. Statistically the flame can be stationary and physically at the stationary state the flame location is balanced with the inflow mass flux, i.e. the incoming flow speed, the fuel consumption rate, i.e. the turbulent flame speed, and the wall boundary condition as well. Especially the wall temperature is crucial for the flame-wall interaction. The results of direct numerical simulation (DNS) demonstrates that if the wall temperature is low enough, the flame surface turns to be broken because of the excessive heat loss to the cold wall. The wall heat flux increases when flame approaches to the cold wall. However, once the flame quenches, the normal heat transfer to the wall starts decreasing, which presents roughly the flame quenching distance coincides with the maximum heat loss point. The flame dilatation is determined by the heat generation from reaction and heat loss to the wall. With the adiabatic wall boundary condition, the dilatation at the flame remains to be positive because of the net heat release by reaction. Differently for case with the cold wall boundary condition the dilatation at the flame decreases sharply to be negative because of the excessive wall heat loss till the flame quenching, after which, the dilatation at the flame increases from negative to zero at the cold wall. In addition the alignment relation between the flame normal and principal axes has also been investigated. Relatively the alignment tendency change is weak with

respect to the wall boundary conditions, which can be explained by the dominant influences of the flame stretch and the heat loss close to the wall.

857 - 3-D Flame Patterns in a Backward Facing Step Mesoscale Combustor for Non-Adiabatic Wall Conditions

M. Malushte, S. Kumar

Experimental investigations on flame dynamics in a backward facing three-step mesoscale combustor with premixed *LPG-air* mixture are reported for a range of mixture equivalence ratios and inlet velocities. The effect of various governing parameters such as equivalence ratio and mixture velocities along with diameters and length of heat recirculating cup on flame dynamics is investigated in detail. The mixture inlet velocities are varied from 1 - 8 m/s and equivalence ratios from 0.6 - 1.4. Various stable and unstable flame propagation modes are observed for the range of conditions investigated. Various interesting rotating and pulsating flame (2-D and 3-D) propagation modes are observed. The details of these modes are analyzed with the help of a high speed camera and it is proposed that these flame modes are formed due to combined effect of hydrodynamics, thermos-diffusive instabilities and flame-wall coupling.

939 - Heat Flux and Flow Topology Statistics in Oblique Quenching of Turbulent Premixed Flames by Isothermal Inert Walls

J. Lai, N. Chakraborty

The statistical behaviors of wall heat flux, and flame quenching distance in the case of oblique quenching of a turbulent premixed V-flame flame by isothermal inert walls have been analysed in terms of the distributions of flow topologies and their contributions, using three-dimensional compressible Direct Numerical Simulations (DNS) data. The flow topology distribution is characterised in terms of the invariants of the strain rate tensor, which divides turbulent flow structures into 8 generic canonical configurations (i.e. S1-S8). The statistics of wall heat flux, flame quenching distance and flow topology distribution have been compared to the corresponding quantities for the Head-on Quenching (HOQ) of a statistically planar premixed flame with the same values of turbulence intensity and integral length scale to flame thickness ratio as that of the inlet values in the V-flame configuration. It has been found that the maximum (minimum) wall heat flux (Peclet number) in the case of oblique flame quenching assumes a greater (smaller) value than in the corresponding turbulent HOQ case. Although the volume fractions of S2 and S7 topologies assume high values within the flame front, the focal topologies S1 and S4 have been found to be the significant contributors to the wall heat flux in the case of oblique flame quenching. By contrast, nodal topologies S2 and S3 remain the major contributors to the wall heat flux when it attains large magnitude in the HOQ case, but all topologies contribute comparably to the wall heat flux at a later stage of flame quenching.

16:00 Turbulent Reacting Flows 1

985 - On the Supersonic Flame Structure in the Hyshot II Scramjet Combustor

C. Fureby

Understanding of the multi-disciplinary physical processes in the flowpath of a scramjet is crucial for the enabling of this technology, considered the most promising for hypersonic flight. The flow in such engines remains supersonic throughout, resulting in flow residence times of O(1) ms. Within this short time interval, the fuel and air must mix, ignite and combust prior to discharging through the nozzle. In this study, we combine results from high-fidelity Large Eddy Simulation (LES), using finite-rate chemistry models and skeletal reaction mechanisms, with experimental data and visualization to elucidate the key features of the flow and combustion processes of the HyShot II combustor at 27 km altitudes. Good agreement between LES and experimental data is achieved, indicating that LES captures the essential physics. More specifically, it is observed that the flame typically resides in the region $10^2 < \text{Re}_t < 10^4$ and $10^{0.1} < \text{Da}_t < 10^2$, and experience significant turbulent Ma numbers, Ma_t, which may have a significant effect on the turbulent flame structure. The observation that the most probable flame regime spans several zones suggests that methods capable of handling various, *a priori*

unknown, flame topologies, such as finite rate chemistry LES methods should be employed in simulations.

1002 - Extinction in Non-Premixed Ethanol Spray Flames Using Direct Numerical Simulation J.C. Tang, H. Wang, E.R. Hawkes, M. Bolla

Results from a parametric study of flame extinction with varying Stokes number using direct numerical simulation are presented in order to investigate the effect of Stokes number on flame extinction in non-premixed spray flames. Two planar, non-premixed ethanol spray flames were simulated at a constant Reynolds number of 6000 and with Stokes numbers 2.5 and 20. Peak flame extinction varies from approximately 30% to 50% as the Stokes number is increased. The effect of Stokes number rate. This increased extinction is a result of a strong interaction between the droplets and the flame surface. The evaporation of droplets weakens the flame due to evaporative cooling and reaction of the fuel with OH in the reaction zone.

1157 - Dynamic Pressure Characterization of a Dual-Mode Scramjet

C. Aguilera, A. Ghosh, K.H. Shin, K.H. Yu

The dual-mode regime of a laboratory scale scramjet combustor with a cavity flame holder was experimentally characterized to study the combustion dynamics associated with scramjet-to-ramjet transitions. Combustor equivalence ratios in the 0.04-0.20 range were tested using hydrogen fuel injected through a wall orifice. Static pressure distributions demonstrated that the combustor undergoes thermal choking for a combustor equivalence ratio between $0.10 < \Phi < 0.12$. Below this threshold, the combustor operated in scramjet mode featuring a pressure spectrum with a wide range of low amplitude frequency components. Around the transition threshold a well-defined and dominant pressure oscillation appeared peaking at a frequency of 1290 Hz. For the highest two equivalence ratios above the transition threshold, the amplitude and frequency of these flame oscillations subsided but the pressure spectra maintained a broadband characteristic shape centered around a frequency of 1000 Hz. This behavior was correlated to upstream-downstream flame front movements visualized in a sequence of schlieren images.

1081 - Development of a Multiscale Adaptive Reduced Chemistry Solver (MARCS) for Computationally Efficient Combustion Simulations

W. Sun, L. Wang, T. Grenga, Y. Ju

The Multiscale Adaptive Reduced Chemistry Solver (MARCS) is developed by integrating the Correlated Dynamic Adaptive Chemistry and Transport (CO-DACT) method with the Hybrid Multi-Timescale (HMTS) and G-Scheme methods, and the Full Speed Fluid Solver to conduct the efficient combustion modeling with detailed chemical kinetics. The preliminary results of ignitions and flame propagations in this paper demonstrate that the computational efficiency can be improved by orders of magnitude using CO-DACT method with HMTS and G-Scheme methods. In the final paper and presentation, MARCS will be applied to the simulations of a two-dimensional jet flame and an oblique shock inducing auto-ignition with detailed mechanisms and transport to demonstrate the efficiency. Detailed turbulence/chemistry interactions on low temperature ignition and ignition to flame and detonation transition will be investigated.

9:00 Plenary Lecture 2

PL2 - Combustion Chemistry Developments Between Experiments, Modeling, and Theory Katharina Kohse-Hoeinghaus, Universität Bielefeld, Germany

Current research towards cleaner and more efficient processes in combustion builds significantly on the development of combustion models and their experimental validation. The combustion community increasingly establishes more or less detailed reaction mechanisms and combustion models for individual fuels or for yet underexplored operation conditions. Key issues include the mechanisms at low temperatures and/or high pressures, for conventional and alternative fuels or their mixtures, and for the formation of toxic species and soot emissions. While much of this research is fundamentally interesting, guidance may be desired regarding realistic expectations, for example when the pertinent combustion chemistry must be adapted to tractable sizes for technical environments. From an experimentalist's perspective, it is important to understand the potential of laboratory measurements for mechanism validation and the interplay between kinetics and diagnostics.

Recent collaborative examples will include species measurements in flames and reactors, especially to understand the oxidation behavior of individual fuels and dual fuel mixtures, and will include recent advances in isomer-selective detection. Discussion of some potentially controversial aspects and perceived trends will be suggested regarding species identification and quantitative concentration measurements as well as model validation and improvement.

10:30 Chemical Kinetics and Reaction Dynamics 3

1033 - Effect of CO2 Dilution on the Burning Velocity of Equimolar Syngas Mixtures at Elevated Temperatures

R.J. Varghese, S. Kumar, H. Kolekar

Laminar burning velocities of equimolar (H2/CO = 1) syngas-air mixtures with different CO2 (60, 70%) dilutions were accurately measured using preheated diverging channel technique. Experiments with syngas-air mixtures having 60% CO2 by volume were carried out for validation of the experimental facility. The burning velocities at ambient conditions were determined for various (equivalence ratio = 0.7 - 1.3) and a range of elevated temperatures (350 - 650 K). Effect of further addition of CO2 (70%) was studied both experimentally and numerical predictions using a chemical kinetic mechanism (GRI Mech 3.0). The predictions are in agreement for the 60% CO2 dilution of syngas, however, interesting to note that the experimental results differ significantly for 70% dilution. The flame structure was analyzed to isolate the prominent reactions. ROP analysis showed the further investigation of 80% reduction in peak ROPs' of H and OH radicals compared to 60% dilution is necessary. The important reactions remains the same for both dilutions however, the reaction with highest positive sensitivity coefficient shifts from R35 (H + O2 + H2O = HO2 + H2O) to third body reaction R33 (H + O2 = HO2 + M).

1052 - Influence of Microscopic Stochastic Properties on the Auto-Ignition of Hydrogen / Oxygen Mixture

C. Yang, Q. Sun

The microscopic stochastic nature of chemical reactions can influence combustion phenomenon like auto-ignition in both individual realization and statistically. Microscopic reaction process can be determined using the Chemical Master Equation and simulated through a particle Monte Carlo method based on this equation. Through plenty of microscopic simulations of H2-O2 auto-ignition, the microscopic fluctuation of ignition delay time is found to be related to the system volume (V) and initial temperature (T). Its standard deviation of ignition delay time has a power law relation with the volume. A detailed expression for the deviation is derived analytically, which agrees very well with simulation results. We also show that the fluctuation in radical concentrations influences the statistical value of combustion process at the micron scale.

982 - Reduced Order Models for Shock-Induced Combustion of Fuel Mixtures

D.A. Schwer, K. Kailasanath

Unlike most previous detonation tubes and engines, most experimental RDE rigs inject fuel and oxidizer separately into the annular combustion chamber of an RDE. This produces a stratified mixture with local pockets of fuel-rich and fuel-lean premixture, which can significantly affect the stability and efficiency of the detonation wave. In addition, for hydrocarbon RDEs, it may prove attractive to use a mixture of different fuels (for example, hydrogen mixed with ethylene), which can significantly alter its reactivity and thus the stability of the detonation wave and flame holding characteristics. Modeling both of these effects are challenging but necessary if modeling is to play an important role in designing RDEs. Due to the size and complexity of RDEs, detailed kinetic models are not feasible to use for simulations of RDEs. The present work develops a reduced-order model based on the hydrogen-air induction-time parameter model to simulate RDEs with both stratified premixtures and fuel blends. A reduced order model is created for hydrogen-air for a range of equivalence ratios, and results show how well the model works based on detonation wave velocities, temperatures, and pressures, as well as detonation cell size.

1175 - Laminar Burning Velocities of Spherically Expanding Hydrogen/Air Mixtures for Temperatures Up to 423 K at Ambient Pressure

J. Beeckmann, H. Pitsch

This paper presents experimental data of hydrogen / air laminar burning velocities extracted from spherically expanding flames for varying initial temperatures up to 423K under ambient pressure. The data is compared to data found in the literature. Simulations of laminar burning velocities are performed with two different mechanism as typical representatives for the hydrogen oxidation chemistry. One agrees very well with the experimental data presented here and the other mechanism is overpredicting, although, interpreting the literature, the opposite might be expected. Possible reasons for this are addressed and discussed.

10:30 Turbulent Flames 1

949 - A New Measured Regime Diagram of Turbulent Premixed Combustion, Based on Images of Flame Structure

A.W. Skiba, T.M. Wabel, J.F. Driscoll, C.D. Carter, S. Hammack

It is proposed to replace the predicted Borghi regime diagram for turbulent premixed flames with a new Measured Regime Diagram that better fits the present measurements and those from previous studies. Thicknesses of preheat and reaction layers were measured along with the probabilities of broken and distributed reactions for 27 cases using CH, OH and formaldehyde laser imaging diagnostics. A new Michigan Hi-Pilot burner provides extreme turbulence levels (u'/S_L) up to 243 and integral scales up to 43 mm, which are 10 times that of previous studies.

Two boundaries on the predicted Borghi diagram do not agree with the measurements: the boundaries of broadened preheat layers (BP) and broken reactions (BR). Instead, we propose a new BP boundary that shows good agreement with the measurements. It is explained by replacing the idea that Kolmogorov eddies must fit inside the flame with the idea that broadening occurs when the turbulent diffusivity exceeds molecular diffusivity. One implication for flamelet modeling is that the measured BP-TR regime (of Broadened Preheat, Thin Reaction layers) extends over a much larger range than is predicted by the Borghi diagram. Broken reactions, which define the upper boundary of the BP-TR regime, were not observed even for turbulence levels u'/S_L of 243, which is five times the predicted value. Thus flamelet models are valid even for extreme levels of turbulence. The preheat layer was broadened by a factor of 14 while, in contrast, the reaction layer was essentially not broadened. For several special cases of stratified flames, both broken and partially-distributed reactions were allowed to be entrained into the hot products by reducing the outer co-flow; these cool pockets created broken reactions.

1058 - Influence of Turbulence on the Propagation of C7H8/Air Flames at Atmospheric Pressure and Temperature

A. Lefebvre, M. Nait-Daoud, N. Chaumeix

The reduction of pollutant emissions and energy diversification become a world challenge which require the development of new combustion processes and new combustibles. Otherwise, the combustion stays a major source of atmospheric pollutants emissions, like carbon monoxide and dioxide, unburned fuel and nitrogen oxide. Hence, in the field of people and goods transport, engine conception is dictated by the efficiency, the reduction of consumption and emissions, while keeping or increase the power. In such engines, the combustion process is driven by the turbulent flow inside the combustion chamber. The understanding of the complex interactions between the reaction rate of a combustible and the flow is hence of first order. The aim of this work is to characterized a new configuration of turbulence generation where the position and the size of the fan have been modified into this large spherical vessel. First a complete study of PIV measurements is presented to determine the turbulence statistic. Secondly, preliminary results of C7H8/air flames at atmospheric pressure and temperature are presented and prospects are announced.

997 - Combustion and Emission Characteristics of Premixed and Non-Premixed Ammonia/Air Turbulent Swirl Flames at the High Pressure and Temperature

K.D.K.A. Somarathne, A. Hayakawa, H. Kobayashi

The present study is dedicated to understand the combustion and emission characteristics of turbulent premixed and non-premixed ammonia/air swirl flames at the high pressure and temperature. Even though ammonia has much lower laminar burning velocity, the recent studies have illustrated that by introducing swirl flow, and thereby making a recirculation near the downstream of swirler ammonia/air turbulent premixed flames have successfully achieved a stable combustion at the atmospheric pressure. In addition, those studies have elucidated that NO generation can be significantly reduced by using the rich flame condition and there is an equivalence ratio in rich flame condition in which NO and unburnt ammonia emissions are minimal and in a same order, and thus this would be the best operating point for the selective catalytic NO emission reduction (SCR) process in the downstream. However, to the best of author's knowledge, there is no any comprehensive study on turbulent ammonia/air flames at the high pressures, which is essential for the design of the gas turbine combustors. Accordingly, a relative simple test cases were chosen as affordable tests to evaluate the feasibility of more complex gas turbine combustors, and, in the present study, large eddy simulation (LES) with a finite rate chemistry is performed in a three-dimensional computational domain.

The space and time averaged emissions (STAE) were evaluated at the exit of a cylindrical combustion chamber for various equivalence ratios and high pressures up to 0.5 MPa at the initial mixture temperature of 500 K. The study found that NO emission is significantly decreased with an increase in pressure irrespective to the combustion type because, at the high pressure, third body reaction of OH + $H + M \Rightarrow H_2O + M$ plays significant role on the reduction of OH concentration, and thereby reduction of NO emissions. But STAE of NO in non-premixed flames are slightly higher than that of the premixed cases at same equivalence ratio. Because, in non-premixed flames, NO production is depended on the local equivalence ratios of the flame region, and thus, there is a significant NO production in the lean flame regions around the wall boundaries owing to higher concentration of OH even in the overall-rich flame conditions. However, similar to the premixed flames, NO emission decreases with the increase in overall equivalence ratio. Unburnt ammonia emission also reduces with an increase in pressure in the case of rich conditions, possibly because of the increase in pressure leads to the decrease in chemical characteristic time, and thereby increase in the overall Damköhler Number. Eventually, this study found that pressure effect is very significant on the NO and unburnt ammonia reductions of ammonia/air combustion.

1176 - Fuel Similarity and Turbulent Burning Velocities of Stoichiometric Iso-Octane, Lean Hydrogen, and Lean Propane at High Pressure

M. Nguyen, L. Jiang, S. Shy

This paper explores general correlations of high pressure turbulent burning velocities (S_T) of spherical flames using a variety of fuel/air mixtures with different effective Lewis number (*Le*), including (i)

stoichiometric iso-octane at high temperature (T = 423 K) with $Le \approx 1.43$, (ii) lean hydrogen at the equivalence ratio $\varphi = 0.6$ at 298 K with $Le \approx 0.58$, and (iii) lean propane at $\varphi = 0.7$ at 298 K with $Le \approx 1.62$. Experiments are performed in a dual-chamber, constant-pressure, constant-temperature, fanstirred cruciform explosion facility capable of generating a sizable near-isotropic turbulence. Schlieren images of statistically spherical expanding turbulent flames for these mixtures are recorded to evaluate the mean flame radius $\langle R(t) \rangle$ and the observed flame speeds, $d \langle R \rangle / dt$ and S_F (the slope of $\langle R(t) \rangle$), where S_F is found to be equal to the average value of $d \langle R \rangle / dt$ within 25 mm $\leq \langle R(t) \rangle \leq 45$ mm. Using the density correction and Bradley's mean progress variable $\langle c \rangle$ converting factor for schlieren spherical flames, $S_{T,c=0.5} \approx (\rho_b/\rho_u)S_F(\langle R \rangle_{c=0.5})^2$ can be obtained, where the subscripts b and u indicate burned products and unburned reactants. We discover that all scattering $S_{T,c=0.5}$ data with different values of Le together with previous methane/air mixtures at $\varphi = 0.9$ at T = 300 K and 423 K with $Le \approx 1$ can be all nicely collapsed onto a general correlation: $S_{T,c=0.5}/u' = 0.092(DaLe^{-1})^{0.5}$ with small variations, where the Damköhler number $Da = (L_1/u')(S_L/\delta_L)$. L_1 , u', S_L , and δ_L are the integral length scale of turbulence, the rms turbulent fluctuating velocities, the laminar burning velocity, and the laminar flame thickness, respectively.

10:30 DDT 1

1109 - Flame Acceleration and Deflagration-to-Detonation Transition Through an Array of Obstacles

H. Xiao, R.W. Houim, E.S. Oran

The flame acceleration and deflagration-to-detonation transition (DDT) in a channel with an array of cylindrical obstacles have been numerically studied by solving the Navier-Stokes equations for an unsteady, fully compressible, and chemically reacting gas. The objective is to understand the mechanisms leading to flame acceleration and DDT through an array of obstacles in the presence of boundary layer effects. The equations are solved on a dynamically adapting grid using a Godunov algorithm with HLLC fluxes, third-order accurate in space and second-order in time. The results of the numerical simulation were compared with experimental data. The flame and flow development agrees well with the experimental observations. The key features of flame acceleration and detonation propagation, including the flame-front evolution, oscillating flame-tip speed, and detonation failure and re-ignition, in the experiment were reproduced in the numerical simulation. This will allow us to gain an insight into the physical processes and mechanisms controlling the flame acceleration and DDT. The numerical calculations shows that the early flame acceleration results from the rapid expansion of the flame into the background flow and stretching in the wakes of cylinders. As shock waves are generated by the accelerating flame, more flame instabilities are produced due to flameshock interactions. This results in a large increase in the flame surface area and faster flame acceleration. Strong leading shocks were produced when the flame becomes turbulent. The initiation of detonation involves a collision of shocks in the shocked boundary layers at the flame tips, which appears to be related to DDT mechanism of shocking focusing.

The computation described here is only one of a series that we have performed to explore flame acceleration and DDT through an array of obstacles. A more extensive group of computations, which focus on obstacle shapes and blockage ratio, will be discussed in the presentation.

959 - Flame - Shock Wave Dynamic Studies at DDT in Diluted Stoichiometric Acetylene-Oxygen Mixtures

Y.A. Baranyshyn, P.N. Krivosheyev, O.G. Penyazkov, K.L. Sevrouk

Significant impact on the formation and characteristics of the detonation wave has a flame acceleration following the leading shock wave in the gas. Besides conventional measurement techniques, different optical measurement techniques (the schlieren techniques, the laser-induced fluorescence) are using to study and visualize this phenomenon. They are useful, but obtained information is usually two-dimensional and line-of-sight integrated.

In our work the experimental studies of DDT in a stoichiometric acetylene-oxygen mixture with 70% of argon dilution and with 60% of nitrogen dilution at different initial pressures were carried out.

Simultaneous registration of the locations of reaction zone near the wall in four directions along the tube and the additional pressure control at the same cross-sections provide the quantitative data on dynamics of the shock wave and the flame velocities, the spatial flame shape, the length of the induction zone between the shock wave and the flame front. As the result the characteristic values of these parameters and the features of the process were determined.

1017 - Stages of Flame Acceleration and Detonation Transition in a Thin Channel Filled with Stoichiometric Ethylene/Oxygen Mixture

H.P. Chan, M.H. Wu

Complete evolvements of reaction and shock waves of stoichiometric ethylene and oxygen mixture in a 1 mm x 1 mm channel were successfully resolved using a high-speed schlieren system. Four reaction propagation stages named, in the order of appearance, 1st FA, quasi-steady, 2nd FA and 3rd FA, were identified prior to the velocity surge associated with detonation transition. A leading shock developed ahead of the flame during the transition from 1st FA to the quasi-steady stage. The flame was stretched and oblique shocks were formed between the flame front and the walls in the 2nd FA stage. A precursor shock right in front of the flame which later developed into a staggered series of oblique shocks structure was the typical schlieren pattern observed during the 3rd FA stage. Growth rate of the reaction front velocity was found to follow power law in the 2nd FA stage, while the slope was linear in the 3rd FA stage, when the reaction propagation velocity reached ~1500 m/s.

792 - Cylindrical Flame Acceleration and Deflagration-to-Detonation Transition in Confinement Space

W. Han, N. Du, Z. Liu, W. Kong

In confinement space the propagation of a cylindrical flame created by weak circle source is simulated by a high-resolution code. It is first found that for the lower initial temperature and pressure globally cylindrical flame can accelerate and eventually turbulent flame, while the transition to detonation is not observed. As increasing initial temperature and pressure, the transition to detonation can appear near wall. The numerical results are significant for explaining the super-knock phenomenon in engine combustion chamber.

10:30 Detonation Structure

1085 - A Note on the Averaging Analysis for One-Dimensional Pulsating Detonations

X. Mi, H.D. Ng, C.B. Kiyanda, A.J. Higgins, N. Nikiforakis

One-dimensional pulsating detonations with increasing instabilities towards chaotic behavior are computationally simulated, and their mean wave structure are obtained using two different averaging approaches, i.e., in a reference frame moving at the average propagation velocity and a wave-attached reference frame. Performing the averaging in a reference frame moving at the average velocity, the result is shown to be sensitive to the sampling length. Using the wave-attached analysis, the global structure qualitatively resembles the standard ZND profile, but significantly deviates from the ZND profile for the case of high chaotic pulsations.

1134 - Mean Structure of Unstable Pathological Detonations

X. Mi, H.D. Ng, C.B. Kiyanda, A.J. Higgins, N. Nikiforakis

Pathological detonations have been numerically simulated for three cases of different propagation behaviors: 1) steady propagation, 2) periodically pulsating propagation, and 3) highly chaotic pulsation. For each case, a time- and density-weighted mean wave structure has been obtained and compared with the corresponding ZND profile. While the mean structure for the periodically pulsating cases agrees well with the ZND solution, that resulting from the highly chaotic case significantly differs from the ZND profile with an elongated hydrodynamic thickness. Further analysis will be performed to examine the hypothesized role played by the relaxation processes of the fluctuating quantities. In future efforts, this study will be extended to two-dimensional pathological detonation systems where transverse instabilities are present.

870 - Structure of Detonation Propagating in Lean and Rich Dimethyl Ether-Oxygen Mixtures *R. Mével*

In the present study, the structure of detonations propagating in lean and rich dimethyl ether-oxygen, DME-O2, mixtures has been investigated using steady one-dimensional and unsteady two-dimensional numerical simulations. The origin of the non-monotonous energy release profile in rich DME-O2 mixtures has been explained based on the analyses of the energy release rate per reaction and of the rate of production of the major species. The numerical soot foils and schlieren fields obtained for DME-O2 mixtures demonstrated significant differences as compared to those obtained for H2-NO2/N2O4 mixtures which exhibit non-monotonous energy release profile and a clear double cellular structure. Chemical kinetics considerations tend to indicate that the structure of the energy release profile of detonation in rich DME-O2 mixtures do not fulfill the critical conditions for the existence of a double cellular structure.

1041 - Influence of Water Sprays on a Multi-Cellular Regular Detonation

G. Jarsalé, F. Virot, A. Chinnayya

This paper presents preliminary results dealing with a detonation propagation in Φ C2H4+3O2+ZAr, for an equivalence ratio Φ ranging from 0.8 to 1.1, with an argon dilution Z = 28 which refers to a 90% dilution in mass, all mitigated with a fine water spray reaching a water mass fraction of 6.4 to 9.2% in mass. A spray investigation revealed an arithmetic and Sauter mean diameter of the distribution of 10 μ m and 83-98 μ m respectively.

Detonation velocity and cellular structure analyses show a significant velocity decrease of 170-240 m/s between CJ theoretical values and data of mixtures laden with a 6.4% of water, linked to a very strong enlargement of the cell structure (ten to twenty times), and to a worsening of the cellular structure regularity. The addition of this amount of water has also a visible impact on the pressure decrease downstream of the leading front shock, and increase the global pressure fluctuations. The detonation extinction limit is found to be between the 6.4 and 9.2% water mass fraction.

Early observations highlight that the detonation cellular structure is found to be more regular with argon dilution in comparison with nitrogen dilution, as expected. The use of an equivalent wet mixture reveals a decrease of the detonation velocity of more than 10% for C2H4/O2/Ar mixtures. As a comparison, the experiments with more irregular dry detonation mixtures with air seem to show a smaller decrease in the detonation velocities.

10:30 Combustion Stability, Instabilities 1

816 - The Origin and Evolution of Mechanical and Thermodynamic Disturbances Caused by Localized Energy Deposition in Gaseous Volumes

D.R. Kassoy

Transient, spatially resolved thermal energy deposition into inert and reactive gas volumes is the source of thermodynamic and mechanical disturbances. Thermo-mechanical concepts and modeling have been used to develop a quantified cause-effect relationship. When the energy deposition is "sufficiently" small the disturbances are described by classical acoustic wave equations. In contrast the mathematical models used to describe thermo-mechanical physics incorporate a much wider range of energy deposition. Examples of these phenomena include shocks generated by lightning and explosions, detonation initiation, internal combustion engine knock, blast waves associated with supernovae, transient pressure variations in liquid propellant rocket engines and perhaps, coronal mass ejections from the Sun.

828 - Subcritical Thermoacoustic Bifurcation in Turbulent Combustors: Effects of Inertia

G. Bonciolini, D. Ebi, E. Boujo, N. Noiray

Thermoacoustic coupling is a recurring issue in many combustion systems, such as gas turbine combustors or rocket engines. When a strong acoustic limit cycle is triggered in a real engine, the corresponding high pressure levels can be detrimental for its mechanical integrity. This fact might prevent the user to operate it at its maximum performance point. The system stability depends on the operating condition at which the machine is run, e.g. on inlet temperature, pressure or air/fuel ratio. In

some cases, the system experiences a subcritical bifurcation when one of these parameters is varied, switching suddenly from a stable operation to a high-amplitude limit cycle.

In this paper, experimental data obtained from a lab-scale, fully premixed, atmospheric combustor showing this phenomenon will be presented. The complex system physics is then reproduced by a simple ad-hoc designed model, represented by a non-linear noise-driven oscillator.

To highlight the peculiar transient dynamics of the system, the bifurcation parameter has been varied over time both experimentally and in simulations of the model.

The results agree in showing how the system experiences inertial effects, delaying the bifurcation when the control parameter is ramped. The entity of this delay can be quantified through the Mean First Passage Time concept. It can be observed that the inertia is more relevant in case of a fast change of the control parameter.

This fact has a practical impact when one is mapping the operative points of a new combustion system: excessive ramp speeds cause the system to jump later (in terms of linear growth rate) to the limit cycle and therefore with higher pressure level, and a longer time is then needed to bring it back to a safe operating condition.

904 - The Effects of Lewis Number on the Combustion Limit, Near-Limit Extinction Boundary, and Flame Regimes of Low-Lewis-Number Counterflow Flames Under Microgravity

T. Okuno, H. Nakamura, T. Tezuka, S. Hasegawa, M. Kikuchi, K. Maruta

Microgravity counterflow experiments and 1-D counterflow computations using detailed chemistry with CH₄/O₂/Kr (*Le* = 0.75) and CH₄/O₂/Xe (*Le* = 0.50) mixtures, and 3-D transient computations using the diffusive-thermal model were conducted to investigate the effect of Lewis numbers on the combustion limit, formation of sporadic flames and the flame regimes of stretched flames. For mixtures at *Le* = 0.5, sporadic flames were observed both experimentally and computationally at extremely low stretch rates (0.8 s⁻¹ in experiments, and 0.18 s⁻¹ in 3-D computations). For *Le* = 0.75 mixtures, sporadic flames were not observed both experimentally and computationally. The experimental extinction points agreed with the 1-D computational results for *Le* = 0.75 mixtures. In addition, the experimental extinction points did not agree with the 1-D computational extinction curve in the region where sporadic flames were observed for mixtures at *Le* = 0.5. The expansion of the combustible region due to the formation of sporadic flames was found to be in qualitative agreement with computational results obtained in a previous study.

765 - On the Effect of Pressure on Intrinsic Flame Instabilities in Lean Hydrogen-Air Mixtures – Part I: Detailed Chemistry Based Direct Numerical Simulation

J. Hasslberger, P. Katzy, T. Sattelmayer

The promoting effect of intrinsic flame instabilities on explosive combustion is generally known. Most detailed computational studies are limited to generic configurations however. In the present numerical investigation, direct qualitative and quantitative comparison with experimental data from a laboratoryscale explosion channel is provided. Characterized by Lewis numbers clearly smaller than unity, lean hydrogen-air mixtures are particularly prone to intrinsic flame instabilities. An imbalance of heat conduction and species fluxes leads to the development of a cellular flame structure, known as the thermal-diffusive instability. Increased flame surface area and interconnected flame stretch effects significantly affect the flame speed. Experimental evidence suggests a strong influence of pressure on the phenomenon. However, a thorough quantification is currently missing. One difficulty arises from the fact that the thermal-diffusive instability is superimposed by the hydrodynamic Landau-Darrieus instability. Additional insight is thus gained by manipulation of the mathematical model to separate different effects. It is shown that pressure variation does not only affect the burning velocity but also the cellular structure of the flame in sufficiently lean hydrogen-air mixtures. The higher the pressure, the smaller the cell size. Flame surface area increases accordingly. The diminishing effect of elevated pressure on (laminar) burning velocity is a standard in modeling whereas the promoting effect of enhanced flame wrinkling via intrinsic instabilities is usually neglected. Burning laws without such correction might lead to an underestimation of flame speed for under-resolved explosion simulations.

13:50 Fire Dynamics

1005 - Smoldering Spread Velocity Along a Thin Solid in a Narrow Channel

K. Kuwana, K. Suzuki, Y. Tada, G. Kushida

Smoldering spread often occurs at an early stage of fire, and understanding its mechanism helps us predict the initial fire growth rate. In this paper, smoldering spread along a thin solid in a narrow channel was studied with the major focus on predicting the spread velocity. A number of different series of experiments were conducted, and the spread velocities were measured. A linear stability analysis was then conducted to identify a governing parameter, F. It was shown that all the experimental data can be expressed by a single function of F. Finally, an equation was derived for predicting the dependence of spread velocity on F. It was found that the equation can correlate all the numerical and experimental data reasonably well.

993 - The Critical Conditions for the Onset of Pool-Fire Puffing

W. Coenen, D. Moreno-Boza, A.L. Sánchez

Pool fires are known to exhibit a self-sustained oscillatory behavior, shedding large toroidal coherent structures at a well-established frequency, a phenomenon referred to in the literature as "puffing". This behavior influences the rate of air entrainment, the radiated heat output, the flame height and also the spreading of the flame. Pool-fire puffing has been studied extensively in the literature, and it is well known that under normal conditions of temperature and pressure typical hydrocarbon fuel pools of a few centimeters in diameter puff with a frequency on the order of 10 Hz. Nevertheless, no detailed account has been given of the critical conditions for the onset of puffing. Following the recent analysis of flickering diffusion flames (Moreno-Boza et al., J. Fluid Mech. 798, 2016), we consider the puffing of pool fires as the manifestation of an axisymmetric hydrodynamic global instability, the onset of which can be determined by means of a linear global stability analysis. Our description of small laminar pool fires accounts for the non-unity Lewis number and vaporization characteristics of typical liquid hydrocarbon fuels. In the description, once the thermochemical parameters corresponding to a certain fuel have been fixed, the only remaining governing parameter is the Rayleigh number Ra. We show that above a certain critical value Rac, a global instability of the flow sets in, leading to periodic oscillations of the flow field with a frequency that decreases with Ra. For the specific case of methanol, our computations find Rac = 10500, which, on Earth in an air atmosphere under normal temperature and pressure, is equivalent to a critical pool diameter of 1.4 cm. Furthermore, the puffing frequency under these conditions is found to be 9 Hz.

1047 - Horizontal Flame Spread Along a Thin Paper-Disk in a Narrow Space

T. Daitoku, T. Takahashi, T. Tsuruda

Flame spread along combustible material must be accurately identified in fire hazards. Heat and mass transfer phenomena, effects of flow, and chemical reaction control flame spread. Flame spread has been studied in various conditions, for example, flame spread over liquids and solids. In solid fuel combustion, it was reported finger-like smolder spread over a thin cellulosic fuel with external airflow in microgravity and the fingering propagation along a thin solid in a narrow space with external airflow in normal gravity. The objective of this study is to obtain fundamental knowledge for the flame spread characteristics of thin solid fuel in narrow gaps. In this research, the behavior of leading edge of flame in the horizontal observation was visualized. Furthermore, we discussed relationship between flame spread and horizontal flow along filter paper.

1011 - Traveling Vortex in a Natural Convection Field

T. Tsuruda

Natural convection governs the heat, mass, and momentum transfers of fire in an enclosure. Real scale room fire has large ceiling height that is large enough to be turbulent. In turbulent flow, the velocity vector which has its scalar and orientation fluctuates with time. A simple numerical simulation of a square space heated from the floor produces a typical natural convection field. If a vortex blob locates between adjoining points, the velocity vectors at these pints cross with an angle. For most part of flow field, the velocity vectors does not cross and the angle is zero. Once flow field is given, by taking the inner product of these velocity vectors, the crossing angle is determined. Inner product of velocity

vectors gives the crossing angle which is an index to determine the presence of vortex blob. Using the distribution of crossing angle, a uniform region is seen. The trace of vortex blobs shows a series of behavior, a pair, two pairs, 10-30, and 50-300 of vortex blobs in the control volume with time.

13:50 Turbulent Flames 2

915 - Large Eddy Simulation of Supersonic H2-O2 Combustion

U. Guven, G. Ribert

The proposed three-dimensional simulation is related to the supersonic combustion of H2/O2. The application under study corresponds to the early phase of ignition in a rocket-like engine. The configuration is a sonic jet of hot burnt gases under-expanding into a combustion chamber filled with gaseous hydrogen. Two and three-dimensional simulations are performed to assess the numerical strategy, define the mesh requirements and help for the choice of the kinetic scheme for H2/O2 combustion. The large-eddy simulation tool is used with a reduced chemistry (5 species and 3 global steps) on a mesh resolution fine enough to use the laminar model assumption ($\Delta x = 25 \,\mu$ m, 680 millions of points). Pope criterion and subgrid scale Damköhler number (Da) are provided with various definitions for Da to validate the retained procedure for three-dimensional simulations. The sequence of ignition is detailed revealing the flame behavior and shocks arrangements. A diffusion flame develops in the supersonic mixing layer formed by the igniter flow and hydrogen injections. The flame structure is recovered with a counterflow flame configuration. A comparison with a non-reacting case shows that the driving physical mechanism is mainly linked to the aerodynamics of the igniter jet.

1074 - Dependence of Limiting Oxygen Index of Buoyant Turbulent Diffusion Flame on Fuel *D. Zeng, Y. Wang*

Recently, there has been a growing interest in water-mist fire suppression systems driven by its low water demand and minimal environmental impacts. Fire modeling has been increasingly used to evaluate water mist fire suppression system. Flame extinction mechanism is important for numerical model to handle gas-phase flame extinction in the presence of water spray. This work features the measurement of limited oxygen index, or the oxygen concertation at flame extinction, of buoyant, turbulent diffusion flames fueled by methane, ethylene, propane, and propylene. Flames were generated from a porous burner and surrounded by a co-flow oxidizer in a water-cooled compartment. Nitrogen gas was added to the air until reaching flame extinction. Combustion efficiency reduces slowly with a decreased oxygen concentration in co-flow, then quickly decreases when the oxygen concentration reached close to the global extinction limit. Limited oxygen index shows values in the following order: methane > propylene > propane > ethylene. This trend can be reasonably explained by the kinetic simulation of opposed-flow flames, which shows that fuel with smaller global extinction limit has lower maximum flame temperature at the same strain rate.

1125 - The Reattachment Process of Turbulent Lifted Diffusion Jet Flames Induced by Repetitive D.C. Electric Pulse Discharges

T.W. Chang, H.Y. Li, T.S. Cheng, Y.C. Chao, M.H. Shen

Among the recently prevailing flame stabilization enhancement by electric field and plasma, repetitive D.C. electric pulse discharge is proposed for the study of the reattachment process of turbulent lifted diffusion jet flames. The examined parameters such as pulse repetition frequency (PRF) and applying electric polarity are investigated experimentally. The experimental results show that the more effective stabilization in terms of a decrease in mean liftoff height and an increase in reattachment velocity can be obtained by increasing PRF, which even results in flame reattachment. Moreover, according to a sequence of instantaneous flame images captured by high-speed camera, the flame reattachment can be divided into two different types of electric-discharge process, referred to an electric field force dominated by ionic-wind effect in the early stage before corona discharge and followed by electric corona discharge characterized by kinetic enhancement when the reattaching flame moves close to the electrode. Flame base trace and PIV results also indicated that flame could reattach to the burner rim for the higher PRF case (above 800 Hz) with applying positive polarity, resulting from the drastic increase in displacement speed and the higher instantaneous gas velocity at flame base locally. This

implies that the propagation speed of flame base after initiating the corona discharges is enhanced beyond the laminar burning velocity for high PRF and positive polarity, thus, leading to flame reattachment.

858 - Combustion Characteristics of Transverse Hydrogen Jet in a Supersonic Compact Inlet/Combustor Model

Z.W. Huang, G.Q. He, F. Qin, X.G. Wei, S. Wang

This paper studies combustion characteristics of hydrogen in a compact supersonic inlet/combustor model numerically. Three-dimensional compressible large eddy simulation (LES) based on an Open Source Field Operation and Manipulation (OpenFOAM) solver is performed on a hydrogen-fueled combustor under the nominal inflow conditions of flight Mach number at 8.0. The partially stirred reactor (PaSR) combustion model is adopted to account for the sub-grid turbulence-chemistry interactions. A skeletal mechanism for hydrogen combustion process on structured hexahedral grids. Special attentions are paid on the inlet-induced shock / the injector-induced shock, / the injector-induced shock / the central reacting layer, and the injector-induced shock / flame interactions. The combustion efficiency is calculated. The combustion process in the model configuration is intrinsically unstable under such high speed flow conditions.

13:50 Detonation Initiation

1059 - Numerical Simulation of Detonation Initiation by Shock-Multiple Discrete Flames Interaction

A.L. Gunter, H.D. Ng, C.B. Kiyanda, K.C.T. Yuk, X.C. Mi, N. Nikiforakis

In this work, the deflagration-to-detonation transition via the interaction of a weak shock with a series of discrete laminar flames is simulated numerically using the unsteady reactive Navier-Stokes equations with one-step Arrhenius chemistry. The numerical setup aims to mimic an array of laminar flames ignited at different spark times, artificially inducing chemical activity to stimulate the coupling between the gas dynamics and the chemical energy release for the transition of deflagration-to-detonation. The interaction of the weak shock with the first cylindrical flame demonstrates very good agreement with the results obtained by Khokhlov et al. [Combust. Flame (1999) 117: 323-339] and that a single weak shock—flame interaction was not enough to cause prompt DDT. However, the simulation results show that a series of shock-flame interactions, producing compression waves which are amplified through the heat release and wall reflections, eventually create a hot spot ahead of the flame brush. This localized hot spot leads to the onset of a detonation wave. A parametric study is on-going in order to assess the influence of various components of the numerical model on the transition event and to explore any scaling relationship among different physical parameters.

983 - Growth to Detonation in Hexanitrostilbene (HNS)

J.D. Olles, R.R. Wixom, R. Knepper, A.S. Tappan, C.D. Yarrington

Explosive properties, such as run-distance or detonation velocity, are typically found using wedge tests or embedded gauges. The growth to detonation and equation of state of an explosive are crucial for predicting performance and parameterizing hydrodynamic simulations. The short distance for growth to detonation in some explosives renders most conventional tests inadequate. By instead using thin vapor-deposited films and initiating with an electrically driven flyer, hexanitrostilbene (HNS) has been observed to grow from an inert shock to full detonation within 100 microns. The plastic flyers (Parylene-C) used to initiate the thin HNS films are driven to a few km/s by exploding a thin metal foil via a high voltage capacitive discharge unit. By varying the size of the flyer and the discharged voltage supplied to burst the foil, the impact conditions are modified. To quantify the flight of the flyer; frequency shifted photonic Doppler velocimetry (PDV) is used and analyzed with short-time Fourier transform methods along with other digital filtering schemes. The measured impact and shock durations correlate well to shock physics simulations.

956 - Effects of Disturbance on Direct Detonation Initiation in H2/O2/Ar Mixture

Y. Wang, C. Qi, R. Deiterding, Z. Chen

Two-dimensional numerical simulation for direct detonation initiation in $H_2/O_2/Ar$ mixture is conducted. Detailed chemistry is considered and structured adaptive mesh refinement is used to efficiently resolve the detonation development. A disturbance is introduced on the surface of high pressure and high temperature initiation region. The influence of disturbance on direct detonation initiation is examined. It is observed that the disturbance induces complex shock wave interaction, which promotes autoignition and onset of detonation. Disturbances with different wave lengths are considered. It is found that the wave length of the disturbance has great impact on direct detonation initiation. The smaller the perturbation wavelength, the more complex the shock wave interaction and thereby the shorter the detonation development time. Therefore, disturbance with small wave length promotes the onset of detonation.

It is noted that symmetrical reflective boundary conditions are used for the upper and bottom walls, where the normal flow speed is zero while the tangential flow speed is not zero. Simulation for nonslip wall will be conducted and the effects of wall boundary will be examined. Besides, periodical boundary conditions will also be used for the upper and bottom walls and thus the effects of wall confinement will be examined. These results will be presented during the conference.

13:50 Detonation Limits

1042 - Nonlinear Dynamics of Gaseous Detonations with Losses

A. Sow, A. Kasimov, R. Semenko

We investigate nonlinear stability of steady state solutions for gaseous detonations in systems with heat and momentum losses. A high resolution shock-fitting numerical method is used for the study. We explore the stability of both high velocity solutions with small velocity deficits and low velocity setvalued solutions that were recently found by Semenko et al. (Shock Waves, 2016). It is found that the low velocity solutions exhibit very slow transients early in the development of instability indicating that the existence of set-valued solutions plays a stabilizing role in the detonation dynamics.

1031 - A Study on Suppression of Detonation Propagation by Inert Gas Injection

K. Ishii, K. Seki

Behavior of detonation transmission into an inert gas zone has been experimentally studied using a test section in which an inert gas is injected into a stoichiometric hydrogen-oxygen mixture. Effects of length of the inert gas zone and types of the inert gas of nitrogen, argon, and helium on propagation of the flame and the transmitted shock wave have been evaluated from measurement of the shock and flame speed. Hydrogen injection has been also tested. The experimental results show that for the inert gas of nitrogen and argon the velocity of the transmitted shock wave decreases with increase in length of the inert gas zone and that flame extinction is observed for length of the inert gas zone longer than about 1.0 m in the case of injection of nitrogen and argon. Nitrogen is found to be the most appropriate for suppression of detonation propagation and prevention of flame propagation among the tested inert gases.

1129 - Effect of Spatial Inhomogeneities on the Propagation Limit of Gaseous Detonations

X. Mi, A.J. Higgins, H.D. Ng, C.B. Kiyanda, N. Nikiforakis

The study investigates the effect of a spatially random distribution of reactive sources on the propagation limit of gaseous detonations. A two-dimensional detonation system governed by singlestep Arrhenius kinetics and an inert, yielding confinement is computationally examined. The inert confinement is implemented as a layer of gas with the same initial pressure and density as those in the reactive region, but with zero concentration of reactant. In the detonable mixture, reactive sources are initialized in discretely located, square-shaped regions and separated by inert gaps. Although the reactive sources are randomly distributed, the overall spatial discreteness and average heat release can be maintained at specific values. In this system with a yielding confinement, detonation waves experience losses due to lateral expansion behind a curved shock front and, thus, propagate at a velocity lower than the ideal Chapman-Jouguet (CJ) velocity. As the thickness of the reactive layer decreases,

the deficit in propagation velocity increases; below a critical thickness, detonations can no longer propagate in a self-sustained manner. In this study, the critical thickness for a steady propagation is determined for a homogeneous reactive medium and a mixture with randomly distributed, discrete reactive sources. The effects of naturally developed cellular structure in a homogeneous system on the propagation limit are compared with those of the randomly distributed reactive sources. The resulting critical thickness and velocity deficit are compared with those predicted using a quasi-one-dimensional, ZND-like model based on the assumption of a smoothly curved shock front.

13:50 Combustion Stability, Instabilities 2

1131 - Experimental Study of the Head-on Interaction of a Shock Wave with a Cellular Flame

M. la Flèche, Q. Xiao, Y. Wang, M.I. Radulescu

The focus of the present work is to determine the evolution of a cellular flame after its head-on interaction with a shock wave. Two novel techniques were devised that use a Hele-Shaw cell in order to visualize the mainly two-dimensional cells using high-speed schlieren imaging. The experiment revealed that the early deformation of the flame cellular structure is via the well-known Ritchmyer-Meshkov instability, due to the baroclinic torque mechanism. When the shock wave passed through the interface separating the burned and unburned gas, the flame gets more corrugated. Depending on the shock's provenance, the cusps get either stretched or flattened, and ultimately the cellular structure is reversed. The experiments were found to be in qualitative good agreement with inert numerical simulations of the early deformation of the density interfaces resembling flame cusps.

764 - On the Effect of Pressure on Intrinsic Flame Instabilities in Lean Hydrogen-Air Mixtures – Part II: Experimental Investigation Based on OH-PLIF Technique

P. Katzy, J. Hasslberger, T. Sattelmayer

This work aims to quantify the effect of pressure on flame front wrinkling caused by intrinsic flame instabilities in lean hydrogen-air explosions. Work concerning pressure dependency was conducted, however only for fuels other than pure hydrogen, like methane, ethylene, propane or methane/hydrogen blends. Furthermore, these flames were investigated for a stationary case under conditions with high turbulence intensity compared to this case, where the turbulence level is assumed to be negligible. The goal of this work is to improve hydrogen-air combustion CFD modeling on under-resolved grids in the context of Unsteady Revnolds-Averaged Navier-Stokes simulations (URANS). In this approach, an effect like the observed flame front wrinkling cannot be resolved and must be modeled. The dependency of flame front wrinkling caused by laminar instabilities under pressure variation was investigated in a complementary approach. DNS simulations (Part I) and high-speed OH-PLIF measurements (Part II) of propagating lean hydrogen-air flames were conducted. A reduction of the thermal-diffusive cell size was observed with increasing initial pressure. A quantitative evaluation of the data showed an increase of the wrinkling factor under increasing normalized pressure to the power of 0.18. The dependency identified leads to the conclusion that the pressure influence on flame front wrinkling of a propagating lean hydrogen-air flame should not be neglected in an under-resolved CFD subgrid model.

1130 - Combustion Instability Prediction Using Minimal Experimental or Computational Data

S. Park, A. Ghosh, K. Yu

A simplified description of heat release oscillations is developed that could significantly reduce the amount of experimental or computational data required for predicting combustor stability. Using phase resolved CH* chemiluminescence data from a laboratory scale dump combustor undergoing vortex dominated marginal amplitude instability at 150 Hz, first it is shown that the heat release oscillations can be adequately modeled as sinusoidal perturbations with two spatially varying parameters: (1) the amplitude of the oscillations and (2) the phase offset of the oscillations with respect to a reference pressure signal. A method that requires a substantially small dataset to estimate the parameters is then developed. Using the simplifying observation that the amplitude of heat release oscillation at any given location will be proportional to the average heat release at that location, it is shown that the two parameters can be estimated by simply knowing (1) the average heat release distribution and (2) the

heat release distribution corresponding to the pressure oscillation maxima. Using the estimated values of the parameters, spatio-temporal variations in heat release oscillations can be reconstructed, which in conjunction with pressure oscillation information could be used to obtain local and global Rayleigh indices. Linear stability of the combustor resulting from a perturbation of the stable heat release rate distribution can then be predicted.

754 - Application of Dynamic Mode Decomposition for Stabilization of Reactive Flow in a Subscale Combustor with an Injector

Y.J. Kim, G. Jourdain, C.H. Sohn

The acoustic optimization of a swirl coaxial jet injector is investigated to tackle combustion instabilities. The least damped modes are extracted by applying dynamic mode decomposition (DMD) and the injector length is optimized to damp the second longitudinal mode. The sensitivity of heat release perturbation to velocity perturbation at the frequency of the second longitudinal mode is investigated by combining two concepts of the Crocco's model and the inhomogeneous wave equation, leading to computation of flame transfer function (FTF). The gain of FTF shows that the sensitivity of heat release fluctuation to inlet velocity fluctuation is minimal in the chamber with the optimized injector length. Dynamic mode decomposition combined with the inhomogeneous wave equation and the Crocco's model appears to be a valuable tool to compute efficiently flame transfer function and evaluate the stability of a combustion chamber.

16:45 Minimum Ignition Energies, Flammability Limits

1032 - Evaluation of Flammability Limits of H2/O2 Mixtures in Conditions Relevant to Nuclear Waste Transportation: Pressure and Nitrogen Addition Effects.

N. Kouame, A. Comandini, M. Idir, P. Jean, C. Thomas, N. Chaumeix

The aim of the present work is to assess the risk of explosion in closed containments used for the transportation of nuclear materials or nuclear waste. Indeed, it is very well-known that hydrogen can be produced due to (i) the radiolysis of different materials within the containment, (ii) the thermal decomposition of mainly the organic part in the containment. Since hydrogen has a very low ignition energy and a very wide flammability domain, it is important to determine the risk of ignition of the subsequent mixture produced by the aforementioned mechanisms. The quantity of the hydrogen that can be produced can vary depending on the containment type and on the state of the material/waste being transported. It is then mandatory to have a very good knowledge not only of the flammability domain of hydrogen in air but also for different N₂/O₂ ratios. To do so, an experimental work on the flammability domain of multiple ternary mixtures containing H₂/O₂/N₂ is being conducted at the CNRS-ICARE laboratory within collaboration with the CEA.

The flammability limits of $H_2/O_2/N_2$ will be determined in a spherical bomb equipped with a central ignition at room temperature and for different initial pressure between 0.3 and 4 bar.

The combustion is monitored using 2 different diagnostics: pressure measurements during the combustion test using a piezo-electric pressure transducer (Kistler) and the recording of the flame. The visualization of the flame is obtained via a schlieren diagnostic. A mixture will be considered as flammable when both the imaging and the pressure indicate a successful ignition followed by flame propagation. On the contrary, the mixture will be considered non-flammable when no flame propagation is observed and no increase of pressure inside the vessel is recorded.

1043 - Effects of Composition Fluctuations on the Structure and Development of Laminar and Turbulent Flame Kernels

A. Er-raiy, Z. Bouali, A. Mura

Propagation of turbulent flames in a non-homogeneous mixture of reactants has a large number of practical applications including those relying on constant-volume combustion cycles. The corresponding hetererogeneities concern both temperature and equivalence ratio, which may result from several distinct factors such as the presence of residual burnt gases issued from the previous cycle, i.e., exhaust gases recirculation (EGR), the internal flowfield or the preliminary dispersion and evaporation of a spray of liquid droplets. The present work aims at investigating some of the effects
that may result from the joint influence of turbulence and mixture heterogeneities on the flame propagation. It is quite clear that the resulting flames (i) have a more complex structure than fullypremixed or diffusion turbulent flames and (ii) still remain neither perfectly understood nor mastered. Since the early investigations conducted by Ishikawa (1983) significant improvements have been made in the application of measurement techniques and diagnostics and some experimental databases that address combustion in heterogeneous environments are now available (Robin et al., 2008; Kamal et al., 2015) but they are still relatively scarce. From the numerical point of view, the use of direct numerical simulation (DNS) has been early considered (Hélie and Trouvé, 1998) and recently generalized, mainly, to explore the effects of equivalence ratio heterogeneites on flame propagation (Chakraborty et al., 2007; Malkeson and Chakraborty, 2011). However, with only a few exceptions (see for instance Jimenez et al. (2002), Pera et al. (2013) or Chevillard et al. (2016)), most of the previous analyses were conducted under the single-step chemistry simplification. The present work thus aims at complementing some of these previous investigations, which were focused on the smallest scales features in such inhomogeneous conditions, through the analysis of a new DNS dataset.

807 - Effects of Fuel Stratification on Ignition Kernel Development and Minimum Ignition Energy

Y. Wang, W. Han, Z. Chen

Ignition and spherical flame kernel propagation in fuel-stratified n-decane/air mixtures are studied by 1D simulation. The effects of fuel stratification on critical ignition condition and spherical flame kernel propagation are examined. For fuel-stratified n-decane/air mixture, both the ignition kernel propagation and the MIE are strongly affected by the equivalence ratios, f_{in} and f_{out} as well as the stratification radius, R_s . Six distinct flame regimes are observed for successful ignition in fuel-stratified mixture. It is found that the ignition kernel propagation can be induced by not only the ignition energy deposition but also the fuel-stratification. For fuel-lean n-decane/air mixture, fuel-stratification can greatly promote ignition kernel propagation and reduce the MIE. Effective ignition enhancement through fuel stratification can be achieved by choosing proper values of inner equivalence ratio and stratification radius. This indicates that fuel-stratified ignition can be used to prevent ignition failure at ultra-lean conditions in internal combustion energies and to achieve reliable high-altitude relight in jet engines.

16:45 Explosion Safety 2

4300 - Understanding the Effect of Multiple Adjacent Vent Panels on Explosion Overpressures

C.R.L. Bauwens, S.B. Dorofeev

The objective of this study is to perform a systematic comparison of the effect of multiple adjacent vent panels on vented explosion overpressures by varying the number of panels present while maintaining a constant overall vent area for both back and center ignition locations. These results will quantify the impact of an obstructed vent opening, as well as generate further data for the development and validation of engineering tools to predict the consequences of vented explosions.

1026 - Re-Ignition by Hot Free Gas Jets - A Parameter Study

F. Seitz, R. Schießl, D. Markus

Re-ignition by hot gas jets plays an important role in desired combustion. However, it can also be a potential risk as ignition source in the field of explosion protection. To prevent this, one frequently applied safety measure is the protection type flameproof enclosure. The flameproof enclosure prevents a flame transmission (in case of a malfunctioning) from inside a pressure resistant housing to the potentially explosive ambience. Nevertheless, hot exhaust gas may emerge from inevitable gaps within the enclosure. Here, they mix with cold ambient gas (fuel/air). If the conditions leading to ignition are fulfilled, re-ignition of the ambient gas by the hot gas jet occurs. This process is highly stochastic and complex involving a strong coupling of molecular mixing of two gas streams and chemical reactions. The ignition process is significantly influenced by various parameters (pressure, temperature, species concentrations, etc.). Due to its turbulent transient nature, even small variations of these parameters might influence the ignition process.

To gain more insight into hot jet re-ignitions allowing the phenomenon to become more predictable in

terms of safety, the main physical quantities influencing the ignition process are studied by means of empirical tests at simplified model systems. In this work, technical parameters which can be controlled more accurately compared to the physical quantities (gap diameter and - length and ignition location of the pre-ignition) are varied and their influence on the re-ignition frequency studied.

1120 - Influence of Congestion on Vented Hydrogen Deflagrations in 20-Foot ISO Containers: Homogeneous Fuel-Air Mixtures

T. Skjold, H. Hisken, S. Lakshmipathy, G. Atanga, M. van Wingerden, K.L. Olsen, M.N. Holme, N.M. Turøy, M. Mykleby, K. van Wingerden

The paper presents the results from an experimental campaign on vented hydrogen deflagrations in 20foot ISO containers. The work is part of the project "Improving Hydrogen Safety for Energy Applications through pre-normative research on vented deflagrations", or HySEA (www.hysea.eu), supported by the Fuel Cells and Hydrogen Joint Undertaking (FCH JU). Thirty-four full-scale tests have been completed with homogeneous hydrogen-air mixtures: 14 tests with venting through the doors of the containers, and 20 tests with vent openings in the roof. The results demonstrate strong effect of congestion on vented deflagrations, especially for the more reactive mixtures. The experimental data will be used for validating both CFD tools and engineering models.

16:45 The Current Status and Future Outlook on Gaseous Detonation Research 3

793 - Autoignition and Detonation Development From a Hot Spot in Hydrogen/Air Mixture *Y. Gao, Z. Chen*

Autoignitive reaction front propagation and detonation development from a hot spot in hydrogen/air mixtures are investigated numerically. Five different modes are identified in the plot based on two nondimensional parameters, ξ and ε . The detonation development is induced by the coherent coupling between pressure wave and chemical reaction, which can be explained by the SWACER mechanism and reactivity gradient theory. It is found that detonation development regime is fuel-dependent and thereby the detonation peninsula might not work for different fuels. Besides, different shapes of detonation development regime are observed for different values of initial pressure, temperature and equivalence ratio. The initial temperature, initial pressure, and equivalence ratio all can affect the detonation development regime for specific fuel at specific initial temperature, initial pressure, and equivalence ratio.

1072 - An Evaluation of Ignition Criteria Through State Classification and Detailed Simulation *K.P. Grogan, M. Ihme*

State classification techniques are employed to investigate several thermochemical features that have been proposed to demarcated weak and strong ignition regimes by various authors. Experimental data from shock tubes, rapid compression machines, and detonations is aggregated from the literature for this purpose. Good correspondence between the learned decision boundaries and the experimental data is found. Additionally, detailed simulations are compared to the decision boundaries and agreement was found as well. Also, it is found that the features that characterized the combustion timescale and sensitivity performed the best for all configurations examined. Interestingly, the Prandtl number is found to be significant for all configurations except for the rapid compression machine. Finally, no significant improvement is found in the test error for more than two features, which suggests that the correct classification of the combustion process is likely low-dimensional.

1247 - The Role of Flame-Generated Turbulence in the Deflagration-to-Detonation Transition *A.Y. Poludnenko*

One of the key prerequisites of the deflagration-to-detonation transition is the significant flame acceleration capable of producing shocks of sufficient strength to ignite a detonation. In unconfined, and to some extent semi- confined, systems it is generally understood that turbulence is the only, or at least the primary, driver of such flame acceleration. At the same time, both such turbulence as well as the associated mechanisms capable of generating turbulent velocities of sufficient intensity remain poorly understood. In this talk, I will discuss the role that flame-generated turbulence can play in the

DDT process. In particular, I will discuss recent findings obtained with direct numerical simulations, which show that in the presence of large pressure gradients, a flame can generate turbulent intensities up to 100 m/s even in the absence of any upstream turbulence or large-scale turbulence generation. Furthermore, such turbulence levels are sufficient to support flame acceleration to transonic and supersonic velocities with respect to the upstream fuel. I will briefly discuss the implications of these effects for LES models. Finally, I will also comment on the experimental challenges involved in studying this problem.

16:45 Dust Explosions 2

1096 - Potential Accelerating Effect of Thermal Radiation in Dust Flame Propagation: Some Experimental Evidence

C. Proust, R.B. Moussa, M. Guessasma, K. Saleh, J. Fortin

The role of thermal radiation in premixed flame propagation has been a matter of debate for decades. In this paper, new experimental results are presented illustrating the promoting role of thermal radiation exchanges through the flame front. In addition suspected large flame acceleration due to this promoting role was observed perhaps for the first time.

768 - Flame Propagation in Nano-Metal Dust Explosions

W. Gao, M. Bi, T. Mogi, R. Dobashi

Experiments were conducted to reveal the combustion behaviors of 40 nm titanium, aluminium and iron particles in dust explosions. Results showed that 40 nm titanium, aluminium and iron dust flame were all developed as approximately spherical flame and characterized by discrete single glowing burning particles uniformly distributed in the combustion zone. The average pulsating flame propagation velocities of 40 nm titanium, aluminium and iron dust clouds were 0.565 m/s, 0.189 m/s and 0.035 m/s, respectively. By analysing the combustion products, it could be inferred that 40 nm titanium, aluminium and iron particles burnt in liquid-phase, gas-phase, and solid-phase, respectively. And 40 nm titanium combustion products contained 43% TiO₂(Ti⁴⁺), 27% Ti₂O₃ (Ti³⁺), 21% TiO (Ti²⁺) and 9% TiN (Ti³⁺), 40 nm aluminium combustion products contained 100% Al₂O₃ (Al³⁺), and 40 nm iron combustion products contained 49% Fe₂O₃ (Fe³⁺), 26% Fe₃O₄ (Fe³⁺/Fe²⁺), 15% FeO (Fe²⁺) and 10% iron nonoxides.

1049 - Investigation on the Diffraction of a Medium Scale Gaseous Deflagration Pressure Wave Behind a Protective Wall

L. Heudier, G. Lecocq, Y. Grégoire, C. Proust

Medium-scale experiments with gaseous deflagration and a blast wall were performed. The experimental setup is a 1.5 m diameter polyethylene hemispherical balloon erected on a metal plate. The 3x6 m wall is located at 10 m. Numerical modeling was performed using the open source CFD tool OPENFOAM. A modified version of the rhoCentralFoam is used with the Tadmor and Kurganov scheme. The physical closure of the chemical source terms is written to ensure the volume of burnt gases increases spherically, the time evolution of the radius being set by the modeler. Blast parameters are examined in free-field, on the front and rear faces of the wall as well as in its shade. A competition between reduction of overpressure with the increase of distance due to overturning of the obstacle and overlapping of blast waves behind the obstacle is observed both in calculations and in the experiments.

16:45 Reactive Systems 1

818 - The Inability of Heterogeneously Reacting Particles to Ignite Below a Critical Size

M. Soo, S. Goroshin, J. Lightstone, D.L. Frost, J.M. Bergthorson

The word "ignition" is often used colloquially to describe the initiation of a reaction leading to selfsustained combustion in an energetic material or condensed-phase fuel system. In the context of the combustion of particles in gaseous suspensions, however, "ignition" has a precise definition that is often misconstrued as a general term for the initiation of reaction. Ignition for a particle is classically defined as the critical transition from a regime where the reaction rate is controlled mainly by kinetics

to a regime controlled mainly by diffusion. For many metal (and metalloid) fuel particles, ignition behavior is, arguably, heterogeneous in nature. Accordingly, the basic physical behaviors of metal particle ignition can be understood from the classic theory of heterogeneous ignition. The theory provides a fundamental understanding of the combustion physics for metal particles as a minimalistic model. The simplicity of the model makes it a valuable tool for developing an intuition of the expected changes in combustion behavior as a function of the various physical and chemical properties of the fuel. One particularly illuminating variation on the heterogeneous ignition analysis is the determination of steady-state particle temperature as a function of the initial temperature of the gas. Using this thermal states analysis, it can be clearly shown that, as the initial particle size approaches a critical value, the phenomenon of ignition will degenerate. Below this critical size, the notion of characteristic measurable quantities like "ignition temperature" and "ignition delay" for individual particles are illdefined since there is no clear critical transition from kinetic to diffusion regimes that classically indicate ignition. The purpose of this paper is to show the utility of the steady thermal states analysis to understand this phenomenon.

1119 - The Vaporization-Controlled Inertial Regime in Nonpremixed Counterflow Spray Combustion

J. Carpio, A. Linan, D. Martínez-Ruiz, A.L. Sánchez, F.A. Williams

Improvements in understanding of combustion processes for fuel sprays in nonuniform flows are needed for advancing engine technologies that employ liquid fuels. Comprehension can be enhanced by identifying different combustion regimes on the basis of appropriate nondimensional parameters and studying how the combustion occurs in each regime. The Stokes number of the droplets in the spray is a key parameter affecting the combustion process. By focusing on nonpermixed counterflow configurations as representative of sprays for many applications, it has recently been shown that, in addition to the known regime at small Stokes numbers, in which nonpremixed spray combustion occurs in the mixing layer between an oxidizer gas stream and a stream of inert gas carrying the fuel droplets, there is a vaporization-controlled inertial regime at Stokes numbers of order unity and larger, in which the droplets penetrate into the oxidizer stream because of their higher inertia and vaporize there, leading to the combustion occurring well into the oxidizer stream. Since the combustion characteristics are poorly understood for that regime, the present work employs numerical methods to help to clarify flame structures that may arise there. It will be shown that, perhaps unexpectedly, when the Stokes numbers reach values on the order of St=3 or greater, a cold fuel stream impinging on a hotter air stream may exhibit two very different types of steady-state combustion behavior, depending on how the interaction process is initiated. The characteristics of each of these will be shown, as well as the characteristics of combustion in the vaporization-controlled inertial regime at Stokes numbers below those at which the dual solutions are obtainable.

876 - Propagation Limits of Flames in Binary-Fuel Mixtures

J. Palecka, S. Goroshin, J.M. Bergthorson, A.J. Higgins

Flame quenching due to heat losses in narrow channels was studied for the combustion of binary fuel mixtures occurring in heterogeneous combustion. A simple one-dimensional analytical model assumes that the reaction starts at some ignition temperature associated with each fuel and proceeds at a constant rate in a step-like manner. The model predicts three different flame configurations: a) a flame front consisting of the first burning fuel with the second playing the role of an inert additive, b) a double-front structure where the first and the second fronts are detached and have their own distinctive preheat zones, and c) an overlapping front structure where the combustion of both fuels occurs within the same flame zone. The model also predicts that the occurrence of each flame structure depends on the ratio of concentrations of each fuel as well as the level of heat losses. The flame modes predicted by the model correspond to an experimentally-observed flame behavior during the combustion of hybrid aluminum-methane mixtures in narrow channels.

9:00 Plenary Lecture 3

PL3 - Dynamics of ammonia combustion

Hideaki Kobayashi, Tohoku University, Japan

Ammonia, which contains 18wt% hydrogen, is one of the hydrogen carriers in the hydrogen energy community. On the other hand, in the combustion community, ammonia can be considered as a potential carbon-free fuel when it is produced using renewable energy or even when it is obtained from natural gas or lignite with CCS. Ammonia has advantages in transportation and storage since its thermal properties are almost the same as those of propane in terms of boiling point temperature and pressure and also because the necessary infrastructure has already been established in the past 100 years. Although research on the practical use of ammonia as a fuel was performed in the 1960s, results were not sufficiently successful because of its very low combustion efficiency. Lately, utilization of ammonia as a carbon-free fuel is again of interest, and research projects on ammonia combustion have started in Europe and Japan.

The Cross-ministerial Strategic Innovation Promotion Program (SIP), 'Energy Carriers', in Japan, which was started in 2014, deals with ammonia combustion for gas turbine power generation, reciprocal engines, and industrial furnaces, as well as with pulverized coal power generation in which a certain amount of pulverized coal is replaced by ammonia. In the project, 41.5 kW power generation with a 100% ammonia fueled micro gas turbine succeeded in 2015 [1].

Challenges of ammonia combustion from the point of view of combustion fundamentals include low combustibility, i.e., low burning velocity of 7 cm/s at most, high ignition temperature, narrow flammable range, etc., and fuel NOx emission, as well as low radiation heat transfer when used for industrial furnaces. Research on combustion dynamics and the structure of ammonia flames combined with flame chemistry is essential to overcome these difficulties and to improve the design of systems using ammonia as a fuel. In this lecture, the characteristics of ammonia combustion in terms of flame dynamics and chemistry and recent progress in R&D of practical ammonia combustion systems are presented.

[1] O. Kurata, N. Iki, T. Matsunuma, T. Inoue, T. Tsujimura, H. Furutani, H. Kobayashi, A. Hayakawa, Performances and Emission Characteristics of NH3-air and NH3-CH4-air Combustion Gas-Turbine Power Generations, Proceedings of the Combustion Institute, Vol. 36, (2017), pp. 3351-3359.

10:30 Explosions and Combustion in IC Engines

1143 - Direct Numerical Simulation of Two-Stage Combustion and Flame Stabilisation in Diesel Engine-Relevant Conditions

D. Dalakoti, E.R. Hawkes, M.S. Day, J.B. Bell

We present preliminary results from a three-dimensional (3D) direct numerical simulation (DNS) of a spatially developing turbulent lifted flame in diesel engine-relevant thermochemical conditions with multiple step chemistry. The simulation is broadly based on the experimental flame known as Spray A, a target flame of the Engine Combustion Network. The configuration has been modified to make DNS feasible, namely we consider an equivalent gas jet with a lower Reynolds number of 15,000 but a similar global Damköhler number. The configuration consists of a round jet of n-dodecane injected into an environment with 60 bar pressure and 900 K ambient temperature, which contains 15% oxygen and 85% nitrogen by volume. The overall structure of the flame shows two-stage combustion and is broadly consistent with proposed conceptual models of diesel spray combustion. Low-temperature chemistry occurs in the rich premixed core and in a shrouding diffusion flame. The analysis presented here focuses on the leading edge of the high-temperature flame. The leading edge is observed to be principally composed of a connected and highly convoluted structure. Upstream of this structure, ignition kernels are occasionally observed that are advected downstream and connect with the main flame. Unexpectedly, flame extinction holes are also observed, which are connected with high

dissipation rates that exceed extinction limits. Flame holes are also observed to arise from flame propagation around unburned regions and upstream flame reconnection to create a hole.

995 - Shock Wave and Flame Front Induced Detonation in Rapid Compression Machine Y. Wang, S. Xiang, Y. Qi, R. Mével, Z. Wang

Super-knock constitutes the major obstacle for the development of more efficient, high energy-density spark ignition internal combustion engine, ICE. Whereas a large number of studies have employed onedimensional simulations to investigate the dynamics of end-gas auto-ignition and combustion wave propagation in reactivity gradients, two-dimensional simulations are needed to unravel the initiation of detonation under the highly complex conditions encountered in ICE. In the present study, experimental work in a RCM and two-dimensional numerical simulations with realistic chemistry are combined to investigate detonation initiation through the so-called shock wave and flame front induced detonation process (SWFID). It was shown that the shocks interaction at the density interface between the fresh gas and the burnt gas originating from the spark plug enables the end-gas flame front to accelerate and couple with the shock front to initiate a self-sustained detonation wave.

1008 - Effects of Fuel/Air Mixture Distribution on End-Gas Autoignition and Pressure Wave Generations in Knocking Combustion

T. Satoh, H. Terashima, N. Oshima

Effects of fuel/air mixture distribution on mechanisms of end-gas autoignition and pressure wave generation in knocking combustion are numerically investigated, for which the compressible Navier-Stokes equations with detailed chemical kinetics of *n*-heptane (373 species and 1071 reactions) are directly solved with a one-dimensional constant volume reactor. Three fuel/air mixture distributions are considered in this study with combinations of rich and lean gas mixtures in several initial temperature conditions. In a case that the reactor initially consists of rich mixture gas for the left region and lean one for the right region, two end-gas autoignition events are uniquely observed, leading to two large peaks in the pressure time histories. The first autoignition takes place in the rich gas region formed in front of a propagating flame, while the second one occurs in the lean gas region near the end-wall. Resultantly, larger knocking intensity is produced in this mixture condition. On the other hand, the other two cases, e.g., lean gas for the left and rich one for the right or a uniform mixture distribution, only show a single peak in the pressure histories due to end-gas autoignition near the wall, resulting intensities. Thus, the present result demonstrates the importance of fuel/air mixture distributions and pressure wave generations influenced by the fuel/air mixture distributions.

929 - Autoignition of End Gas in a Rapid Compression Machine Under Super Knock Conditions

Y. Qi, Y. Wang, H. Liu, J. Wang, Z. Wang

Super knock (detonation) is generated using spark ignition induced end gas autoignition for stoichiometric iso-octane/O2/N2 mixture in a rapid compression machine. The combustion process is recorded by high speed photography synchronizing with pressure data acquisition. Two autoignition events with very short time interval are sequentially observed in end gas area, which has not been reported in previous engine researches. The first autoignition can generate a weak shock wave propagation in the combustion chamber and cause a relatively low amplitude pressure oscillation. The second autoignition can lead to a detonation. Based on the pressure traces, the ignition delay evolution curve of the end gas is calculated, which almost does not pass through the NTC region for lower temperature condition (TEOC = 641 K). For higher temperature conditions (TEOC = 681 K and TEOC = 729 K), only a small parts of ignition delay evolution curves pass through the NTC region.

909 - Measurement of the Carcinogenic Polyaromatic Compounds in the Exhaust Gases of a Gasoline Internal Combustion Engine

M.S. Assad, O.G. Penyazkov, I.N. Tarasenko

This work is devoted to a quantitative analysis of 16 compounds of polycyclic aromatic hydrocarbons in exhaust gases exhausted into the atmosphere by an automobile four-stroke four-cylinder gasoline engine operating as in an idle-running regime, so in the regime of load. The concentrations of the

polycyclic aromatic hydrocarbons in the gas samples taken at two points of the engine exhaust pipe (upstream and downstream of a catalytic neutralizer, delivered in a complete set by a factory) were determined by the gas-chromatography and mass-spectrometry methods. The combustion products of ON-92, ON-95 and ON-98 gasolines were analyzed. It has been established that the combustion products exhausted into the atmosphere by a gasoline engine contain carcinogenic polycyclic aromatic hydrocarbons that bring the threat to the people contacting with them. The concentrations of some of these substances (especially of benz(a)pyrene) in the exhaust gas of an automobile engine are very high-they exceed the reference values, recommended by the World Health Organization (0.12 ng/m³) and the European Union (1 ng/m³) for the atmospheric air of an inhabited locality by hundreds times.

10:30 Chemical Kinetics in Shock Tubes, in Memory of Paul Roth

795 - Ignition Delay Time Study of Aromatic LIF Tracers in a Wide Temperature and Pressure Range

J. Herzler, M. Fikri, C. Schulz

Ignition delay times of the LIF tracers 1,3,5-TMB and anisole were determined at 10, 20, and 40 bar at lean (phi= 0.5) and stoichiometric conditions in the 770–1600 K temperature range and compared to simulations with various mechanism from literature and with experimental values for 1,3,5-TMB at 10 and 20 bar. The measured 1,3,5-TMB data agree very well with simulations with the mechanism of Gudiyella and Brezinsky whereas the mechanism of Diévart et al. predicts too long ignition for lower temperatures. Simulations with both mechanisms exhibit significantly too slow ignition delay times for phi = 1, 40 bar and low temperatures. A comparison of the anisole measurements and the simulations with the mechanism of Ranzi et al. shows a very good agreement for all data with the exception of the experiments at temperatures below 1000 K at phi = 1 where the mechanism of Nowakowska et al. predict too long ignition delay time for all conditions. A comparison of the 1,3,5-TMB measurements of this work with data of Diévart et al. at 10 and 20 bar show a very good agreement whereas experiments of Rao et al. at 20 bar exhibit slightly faster ignition delay times.

1004 - High Speed Imaging of Inhomogeneous Ignition in a Shock Tube

A.M. Tulgestke, S.E. Johnson, D.F. Davidson, R.K. Hanson

Inhomogeneous ignitions of real and surrogate fuels were imaged following small particle explosions in two shock tubes. Experiments were carried out at low temperatures (900-1000 K) and low pressure (1-2 atm). Particles within the shock tubes were found to match the material of the diaphragm burst during the experiment. The particles were found to arrive near the end-walls of the shock tubes less than 5ms after reflection of the incident shock wave. Particle explosions were observed for several milliseconds after arrival of the particles, often leading to inhomogeneous ignition of the gaseous fuel. Flames formed from particle explosions grew to consume all of the fuel within the cross-section of the shock tube. These flames were found to influence line-of-sight measurements made from the sidewalls of the shock tubes. The diaphragm material used to create shock waves was varied between Lexan and steel. Distinctly more particles were observed during experiments using steel diaphragms than those using Lexan diaphragms. Both diaphragm materials generated particles which exhibited explosive behavior and lead to flames.

911 - Experimental Study of Nitromethane Oxidation: CO and H2O Time-Histories Behind Reflected Shock Waves

O. Mathieu, C. Mulvihill, E. Petersen

To further develop and validate a detailed nitromethane combustion chemistry model, the time histories of CO and H_2O were followed using laser absorption techniques behind reflected shock waves. Two shock tubes were used (one for each laser diagnostic) during this study. Carbon monoxide was measured with a quantum cascade laser (QCL) from Alpes Lasers to generate light at 4566.17 nm while a tunable diode laser (TDL) from Toptica Photonics was used to generate light at 1388.140 nm, to access the H_2O transition at 1388.1389 nm within the v_1+v_3 fundamental band. Mixtures diluted in 99% Ar were investigated at stoichiometric condition for CO and at 3 equivalence ratios for H_2O : 0.5, 1.0,

and 2.0. Pressure behind reflected shock waves was maintained around atmosphere during the course of this study.

A peculiar profile with two growth periods was observed for both species monitored. The first growth appeared right after the arrival of the reflected shock wave in all cases, whereas the timing of the second growth was temperature dependent. Modern detailed kinetics mechanisms capture this unique profile but could still be improved. This study shows that an accurate determination of the rate of reaction for $CH_3 + NO_2 \rightleftharpoons CH_3O + NO$ is necessary to obtain better predictions for nitromethane combustion.

1045 - Combustion Properties of n-Heptane/Hydrogen Mixtures

A. Comandini, K. Brialix, N. Chaumeix, J. MacLean, G. Ciccarelli

The objective of the present study is to analyze the effects of hydrogen addition on the fundamental combustion properties of n-heptane, a common component used in fuel surrogate formulations. Laminar flame speeds and ignition delay times of different n-heptane/hydrogen/air mixtures were measured over a wide set of conditions using spherical bomb and shock tube techniques, respectively. The new data were used to validate suitable chemical kinetic models for subsequent detailed analysis of the role played by hydrogen in the n-heptane oxidation kinetics.

10:30 Detonation Engines 2

992 - Rotating Detonation Wave Mechanics Through Ethylene-Air Mixtures in Hollow Combustors, and Implications to High Frequency Combustion Instabilities

V. Anand, A.S. George, C.F. de Luzan, E. Gutmark

Recent investigations into the rotating detonation phenomenon have involved its inception and sustenance in hollow combustors, in contrast to the traditional annular rotating detonation combustor (RDC) designs. Despite this proof-of-concept, the mechanism of propagation of detonation waves in hollow combustors is unclear. On the other hand, the decades-old issue of high frequency combustion instabilities, especially in rocket engines, has been known to produce distinct shock waves that are insync with regions of intense combustion, the reason for which is widely attributed to the Rayleigh criterion. In this paper, we argue that there is a considerable overlap in the physics behind the reported rotating detonations in hollow RDCs and the high frequency tangential combustion instabilities that are known to wreak havoc on engines. To support this notion, an atmospheric hollow combustor is experimentally tested to attain the baseline performance. It is then 'transformed' into a hollow RDC by a simple geometric alteration. Some properties of this rotating the ideal Chapman-Jouguet speeds and peak detonation pressures exceeding 20 bar, or in an unstable fashion with considerable velocity and pressure deficits—not exceeding 2 bar, but propagate at about 80% of the ideal speed.

1084 - Experimental Observations of Semi-Confined Steadily-Rotating Detonation

V. Rodriguez, P. Vidal, R. Zitoun

This work presents some experimental observations of the dynamical behaviors of a detonation along the concave outer wall of a cylindrical chamber without inner kernel. This geometry is helpful for understanding the possible detonation configurations in the combustion chamber of a rotating detonation engine (RDE). The experiments were carried out in a concave cylindrical chamber with an 80-mm outer-wall radius and a 270° run angle. The detonation entered the chamber from a straight channel connected to a 2-m long, 50-mm diameter tube in which a CJ detonation was initiated. The top and bottom flat faces of the chamber were lined with soot-covered plates to record the detonation behaviors. Depending on the initial pressure, a steadily-rotating detonation was observed along the concave outer wall. The records show that the larger the initial pressure, the thinner the rotating-detonation layer, and that the closer to the outer wall, the smaller than the in the layer were always smaller than their value at the channel entry and smaller than the mean cell width for the multicellular Chapman-Jouguet (CJ) detonation front at the same initial pressure. This would indicates either that the rotating detonation front as sociated with the detonation transmission from the straight channel

to the chamber led to an increase of the initial pressure in the chamber before the rotating detonation could be installed. Nevertheless, these results demonstrate that a semi-confined detonation can rotate very rapidly in a narrow layer along a curved wall, with the consequence that not all the fresh mixture in the chamber is burned. This may participate in the set of explanations for the differences between some observed and predicted performances of RDEs.

1066 - 3D Numerical Study on Continuous Detonation Engine Using Reactive Navier-Stokes Equations

L. Zhang, S. Zhang, J. Wang

This paper investigates the influence of no-slipping boundary conditions, viscous and thermal conduction in three-dimensional numerical simulation of a continuous detonation engine (CDE). Three-dimensional reactive Navier-Stokes (N-S) equations with a one-step Arrhenius chemistry model are solved using direct numerical simulation (DNS) with no-slipping boundary conditions. A pre-mixed stoichiometric hydrogen-air mixture is injected from the head. The influence of no-slipping boundary conditions, viscous and thermal conduction are often absent in conventional CDE simulations due to the use of Euler equations. We get some different phenomena via a comparative analysis of the simulation results with the reactive N-S equations and the reactive Euler equations. It is found that When we consider the detonation wave velocity, the influence of no-slipping boundary conditions and viscosity can be ignored. The detonating front has a lower energy and the height is higher when the reactive N-S equations are used. We can also get the velocity boundary layer and the temperature boundary layer.

1037 - Detonation Regimes in a Small-Scale RDE

S. Hansmetzger, R. Zitoun, P. Vidal

The detonation regime is currently considered as one of the alternatives to the conventional constantpressure combustion mode for propulsive systems with high thermal efficiency. Its main interest is that high-pressure and high-temperature products are generated on very short time and distance. One possible implementation is the rotating detonation engine for which the combustion chamber is the annular space between an inner kernel and an outer cylindrical wall. An uninterrupted supply of fresh reactive gas then enables the detonation to continuously rotate in the annular space. A few works indicate that the inner geometry of the chamber and the mean width of the cells - that characterizes the unstable local structure of detonation fronts in gases - greatly influence the properties of the rotating detonation.

This experimental investigation focuses on the effects of the length and of the shape of the inner kernel. The chamber was 90-mm long with a 70-mm outer-wall diameter d_0 . Three kernel configurations were considered, i.e., a long cylinder, a short cylinder and a short converging cone. The long cylindrical kernel had the same length as that of the chamber (90 mm), and the short cylindrical and conical kernels were 30-mm long. The diameter of the long and of the short cylindrical kernels was d_i =50 mm. The short conical kernel has diameter decreasing from d_i =50 mm at the chamber entry to d_e =42 mm. The reactive mixtures were composed of C₂H₄, O₂ and N₂ with several equivalence ratios in the interval [0.8-1.5] and with the three N₂ dilutions 50%, 30% and 0%. The mass flow rate was varied in the interval [50-112] g/s.

Two detonation regimes were obtained, with one or two detonation fronts. Decreasing the length of the cylindrical kernel was found to induce the transition from 2-fronts to 1-front detonation regimes, the increase of the front velocity from 55% to 70% of the Chapman-Jouguet velocity (D_{CJ}), and the increase of the pressure, at the chamber outer wall, from 2 bar to 4 bar. Using the short conical converging kernel was observed to significantly improve the properties of the 1-front detonation regimes with velocities about 80% of D_{CJ} and pressure peaks of 8 bar, the best performances for the three considered configurations of kernel. The interpretation is that too long kernels hinder the evacuation of the burnt gases, and so the actual mixture in the chamber does not contain enough fresh gases for an optimum detonation process. High-speed camera visualizations were performed to confirm the results from the pressure transducers and to obtain the additional information that the detonation front appears stronger at the chamber outer wall than at the kernel surface.

Acknowledgment:

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1117 - Baffled Tube Ram Accelerator Combustion

C. Knowlen, T. Byrd, J. Dumas, N. Daneshvaran, A.P. Bruckner, A.J. Higgins

The baffled-tube ram accelerator is a device that has the potential to accelerate axisymmetric projectiles in the velocity range of 0.5 to 3 km/s. Preliminary experiments in a 38-mm-bore device demonstrated that only about 30 to 50% of the theoretical thrust is attained using a baffle geometry that is effectively a solid washer with a center hole bored out with a slight projectile clearance. Recent transient CFD modeling results indicate that significant improvements in thrust generation capability can be realized by inclining the baffles toward the approaching projectile. With this configuration, reactive flow simulations showed that the combustion goes to completion closer to the projectile base than in the original baffle orientation, resulting in a doubling of thrust. Newly fabricated baffles based on this concept are undergoing testing. The results of these upcoming experiments with the new inclined baffle design will be presented.

10:30 Detonation Boundary Interactions 2/ Detonation in Narrow Channels

988 - Interaction of a Condensed-Phase Explosive Detonation with a Compliant Boundary

J.B. Bdzil, M. Short, C. Chiquete

We discuss the interaction of a condensed-phase explosive detonation with a compliant, inert material boundary. The focus is on the rarefactions introduced into the detonating explosive by low-density inert materials, and how detonation dynamics and propagation are affected.

1107 - Detonation Propagation in a Linear Channel with Discrete Injectors and Side Relief *J.R. Burr, K.H. Yu*

The potential thermodynamic gains associated with pressure gain combustion cycles have resulted in a steady rise in interest in combustors like the pulse detonation engine (PDE) and rotating detonation engine (RDE). The objectives of this study are to experimentally investigate the nature of a detonation wave propagating across transversely injected reactants in a canonical channel set-up simulating an unwrapped RDE configuration and to provide detailed experimental data that can not only increase the fundamental understanding of the RDE flow structure but can also be used for CFD validation. The approach is to simplify the experimental environment by examining the transient propagation of a detonation wave in cross-flowing reactants through a novel linear channel facility instead of the annular RDE arrangement. Studying the detonation wave propagation in a straight channel allows for the use of high-quality optical measurements that are much more difficult in a curved annulus.

922 - Hydrogen-Oxygen-Argon Detonation Diffraction in a Narrow Channel

R. Mével, Q. Xiao, M.I. Radulescu

Despite six decades of extensive investigation, the detonation diffraction critical conditions have not yet been predicted from first principles and only semi-empirical models are available to estimate the critical tube diameter. The present study aims at providing a well-defined experimental and numerical framework to help establishing a quantitative theoretical model to predict the critical conditions for diffracting detonation failure and re-initiation. More than 100 diffraction experiments were performed in a narrow channel facility for a 2H2-O2-2Ar mixture at P1=10.3-23.4 kPa and T1=298 K. The diffraction experiments were analyzed in terms of probability of successful transmission as a function of initial pressure. Numerical simulations were performed with a realistic reaction model. Qualitative agreement with the experimental results was demonstrated but the critical pressure for detonation failure could not be quantitatively reproduced. Simplified combustion models were used to estimate the respective effect of shock front curvature and volumetric expansion behind a decaying shock on diffracting detonation failure. It was found that the expansion was the dominant process responsible for the increase of ignition delay-time and possibly for detonation failure.

822 - Experimental Study on Behavior of Methane/Oxygen Gas Detonation Near Propagation Limit in Small Diameter Tube: Effects of Equivalent Ratio

K. Yoshida, T. Inoue, Y. Morii, K. Murakami, N. Tsuboi, A.K. Hayashi

The unstable behavior of the detonation is an important issue in predicting detonation limits and safety problems. However, a theory for the prediction of the detonation limits does not exist. There are many reports about detonation propagating limit in hydrogen/oxygen mixtures. However, there are few reports about the effect of the equivalent ratio near propagating limits in methane/oxygen mixtures. The purpose of this study is to obtain the knowledge on the unstable phenomenon of detonation near the propagation limit by using the data from records of smoked foil experiments and detonation velocity measurements in methane/oxygen gas mixture for various initial pressures and equivalent ratios. Regardless of the equivalent ratio, the experimental detonation velocity is 60 - 80 percent of the C-J velocity for $\alpha < 1.0$. On the other hand, the detonation velocities correspond to the theoretical C-J velocity for $\varphi = 0.6, 0.8$, and 1.0, and the detonation velocities are approximately 95% of the C-J velocity for $\varphi = 1.2$ and 1.4 mm. For $\alpha > 1.1$, the difference between the maximum and the minimum values is small. The behaviors of the detonation velocities are stable. The oscillation of the detonation velocities for $\alpha < 1.0$ is observed. The detonation velocities vary between 0.2 D_{CI} and 1.6 D_{CI} . For $\alpha < 1.0$ 1.0, patterns disappear. For $\alpha > 1.0$ and the all equivalent ratio, the detonation propagates with the cellular patterns. However, the stable and unstable propagation are observed for $\varphi = 1.4$ and $\alpha = 1.2$. The parameter α is important in determining the propagation mode for the gaseous detonation near the propagation limit. The appearance of the cellular structure is observed under the over-driven velocity region. In the region where the cellular structure is not observed, the experimental detonation velocities become smaller than the C-J velocities. The oscillation of the detonation velocities is due to the instability of the cell patterns. The criterion $\alpha = 1.0$ is important in dividing the features of detonations near the detonation propagation limit. This criterion means that the detonation cell width is equal to the inner perimeter of the tube. The re-ignition and disappearance causes the variation in the detonation velocity for $\alpha < 1.0$.

802 - Detonation Limits in Highly Argon Diluted Acetylene-Oxygen Mixtures

B. Zhang

In this study, the velocity deficits and detonation limits of highly argon (70% and 85% vol.) diluted stoichiometric acetylene-oxygen mixtures in a small diameter circular tube (D = 36 mm) and three annular channel widths (w = 2, 4.5 and 7 mm) were investigated. Fiber optics were used to measure detonation velocity along the test section. Smoked foils were employed in the circular tube to record the cellular detonation structure, and the detonation cell sizes at different initial pressure for those two mixtures were systematically measured. It has been suggested that the highly argon diluted acetyleneoxygen mixture is considered as a stable mixture, the cellular instabilities do not play a prominent role in the propagation of detonation, therefore the failure mechanism responsible for the limit phenomenon is due to the losses at the boundary layer behind the leading shock front of the detonation wave. In addition, the flow divergence in the reaction zone near the limits results in curvature of the detonation front, hence, leading to a detonation velocity deficit and its eventually failure. The purpose of this study is to explore the velocity behavior of stable mixture due to its different failure mechanism by investigating the scaling law between the hydraulic diameter $(D_{\rm H})$ of the circular tube and annular channels with the characteristic length scale (i.e., cell size λ and ZND induction zone length Δ_{I}) of a stable detonation. The experimental results suggest the detonation velocity decreases with the decreasing of initial pressure, when the initial pressure reaches a critical value corresponding the maximum velocity deficit, the detonation fails and the detonation limit is approached. The present experimental results indicate that the average maximum velocity deficit is approximately 14% of the corresponding CJ value $V_{\rm CJ}$ for the highly argon diluted mixtures in the tubes with different geometries. The scaling between the hydraulic diameter and the cell size $(D_{\rm H}/\lambda)$ or ZND induction zone length $(D_{\rm H}/\Delta_{\rm I})$ gives an average estimation for the highly argon diluted mixtures at the detonation limits 0.66 and 15, respectively.

10:30 Turbulent Reacting Flows 2

1050 - Two-Dimensional Numerical Analysis on Shock Flame Interaction in Premixed Gas of Hydrocarbon/Oxygen with Multi-Step Reaction Model

M. Iwai, K. Yoshida, Y. Morii, N. Tsuboi, A.K. Hayashi

Detonation is a combustion phenomenon propagating with shock waves and has some characteristics, for example hypersonic, high pressure and high temperature. It is very important from the safety engineering to obtain the knowledge of the Deflagration-to-Detonation Transition (DDT), which is one of the initiations of detonation. DDT process is generally separated into two processes, one is the flame acceleration process and the other is the process that local explosions cause a detonation. One of the reasons why flames are accelerated is the shock/flame interaction (SFI). It has been investigated experimentally and numerically. Matsumoto et al. carried out the experiments about the SFI in methane/oxygen/nitrogen premixed gas that the flame interacts with the shock after the flame propagates along some distance. The final goal of our research is to simulate in the same experimental conditions by Matsumoto et al., so we have been carrying out the SFI simulations using the multi-step reaction model, which can capture the flame propagation more accurately than the one-step model. The objective of this paper is to investigate the grid resolution and the qualitative effect of the incident shock Mach number on the shock/flame interaction in hydrocarbon premixed gas. As a preliminary step for the final goal, we simulate the shock/flame interaction in ethylene/oxygen premixed gas, which is relatively lower computational cost than methane/oxygen premixed gas. We solve the Navier-Stokes equations for a system containing premixed ethylene and oxygen gas mixture to consider the effects of the boundary layer because it is important in the DDT. In this study, the grid resolution does not have a large impact on the flame and the bifurcated shock just after the reflection; however, when the flame and the shock propagate to some extent, the combustion speed in the coarse grid is faster than that of in the fine grid. Even if the temperature is about the same, no local explosions occur unless the pressure is high. The flame after the interaction is divided into two regions and the reflected shock and the bifurcated shock appear. The upper flame develops for the high shock Mach number case (Ms = 1.97); however, the upper flame does not propagate for the low shock Mach number case (Ms = 1.61).

978 - Experimental Investigation on the Flame Wrinkle Fluctuation Under External Acoustic Excitation

L. Zheng, S. Ji, Y. Zhang

The flame front wrinkle instability response of laminar premixed conical flames to acoustic excitation is investigated experimentally with a focus on the fluctuation amplitude along the downstream and the response frequency under a various harmonically forced frequencies and sound pressure. By using a high-speed colour camera and a microphone, the acoustic data and the induced flame dynamic characters can be measured simultaneously. As a result, the high sound pressure on the action points induced more severe flame oscillation and it shows more evidently under high harmonic frequency. The fluctuation amplitude grows linearly along the flame length and both frequency and sound pressure has a positive effect on the growth rate. The frequency of the flame boundary displacement at a certain i-axis point correlates well with the excitation frequency. The domain frequency peak becomes more apparent with the increase of sound pressure in each frequency group and under the high sound pressure the derivative harmonic frequencies also can be noticed.

931 - Sub-Grid Scale Modeling of the Equation of State for Fully Compressible Combustion LES

G. Ribert, P. Domingo, L. Vervisch

In Large Eddy Simulation of multicomponent and fully compressible flows, formally the pressure is obtained after filtering the equation of state. In practice, correlations between density, species and temperature are usually neglected to compute the filtered pressure from the resolved fields. Analysing one-dimensional and three-dimensional H2/O2 space- filtered flames, it is found that a large part of the error introduced by the linearisation of the equation of state can be counterbalanced by expressing the mean molar weight of the mixture with the Reynolds filtered species mass fractions, instead of the density weighted ones. An approximate deconvolution/filtering procedure is then discussed to estimate

the Reynolds filtered mass fractions from the density weighted mass fractions, which are the transported quantities in LES flow solvers.

1187 - Reaction Front Characterization in Turbulent Combustion Based on Entropy

Production Field Curvature

R. Schießl, V. Bykov

We present and apply a strategy for reaction front characterisation in turbulent combustion. It uses the chemical entropy production rate as a marker for chemical activity. A characterization of the local geometry of reaction field structures is developed which uses the principal curvatures of the entropy production rate field. Different paradigms for the local geometrical shape of a reaction field structure can be identified by means of ratios of the principal curvatures. These paradigms include the classical two-dimensional flame sheet, but also one-dimensional, one-dimensional filamentary or "worm"-like reaction structures and isolated "dot"-shaped reaction islands.

The method is applied to 3D Direct Numerical Simulation Data of a turbulent nonpremixed flame. It is found that in this data set, the one-dimensional reaction front paradigm is often encountered. These "flame worms" are numerically tracked in a DNS data sample by a path-following algorithm and their overall appearance in 3D space is visualized; it turns out that they often form closed loops.

The appearance of the one-dimensional structures is thought to be related to the decay of twodimensional reaction sheets into one-dimensional structures by the interaction of the turbulent flow field with chemical reaction, but their exact relation to turbulence-chemistry interaction, as well as to other one-dimensional turbulence structures, still needs to be investigated. The results can be used, for instance, to more accurately quantify an effective flame surface of a turbulent flame, and therefore, for improved models of the flame propagation velocity in turbulent combustion.

924 - Effect of Asymmetric Fuel Injection on the Combustion Characteristics of Liquid Fuel Fired Flameless Combustor

S. Sharma, H. Pingulkar, A. Chowdhury, S. Kumar

In the present work, effect of asymmetric location of fuel injection nozzle on the different combustion characteristics has been investigated. A single solid cone type pressure swirl nozzle, N1 has been considered with different high injection pressures (14, 30, and 48 bar) to achieve different fuel flow rates of 2.5 kg/hr (30 kW), 3.12 kg/hr (37.27 kW), and 4.46 kg/hr (53.23 kW). Effect of air preheating has been investigated for the kerosene fuel at a fixed temperature of 800 K. Combustor exhibited more stability in the flameless regime with asymmetrical fuel injection. That helps reducing the NOx emissions. The measured CO and NOx emissions were in the range of 28-161 ppm and 2-32 ppm for all heat inputs and equivalence ratio = 0.4 to 0.92), respectively. Measured sound levels were in the range of 93-99 dB and 98-103 dB for the flameless and transition mode respectively.

09:00 Memories of Toshi Fujiwara: Kindness, Splendor, and Physics

1003 - Numerical Analysis on Liquid JP10 Rotating Detonation Engine

A.K. Hayashi, W. Yoshida, M. Asahara, N. Tsuboi

Liquid-gas two phase detonation has not been studied much because of dealing with different phase and complex dynamics although liquid is actual fuel for aerospace vehicles, boat, car, etc. Recently Dabora et al. reported that cyclodecane of its diameter of 2.6 mm deforms, breakups, evaporates, mixes, and burns after detonation passes its mixture. Cheatham and Kailasanath reported an evaluation of thrust performance of liquid JP10 PDE that specific impulse increases as liquid evaporation rate increases. However there a few work on liquid RDE study. One of the most recent work is presented by Anderson et al. to understand liquid injector performance under the transient atmosphere characteristic of RDE. They showed a strong effect of a passing detonation on liquid atomization. In order to get a stable rotating detonation in RDE when liquid fuel is applied, this study will seek the liquid phase influence on rotating detonation structure.

937 - Modelling Mixing Near HE-Air Interfaces in Explosions

A.L. Kuhl, D. Grote, J.B. Bell, V.E. Beckner

We consider the problem of mixing near HE-air interfaces in explosions, where the Detonation Products (DP) are rich in carbon particles. The model consists of gas phase conservation laws (i.e., the compressible Navier-Stokes equations), coupled with a heterogeneous continuum model for the carbon particle phase. The problem is assumed to be point symmetric, so the 1D spherical coordinates are used. The hyperbolic terms are integrated with a 2^{nd} -order Godunov scheme (PPM), while the viscous terms are advanced by a 2^{nd} -order Runge-Kutta method. The particle phase conservation laws are also integrated with a 2^{nd} -order Godunov scheme (for dilute particle systems. Adaptive Mesh Refinement (AMR) is used to resolve steep gradients in the flow. A tabular EOS, based on equilibrium thermodynamics code Cheetah code, is used. Three converged solutions were found: (i) inviscid, (ii) viscous and (iii) two-phase. The blast wave solution (*p*, *rho*, *T*, *u*) scaled gasdynamically (i.e., with the appropriately-defined Peclet and Reynolds numbers. The DP-Air interface is unstable and evolves into a turbulent mixing layer; 3D inviscid AMR simulations of this case will also be presented.

09:00 Laminar Flames 3

1044 - Effect of Multi-Component Transport Model on Soot Prediction in Opposed-Jet Ethylene Diffusion Flames

A. Borg, H. Lehtiniemi, F. Mauss

This paper investigates the differences in soot predictions when using a detailed multi-component transport model instead of a mixture-averaged transport model. Two ethylene/air counter-flow flames of Wang et al. (Proc Combust Inst 26:2359-2368, 1996) were used to investigate the impact of multicomponent diffusion on soot prediction. The soot was calculated with a detailed kinetic soot model. The calculations showed good agreement compared to the experiments of Wang et al. both in absolute values and in the shape of the soot profile. The mixture-averaged transport models predicted approximately 15 percent more soot (in terms of soot volume fraction) compared to the multicomponent transport model, with no corresponding change in soot number density. The heat conductivity was the most sensitive of the transport processes for soot prediction. Heat conductivity decreased the total soot amount when using multi-component transport. The second largest sensitivity was due to the diffusion, which also decreased the soot amount with the multi-component transport model, although to a lesser degree. Smallest sensitivity to the soot volume fraction was found to be the viscosity, which only lowered the soot volume fraction very slightly. The viscosity effects can be related to thermophoresis, heat conductivity affects temperature and chemical reactions, while diffusion coefficients affect surface growth by radical transport to the soot growth layer. Other experiments might result in a different sensitivity of the species transport coefficients.

979 - Impact of Acoustic Excitation Frequency on Laminar Premixed Flame

L. Zheng, S. Ji, Y. Zhang

The response of an air/propane premixed conical flame in a one end closed tube at different excitation frequency (10-600 Hz) is investigated. The flame axial position in the tube can be adjusted, so that the flame response to the varying sound pressure level along the tube can be studied. The flame dynamic wrinkle structure and dilution behaviour under various excitation frequencies are measured simultaneously by a microphone and high speed colour camera. Through digital image processing, a range of flame properties such as the flame wrinkling displacement and the surface to volume ratio have been evaluated. It has been observed that the higher acoustic excitation frequency has a significant effect on flame oscillation characteristics. The variation of the displacement at a single point on flame boundary, the length of the boundary line and the flame surface to volume ratio are also sensitive to the local sound pressure level in the tube. As a result of the sound pressure perturbation and the change of boundary condition, the flame exhibited a varying degree of further air/fuel mixture dilution, which is indicated by the B/G ratio increase through Digital Flame Colour Discrimination techniques (DFCD).

1012 - Elevated Temperature Effects on Laminar Burning Velocity Temperature Exponent of Liquid Fuels

A. Katoch, R. Kumar, S. Kumar

In the present work the meso-scale diverging channel technique is used to measure a fundamental fuel characterization parameter- laminar burning velocity, of ethanol-air mixtures at high unburnt mixture temperatures (350-600 K) and atmospheric pressure. The effect of unburnt mixture temperature was assessed by deducing temperature exponent values from experimental burning velocity data. The measurements for ethanol-air mixtures were carried out for equivalence ratios - 0.8, 1.0 and 1.2. For methanol-air mixtures sensitivity analysis is employed to analyze the effects of key reactions on burning velocity and temperature exponent. PREMIX was employed to compare the experimental results with the San Diego Mechanism for ethanol and Li et al. Mechanism for methanol analysis.

976 - Effects of Applied Electric Fields on Liftoff Height in Laminar Lifted Coflow-Jet Flames *B.H. Seo, K.H. Van, G.T. Kim, N.P. Sapkal, O. Kwon, J. Park, S.H. Chung*

The study has been conducted on laminar lifted nitrogen diluted methane coflow jet flames to elucidate the effects of electric filed to the lifted flame which has a decrease of lifted off height with increasing nozzle exit velocity. Two types of flame behavior were observed nearby the extinction limit without electric filed in previous study; the decrease of lifted off height with increasing nozzle exit velocity within 72.5 $\leq U_0 \leq$ 120 cm/ and flame self-excitation in the range 72.5 $\leq U_0 \leq$ 75 cm/s at 0.45 $\leq X_{F,O} \leq$ \leq 0.55. In this study, the lifted flame in the decreasing lifted off height region with alternate current electric field (AC) exhibit different behavior compared with previous study. While for direct current electric field (DC), the influence on liftoff was minimal. The flame behavior was distinguished into stable and unstable with the variation of applied voltage and frequency at fixed U_0 . In case of $U_0 = 80$ cm/s, stable flame within $V_{ac} \leq$ 1000 V and $f_{ac} > 400$ Hz and unstable flame within $500 \leq V_{ac} \leq$ 1000 V and $f_{ac} < 400$ Hz. In order to show the effect of AC electric field on lifted off height, axial distribution of OH* chemiluminescent intensity passing through the triple point at various frequencies for V_{AC} = 900 V, $V_{CO} = 7$ cm/s, and $X_{F,O} = 0.436$. The results show that increasing f_{AC} rather reduces maximum OH chemiluminescent intensity. This implies that increasing f_{AC} does not enhance edge flame speed. Such a liftoff heights were characterized well by some physical parameters.

09:00 DDT 2

1067 - Effect of Surface Roughness on Deflagration-to-Detonation Transition in Submilimeter Channels

R.W. Houim, E. Oran

Three-dimensional simulations were performed to study the influence of surface roughness on the runup distance and mechanism of deflagration-to-detonation transition (DDT) in submillimeter channels. The channels have a square cross-section and an unobstructed half-height of 300 micrometers. The channel initially contains a stoichiometric mixture of ethylene and oxygen at 300 K and 1 atm. The

surface roughness is approximated using small pyramid-shaped elements to create a rough wall that resembles a knurled surface. The compressible reactive Navier-Stokes equations were solved using a high-order Godunov algorithm with adaptive mesh refinement. The rough walls produce shock reflections and turbulence that does not occur in smooth submillimeter channels. These effects accelerate the flame faster and initiate detonation sooner compared to smooth channels and reduced DDT run-up distance by a factor of 16 when 80 micrometer-high roughness elements were used. The detonation is initiated when unburned material autoignites in the cavities between the surface roughness elements.

759 - Deflagration-To-Detonation Transition in an Unconfined Space

A. Koksharov, V. Bykov, L. Kagan, G. Sivashinsky

This study is motivated by recent theoretical developments in premixed gas combustion revealing positive feedback between the advancing flame and the flame-driven pressure build-up, which results in the thermal runaway when the flame speed exceeds a critical level. The present study is an application of this finding to the problem of deflagration-to-detonation transition (DDT) of a spherical flame expanding in an unconfined environment. As has long been conjectured, in the unconfined system the expected transition might be caused by the flame acceleration induced by the Darrieus-Landau instability (wrinkling). Indeed, it has been shown recently, that for the wrinkled spherical flame the transition may be modeled even within the framework of a one-dimensional formulation by merely replacing the reaction rate term W by Σ^2 W, with Σ being the degree of folding - the ratio of the total area of the wrinkled front fractal dimension. Within Σ -based formulation the transition may be triggered at any initial temperature T₀ and pressure P₀, as soon as R becomes large enough. The present study is an extension of our recent exploration of the Σ -model based on ignition-temperature kinetics and planar geometry over (i) one-step Arrhenius kinetics and spherical geometry, and (ii) multistep hydrogen-oxygen kinetics and numerically more benign planar geometry.

1000 - Propagation Mechanism of Detonations in Rough Walled Tube

J. Li, J. Ning

The paper reports the results of a study of detonation propagation mechanism in rough walled tube. To generate wall roughness, spirals with rectangular cross section of various wire lengths and a pitch of one tube diameter were used. Detonation velocity is measured by photodiodes along the length of the tube as well as a high-speed camera for detonations with weak illumination. A short length of the smoked foil was inserted into the core of the tube at the end to register the core detonation pattern. The experimental results indicates that in rough tubes with spirals, detonation velocity can vary continuously from close to the theoretical Chapman-Jouguet value far from the limits to about 40% V_{CI} where the detonation fails. This contrasts with the detonations in smooth tubes, where the detonation velocity seldom decreases to less than 80% V_{CI} at the limits. It suggests that wall roughness tends to facilitate the self-sustained propagation of detonation waves. We also found that an abrupt drop in velocity exists when decreasing the initial pressure for mixtures with high argon dilution, indicating a transition from a quasi-detonation to a fast deflagration in a rough walled tube, i.e., $d/\lambda=1$.

09:00 Diagnostics, Sensoring 1

1070 - High Speed PIV of Flame Propagation in Obstructed Channels

T. Li, R.P. Lindstedt

Turbulence-chemistry interactions and fuel (or mixture) reactivity directly affect flame acceleration caused by positive feedback mechanisms in obstacles laden channels. The use of more reactive hydrogen enriched fuels is increasingly important due to the desire to use syngas and/or biogas in power generation applications. However, experimental data remains limited due to difficulties in achieving repeatable results. The current study reports highly reproducible experiments performed using strongly hydrogen enriched fuel lean CH4/H2/air mixtures with the flame propagation leading up to a turbulent

explosion quantified using high-speed particle image velocimetry (HS-PIV) and Mie scattering. The time-resolved evolution of the recirculation zone was successfully captured with the explosion overpressure and flame propagation speed also measured. A peak over-pressure of 37 kPa and a flame speed of 190 m/s were obtained. The horizontal and vertical velocity components were calculated at selected spatial locations in the free flow, shear layer and recirculation zone. In the free flow region, u is dominant, while in shear layer u and v are comparable with the thickness of the shear layer was estimated to be 10 mm based on the velocity gradient. The change in the horizontal velocity against height is also reported. It is expected that the data will be useful in risk assessments of explosion hazards and for model development.

1038 - Experimental Assessment of the Displacement and Consumption Speeds in Flame/Vortex Interactions

F. Thiesset, F. Halter, C. Bariki, C. Lapeyre, C. Chauveau, I. Gokalp, L. Selle, T. Poinsot

While the displacement speed is readily measurable, a proper experimental assessment of the consumption speed is challenging as the fuel reaction rate is not accessible. Some studies reveal that surrogates of the heat release such as CO2, CH, OH, HCO can be employed. However, these surrogates are unequally appropriate, and the relationship between fuel reaction rate and measured intensity of these surrogates may not hold in general. Here, we propose a novel approach inspired by previous work on spherical flames, tailored for simultaneous Mie scattering tomography - PIV measurements. The method is tested in a stagnation point premixed flame and in DNS of premixed flame-vortex interaction.

1015 - Extinction Measurements of Soot Particles in a Diffusion Flame When Submitted to a DC Electric Field

P. Gillon, V. Gilard, M. Idir, B. Sarh

We present the influence of a DC electric field on the sooting characteristics of an ethylene diffusion flame of 80 mm long burning in ambient air. The particle volume fraction is deduced from laser extinction measurements on the flame axis. In the case of a stable flame; the application of a downward electric field leads to a decrease of the soot volume fraction inside the flame. Above a certain voltage, flame oscillations are observed which seem to correspond to a transition in the ion current flowing in the flame. In the case of unstable flames, the mean soot volume fraction on the axis of the flame is shown to increase compared to the stable case. The generation of an ionic wind issuing from collisions of ions and electrons with neutral molecules could explain these effects. By slowing the ascending gas flow, the ionic wind which perturbes the shear layer between the flame front and air can be at the origin of a flickering phenomenon characterized by flame length oscillations, and in turn affects the soot formation mechanism.

1124 - High Speed PIV Analysis of the Combustion Regimes During Autoignition of Homogeneous Fuel - Air Mixtures in a RCM

C. Strozzi, A. Delicourt, M. Bellenoue, J. Sotton

The present work deals with the characterization of combustion regimes observed during autoignition of fully premixed iso-octane – air mixtures in a Rapid Compression Machine (RCM). After validating the ignition delays measured for these mixtures, high speed PIV is employed to monitor the development of the different combustion regimes during auto-ignition of a lean iso-octane air mixture at pressures of 20 and 27.7 bar at the end of compression. However, if the fuel air mixture is fully premixed, aerothermal processes naturally present during compression of flat piston RCMs generate temperature heterogeneities. Amplitude of the local thermal gradients may lead to different processes, like deflagration or auto-ignition fronts for instance. These both regimes were investigated in the RCM by high speed Particle Image Velocimetry (PIV) with prospect of the measurement of the reactive front velocity relative to the unburned mixture. The diagnostic method brings useful data about the aerothermal processes and the way they are affected by heat release. In particular, the velocity field is weakly affected when combustion process is driven by deflagration, whereas propagation of autoignition fronts at 40 m/s drastically changes the internal aerodynamics inside the vessel. Finally, the diagnostic method is found promising for further studies of autoignition combustion regimes in RCMs.

09:00 Reactive Systems 2

1094 - Near-Structure Air Blast Simulations Using Zapotec, A Coupling of CTH and Sierra/SM *A. Gullerud*

The ability to conduct simulations for air-blasts and their subsequent interaction with structures is vital in the study of a range of security and safety concerns. For significant stand-offs between the blast and the structure, a range of analytic/simplified simulation techniques can provide suitable results, e.g. conwep [1] for simple geometries. However, for blasts which originate close to the structure or with complex geometries, the interaction of the explosive products, air shock, structure geometry, and material failure necessitate the use of more complex computational frameworks. Zapotec, an Euler-Lagrange code which couples the hydrocode CTH with the structural transient-dynamics finite element code Sierra/SM, provides such a framework. This presentation includes a short overview of the Zapotec code methodology, and then compares Zapotec simulations to two simple test series which investigate structural response to explosive detonations with small standoffs where analytic/simplified simulation techniques can fail. The Zapotec simulations compare well to the experimental results in both cases, giving confidence in the use of Zapotec for near-structure air-blast scenarios.

903 - Raman Study of Structural Change in 1,3,5-Triamino-2,4,6- Trinitrobenzene Under Non-Hydrostatic Pressure

X. Sun, C. Gao, Z. Sui, R. Dai, Z. Wang, X. Zheng, Z. Zhang

Raman spectroscopy was applied to study the structure evolution of TATB powder under nonhydrostatic pressure. The variation of Raman vibrational modes of TATB is analyzed at low pressure. A new Raman peak that represents the NH₂ out-of-plane twist vibration mode occurs at 860 cm⁻¹. The peak intensity increases gradually with increasing pressure and the adjacent NH₂ rocking vibration and NO₂ shear vibration mode gradually weakened and disappeared completely at 10.6 GPa. Raman peak shifts with increasing pressure show a clear discontinuity in the range of 5-8 GPa. The results reveal that there is a structural phase transformation in TATB around 5 GPa. During loading compression, the color of TATB undergoes a series of changes. After releasing pressure, the change of TATB is reversible, indicating that the molecular structure of TATB has not been destroyed and chemical stability is still maintained.

1114 - Porous Wall Fed Liquid Fuel Nonpremixed Swirl-Type Tubular Flames

V.M. Sauer, D. Dunn-Rankin

A tubular flame is a classical configuration used in fundamental studies in combustion science. The most common tubular flame configurations, i.e., the swirl type and the counterflow type, have been mainly applied to the analysis of premixed systems. A nonpremixed version of counterflow-type tubular flames has also been developed, but the majority of the studies are limited primarily to gaseous fuels. The present study examines a liquid fueled nonpremixed swirl-type tubular flame. A permeable material is used to deliver vaporizing fuel into the combustion chamber for the chemical reaction with the swirling air coming from the bottom inlet. Stability limits and temperature measurements of the external burner wall are performed. Experimental results show the feasibility of the proposed configuration.

1024 - Behavior of Explosive Bubbles Behind an Underwater Shock Wave

N. Watanabe, K. Ishii

In the present work, an underwater shock wave driven by detonation travels in water containing explosive gas bubbles. The bubbles are made of a stoichiometric ethylene-oxygen mixture. Behavior of the bubbles is visualized with a high-speed camera using the shadowgraph method. Pressure rise due to bubble expansion is measured with a pressure probe. As a result, behind the underwater shock wave, the bubble starts to shrink resulting in combustion, and then expands, which is followed generation of a shock wave. The maximum pressure of 54 MPa was obtained after the shock-bubble interaction.

11:10 Chemical Kinetics and Reaction Dynamics 4

1055 - Reduction of Detailed Chemical Mechanisms by Entropy Production Analysis in the Presence of Irreversible Reactions

L. Acampora, M. Kooshkbaghi, C.E. Frouzakis, F.S. Marra

This paper introduces a generalized formulation for the entropy production analysis devoted to the reduction of detailed chemical mechanisms. A general formulation of the entropy produced by the chemical reactions is introduced. This formulation holds also for irreversible reactions, when the principle of detailed balance is violated. An index that represents the relative importance of each reaction with respect to the total entropy production is defined. As a result, an algorithm has been developed to generate reduced mechanisms involving both irreversible reactions or ad hoc estimated reverse rates. The new approach is then exploited to obtain a skeletal mechanism for n-dodecane starting from the detailed reaction scheme developed by the CRECK group, a mechanism composed mainly by irreversible reactions.

774 - On the Dynamics of Ignition Process Behind Reflected Shock Waves Under the Influence of Bifurcation

O. Pryor, S. Barak, E. Ninnemann, S. Vasu

Shock tubes are typically used to measure ignition delay times - a fundamental property of fuels that is a function of temperature, pressure, and mixture concentrations. Bifurcation occurs because the boundary layer is not able to negotiate the pressure rise across the reflected shock when brought to rest relative to it, and is therefore trapped and carried along at the foot of the shock. Bifurcation features normally appear in diatomic and polyatomic gases (such as fuel/air mixtures, mixtures with CO₂) but not in argon diluted mixtures and its features have been well-known through experimental visualization utilizing color schlieren and side-wall pressure measurements. Bifurcation has been modeled in many computational studies. Bifurcation affects determination of time zero because of the uncertainty in determining the arrival of the normal shock wave at the sidewall location and its effects are severe as one moves away from the end-wall and also for short ignition delay times (<100 ms). In addition, it is commonly assumed that bifurcation should not affect the core portion of the post-shock region, which comprises most of the flow area [4]. However, a comprehensive study using multiple diagnostics to verify the influence of bifurcation and inhomogeneity on chemical kinetics is lacking in the literature though similar studies in rapid compression machines have been carried out. In this work we focus on studying H₂/CO ignition under the influence of bifurcation in heavily CO₂diluted mixtures near 1000K for pressures less than 5 atm. Multiple diagnostic techniques (pressure, sidewall emission, laser absorption, and high-speed imaging) are used to determine accurate ignition delay times when bifurcation is present. The mixtures used contained varying amounts of H2, CO, CO2, O2, and Ar to control the reactivity and bifurcation levels.

1068 - Effects of Variation in Sample Mass, Gas Flow and Lid on Chemical Reactions During STA Measurements

D. Lázaro, M. Lázaro, A. Alonso, D. Alvear

Thermal analysis are a family of experimental techniques which are widely used to study chemical reactions of many materials and specially to analyse polymers decomposition. The chemical reactions that occur during thermal decomposition are often highly dependent on the conditions of the tests and sample.

This work aims to analyse the main parameters needed to guarantee the validity of the results such as the sample mass, use of lid and gas flow. In order to assess influence in different sort of chemical reactions, the polyvinyl chloride (PVC) was studied using Simultaneous Thermal Analysis apparatus. As PVC has a large number of different kinds of chemical reactions, the results could be extrapolated to other materials.

Since results showed the impact of each different boundary conditions in the thermal decomposition, some useful recommendations have been defined.

11:10 Turbulent Flames 3

1159 - Combustion in a High-Swirl Turbulent Jet Undergoing Vortex Breakdown. Investigation by PIV and HCHO PLIF

L.M. Chikishev, V.M. Dulin, A.S. Lobasov, D.M. Markovich

The paper reports on results of the experimental study of regions of local heat release in strongly swirling premixed methane/air turbulent flames. The measurements were carried out for the jet-flames with different equivalence ratios ($\phi = 0.7$, 1.4 and 2.5) by using planar laser-induced fluorescence of formaldehyde, excited by laser radiation with 355 nm wavelength, and stereo PIV technique. Shape of intensive heat release region for the lifted flame of the fuel-rich mixture ($\phi = 2.5$) was found to be considerably different from that for the inverted flames for $\phi = 0.7$ and 1.4. For all three equivalence ratios, large-scale deformations of the flame front were detected. According to the PIV data the flame front deformations were induced by vortices in the inner (around the central recirculation zone) and outer (between the annular jet core and the surrounding air) mixing layers, induced by flow precession.

1156 - Experimental Measurements of Turbulent Burning Velocity in Gas Explosions with Two Obstacles of Variable Spacing: Implication to Gas Explosion Scaling

A. Na'inna, H. Phylaktou, G. Andrews

For a significant interpretation of results from small scale tests and for application to actual size explosion hazards, the understanding of the influence of which is determined by the presence of turbulence initiators (obstacles) in gas explosions is necessary. The S_T used in gas explosion scaling from small to large scale has a direct influence of *l*. Thus, the present work measures S_T experimentally in gas explosions with two obstacles of variable spacing with a view to looking at its implication to gas explosion scaling. The newly obtained correlation is given as $S_T/S_L = 2.99R_l^{0.36}$.

The empirical S_T correlation shown above have demonstrated a dependence on which is significantly higher than most of the S_T models in the literatures. Even though, the variation in is small in absolute terms, the resultant estimates, mostly overpressures are significantly different and could make a barrier between safe and unsafe designs.

From the newly measured S_T , a blast overpressure correlation with explicit dependence on the geometric configuration, pressure loss characteristics (effectively the blockage ratio of the obstacles) and mixture properties was derived as, $P \propto [(C_T K^{0.5})^{0.54} l^{0.54}][E^{2.54} S_L^{2.54} v^{-0.54}]$

Also, the relevant S_T models used for gas explosion scaling and CFD codes (FLACS and FLUENT) were expanded to formulate gas explosion overpressure. The explosion overpressure correlations were validated against a limited suitable experimental data for both laboratory scale and a large scale that is 20 times bigger than the small scale. For both methane and propane-air mixtures, the calculated overpressures were in a close agreement with the experimental data especially for models with higher exponent. This agreement is very promising as it reveals that from using geometry at laboratory scale in the present research to calibrate an overpressure correlation, then the effects of different blockage ratios, gases and scales for the same overall geometry could be successfully predicted.

1001 - Disturbance Energy Analysis of Turbulent Swirling Premixed Flame in a Cuboid Combustor

K. Aoki, M. Shimura, Y. Minamoto, M. Tanahashi

Combustion oscillation induced by thermoacoustic instability is one of the most critical problems in practical combustion systems operated with lean premixed combustion technologies employed for reducing NO_x emission. It still remains challenging to accurately predict the onset of combustion oscillation and to control a combustion field due to the presence of turbulence in practical combustors and complexity of interactions between flame, acoustic, velocity and other scalar fluctuations. In order to gain insight into critical factors in the combustion instability, an exact disturbance energy equation derived from governing equations without any physical assumptions is examined using results of direct numerical simulation (DNS) of turbulent swirling premixed flame in a cuboid combustor. The DNS in this study is conducted for two swirl number conditions (S = 0.6 and 1.2) employing a detailed kinetic mechanism for hydrogen-air combustion. The DNS results for the lower swirl number case show that large-scale helical vortical structures are dominant in upstream region, whereas fine-scale eddies

Thursday

caused by turbulence transition distort the flame surfaces in downstream region. As for the higher swirl number condition, a significant convolution of flame surface is caused by a large-scale ring-shaped vortex near the inlet, and small-scale eddies also contribute to distortion of flame surfaces in downstream region. Disturbance energy analysis of the DNS results shows that source terms related to entropy fluctuation (D_s) and heat transfer fluctuation (D_O) have significant magnitude and behave as a production and sink terms, respectively. Further investigation into D_s reveals that terms including momentum fluctuation are the most dominant source of disturbance energy and that these terms are strongly affected by swirling intensity. On the other hand, the effect of the swirl number on the other terms included in D_s are not significant, implying that higher swirl number could make the difference between the terms including momentum fluctuation and the other terms in D_s more significant. Analysis of D_Q shows that a term caused by heat conduction is the most dominant sink term. Another term including a product of temperature fluctuation and heat release rate fluctuation, which is analogous to a modified Rayleigh term, is the second most dominant term in D_Q and it only behaves as a sink term in the present computational cases. The sink term caused by heat conduction is strongly affected by swirling intensity, while the effect of the swirl number on the Rayleigh like term is not significant. Further investigation into the heat conduction term reveals that the dissipation of the disturbance energy mostly comes from fluctuation of temperature gradient caused by flame distortion by eddy motions. Thus, a flow field with higher swirling intensity could increase the contribution of the heat conduction term as a sink term through stronger turbulent motions. The results in this study suggest that the source term D_Q could be reduced to a simpler form keeping only the dominant dissipative term and the heat release term.

11:10 Detonation Engines 3

1133 - Small Size Rotating Detonation Engine: Scaling and Minimum Mass Flow Rate

C.B. Kiyanda, S. Connolly-Boutin, V. Joseph, X. Mi, H.D. Ng, A.J. Higgins

Rotating detonation engines (RDE) have been investigated since the mid-1960s with a renewed interest in the last 10 years. There is evidence that for an RDE to successfully operate, there exists a minimum mass flow rate for a given engine size. Determining the scaling of this minimum mass flow rate will help determine the range of applications of the RDE concept as a viable propulsive system. Based on geometric constraints, the minimum mass flow rate of a 76.5 mm outer diameter annulus RDE operating with either a mixture of $2H_2+O_2$ or H_2+N_2O is determined. This minimum mass flow rate estimation is seen to reproduce the order of magnitude of limits reported in the literature for similar mixtures.

1080 - Experimental Study on a Rotating Detonation Turbine Engine with an Axial Turbine

H. Rhee, C. Ishiyama, J. Higashi, K. Akira, K. Matsuoka, J. Kasahara, A. Matsuo, I. Funaki

In this study, for the first step of developing a rotating detonation turbine engine (RDTE), we designed, fabricated, and tested an RDTE. We have confirmed that the revolutional speed of the engine increases by the operation, and we have obtained a prospect for the self-sustained operation. For analyze the experiment, we measured a change of temperature, pressure and revolutional speed by the sensor which installed in an RDTE. We performed two kinds of experiment, hot flowtest and cold flow test with 0.2 s combustion. In the case of hot flow test, experiment was performed in the condition that rich of $\varphi = 1.52$ and lean of $\varphi = 0.96$. The result of hot flow test, lean test shows higher increase in temperature and revolutional speed rather than rich test. Maximum temperature in lean test was about 3000 K and maximum revolutional speed in lean test by high-speed camera. The high-speed photograph prove that the speed of detonative wave was $0.916D_{CJ}$. By above reason, the wave which was seen in combustor is close to detonation wave. Lastly, we confirmed that the possibility of pre-rotating a turbine by the injection of high-pressure gas.

769 - Spectra Signals of Gas Pressure Pulsations in Nozzles

V.A. Levin, N.E. Afonina, V.G. Gromov, I.S. Manuylovich, A.N. Khmelevsky, V.V. Markov

Annular and dual slotted linear nozzles with the internal deflector are considered as perspective for realization a pulsing, including the detonation, regime of fuels combustion The study of pressure pulsation signals are topical to determination the dependence the spectral composition of pulsations from geometric nozzles parameters and the flow conditions in them in order to govern by frequency of a process. Also of interest is clarification the degree of influence of gas pressure pulsations in the flow on the thrust characteristics of these nozzles. The paper presents the results of computational and experimental study of dependences of frequency and oscillations amplitude of flow parameters in annular and dual slotted linear nozzles from the conditions at the inlet and the outlet of the nozzle and its geometry. Experiments with annular nozzles were conducted in a pulsed aerodynamic setup using as the working gas the combustion products of acetylene-air mixture. Calculations were made on the basis of the Navier-Stokes equations for multicomponent reactive gaseous medium using a singletemperature chemical nonequilibrium model including all main products of the combustion of a stoichiometric mixture of acetylene in air. As a result of investigation the dependences frequencies and oscillations amplitudes of the flow parameters in annular and equivalent gas flow dual slotted linear nozzles from the governing parameters were established. We dealt with different pressures at the inlet and exit of nozzles, different sizes of the critical cross-section and different diameters of the annular nozzle. Presented the comparison results of computational and measured spectral composition of quasiperiodic pulsating signal of pressure on the thrust wall of the annular nozzle obtained by the discrete Fourier transform on the time interval 0.5 to 2.5 ms. The calculation predicted the existence of quasiperiodic pulsating regimes of gas flow in a dual slotted linear nozzle and defined the spectral composition of pressure pulsations on the thrust wall and the thrust force developed by the such nozzle.

11:10 Detonation Propagation

1091 - Visualization of Detonation Propagation in a Round Tube Equipped with Orifice Plates *G. Rainsford, G. Ciccarelli*

Self-luminous high-speed photography was used in conjunction to soot foils to visualize detonation propagation in a round tube with repeated orifice plates. Experiments were conducted in a 3.16 m long aluminum combustion channel with a 7.62 cm square cross-section connected to an Acrylic 1.55 m long, 7.62 inner-diameter cylindrical combustion channel. A 50% blockage ratio was maintained throughout the channel using 7.62 cm high, 1.91 cm wide and 1.27 cm long, equally spaced 'fence type' obstacles in the square channel and 5.33 cm diameter Acrylic orifice plates in the tube. Stoichiometric hydrogen-oxygen mixtures at initial pressures of 6-60 kPa were ignited in the channel and synchronized end- and side-view video was recorded through the tube. The square channel had a higher detonation limit than the round tube, which is consistent with the d/λ criteria based on the difference in obstacle opening size, d. A higher velocity deficit was observed in the round tube, which was attributed to the greater shock diffraction and resulting detonation decoupling that occurs. The detonation wave undergoes three-dimensional diffraction in the round tube, compared to the twodimensional diffraction in the square channel. Three distinct quasi-detonation propagation modes were observed in the round tube: single hot spot ignition on the tube wall (7-15 kPa), multi-head detonations (20-45 kPa) and continuous detonations (50-60 kPa). The video results corroborate the interpretation of the detonation propagation mechanism proposed solely on soot foils by Ciccarelli and Cross (2015). Single head-spin was not observed, instead the stable propagation mechanism near the limit involved ignition at a single hot-spot on the wall that alternated diametrically between orifice plates.

1135 - Single-Head Detonation Propagation in a Partially Obstructed Square Channel

M. Kellenberger, G. Ciccarelli

There are three distinct propagation regimes that will be discussed using the aid of schlieren images and soot foil records, which will be compared to results previously obtained in a narrow aspect ratio channel. Two of the regimes (fast flame and continuous detonation) were observed in a narrow channel.

The third, a single-head propagation regime, was not observed in the narrow channel and indicates that transverse wave propagation plays an important role in this mode. Tests investigating the threedimensional behaviour of propagating supersonic combustion waves were performed in an obstructed square channel. At pressures below 10 kPa, only fast flame propagation was observed, whereas above 25 kPa continuous detonation propagation was observed with weakening at the obstacle. Between these pressures, various forms of discontinuous detonation propagation was observed, with single-head being the most stable and reproducible in the pressure range of 17 to 23 kPa. This single-head should not be mistaken with a single-head spin in an unobstructed rectangular duct observed by Lee et al. (1969). The present single-head wave was found to propagate by the reflection, initiation, and subsequent failure of overdriven detonation waves across the channel width.

991 - Detonation Propagation in Rough Tube

Y. Liu, J.H. Lee, H. Tan

Wall roughness is found to have a large influence on the propagation of detonation waves and the propagation mechanism in rough tube is very complex. Experiments of detonation in a rough tube were conducted for both stable ($C_2H_2+2.5O_2+70\%Ar$) and unstable ($C_2H_2+5N_2O$) mixtures. Velocity measurement and smoked foils were used to observe the effect of roughness on the detonation propagation. The results indicate that the detonation propagation has a large velocity deficit at some critical pressures and there is an abrupt jump to a different regime of high speed deflagration at about 40% CJ velocity. Smoked foil records indicate tube roughness has a destructive interference with the cellular structure reducing a multi headed wave to a single headed spin wave. In the high speed deflagration regime, cell structure is absent indicating a different mechanism of propagation.

11:10 Turbulent Reacting Flows 3

883 - Direct Numerical Simulations of Shock-Scalar Mixing Interaction

R. Boukharfane, Z. Bouali, A. Mura

Due to the short residence time of air in supersonic combustors, achieving efficient mixing in compressible turbulent reactive flows is crucial for the design of supersonic ramjet (Scramjet) engines. In this respect, improving the understanding of shock-scalar mixing interactions is of fundamental importance for such supersonic combustion applications. In these compressible flows, the interaction between turbulence and shock wave is reciprocal, and the coupling between them very strong. Amplification of velocity fluctuations and substantial changes in turbulence characteristic length scales are the most important outcomes of this interaction, which may deeply influence scalar mixing between fuel and oxidizer (Huh and Driscoll, 1996). A basic understanding of the physics of such complex interactions has already been obtained through the analysis of relevant simplified flow configurations, including (i) shock wave propagating through density-stratified media (Layes et al., 2007), (ii) shock wave-mixing layer interaction (Morgan et al., 2013), and (iii) shock wave-vortex interaction (Grasso and Pirozzoli, 2000). The primary goal of the present study is to extend previous analyses to the case of shock-scalar mixing interaction, which is directly relevant to supersonic combustion applications. The turbulent mixing of a passive (i.e., inert) scalar in the presence of a shock wave are thus investigated with a special focus on the transport equations of the variance and mean scalar dissipation rate (SDR) of the mixture fraction.

980 - High-Order Numerics for Simulating Turbulent Deflagration Fronts Over Coarse Meshes E. Bossennec, G. Lodato, L. Vervisch

The information brought by the nodal decomposition of scalar signals in high-order spectral differences is used to calibrate artificial diffusivity in order to control the artificial thickening of reactive scalars in premixed flames computed over coarse meshes. The estimation of a sub-grid scale wrinkling factor from a nodal decomposition of the scalar gradient in a Legendre polynomial base is also studied for turbulent flames. The discussed methodology is tested in one- and three-dimensional canonical flows. The results obtained confirm the potential of the approach.

1090 - Fully-Implicit Density-Based Algorithms for Simulations of Arbitrary Gas Mixtures

L. di Mare, F. Wang, F. Ferraro, F. di Mare

A robust and straightforward extension of Roe's approximate Riemann solver to chemically reacting flows is presented in this paper. Flux-difference-splitting and flux-splitting methods for general, reacting gas mixtures are obtained via a formulation based on the excess internal energy of the mixture with respect to its ideal, thermally perfect gas state. A practical, fully implicit algorithm is derived. Detailed derivations of the Roe-average state, as well as of the transformation Jacobians are shown for the case of a reacting mixture of ideal gas species with variable specific heats. The algorithm is suitable for models with detailed thermochemstry as well as reduced models, e.g. based on progress variables. Results are presented from a strange-wave shock-flame interaction case in air-ethylene.

13:50 Ignition 2

932 - Effect of Low Initial Pressures on Ignition Properties of Lean n-Decane/Air Mixtures for Laser Induced Breakdown

S. Rudz, P. Tadini, F. Berthet, P. Gillard

Nowadays, laser-induced spark technique is considered as a valid solution for performance improvement of igniters in aeronautical sector. By promising stable ignition of lean mixture in both high and low pressure conditions, its range of application spans from internal combustion to turbojet engines. In addition, besides a more stable combustion, together with lower pollution and fuel consumption, laser-induced igniter might even represent a key technology for the development of scramjet vehicles. In this work, the ignition characteristics of a n-decane/air mixtures for different equivalence ratios (from 0.65 to 1.3) and initial chamber pressure (from 0.2 to 2.5 atm) are analyzed. For each conditions, a minimum ignition energy, accounting for 50% of ignition probability, is defined by means of the Langlie algorithm associated with the fitting a cumulative distribution function of a log-normal law. The achieved results lead to define an empirical relation able to predict the absorbed energy by the ignition of n-decane/air mixture, as well as an energy threshold for each tested configuration.

1108 - Thermomechanics of Laser-Induced Shock Waves in Combustible Mixtures

N.D. Peters, D.M. Coombs, B. Akih-Kumgeh

A combined experimental and CFD study of laser-induced shock waves is presented. Optical breakdown is induced in air, methane/ N_2 , methane/air, and biogas/air using blast wave theory to capture the mechanics of the resulting shock wave. This provides insight into the effect gas composition has on energy release from reactive mixtures during the optical breakdown process. For breakdown in air, CFD simulations are compared with experimental results. The simulated flow also reveals information about the velocity field within the shocked region.

1121 - Direct Numerical Simulation of Ignition by Hot Moving Particles

T. Zirwes, F. Zhang, T. Häber, D. Roth, H. Bockhorn

Ignition by moving hot solid sparks plays an important role in safety-related assessments in process industry and aviation. 3D direct numerical simulations employing detailed reaction mechanisms and molecular diffusive fluxes have been conducted for premixed methane/air and hydrogen/air mixtures at atmospheric conditions to investigate ignition at heated spherical particles in dependence on flow velocity. For low fluid velocities, 2D simulations assuming axial symmetry and full 3D simulations yield the same surface temperatures at the time of ignition. For higher velocities, 3D and 2D results deviate due to asymmetric flow structures caused by unsteady vortex shedding. The simulation results show that the ignition temperatures depend on the square root of the fluid velocity or Reynolds number. A model from literature is applied which correlates the ignition temperature with the Nusselt number and yields the apparent activation energies of the ignition process.

13:50 Explosion Safety 3

1111 - Evaluation of Engineering Models for Vented Lean Hydrogen Deflagrations

A. Sinha, V.C.M. Rao, J.X. Wen

Four engineering models including NFPA-68 [1], EN-14994 [2], Bauwens et al. [3] and Molkov and Bragin [4] are evaluated for their accuracy in predicting the deflagration generated overpressures in vented hydrogen deflagrations. At first the individual model predictions are compared with the available experimental data for lean hydrogen-air deflagrations and later overpressures are predictions for 15%, 18%, 21% and 24% hydrogen vol concentration in the container. NFPA and EN-14994 models have not effectively included the effect of obstacles. The models of Bauwens et al. [3] and Molkov and Bragin [4], which incorporate several physical aspects of the phenomena of vented deflagration, are found to give predictions within the error bands of Eauwens et al. [3] while more discrepancies are found with that of Molkov and Bragin [4].

1. NFPA 68. (2007): Standard on explosion protection by deflagration venting, 2007 Edition, National Fire Protection Association, Quincy, MA 02269.

2. EN 14994 (2007). Gas explosion venting protective systems

3. Bauwens, C. R., Chao, J., & Dorofeev, S. B. (2012). Effect of hydrogen concentration on vented explosion overpressures from lean hydrogen–air deflagrations. International journal of hydrogen energy, 37(22), 17599-17605.

4. Molkov, V., Bragin, M. (2015). Hydrogen–air deflagrations: Vent sizing correlation for low-strength equipment and buildings. International Journal of Hydrogen Energy, 40(2), 1256-1266.

1099 - The Essential Role of Science in Explosives Safety

C.B. Skidmore, K.A. Fleming

Historically, the sudden release of chemical energy in an explosion has been used as a destructive or propelling outward moving force. Towards the end of World War II, scientists and engineers learned to use this force creatively. By focusing the energy inwardly, they were able to rapidly change fissile metal from a subcritical state to a supercritical one. The development of the implosion-assembled atomic bomb during the Manhattan Project required explosives to be used in a new and different way. Rather than using explosives as bursting charges encased within metal shells for military effect, specially-designed charges were assembled so as to entirely encompass the fissile metal. When detonated, the spherically converging pressure wave compressed the fissile metal to a condition of nuclear supercriticality. In order to achieve this, precisely shaped pieces of solid explosives with accurately measured detonation velocities initiated by detonators with minimal timing irregularities (low jitter or high simultaneity) were required. This stimulated the science of high explosives performance to mature rapidly.

As military objectives evolved, more efficient implosion methods were investigated. New explosives were invented and sometimes the power within was released unexpectedly resulting in the tragic loss of human life. Administrative controls such as written operating procedures and remote machining operations were emphasized. In addition, the scope of high explosives science broadened to include a focus on understanding the potential mechanisms for *unintended* initiation. New methods for characterizing the safety of consolidated explosives charges, not just the precursor powdered forms, were developed. This paper recalls three fatal explosives accidents that instantly killed eight people within an eight-month period in 1959 and draws upon decades of experience by the authors in separate countries to emphasize the continuing need for science to play an essential role in explosives safety.

1020 - A Model to Account for the Effects of Friction During Explosive Pinch

R. Timms, R. Purvis, J.P. Curtis

Safety is of paramount importance in the handling, processing and storage of explosives. Mechanical insults resulting from low-speed impact, that crush and pinch an explosive, have been identified as a possible ignition source. However, modelling such an ignition mechanism numerically with

hydrocodes proves to offer some considerable challenges. Here we develop a model for the pinching of an explosive cylinder between two flat plates, which accounts for the effects of friction at the contact between the plates and the explosive. In this formulation it is assumed that as the material is compressed it is in perfect plastic flow under adiabatic conditions. The explosive reaction is modelled using a simple Arrhenius Law. The effects of friction are modelled by prescribing the shear stress at the boundary to be a fixed fraction of the yield stress in shear. We exploit the small ratio of sample height to radius, and a solution is sought as a correction to the uniform straining motion, allowing the heating of the explosive by mechanical dissipation and self-heating due to the reaction to be calculated. The work presented allows us to investigate the effects of frictional heating during compression, and arrive at an improved model of the pinching of explosive material between two flat plates.

13:50 DDT 3

968 - Deflagration-To-Detonation Transition for Hydrogen-Enriched Air Mixtures Through Pressure Wave Focusing in Pipes

S. Bengoechea, J. Gray, J. Reiss, J. Moeck, C. Paschereit, J. Sesterhenn

The use of detonation presents a more efficient alternative of releasing the chemical energy of fueloxidizer mixtures. The cornerstone of pulse-detonation-engines (PDEs) is the ability of producing a reliable deflagration-to-detonation transition (DDT) over a short distance. This is imperative for the application in gas turbines. This report describes the experimental and numerical study of DDT in a pipe obstructed by a single obstacle (an axisymmetric convergent-divergent nozzle). The combustion chamber is filled with a mixture of hydrogen-air, enriched to 40% oxygen (4/9 H2 + 2/9 O2 + 9/3 N2). The effects the proposed configuration has on the onset of detonation for PDEs has been analysed. For this purpose, different scenarios have been confronted, thereby, enhancing the understanding of the processes inside the pipe and bringing closer experiments and simulation by the use of data assimilation techniques. For one of the cases, the necessary parameters for a successful DDT are identified and the results indicate a close to 100% rate of success in the transition. This deterministic and reliable behaviour paves the way for a potential use in PDEs.

1027 - Numerical Study on Effects of Obstacle Shape on Detonation Transition Mechanism

A. Ago, T. Niibo, N. Tsuboi, A.K. Hayashi

In this paper, the numerical simulations on DDT (Deflagration-to-Detonation Transition) in the twodimensional channel with the repeated obstacles are performed for various BR (Blockage Ratio: the value obtained by dividing the height of the obstacles by the channel width) values.

According to past studies, it is found that detonation transition can be promoted when obstacles are installed the channel inner wall. In 2000, Dorofeev et al. introduced the characteristic geometric dimension *L* into the distance between obstacles installed at equal intervals in the channel. They showed that when the value (L/λ) obtained by dividing the length *L* by the detonation cell width λ exceeds 7, the detonation occurs. Although DDT has been investigated by many researchers, DDT has not been predicted theoretically because the DDT mechanisms change by physical conditions, for example, channel sizes and wall conditions.

This research intends to find out the mechanisms of the detonation transition in the channel with obstacles in order to understand the physical phenomena such as shock wave, turbulent flame, and local explosion caused by self-ignition by using the numerical analysis. In particular, two patterns of obstacles height are used to investigate the detonation transition mechanisms. In this paper, the calculation domain size is based on the one-twentieth scale of the experimental device used by Dorofeev et al. and two cases of obstacle heights are used in order to compare with their experiments. In the channel with repeated obstacles, a stoichiometric premix gas of hydrogen/oxygen is filled and a small energy source near the left end of the channel is located.

As a result, for BR = 0.3 and 0.45, the deflagration transits to the detonation. When the detonation transition occurs, the flame is largely disturbed. Then the flame is accelerated by the repeated local explosions, the compression and expansion in the flow path, and strengthened shock wave. And it is found that opportunities for DDT are different depending on the height of obstacles. Also, even if local

explosions occur, detonation transition is failed, and for BR = 0.45, the detonation transition is delayed as compared with BR = 0.3 because of high obstacles. Comparing with the experimental results, it is found that the effects of the geometry scaling, the ignition source, the wall condition, and three-dimensional depth should be estimated.

1022 - Quasi-Detonation in Matrix of Cylinders

P.N. Krivosheyev, A.O. Novitski, O.G. Penyazkov, K.L. Sevrouk

The propagation of fast deflagration and quasi-detonations in a layer comprised of matrix of 8-mm steel cylinders has been studied experimentally using high speed self-luminous observations.

13:50 Detonation Diffraction 1

1110 - Propagation Characteristics of 2H2/O2/2Ar Detonations in Channels with Constant Area Divergence

Q. Xiao, J. Chang, M. la Fleche, Y. Wang, M.I. Radulescu

Detonations propagating in channels with cross-sections increasing exponentially (exponential horns) have been shown to propagate at a constant average speed by Borzou and Radulescu. The magnitude of the lateral flow divergence controlled this speed. Beyond a critical value of flow divergence, detonations were not possible. Their previous studies showed that predictions made with the steady ZND model for the velocity deficit in the presence of lateral divergence disagreed with the experiments, with larger departures for more unstable detonations. The present study revisits their work for a much more stable mixture of $2H_2/O_2/2Ar$, with better known kinetics. The results of the present study show that indeed constant average speeds can be obtained for a fixed flow divergence. The variation of velocity deficits with flow divergence was found in excellent agreement with the predictions made with the steady ZND model with lateral divergence using the San Diego chemical mechanism for moderate divergence and small velocity deficits than predicted by the steady model, at larger lateral divergence. Visualization of the reaction zone structure revealed the presence of transverse detonations in the cellular structure. It can be speculated that these transverse detonations provide the mechanism for promoting the propagation of the cellular detonations.

984 - Propagation of a Detonation in a Converging Conical Channel

I.H. Hung, J.H. Lee

The present paper is an experimental study of a detonation propagation in a converging conical channel of cone angles of 6 degrees and 10 degrees. In the present study, we explore the amplification of converging detonations in gaseous mixtures generated in a small angle conical tube. Experiments were carried out in a round detonation tube which has a constant area section in which a fully developed steady C-J detonation is formed prior entering the converging section. Stoichiometric acetylene-oxygen mixture are used from initial pressures of 3 kPa down to 0.5 kPa as well as acetylene-oxygen mixture with 70% argon dilution from initial pressures of 16 kPa down to 4 kPa. The velocity measurement indicates an acceleration of the detonation from its C-J value as it propagates into the converging channel and also a progressive decrease in cell size is observed.

791 - Mechanism for Dynamical Stabilization of Detonation in Expanding Channels

X. Cai, J. Liang, R. Deiterding, Z. Lin, S. Liu

The mechanism of stabilization of detonation in expanding channels is investigated solving the reactive NS equations and one-step two-species reaction model using the hybrid high-order WENO-CD scheme based on the SAMR framework. The results show that generation and consumption of the unburned jet are enhanced for rapid periodical heat release due to the turbulent mixing resulting from large-scale vortices along the unburned jet, which can contribute significantly to propagation maintenance through chemical energy provision. In addition, further detonation attenuation is suppressed due to the formation of the hydrodynamic throat. These two effects combined together can lead to dynamical stabilization of detonation in expanding channels after the shutdown of the hot jet.

13:50 Combustion Stability, Instabilities 3

944 - Effects of External Heating on Flame Stability in A Micro Porous Combustor Fueled with Heptane

J. Li, X. Chen, M. Feng, R. Yao, N. Wang

Effects of external heating on flame stability in a micro porous combustor are investigated experimentally. The flammable limits, extinction delay time and low-temperature oxidation are studied. Results show that external heating can extend flammable limits in micro porous combustor and the limits at heating temperature of 525.7 °C is much wider than that at normal state. After stopping external heating, the flame oscillates and then becomes unstable, finally extinguishes. The time between stopping heating and flame extinction is defined as extinction delay time and it increases with heating power. The shortest delay time is 15.7 s at U=9.6 V. When heptane and air are injected into heated porous medium, whose temperature is between 160.1 °C and 488.1 °C, low-temperature oxidation reaction takes place and it contributes to enhancing flame stability in the micro-combustor.

1036 - Tomographic Visualization of Thermo-Diffusive Instabilities of Lean Hydrogen/Air Mixtures

J. Goulier, N. Kouame, M. Idir, N. Chaumeix

In case of a severe accident in a nuclear power plant with core meltdown, large amounts of hydrogen can be produced by the oxidation of the fuel sheathing with the cooling water or the interaction of the molten corium with the concrete and structure elements. Since hydrogen/air mixtures are characterized with very low ignition energy the presence of a hot surface may lead to ignition and propagation of a slow flame. During its propagation, the flame can accelerate to a fast flame that can cause high pressure loads threatening the integrity of the containment building. Hence, it is mandatory to identify the phenomena that are responsible for this flame acceleration. Promptly after ignition, the surface of the flame wrinkles due to the Darrieus–Landau and the thermo-diffusive instability. The aim of this work is to characterize the wrinkling of the flame surface after ignition responsible for an early acceleration of the flame.

In order to measure the wrinkling of the flame surface, two complementary optical systems will be used, a schlieren imaging system and a laser tomography. A schlieren system is a non-intrusive technic based on the thermal gradient of the flame front where the observed flame is projected onto a screen (line of sight). Using schlieren system, depth of the wrinkled flame surface is hidden. Whereas laser tomography system allows us to observe a cross-section of a flame and therefore the depth of the wrinkles on the flame surface. On the other hand, tomography requires seeding which can impact the flame propagation.

This work will two aims: (i) to quantify the effect of seeding on the propagation of lean hydrogen/air flame, (ii) to estimate the surface of wrinkle of flame during its propagation.

887 - Edge Flame Dynamics - Assisting the Stabilization of Diffusion Flames in Mixing Layers *Z. Lu, M. Matalon*

In this paper we show that the various possible mechanisms of flame stabilization in mixing layers depend on the structure of the edge flame sustained near the splitter plate or further downstream in the flow, its stability (or dynamics), and on the heat exchange between the edge flame and the plate.

16:20 Energetic Materials 1

1054 - Burning Characteristics of Aluminum-Air Flames

R. Lomba, F. Lespinasse, V. Lago, C. Chauveau, F. Halter

Metal particles are highly energetic, and therefore present an interesting potential for carbon-free energy carrier. Its combustion in air, in particular, can lead to elevated specific energies. This work presents an experimental study of aluminum-air flames stabilized on a Bunsen-type burner and obtained using an aluminum powder of whose average particle size is of 7 µm. The experimental setup is shown to produce stable dust suspensions under well-controlled conditions. The flame contour is determined using two different techniques: Abel deconvolution of the AIO emissions, and laser sheet

tomography. The mixture's burning velocity is then obtained using the ratio between the volumetric flow rate and the total flame surface calculated from the flame contour. Flame temperatures are estimated by fitting a theoretical AIO emission spectrum to the experimentally measured emissions. It is observed that both burning velocities and flame temperatures remain stable when the solid fuel concentration ranges from 260 g/m³ to 450 g/m³, and are about 28 cm/s and 3150 K, respectively. Moreover, burning velocities obtained in the burner presented in the current work with the tomography technique are shown to present a lower reproducibility error when compared to previous literature. It is therefore shown that the aluminum powder used presents a specific energy and burning velocities that are comparable to traditional hydrocarbon fuels.

799 - Spherically-Expanding Flames in Hybrid Aluminum-Methane-Oxidizer Mixtures at Atmospheric Pressure

J. Vickery, P. Julien, S. Goroshin, J.M. Bergthorson, D.L. Frost

Spherically-expanding flames propagating through hybrid aluminum-methane-oxidizer mixtures are studied in the present work. Transparent latex balloons are used to contain the dust-combustible gas mixtures, which allows for the flame propagation to occur at constant pressure while also permitting the visual analysis of both the dust dispersal and flame propagation process. In fuel-rich methane-oxidizer combustible gas mixtures (i.e. no excess oxygen in methane flame products), the aluminum acts as an inert diluent at low concentrations, resulting in reduced flame speeds. At a concentration of about 100 g/m³, the flame speed stops decreasing and remains constant with further increases in aluminum concentration, a behavior associated with the formation of an aluminum flame front which thermally couples to the leading methane flame. In mixtures where there is excess oxygen in the methane combustion products, the flame speed monotonically increases with aluminum concentration before also reaching a plateau at higher concentrations. This increase in flame speed at low aluminum concentrations is attributed to the ability of aluminum particles to ignite when oxygen is present to react. When the particles ignite, they burn in the diffusion limited regime where reaction rates are largely independent of the surrounding gas temperatures, which allows for relatively high reaction rates at the relatively low temperature of the methane flame.

948 - Experimental Study on Effect of Large-Sized Granules in Powdery Explosives Under Drop-Weight Impact

Y. Wu, H. Guo, F. Huang, X. Bao

Drop-weight impact experiments are performed on a thin layer of cyclotetramethylenete tranitramine (HMX) and cyclotrimethylene trinitramine (RDX) powdery explosives, which was mixed with a few large-sized crystals and NaCl salt granules. The drop-weight impact machine is equipped with the high-speed photographic systems for observing the experimental process. The influences of large granules on the low-velocity impact response of powder explosives were studied. Experimental results showed that the mixed explosives are more sensitive than pure powdery explosives Hard salt particles could greatly enhance burning probability of powdery explosives because friction between granules and powders, stress concentration and breakage of large granules jointly contributed to heat accumulation at the junction of dissimilar materials.

16:20 Shock Tubes, Ignition Delay Times, Kinetics 1

812 - Ignition Delay Times of Methane/Diethyl Ether Blends Measured in a Rapid Compression Machine (RCM)

S. Drost, M. Werler, R. Schießl, U. Maas

Despite the interest in using diethyl ether as ignition enhancer in combustion engines, there are, to our best knowledge no fundamental studies on the auto-ignition of methane/DEE-mixtures. Therefore, in this work, different methane/DEE-mixtures have been investigated. The experimentally obtained data were used for comparison with a recently published reaction mechanisms for pure DEE/air-mixtures. This work will explain the experimental procedure, present the measured ignition delay times, and study the promoting effect of DEE on methane auto-ignition and in which regimes the mechanisms can

reproduce the ignition delay time, despite the fact that they are originally not made for CH4/DEE/airmixture with a low ratio of DEE/CH4 (5 mol-% to 10 mol-% DEE of fuel).

957 - Experimental and Numerical Study of the Ignition Delay Times of Primary Reference Fuels Containing Diethyl Ether

M. Fikri, Y. Sakai, J. Herzler, C. Schulz

Ignition delay times of lean and stoichiometric mixtures of the primary reference fuel PRF95 doped with DEE (10 and 30 Vol.%) were measured between 650 and 1250 K at pressures of 10 and 40 bar. The experiments show that DEE drastically increases the reactivity of the base fuel. The model for gasoline surrogates of Cai and Pitsch (Combust. Flame 2015) was embedded in a new DEE mechanism of Sakai et al. (Combust. Inst. in press), in which important low-temperature species such as QOOH and O_2QOOH were considered. The prediction of the measured ignition delay time data by the new model was very good.

1149 - Ignition Delay Time Measurements of Sarin Surrogate (TEP, DMMP)-Based Mixtures in a Heated Shock Tube

O. Mathieu, W.D. Kulatilaka, E.L. Petersen

To defeat a potential terrorist attack involving chemical warfare such as Sarin ($C_4H_{10}FO_2P$), the most likely scenario relies on the use of a conventional weapon with an energetic material payload. However, little is known on the high-temperature chemistry of Sarin. To provide capabilities for eliminating the threat efficiently or, at least, to mitigate its effects, it is therefore necessary to understand the detailed combustion chemistry of Sarin over a wide range of conditions. To help in refining and developing detailed kinetics models, ignition delay times of various mixtures based on common Sarin surrogates, namely dimethyl methylphosphonate (DMMP, C₃H₉O₃P) and tri-ethyl-phosphate (TEP, C₆H₁₅O₄P) were measured. Mixtures of simulants and O₂ diluted in 99% Ar were investigated at 3 equivalence ratios: 0.5, 1.0, and 2.0 for TEP and at an equivalence ratio of 0.5 only for DMMP. To assess the effect of the simulants on the combustion chemistry of hydrocarbons, mixtures of methane/oxygen diluted in Ar and seeded with DMMP or TEP were also investigated at the same 3 equivalence ratios. The amount of Sarin surrogate added corresponded to 10% of the fuel concentration. Finally, a fuel lean mixture of H₂/O₂ seeded with DMMP or TEP was also studied. Results showed an unusual behavior on the OH* profile when the stimulants were studied alone, where the appearance of the OH* always occurred shortly after time zero and rise to a maximum that varies significantly with the temperature. When added to either H₂ or CH₄ mixtures, the OH* profiles present the same behavior as for the neat mixtures, but the reactivity is changed noticeably in most cases. The comparison between the two Sarin surrogates demonstrates stark differences in their reactivity, for all conditions and mixtures investigated. This difference shows that proposing an accurate combustion model for Sarin probably necessitates studying several Sarin surrogates; each Sarin simulant representing one part of the structure of Sarin. The data presented herein will be useful to validate and develop chemical kinetic models for DMMP and TEP, and once these models have been developed and validated on a common base, it will be possible to assemble with more confidence a detailed kinetics model for Sarin.

1075 - Ethene / Dinitrogen Oxide - A Green Propellant to Substitute Hydrazine: Investigation on Its Ignition Delay Time and Laminar Flame Speed

C. Naumann, T. Kick, T. Methling, M. Braun-Unkhoff, U. Riedel

The fundamental combustion properties of ethene/dinitrogen oxide mixtures that have the potential to substitute hydrazine/dinitrogen tetroxide in chemical propulsion systems was investigated. Ignition delay times of shock heated stoichiometric C2H4/N2O mixtures diluted 1:5 with nitrogen were measured at initial pressures of 1, 4 and 16 bars, resp., as well as laminar flame speeds of C2H4/N2O mixtures diluted 1:2 with nitrogen at atmospheric and at elevated pressures. Initially, the predictive capability of an adapted public domain reaction mechanism based on the GRI 3.0 was tested. Finally, a linear transformation model approach was applied to a subset of five nitrogen reactions and the collision enhancement factor of N2O in order to achieve an optimized version of the adapted reaction scheme consistent with the measurements.

16:20 Detonation Engines 4

1046 - Numerical Investigation on the Behavior of Detonation Waves in a Disk-Shaped Rotating Combustor

Y. Sato, A. Matsuo, J. Higashi, C. Ishiyama, K. Matsuoka, J. Kasahara

Behavior of detonation waves in a disk-shaped rotating combustor is numerically investigated. A calculation target is the disk-shaped Rotating Detonation Turbine Engine (RDTE) that Nagoya University experiments with. The disk-shaped RDTE has a centrifugal compressor, a combustor, and a radial turbine on the same disk. In this study, the turbine is neglected for simplicity. First, the effect of the combustor shape is examined. A rectangular domain and an annular domain correspond to a conventional double cylindrical combustor and the present disk-shaped combustor respectively. The pressure and temperature of the annular domain are lower than those of the rectangular domain because the flow field is more influenced by expansion. The detonation propagation velocity is almost the same as the CJ velocity in both cases. The detonation wave height and the injection rate are higher in the annular domain. Second, the effect of the disk rotation is examined. Premixed jet pillars tilt to the left in the clockwise cases and to the right in the counterclockwise cases compared with the stationary case because of the Coriolis force. Therefore, the detonation propagation angular velocity relative to the disk becomes higher in the clockwise cases and lower in the counterclockwise cases. The detonation wave height and the normalized mass flow rate become higher in the rotating conditions. The turbine inlet angle is smaller when the rotating direction of the disk and detonation is opposite and it would be preferable for the turbine.

1103 - Numerical Investigation on Detonation Behavior in a Disk-Shaped Rotating Detonation Combustor

Y. Kumazawa, A. Matsuo, S. Nakagami, K. Matsuoka, J. Kasahara

The numerical simulation for the detonation wave propagation in a disk-shaped rotating detonation combustor is conducted. The purpose of this paper is to clarify the effect of wall curvature and the combustor height on the detonation behavior. Governing equations are two-dimensional Navier-Stokes equations with reduced kinetic reaction model for C_2H_4 - O_2 . The length of outer radius $r_{out} = 25.46$, 50.93 mm and the calculation region height h = 10.24, 20.48 mm are used. Injection gas is stoichiometric premixed condition and imaginary conversing nozzle is adopted. The following knowledge is obtained through the calculations. The value of h/r_{out} is the dominant parameter for the detonation behavior, not the curvature of the outer wall having the injection port, in the disk-shaped rotating detonation combustor. When h/r_{out} is small, detonation waves keep steady propagation. On the other hand, the detonation cannot be observed in $h/r_{out} = 0.82$. The pressure peaks is lower than other h/r_{out} cases, and the pressure at non-injection region is higher.

1097 - A Numerical Study of H2-Air Rotating Detonation Combustor

S. Yellapantula, V. Tangirala, K. Singh, J. Haynes

One of the major technical challenges encountered while developing rotating detonation combustor (RDC) for propulsion or energy generation applications can be relatively poor combustion efficiency (relative to deflagration based combustion) and resulting high levels of emissions especially in combustors with smaller residence times. In the current computational study, an attempt has been made to improve our understanding of mechanisms behind emissions and poor combustion efficiency. The primary motivation for this computational research stems from the need to perform trade studies of RDC to understand the effect of operating and inlet parameters on the RDC performance metrics.

Results from three-dimensional simulations of a H2-air atmospheric RDC are presented in this study. Starting from an ignition kernel in the initiator tube unsteady simulations are performed in a way to reflect the operation of the RDC in the experimental studies. Focus of this study is devoted towards understanding:

Detonation diffraction from the initiator tube into the channel annulus; Influence of fill height and bifurcation of detonation into multiple fronts; Impact of fuel-air mixing on detonation stabilization.

1106 - Generation of Detonation in a Supersonic Flow of Combustible Mixture with Use of Bended Channel

V.A. Levin, I.S. Manuylovich, V.V. Markov

The problem of detonation initiation in a supersonic flow of stoichiometric propane-air mixture occupying the entire cross-section of a plane or 3D bended channel is considered. Detonation is initiated as a result of the formation of shock wave configurations associated with the flow turn in the channel. The time-dependent flow patterns are obtained and their dependence on the problem parameters (incoming flow velocity, channel width, channel turn angle, and radii of curvature of the walls at the bend location) is investigated. The flow regime diagram is constructed in the velocity-channel turn angle plane. The numerical calculations show that the radius of curvature of the channel bend has almost no effect on the position of the critical curves separating different flow regimes. It is established that the detonation propagation pattern depends on the ratio of the channel width to the radius of curvature. The investigation is carried out using the special software package intended for solving the problem considered.

16:20 Detonation Failure and Propagation

908 - Detonation Failure in Stratified Layers - the Influence of Detonation Regularity

A.V. Gaathaug, K. Vaagsaether, D. Bjerketvedt

The detonation propagation in stratified layers of reactants bound by one solid and one inert boundary is of interest from a safety perspective. This study has started to investigate the failure of detonation as it propagates into a stratified reactant layer. The idea behind the study was to investigate if detonations with irregular cellular structure can propagate further into the reactant layer compared to detonations with regular cellular structure. The regularity was studied by varying the heat of combustion and an activation energy. A finite volume 2D CFD method was used, by solving the Euler equations and using a two-step reaction model. The first reaction was an isothermal reaction in the induction zone, while the second reaction was the exothermic reaction. The activation energy of the first reaction was changed to investigate the regularity of the detonation. The computation was simplified to get 10 cells in the induction zone. This was achieved to adjust the pre-exponential factor of the induction zone reaction. A developed detonation was used as an initial condition, and a layer of inert was inserted in the computational domain. The more stable detonations failed as the triple points diffracted into the inert

layer, while the more irregular detonations were able to generate new triple points in the reactant layer but eventually failed as well.

776 - Effect of Vertical Concentration Gradient on Detonation Behavior with Detailed Reaction Mechanism

W. Han, W. Kong, N. Du, Z. Liu

A detonation propagating in H_2 -O₂ mixture with concentration gradient is simulated by a highresolution code based on the fifth-order Weighted Essentially Non-Oscillatory (WENO) scheme in spatial discretization and the 3rd-order Additive Runge-Kutta scheme in time discretization and detailed chemical kinetics model. It is found that concentration gradient enhances largely the instability of the detonation, leading to galloping behave. In the propagation, reinitiaition can be triggered by the local explosion in the fuel-lean layer and the resulting transverse detonation makes the explosion wave propagate and decay into inert shock in the fuel-rich layer. The possibility of the detonation survive is enhanced due to both the occurrence of the spontaneous local explosion and the presence of the transverse detonation, although the instability of the detonation globally increased by the transverse concentration gradient.

1013 - Experimental Investigation of Detonation Failure and Re-Initiation in Non-Uniform Compositions

S. Boulal, P. Vidal, R. Zitoun, T. Matsumoto, A. Matsuo

In many situations of practical interest, accidental or intentional reactive mixtures present nonuniformities of composition. For example, the explosive clouds formed with the air after leaks from tanks or ducts involve spatial distributions of composition. In detonation engines (PDE, RDE), the

mixture non-uniformities result from the imperfect mixing of the fuel and of the oxidizer, and to the presence of residual burnt gases. This work is an experimental investigation into the dynamical behavior of detonation in non-uniform mixtures of propane, oxygen and ethane at initial pressure and temperature of 200 mbar and 290 K, respectively, with non-monotonic distributions of Equivalence Ratio parallel to the direction of detonation propagation. Compositions gradients were realized by means of a planar successive injections of the mixture components. The non-uniform distributions in a 665-mm-long, 50x50-mm²-cross-section vertical chamber were then controlled by molecular diffusion with the diffusion time defining the composition gradient. A Chapman-Jouguet multicellular detonation was transmitted at the chamber bottom-end from a 3.6-m-long driver tube connected to the chamber. Sooted plates and schlieren visualizations were used to characterize the unsteady dynamics of the detonation such as failure and re-initiation mechanisms. Supercritical, critical and subcritical behaviors were identified, depending on whether the detonation was transmitted or not from the domain where the equivalence ratio decreased to that where it increased. In regions of decreasing reactivity, the failure criterion previously proposed was found to well predict shock-flame decoupling. A failed detonation can re-initiate depending essentially on the Mach reflections strength of transverse waves at side walls. This detonation re-initiation process could be part of the explanation for the transition to counter-rotating modes observed in Rotating Detonation Engines.

1030 - Numerical Investigation of Detonation Failure in Non-Uniform Compositions and Comparison to Experiments

T. Matsumoto, S. Boulal, A. Matsuo, P. Vidal, R. Zitoun

For safety of industrial processes and specific applications such as detonation engines, detonation behaviors in non-uniform compositions should be analyzed. This study is a numerical investigation into the detonation dynamics in mixtures with composition gradients parallel to the propagation direction with monotonic Equivalence Ratio distributions. First, in order to validate the simulations, comparisons between numerical and experimental sooted plates are presented. The two typical detonation failure mechanisms observed in a previous experimental investigation, i.e., a sudden one through shock-flame decoupling and a progressive one with transition to marginal propagation modes, were successfully reproduced. The then-proposed shock-flame decoupling criterion was numerically implemented and found to provide a good prediction of this type of failure mechanism and therefore, a good validation tool for numerical simulations of detonation marginal propagation was also considered. For the same initial composition distribution, the larger the transverse width, the further the detonation propagation. This work demonstrates the ability of numerical simulations to reproduce the complex dynamics observed in experiments of detonation propagation in non-uniform compositions.

16:20 Reactive Systems 3

1102 - Calculation of Thermo-Chemical Equilibrium Using Phase Diagram Methods

A.E. Gheribi, J.J. Lee

The present work describes a method to perform thermo-chemical equilibrium calculations for reactive systems with a high fraction of condensed-phase products, such as thermites and metal-sulphur mixtures. Equilibrium codes designed for gaseous products such as CEA or CHEETAH use equations of states that are not well-suited for condensed phases and typically become increasingly inaccurate as the fraction of solid or liquid products increases. In contrast, CALPHAD (Calculation of Phase Diagrams) [1]– type software is designed specifically to handle condensed phases and uses polynomial thermodynamic functions to represent the phase diagrams of a wide range of metals, oxides, and salts. This formulation is well-suited for solution-finding in condensed phase space, especially with mixtures of different substances. The method can be used to analyze systems with little to no gaseous products, and can be used for calculations of various combustion modes such as constant pressure flames known as Self-propagating High-temperature Synthesis (SHS) reactions. A particular case of interest was the possible existence of gasless detonation, or heat detonation, and CALPHAD methods were previously

used to analyze this mode of combustion in AI-Fe2O3 mixtures [2]. The presence of several condensed phases in the products leads to complex shock states, and the Chapman Jouguet (C-J) detonation solution is not straightforward for systems with complex phase diagrams which give rise to shock Hugoniot curves that do not have a smooth hyperbolic shape. As a result, a single tangency solution may or may not be possible. The existence of gasless detonation thus depends on additional criteria compared to traditional gaseous detonations. The dependence of the shock states on the condensed phase behavior, and its subsequent effect on the C-J detonation solution are discussed, and three test cases are shown with the Ti-Si, Zn-S, AI-Fe₂O₃-AI₂O₃ systems.

1076 - Turbulent Fuel Droplet Vaporization and the Initial Size Effect: Experimental Data at Elevated Temperature and Pressure

C. Verwey, M. Birouk

The experimental results presented in this paper represent an initial effort to understand the complex relationships between fuel droplet vaporization and several influencing parameters which include droplet initial diameter, turbulence, pressure, and temperature. Droplets with diameters ranging between 110 and 730 μ m have been successfully generated and examined. The effectiveness of turbulence increases with pressure at all droplet sizes, whereas the inverse scenario happens with temperature. Furthermore, conditions under which *d2-law* behavior deviates from linearity are identified.

958 - Numerical Investigation on the Initial Development of Layered Coal Dust Combustion *K. Shimura, A. Matsuo*

The flame acceleration mechanism of layered coal dust combustion inside the 2D narrow channel is numerically investigated by using Particle-In-Cell method based on solid/gas two-phase theory to treat discontinuous particle behavior. Particles are layered at the bottom in inert air, and strong shock wave generated by gaseous detonation is used to initiate layered dust combustion. The flame acceleration and supersonic propagation appear after 15 ms from initiation and their structure is similar to diffusion flame. The advection velocity of this flame exceeds the propagation velocity of leading shock wave initially set to initiate the combustion. The mechanism of flame advection is as follows. First, the reaction front is formed at the contact surface between atmospheric air and devolatilized CH4. Gas temperature increases at the reaction front and dust particles are heated and are ignited. The devolatilization of coal-dust mainly occurs 3 m behind the reaction front and CH4 gas spreads. Then, pressure and gas density dramatically increase and pressure gradient is generated. Finally, devolatilized CH4 catches up the reaction front due to the acceleration by the pressure gradient.

1035 - Impact of Water Mist on Chemical Reaction of Methane/Air/Water-Mist Premixed Flames

S. Nakanishi, Y. Ogami, M. Ito, T. Tsuruda

Measurements of the flame speeds of $CH_4/air/water-mist$ were conducted under the conditions of the wide range of the equivalence ratios and the high water mass fractions. The numerical simulations considering the detailed chemical reactions were also conducted, and the numerical results were compared with the experimental data. Moreover, the effects of the water mist on the chemical reaction were conducted by using the sensitivity analysis.



09:00 Ignition 3

1064 - Flame Speed Measurements in Turbulent Dispersions of Liquid Fuels

P.M. de Oliveira, T. Higuchi, P.M. Allison, E. Mastorakos

This work focuses on the experimental evaluation of flame speed of uniform multi-component fuel dispersions in a turbulent air flow. A spherically-expanding flame was observed by igniting the flame with a laser beam in a spatially homogeneous droplet flow, and visualized using schlieren and OH*-chemiluminescence imaging. Jet A and two other alternative fuels for aviation were investigated. The unburned flame speed was estimated based on the burned flame speed measurements and additional data for each fuel, exhibiting significant differences between the fuels and with changes in the mixture composition and flow parameters. Overall, the experiments have shown a strong dependence of the measured flame speed and the volatility of the fuels, being the lowest for Jet A under the experimental conditions of this work, and directly proportional to the turbulence levels and degree of prevaporization of the mixture.

910 - A Simulation of Ignition Thresholds for Low Voltage Electrical Contact Arcs in a Hydrogen-Air Mixture

R. Shekhar, C. Uber, U. Gerlach

The contact arc is an electrical discharge which occurs due to the motion of energised electrodes, such as the opening and closing of electrical contacts. This type of discharge is an important ignition source in the field of explosion safety. Although several practical measures exist for managing this risk, all are reliant on empirical data and procedures which are difficult to reproduce and verify. Through the application of modelling and simulation, it is hoped that a fundamental understanding of the contact arc's properties as an ignition source can be developed, paving the way for a more scientifically justifiable approach to managing the explosion risk.

The contact arc has several characteristics that distinguish it from better known arc discharges and high voltage sparks. These include relatively low voltages (up to 50 V) and currents (usually < 1 A). Another important defining characteristic is the duration of the discharge, which can range from 30 us up to several milliseconds, as well as the variation of size and power output over this duration. This has significant implications for the ignition process, as minimum ignition energy is strongly influenced by energy deposition time.

This study examines the relationship between these transient energy deposition characteristics, their associated losses, and ignition thresholds, using a three dimensional reactive flow simulation coupled with an empirical approximation of the discharge. Two common characteristic values, namely the minimum ignition energy and minimum ignition kernel radius, are estimated for different combinations of source parameters. Simulation results are also compared to a classical one dimensional theory.

Simulations showed that both minimum ignition energy and minimum ignition kernel radius vary according to the transient properties of the contact arc. Values of minimum ignition kernel radius were somewhat larger, though comparable in order of magnitude to those predicted by the 1-D theory.

1021 - A Computational Study of the End Gas Autoignition and Shock Development by Flame Front and Local Hot Spot

A. Sow, B.J. Lee, H.G. Im

In the present paper, direct numerical simulations were conducted to probe the interaction between a flame front and a local hot spot in engine configuration. An adiabatic configuration was considered here and the hot spot was represented by a small region with a pressure gradient. H2/air mixture was used in this study. The results show that the presence of local hot spot accelerates detonation development that leads to high pressure pikes which can damage the moving parts of the engine.

In internal combustion applications, effects of heat losses at walls are important; therefore, additional computations considering wall heat losses need to be investigated. Furthermore, combined effects of temperature and mixture concentration will be investigated in order to represent realistic engine conditions. We hope to report on these points during the oral presentation.



09:00 Explosion Safety 4

884 - Electrochemical Reaction Kinetics for CO-CO2 Electrochemical Conversion in the Nickel-Patterned Electrode

Y. Luo, Y. Shi, W. Li, N. Cai

In this study, the possible mechanism of CO-CO2 electrochemical conversion was proposed according to existing reference, and the rate-determining steps were analyzed based on the analytical calculation and experiments in the nickel-patterned electrode to understand the relation between the electrochemical pathway and carbon deposition/consumption. The analytical calculation shows that carbon deposition/consumption was likely to be relevant to the electrochemistry in the nickel-patterned electrode, especially in SOEC mode. In SOFC mode, CO electrochemical oxidation into CO2 was more probably the major electrochemical reaction while adsorbed carbon also could be oxidized into CO. In SOEC mode, the reaction rate of CO2 electrochemical reduction could be inhibited due to difficult CO2 adsorption, hence, CO reduction into carbon could be more probably the major electrochemical reaction rate of more probably the major electrochemical reaction in the nickel-patterned electrode.

826 - Blast From Pressurized CO2 Released Into a Vented Chamber

P.M. Hansen, A.V. Gaathaug, D. Bjerketvedt, K. Vaagsaether

This paper presents results from small-scale experiments on the release of saturated pressurized CO_2 from a high-pressure reservoir at temperature 19 °C into a vented atmospheric chamber. The main goal was to investigate the effect of vent opening and initial liquid content on the measured pressure and calculated impulse response in the atmospheric chamber. In addition, an objective was to study if the volume increase resulting from the rapid boiling would contribute to shock strength in the current test geometry. The contribution includes experimental results from two different vent-opening areas (100 and 10 cm²) and two different liquid portions (vapor only and a liquid/vapor mixture). The rapid phase transition (boiling) did not contribute to the initial shock strength in the current test geometry. The boiling process seemed too slow or the release rate from the high-pressure reservoir was to low to contribute to the measured peak pressure, which was in the range 0.15-0.20 barg. The test runs with a liquid/vapor mixture CO_2 in the high-pressure reservoir, showed a significantly higher impulse (time integrated pressure response) compared to test runs with vapor phase only. Reducing the vent opening on impulse was evident in the test runs with vapor only, but not so clear in the test runs with the liquid/vapor mixture.

943 - Flame Spread Over Electrical Wires with Various Diameters Under Applied AC Electric Fields

S.H. Park, S.J. Lim, J. Park, O.B. Kwon, O. Fujita, S.H. Chung

An experimental study on spreading flame over electrical wire, which was insulated by Polyethylene (PE) and had different diameters, was conducted with applied AC electric field. The result showed that the flame spread rate decreased in increase of the diameter of insulator at a fixed electric field. The flame spread rate exhibited increase or decrease tendency with applied AC electric field, having three distinct regimes depending on applied voltage and frequency. In each regime, the flame spread rate was characterized by applied electric field, and wire dimension and its behaviors could be explained by a thermal balance mechanism.

09:00 Detonation Modeling

914 - Numerical Computation of Linear Stability of Detonations

D.I. Kabanov, A.R. Kasimov

Linear stability of detonation waves is analyzed by means of numerical calculation of time-dependent solutions of linearized Euler equations. No assumption of normal modes is used which helps avoid solving singular systems of ordinary differential equations that arise in normal mode analysis. Here we present the method for the case of one-dimensional flow of an ideal chemically reacting gas with one-
step irreversible reaction $A \rightarrow B$. Neutral stability boundaries in the plane of heat release vs activation energy are calculated and compared with predictions by normal mode analysis.

892 - A Full Scale Hydrodynamic Simulation of Detonation and Deflagration in an Energetic Component System

B. Kim, J.J. Yoh

A full scale hydrodynamic simulation which necessary to accurately reproduce shock-induced detonation is conducted to analyze the reacting flow of an energetic component system. An explosive train configuration composed of detonator (HNS+HMX) / bulkhead (STS) / acceptor (RDX) / pyrotechine propellant (BKNO3) was considered to measure the release pressure wave into 10 cc enclosed chamber for quantifying the inherent oscillatory flow induced by the interferences between shock and rarefaction waves. The pressure fluctuation measured from experiment and calculation was investigated to further validate a peculiar peak at a specific characteristic frequency ($\omega = 8.3 \text{ kHz}$) representing intrinsic oscillation in the chamber. Since the present methodology for analyzing the energetic component system involving detonation of high explosives, deflagration of propellant, and deformation of confinement system is quite straight forward, one needs to properly implement the outlined formulation into a shock physics code for a full scale hydrodynamic simulation involving such energetic components.

1122 - A Toy Model for Detonations and Flames

L.M. Faria, S. Lau-Chapdelaine, A.R. Kasimov, R.R. Rosales

We propose a new toy-model for combustion which includes, when restricted to the corresponding limits, both diffusion flames and weakly nonlinear detonations. The equations, although simpler than the Navier-Stokes system, still pose an interesting challenge. For a fixed set of physical parameters, exact traveling wave solutions can be found which resemble either a diffusion flame, or a detonation. Through numerical simulations we investigate the stability properties of such traveling waves and examine their long-time behavior.

09:00 Detonation Diffraction 2

962 - Propagation Behavior of Diverging Cylindrical Detonation in Mixture with Reactivity Change

T. Okada, A. Matsuo, J.H. Lee

The aim of this work is to clarify the propagation mechanism including local re-initiation and quenching of a diverging cylindrical cellular detonation front. In this paper, the effect of the activation energy and shock front disturbances on propagation behavior of cylindrically expanding detonation wave is investigated. As a result, the activation energy affects both the onset and propagation behavior of a diverging cylindrical detonation. Firstly, the critical energy for lower activation energy case tends to be lower than the value for higher activation energy case. Propagation behavior in the 1st stage depends more on the source energy. Secondly, shock front disturbances formed in the 1st stage affect the propagation more than the activation energy and the source energy in the transition stage. In the 1st and transition stage, it is easier for diverging cylindrical detonations to propagate in the lower activation energy. Finally, once the detonation propagates into the 2nd stage, the activation energy is the most dominant factor of the diverging cylindrical detonation propagation behavior.

1112 - Prediction of the Critical Curvature for LX-17 with the Time of Arrival Data From DNS

J. Yao, L.E. Fried, W.C. Moss

We extract the detonation shock front velocity, curvature and acceleration from time of arrival data measured at grid points from direct numerical simulations of a 45 mm rate-stick lit by a disk-source, with the ignition and growth reaction model and a JWL equation of state calibrated for LX-17. We compute the quasi-steady (D, kappa) relation based on the extracted properties and predicted the critical curvatures of LX-17. We also proposed an explicit formula that contains the failure turning point, obtained from optimization for the (D, kappa) relation of LX-17.

781 - The Methods of Control of Stabilized Detonation Location in a Supersonic Gas Flow in a Plane Channel

V.A. Levin, T.A. Zhuravskaya

Using a detailed kinetic model of chemical interaction, detonation stabilization in a stoichiometric hydrogen-air mixture flowing at a supersonic velocity into a symmetric plane channel with constriction the outflow section of which is more than the inflow one, and possibility of control of stabilized detonation location in the flow have been studied.

In case of detonation initiation by energy input, the investigation of conditions of formation in the channel of a thrust developing flow with a stabilized detonation wave was carried out. The effect of variations of the inflow Mach number, the dustiness of the inflowing gas mixture and the width of the outflow channel cross section on stabilized detonation location was examined with the purpose of thrust increase. Several methods of controlling of detonation location in the flow have been proposed. The possibility of formation of the thrust developing flow with stabilized detonation in the channel under consideration without any energy input has been detected.

09:00 Spherical Explosions

1007 - Effects of Endothermic Chain-Branching Reaction on Spherical Flame Initiation and Propagation

H. Li, H. Zhang, Z. Chen

This work aims to determine how the endothermicity of chain branching reaction influences the premixed flame initiation and propagation. A theoretical model containing endothermic chainbranching reaction and exothermic recombination reaction is derived and the simplified Zel'dovich-Liñán model is used. Unlike previous studies, we consider the endothermicity of the chain-branching reaction. Within the framework of large activation energy and quasi-steady assumptions, the analytical solutions for the distributions of fuel mass fraction, radiation mass fraction and temperature are obtained and a correlation describing spherical flame propagation is derived. Based on the correlation, the effects of endothermic chain-branching reaction on stretched spherical flame propagation speed, Markstein length, unstretched planar flame speed, ignition kernel development and critical ignition conditions are examined. As the endothermicity of the chain-branching reaction increases, the flame propagation speed decreases while the Markstein length increases, indicating that the stretched flame is more sensitive to stretch rate. As for the ignition process, the critical ignition power and the critical ignition radius both increase monotonically with the endothermicity of the chain-branching reaction. Therefore, the endothermicity of the chain-branching reaction inhibits the ignition process. For both premixed spherical flame propagation and initiation, the effects of endothermicity become stronger for weaker flames.

867 - Dynamic Behavior of Spherically Expanding Flame of H2/Air/CO2 Mixture in a Closed Chamber

T. Katsumi, K. Aiba, Y. Itakura, S. Kadowaki

As the first step to understanding flame propagation characteristics of hydrogen-based multicomponent mixture, combustion experiments of $H_2/air/CO_2$ mixtures were conducted in a closed chamber. Previously, we established an experimental apparatus and performed combustion experiments of H_2/air mixtures in the closed chamber which has four large windows 300 mm in diameter. In the previous experiments, flame propagation behaviors of H_2/air mixture were observed by schlieren photography using a high-speed video camera, and flame propagation velocities were measured analyzing the schlieren images. In this study, we also obtained propagation characteristics of spherically expanding flames of $H_2/air/CO_2$ mixtures varying the equivalence ratio and CO_2 concentration at the same experiment apparatus as the previous study. Based on the results, we examined influences of mixture composition on flame propagation velocity, cellular flame structure, and onset flame radius of flame acceleration. Moreover, we proposed a simple calculation model of the flame propagation velocity.

10:45 Ignition 4

907 - Experimental Investigation of the Electrical Characteristics of Low-Voltage Contact-Arcs in Hydrogen-Air Mixture

C. Uber, R. Shekhar, U. Gerlach

Low voltage discharges occurring between opening electrical contacts are a potential ignition source in flammable gas mixtures. For safe operation in hazardous areas equipment is approved according to an international standard. For deriving the limit values in the standard and if necessary in practice, a so called spark test apparatus (STA) is used [1], which generates these discharges between contacts in the gas mixture with the electrical energy of the test equipment. However, the results are unreliable and must be improved.

For this reason, electrical discharges between opening contacts in flammable gas mixtures are investigated. The relationship of the distance of the electrodes and the voltage of the discharge for different current values of a constant current supply is determined and plotted. Differences between igniting and non-igniting discharges of the first measurements will be shown. The measurement is very challenging because the short duration of the discharges (microseconds), small dimensions (micrometers) and low radiation.

The goal is to investigate the opening process in the STA in order to obtain a voltage-length curve of the discharge as well as the geometric distribution of its energy transfer into the gas. These relationships can be used for a simulation of the ignition to enable the long-term development of an alternative to the STA.

926 - A Rapid Compression Machine Study of n-Decane Ignition at Intermediate Temperatures V.V. Leschevich, O.G. Penyazkov, S.Y. Shimchenko

Ignition of homogeneous stoichiometric n-decane/air mixture was investigated in rapid compression machine at pressures 0.6-1 MPa within the temperature range of 820-900 K. The objective of this study is to extend the range of available experimental data for n-decane auto-ignition at intermediate temperatures and to sew the new data together with the data obtained by shock tube at high temperatures. Volumetric and insensitive to burning contaminating particles ignition was observed simultaneously in several places of the combustion chamber. The significant difference of ignition delay times measured in multiple runs under identical conditions was found. The end and side wall light emission observation showed that more rapid ignition can be attributed to low-intensity light that can appear in the combustion chamber at different time moments in repeated experiments. Due to sensitivity limitation of CCD sensor of the high-speed camera, the source of this light was not established. The longest of ignition times measured from repeated runs were selected as representative data and compared with the reported literature data. Discrepancies are noted and discussed. Current data are well jointed with previously obtained at high temperatures shock tube data for the similar mixture density and together exhibit a monotonically increasing trend of ignition delay with a decrease in temperature. No evidence of the onset of the NTC-like behavior for ignition delay for stoichiometric n-decane/air mixture is seen for studied range of pressures.

1006 - Investigation of the Flame Kernel Propagation After Ignition by a Low Energy Electrical Discharge

S. Essmann, D. Markus, U. Maas

In safety engineering and process industry, electrostatic discharges frequently pose a risk as ignition sources for burnable gas/air mixtures. When the ignition energy is close to the minimum ignition energy, loss processes play an important role. In this energy region, ignition is a stochastic process in practice so that there is only a limited probability of ignition. Detailed knowledge about the underlying physical and chemical processes is often lacking. On the other hand, global parameters like the energy of an electrical discharge are useful for real-world situations. Therefore, we investigate the properties of the electrical discharges based mainly on the discharge energy as the independent variable.

In this study, we investigate the ignition by electrical discharges near the MIE experimentally. First, high speed schlieren videos of the early flame propagation following the discharge are recorded for three burnable gas/air mixtures and several energy levels. The effects of discharge energy on the

propagation speed and the reproducibility are discussed. Second, optical emission spectroscopy (OES) is employed to the discharges. The vibrational and rotational temperatures are determined from the comparison of experimental spectra with numerical ones.

1100 - Hot Surface Ignition Dynamics in Hydrogen-Air Mixtures Near the Flammability Limits L.R. Boeck, J. Melguizo-Gavilanes, J.E. Shepherd

The dynamics of ignition from a hot surface near the flammability limits of premixed hydrogen-air were investigated in a combined experimental and numerical study. Surface temperatures during heating and at ignition were measured by 2-color pyrometry, and gas temperatures were determined by high-speed Mach-Zehnder interferometry. Numerical simulations with detailed chemistry were performed using the low Mach number, variable-density reactive Navier-Stokes equations with temperature-dependent transport properties. Differential diffusion effects were also included in the numerical model. In addition to the known cyclic (puffing) combustion phenomenon, singular ignition events (single puff) near the lean flammability limit were observed. An ignition kernel forms at the top of the hot surface, and a flame travels upward within the thermal plume. Since the flame only expands weakly in the horizontal direction, a propagating vortical structure forms as a result of the interaction of the flame-induced flow with the vertical buoyant flow. The flame anchors at the hot surface edges, feeding a hot plume with combustion products. Despite high surface temperatures, no further ignition events occur. A layer of non-flammable mixture develops around the hot surface and shields it from the fresh surrounding mixture. The described ignition phenomenon does not lead to a significant pressure increase in the closed combustion vessel. Towards the rich flammability limit puffing flames or single puff ignition were not observed.

10:45 Shock Tubes, Ignition Delay Times, Kinetics 2

788 - Experimental Measurement of Ignition Delay Times of Thermally Cracked n-Decane in Shock Tube

S. Pei, H. Wang, X. Zhang, S. Xu, L. Wang, G. Liu

The ignition characteristics of endothermic hydrocarbon fuels (with different pyrolysis degrees) were investigated in a shock tube using *n*-decane as model compound. Six component surrogates (CH₄/C₂H₄/C₂H₆/C₃H₆/C₃H₈/n-C₁₀H₂₂, marked as cracked *n*-decane) for thermally cracked *n*-decane were proposed based on the chemical compositions from the thermal stressing of *n*-decane on electrically heated tube under 5 MPa. Ignition delay times were measured behind reflected shock waves over temperature range of 1296-1915 K, pressure of 1-2 atm and equivalence ratios of 0.5-2.0. *n*-Decane showed shorter ignition delay time than cracking gas at 1 atm, demonstrating higher reactivity. For cracked *n*-decane, it was found that thermal cracking could improve the ignitability at certain conditions with a limited degree, i.e. at T>1480 K for x=37.97% and x=17.61% and at T<1480 K for x=62.15% (x represents conversion of thermal cracking of *n*-decane) in this work. Unimolecular decomposition reactions of *n*-decane producing active radicals and H-atom would help chain initiation via H-abstraction reaction for unreacted fuels. This initial stage might accelerate ignition by activating cracking gas at these conditions. The empirical correlations for the ignition delay time of cracking gas and *n*-decane were also analyzed. Two models were also used to simulate the experimental data and showed good agreement with experimental results.

1118 - Numerical Investigations of the Impact of Tailored Driver Gases and Driver Inserts on Shock Tube Flows

D.M. Coombs, B. Akih-Kumgeh

Numerical simulations of shock tube flows with tailored driver gases and driver insert geometry are presented. The thermodynamic conditions in the post-reflected shock region in an Argon driven gas are simulated using 4 driver mixtures of Helium and Nitrogen. In addition a shock tube geometry with a driver insert contour is simulated for one of the driver gas mixtures. The variations in post-reflected shock conditions due to deviation from the perfectly tailored driver gas and the impact on combustion chemical kinetics is presented. The effects of the combination of driver gas tailoring and the driver

insert on the shock tube flow are discussed. It is shown that deviations from the tailored driver gas condition in combination with driver inserts can increase shock tube test times.

928 - Chemical Reaction Mechanisms Validation Based on Ignition Delay Time of C1-C5 Hydrocarbons

W. Rudy, A. Jach, A.A. Pękalski, A. Teodorczyk

Ignition delay time (IDT) is one of the most important combustion properties of flammable mixture. It is used as an input for modelling diesel engine combustion, knock modeling, gas turbines and any device where high initial temperature and pressure are present. IDT value is also used to calculate induction zone length in ZND detonation model and therefore lets it correlate with detonation cell size or detonability parameters like KSI and RSB. Taking into account the importance of the IDT value in many areas of modeling the proper selection of the chemical reaction mechanism becomes crucial. The main aim of the analysis presented in this paper is to quantify the quality of the available chemical reaction mechanisms by comparing numerical IDTs with the experimental ones. The simulations were performed with use of freeware Cantera code simulating IDT in C1-C5 hydrocarbon fuels mixed with air or oxygen and diluted with argon. The analysis results on 1866 experimental points pointed out the machanisms which give IDT the least deviation from the experimentally obtained values. The results may be used as an initial guide for selecting reaction mechanism for modeling combustion of particular fuel and for further analyses.

10:45 DDT 4

1087 - Exploration of Turbulence Driven Deflagration to Detonation of Fast Flames

J. Chambers, K. Ahmed, A. Poludnenko

One of the fundamental mechanisms for detonation initiation is turbulence driven deflagration to detonation transition (DDT). The research experimentally explores the physical mechanisms of turbulence driven fast deflagration flames transitioning to detonation. The flame structural dynamics and reacting flowfield are characterized using simultaneous high-speed particle image velocimetry, chemiluminescence, and schlieren measurements. The investigation classifies the fast flame propagation modes at various regimes. The study further examines the conditions for a turbulent fast flame at the boundary of transitioning to quasi-detonation. The local measured turbulent flame speed is found to be greater than the Chapman–Jouguet deflagration flame speed which categorizes the flame to be at the spontaneous transition regime and within the deflagration-to-detonation transition runaway process.

1078 - The Influence of Turbulent Mixing on Deflagration to Detonation Transition

B. Maxwell, M.I. Radulescu, A.A. Pękalski

In the current study, the influence of turbulent mixing on Deflagration to Detonation Transition (DDT) is investigated using a state-of-the-art numerical simulation strategy and compared to shock tube experiments accordingly. Specifically, detonation attenuation by a porous medium, and the subsequent re-initiation for methane-oxygen, a moderately unstable mixture, is considered. The modelling procedure adopted was a grid-within-a-grid approach: The Compressible Linear Eddy Model for Large Eddy Simulation (CLEM-LES). The purpose of the investigation was to validate DDT events observed in numerical simulations with experimental observations, and to determine how such events are influenced by changes in the turbulent fluctuations present. It was found, through numerical simulation, that turbulent mixing rates play a major role which contribute to, or mitigate, DDT events. It was found that a sufficient amount of turbulence intensity generation behind the wave front was required in order to maintain wave speeds above the theoretical CJ-deflagration speed, thus allowing for the necessary conditions in order for DDT to occur. It was also found that a further increase in turbulent mixing rates can also have a mitigation effect on DDT. Detonation initiation events were found to be very sensitive to changes in turbulence intensity. Specifically, there exists an optimal range of turbulent mixing intensity in order to provide the necessary conditions, and combustion regime, for detonation to occur.



834 - Numerical Study of Deflagration-to-Detonation Transition in Homogenous and Inhomogeneous Hydrogen-Air Mixtures

R.K. Azadboni, A. Heidari, L.R. Boeck, J.X. Wen

Explosions in homogeneous reactive gas mixtures have been widely studied both experimentally and numerically. However, in accident scenarios, combustible mixtures are usually inhomogeneous. The present numerical investigation aims to study flame acceleration and transition to detonation in homogeneous and inhomogeneous hydrogen-air mixtures with two different average hydrogen concentrations in a horizontal obstructed channel, filled with hydrogen-air mixture. A density-based solver was implemented within the OpenFOAM CFD toolbox. The Harten–Lax–van Leer–Contact (HLLC) scheme was used for accurate shock capturing. The numerical model initially has been verified by Sod's shock tube problem. A high-resolution grid is provided by using adaptive mesh refinement, which leads to 30 grid points per half reaction length (HRL) in the finest regions near the flame and shock fronts. In agreement with the experimental measurements and observations, it was found that transverse concentration gradients lead to stronger flame acceleration and promote transition to detonation for an average hydrogen concentration in air of 20%, whereas gradients slightly retard both phenomena for a 30% mixture.

10:45 Detonation in Non-Uniform Mixtures

1009 - Self-Sustained Oblique Detonation in a Non-Uniform Mixture

K. Iwata, S. Nakaya, M. Tsue

In order to investigate the physics of self-sustained oblique detonation in a fuel concentration gradient stabilized behind a hypersonic projectile, axisymmetric two-dimensional simulation was conducted with a detailed chemical kinetic mechanism of $H_2/O_2/Ar$ mixture. The concentration gradient was artificially given according to the Gaussian distribution. It was revealed that Chapman-Jouguet (C-J) oblique detonation was maintained in a relatively mild concentration gradient, with a curved front whose local wave angle closely matches C-J value of the incoming local equivalence ratio. However, when a strongly fuel-rich/fuel-lean region exists, oblique detonation ceases to be maintained resulting in the decoupling between the shock and flame front. This decoupling was accompanied by a sudden drop in the incident shock angle in the fuel-rich mixture, while a minor difference of C-J angle and inert shock angle in the fuel-lean mixture resulted in a smooth change along C-J values. Also, in the fuel-rich region, a flat wave front with a nearly constant angle was encountered due to a weaker interaction of the shock and flame front caused by a longer induction length.

987 - Numerical Study of a Gaseous Detonation Propagation Across a Density Interface

K.C.T. Yuk, X.C. Mi, J.H. Lee, H. Teng, H.D. Ng

The present paper studies numerically the transmission of a gaseous detonation wave across an abrupt change in density of the reactant medium. Both one-dimensional and two-dimensional simulations using the reactive Euler equations with one-step chemistry are carried out. Additionally, a step increase as well as decrease in density of the reactant are considered. The study is focused on the relaxation process subsequent to the perturbation by looking at different wave interactions and the re-initiation to the final detonation structure corresponding to the new reactant density. This is in an attempt to elucidate the dynamics of the detonation structure and analyze the relaxation length as a mean to provide a measure of its characteristic hydrodynamic thickness.

994 - Numerical Investigation on Characteristics of a Planar Detonation Wave Across Layers of Burned Gas

N. Ohira, A. Matsuo, J. Kasahara, K. Matsuoka

Inside the Rotating Detonation Engine (RDE) chamber, reactants are injected and mixed into burned products. There is certain interval of injection ports and thus rotating detonation waves propagate into injected reactants and burned products alternately. Existence of burned gas would affect the velocity and the stability of detonation waves. A two-dimensional numerical investigation is conducted to research the effect of burned gas on detonation. The numerical target is a planar detonation wave in a channel with constant cross-sectional area. Uniform rectangles of premixed ethylene-oxygen and

burned gas are set by turns in the channel. In the burned gas region, propagation is maintained by the combustion of reactants advected from the premixed gas region. Propagation behavior becomes unstable as the width of burned gas region increases. Due to thermodynamic characteristics, propagation velocity of the leading shock wave is higher in burned gas region than that in premixed gas region. This leads to keeping the overall propagation velocity at around the CJ value in the RDE chamber which includes not only premixed gas but also high-temperature burned gas.

750 - Physical and Mathematical Modeling of Interaction of Detonation Waves in Mixtures of Hydrogen, Methane, Silane and Oxidizer with Clouds of Inert Micro- and Nanoparticles

D.A. Tropin, A.V. Fedorov

In the paper physical and mathematical models for the description of the processes of transition, weakening and suppression of detonation in mixtures of hydrogen, methane, silane with oxidizer and inert micro- and nanoparticles were proposed. On the basis of these models the dependencies of detonation velocity deficit on the size and concentration of inert micro- and nanoparticles were found. It was revealed that the same types of detonation flows exists in the mixture of a gas and nanoparticles, as in gas suspensions with micro particles: 1. stationary propagation of weakened detonation wave at velocities less than Chapman-Jouguet velocity; 2. the detonation wave suppression. Furthermore, it is determined that the mechanisms of detonation suppression by micro- and nanoparticles are quite similar and lies in the decay of a detonation were calculated and it is shown that in reactive gas mixtures with particles with diameter from 10 nm to 1 micron these limits are close. It was found that the tendency of increasing of detonation suppression efficiency with decreasing of the inert particles size in the transition from micro to nano-sized particles is violated.

10:45 Reactive Systems 4

825 - Measurements of Laminar Flame Speeds of Alternative Liquid Fuel Blends

S.F. Samim, S. Ahmed

This work investigates the laminar flame speed of GTL fuel and its 50%-50% blend with conventional diesel, in a cylindrical bomb capable of measuring laminar flame speed, S_N , at different initial temperatures and equivalence ratios. S_N was measured by analysing the pressure signals inside the bomb after combustion. It was found that pure GTL-Diesel has the highest flame speed near stoichiometric conditions. However, at lean and rich mixtures, the flame speed of GTL get slightly lower than conventional diesel. The blended fuel has a lower S_N at lean and rich mixture conditions than those of other fuels. Studying effect of increases with the increase in initial temperature of the mixture almost linearly. However, the blended fuel has the lowest S_N at high temperature.

945 - Diffusion Flame at High Pressure with Air and Water-Laden Methane

A. Jorda, W.A. Sirignano

Water-laden combustion at high pressure is gaining interest for different applications, including rocket engines, methane hydrates, exhaust gas recirculation in engines, or bio-fuels. A counterflow canonical configuration is studied to obtain numerical results in relation to these applications. We analyze different gaseous mixtures of methane and water vapor impinging against air. Results are obtained at pressures ranging from 1 to 100 atm. The one-dimensional similar model for laminar counterflow diffusion flames is used with modifications in the energy equation to account for the proper evaluation of the mixture enthalpy at high densities. Real-gas effects are taken into account with the use of a cubic equation of state. The model is equipped with a detailed reaction mechanism and detailed transport properties are also evaluated for real gases. Results indicate that water addition reduces the flame temperature acting as an energy sink. Extinction occurs when the mass fraction of water in the fuel stream is above 67%. Analysis shows that, for the centimeter scale considered here, radiative transport, turbulence generation, and the Soret effect are negligible in the flame region. The second part of the paper presents the formulation for the two-phase shifting equilibrium when the methane and water are

a two-phase mixture in the counterflow. Results on the second part will be discussed in the oral presentation.

937 - Modelling Mixing Near HE-Air Interfaces in Explosions

A.L. Kuhl, D. Grote, J.B. Bell, V.E. Beckner

We consider the problem of mixing near HE-air interfaces in explosions, where the Detonation Products (DP) are rich in carbon particles. The model consists of gas phase conservation laws (i.e., the compressible Navier-Stokes equations), coupled with a heterogeneous continuum model for the carbon particle phase. The problem is assumed to be point symmetric, so the 1D spherical coordinates are used. The hyperbolic terms are integrated with a 2^{nd} -order Godunov scheme (PPM), while the viscous terms are advanced by a 2^{nd} -order Runge-Kutta method. The particle phase conservation laws are also integrated with a 2^{nd} -order Godunov scheme (represented) as 2^{nd} -order Godunov scheme for dilute particle systems. Adaptive Mesh Refinement (AMR) is used to resolve steep gradients in the flow. A tabular EOS, based on equilibrium thermodynamics code Cheetah code, is used. Three converged solutions were found: (i) inviscid, (ii) viscous and (iii) two-phase. The blast wave solution (*p*, *rho*, *T*, *u*) scaled gasdynamically (i.e., with the cube-root of the charge mass), however, the DP-Air interface and peak temperature were smeared by molecular diffusion effects. Similarity solutions for the latter show that diffusion effects scale with the appropriately-defined Peclet and Reynolds numbers. The DP-Air interface is unstable and evolves into a turbulent mixing layer; 3D inviscid AMR simulations of this case will also be presented.

14:15 Energetic Materials 2

1139 - On Minimum Flash Ignition Energy of Energetic Igniter Using Aluminum Nanoparticles: Effects of 2D Interparticle Distances

J.Y. Yu, Y.P. Chan, Y.C. Hsu, Y.C. Chao

In this study, energetic igniter composed of nitrocellulose with distinct amount of aluminum nanoparticles has been developed. To save the cost, the amount of aluminum nanoparticles related to inter-particle distance should be lowered. According to relevant literatures, nanoparticle interaction influenced by inter-particle distance would significantly affect ignition behavior and ignitor performance. As a result, the minimum ignition energy (MIE) would change as well. Hence, the relationship of inter-particle distance and minimum ignition energy is investigated in this study. Moreover, a 2D model is established to perform theoretical analysis to further eliminate the influence of 3D shape effects on the ignition. Different thermal, optical and spectroscopic instrumentations and equipment are used to measure and examine the material structure and properties, and ignitor performance. The results from experiment and theoretical analysis are compared to counter-validate and demonstrate the findings that the lowest MIE from igniter can be achieved with inter-particle distance being four to five times the particle radius.

1063 - Experimental Investigations of Combustion Enhancement of HAN-Based Green Propellant with K2CO3-Activated Carbon

M.K. Atamanov, K. Hori, E. Aliyev, R. Amrousse, Z.A. Mansurov

The paper is focused on the effects of activated carbon with high specific surface area (SSA) based on vegetable raw materials as a carbonized rice husk (CRH-K₂CO₃) on the combustion performance of hydroxylammonium nitrate propellant (HAN: [NH₃OH]⁷[NO₃]). The structure of activated carbon investigated by SEM, AFM and BET analysis. Were performed the combustion experiments to investigation of the influence of additives on the HAN linear burning rate. The kinetics study of HAN thermal decomposition with the activated carbon were assessed by differential thermal analysis (DTA – TG) at different heating rates. Based on DTA-TG results shown, that the additive of carbon decreases the ignition temperature of HAN on compared to the propellant alone. The carried out EI-MS analysis of the HAN propellant with activated carbon at different heating rates. It was shown the major products and product distribution of HAN decomposition with activated carbon.

817 - Development of Protection Recommendations for Warehouse Storage of Li-Ion Batteries *B. Ditch*

Protection recommendations for warehouse storage of cartoned lithium ion batteries have been developed through fire testing. A unique approach was developed that incorporated different fire test evaluations, ranging from intermediate- to large-scale, with the goal of extending the application of a successful large-scale fire test to additional types of lithium ion batteries. A reduced-commodity (intermediate-scale) test evaluated the flammability characteristics of several large- and small-format lithium ion batteries compared to standard warehouse commodities. Measurements focused on the fire development of each commodity and the time of battery involvement for the lithium ion products during a free-burn rack storage fire test. The results of this testing provided a ranking of the relative hazard of each battery in a warehouse storage setting. The performance of ceiling-level sprinkler protection was then assessed with a large-scale sprinklered fire test using the highest hazard battery.

14:15 Dust Explosions 3

913 - Analysis of Dust Cloud Combustion Using High-Speed Infrared Imaging

F. Marcotte, S. Savary, M.A. Gagnon, V. Morton

Dust cloud combustion is unfortunately at risk in many working environments, jeopardizing several workers. The heat and shock waves resulting from the flame propagation into the dust cloud are harmful and lead to major endangerment or casualties. More precisely, dust cloud (small particles) explosions are even more malicious since they often result from ordinary materials such as coal, flour or pollen. In addition, many metal powdered (such as aluminum oxide and magnesium) can form dangerous dust cloud when they are in suspensions in air. The understanding of this particular type of combustion is critical for the preventive care of sites and workers afflicted to such conditions. This paper presents the results of a dynamic flow analysis of metal particles combustion in a dust cloud. The ignition points, the flow rate as well as the propagation direction of the flow have been characterized using fast infrared imagery.

1126 - Dimensional Scaling for Propagation in Particulate Clouds with Lateral and Volumetric Losses

F. Lam, X. Mi, A.J. Higgins

The dependence of the propagation limit of a reaction-diffusion system consisting of point-like energy sources on lateral and volumetric losses are studied via a numerical construction of analytic solutions. The propagation limit in cylindrical and slab geometries are determined via simulations on statistical ensembles. The critical dimensions, below which the reaction-diffusion wave fails to propagate, are found to vary as a function of a discreteness parameter defined as the reaction time of discrete sources, scaled by heat diffusion time between sources.

891 - Monitoring of a Dust Explosion in a 10 m³ Vessel

Y. Grégoire, C. Proust, E. Leprette, D. Jamois

The present study aims to present INERIS latest works on large scale dust deflagrations in the scope of industrial explosions. Dust dispersion and explosion tests were performed in a 10 m³ parallelepiped with a transparent face. The document is primarily focused on the dust distribution and velocity in this volume, prior to ignition. Two approaches are considered: a local one, and a global one. The local method is performed through the more "classical" analysis of the measurements provided by sensors (turbulence, concentration) placed at points of interest. The global approach consists in the analysis of velocity measurements performed through the transparent face in view of characterizing the flow turbulent intensity. It involves a novel technique of image processing through the computation of the optical flow on the video sequences completed by a statistical analysis on the measured velocity fields.

14:15 Detonation Engines 5

796 - Experimental Investigation on Delay Time of Continuously Detonation Engine

X. Han, S. Zhang, Z. Ma, J. Wang

An experimental study is carried out to investigate the delay time of continuous detonation engine. An annular chamber combustor with an array of injection holes is designed for testing and pressure history is obtained during each shot. According to the analysis of the experimental data, several conclusions are obtained. The pressure history shows that continuous rotating detonation wave can be obtained in the combustor with an array of injection holes when hydrogen-oxygen is used. Delay time obtained in experiments increases when the prefilling time increase, which is an indicator of the volume ratio of gas mixtures pre-filled in the main combustor. Following numerical simulation shows similar trend that delay time increases as the volume ratio of the gas mixtures pre-filled increases.

947 - The Effect of Combustor Width on Continuous Rotating Detonation Wave Fueled by Ethylene

H. Peng, W. Liu, S. Liu

Continuous Rotating Detonation (CRD) fueled by ethylene is achieved in optically-accessible racetrack combustor. By varying the combustor width, operating domain, propagation characteristics, flowfield structure and stability are investigated. Ethylene CRD can be achieved on larger width combustor compared with CRD fueled by hydrogen due to its relatively bigger detonation cell size. In the experiments, CRD Waves propagate mostly as two wave in hetero-rotating mode in combustor with inner body, while they propagate mostly as single wave or two wave in homo-rotating mode in hollow chamber. Based on the high frequency pressure and optical observations, both the propagation modes are detailed. The rotating velocities of the inducing shock wave and combustion flame are calculated by PCB results and optical observations respectively, and they agree generally with each other. It indicates that the inducing shock wave and the combustor flame are coupled with each other. Considering the operating domain and propagation stability, 15 mm wide combustor is the best choice for ethylene CRD in this test. The study will improve the combustor design of CRD Engine fueled by hydrocarbon fuels and enhance the understanding of flowfield structure and flame dynamics of CRD Waves.

898 - Numerical Study of Reinitiation Phenomenon in Continuous Detonation Engine

S. Yao, J. Wang

This article presents a numerical study on the continuous detonation engine (CDE). The simulation explores the phenomenon of reinitiation of detonations in a cylindrical combustion chamber of the CDE. The process is modelled by the three-dimensional reactive Euler equations with an Arrhenius form of the reaction rate for the premixed stoichiometric hydrogen-air mixture. The detonation flow goes through three stages: initiation, quenching, and spontaneous reinitiation. The detonation fronts collide with each other and also have frequent collisions with the outer wall after initiation. While there is a possibility of generating new detonation fronts from the explosion, it is also likely that the explosion will burn out the surrounding reactive mixture and snuff out the detonation maves. The simulation shows that a strong collision between two detonation wave fronts quenches the detonation flow and consequently renders the engine inoperative for an extended period until a spontaneous reinitiation occurs in the flow. The reinitiation is found to be triggered by a rapid and sharp increase of pressure near the chamber wall.

886 - Effects of Pre-Ignition Conditions on Continuous Detonation Engine

S. Yao, S. Zhang, J. Wang

The utilization of detonations for propulsion systems has been explored for decades. Recent research has paid much attention to the continuous detonation engine (CDE), which is also called the rotating detonation engine (RDE). The concept of the CDE was attributed to the work of Voitsekhovskii. The feasibility of the CDE has been tested extensively by Bykovskii et al.

Experimenting on the CDE requires that the combustion chamber is initially filled with some reactants before initiation. The premixed unburned mixture of fuel and oxidizer will then be consumed by the initial detonation wave introduced by, for instance, the pre-detonator. It seems reasonable to guess that

the properties of these pre-ignition gases are unlikely to have a noticeable effect on the initiation process and the final stabilization of the CDE since they will be consumed quickly and then fresh reactants will be supplied continuously. This, however, was proved to be not the case in hindsight. As a matter of fact, interesting phenomena were observed when we varied the properties of pre-ignition gases, e.g., the pressure and temperature. Moreover, the volume of them with which the combustion chamber was initially filled with was also found to have an effect on the stabilization process.

14:15 Diagnostics, Sensoring 2

766 - Embedded Fiber Optic Sensors for Measuring Transient Detonation/Shock Behavior: Time-of-Arrival Detection and Waveform Determination

M.A. Chavez, M.D. Willis, T.T. Covert

Energetic materials research has led to an increased interest with miniaturization of energetic based components to the microscale. This has paved a path for probing fundamental behavior that occurs in explosives on the microscale. Running parallel in the same realm, interest in dynamic pressure loading of inert materials has become increasingly important. Diagnostics that measure these events are relatively large by comparison and generally do not allow unobtrusive interrogation of the physical phenomena of interest in microscopic components or experimental configurations. A typical measurement system employs laser interferometry paired with spectrally coated optical windows to measure the apparent particle velocity induced into the window material by a shock or non-shock event. These experimental configurations are on the order of centimeters in size. Embedded Fiber Optic Sensors are microscopic sized diagnostics that allow probing of the induced apparent particle velocity within reactive environments, such as microscale sized energetic materials undergoing deflagration to detonation transition.

933 - Possibility of Applying Flame Chemiluminescence and Ionization Current to the Combustion Status Monitoring

Y. Ding, D. Durox, N. Darabiha, T. Schuller

The development of a combustion control system has received interests from gas boiler manufacturers in order to ensure an optimized performance despite variations of natural gas compositions. For this purpose, an important parameter to monitor is the air-fuel equivalence ratio. In the present study we are focused on two potential solutions: flame chemiluminescence and flame ionization current. Experiments are performed on a laminar premixed conical flame. The effects of secondary natural gas components (N2, CO2, H2, C2H6, C3H8) are investigated and the validity of CH*/OH* chemiluminescence intensity ratio and ionization current as equivalence ratio indicator is tested.

1034 - Infrared Radiation Measurements at Failure of Mobile Gas Vessels

D. Krentel, M. Rudolph, R. Tschirschwitz, M. Kluge, E. Askar, K. Habib, H. Kohlhoff, G. Mair,

P.P. Neumann, B. Schalau, A. Schoppa, S.U. Storm, M. Szczepaniak

A total of 15 identical, off-the-shelf propane cylinders, without any kind of pressure relieve device, were underfired using three different types of fire (wood, gasoline, propane). This extended abstract contains only results for one type of bonfire. All tested cylinders failed within a time period of 70 s to 152 s and fragmented into up to seven major parts (average: four objects) covering distances of up to 260 m. The infrared radiation of the explosion of the propane air cloud, that occurred in the aftermath of the vessel failure and the release of the propane, was recorded using four bolometers. These measurements were compared with an estimation of the maximum intensity gained by an analysis of the video data and an extended version of the Stefan-Boltzmann law. It is demonstrated, that both methods are in good compliance, and that bolometers are in general also capable to measure radiation pulses of short duration. The dataset gained within this project can help to estimate potential damages to persons, infrastructure and the environment. They can also be used to increase the safety of firefighters and other forces responding to fires involving gas cylinders.

14:15 Reactive Systems 5

923 - A Computational Analysis of Autoignition of H2/Air Mixture with Temperature Fluctuations Using Computational Singular Perturbation

W. Song, E.A. Tingas, S.R. Lee, H.G. Im

Autoignition behavior of a hydrogen-air mixture has been studied numerically to investigate the effects of temperature fluctuation on the ignition delay time at both strong and weak explosion regimes. It was found that regardless of explosion regimes, ignition delay time was always faster when the temperature fluctuation was imposed. The analysis was carried out using tools of computational singular perturbation (CSP) approach. The dominant reactions and variables have been identified and analyzed for both cases under investigation.

1057 - IR Absorption Measurements of the Velocity of a Premixed Hydrogen/Air Flame Propagating in an Obstacle-Laden Tube

R. Scarpa, E. Studer, B. Cariteau, S. Kudriakov, N. Chaumeix

In case of severe accident, in-core metal-water reactions due to fuel temperature increase lead to massive release of hydrogen into the containment of Light Water Reactors, as recently recalled by Fukushima accident.

The safety features currently implemented for severe accident management cannot guarantee that the formation of large flammable clouds can be avoided. In case of hydrogen accumulation, a small amount of energy (such as an electrical spark) is sufficient to ignite the mixture. The explosion of such a cloud may eventually jeopardize the integrity of the containment and damage components important to safety or accident management. Moreover, the extent of this damage becomes more important as the propagation velocity of the reactive wave increases. The empirical flame acceleration criteria developed in the early 2000s by Dorofeev and colleagues provide an effective tool for the analysis of the possible scenarios and it allows the selection of the most relevant situations for which flame acceleration may take place.

The validation of numerical tools capable to simulate the propagation of a premixed hydrogen/air flame in a large geometries is therefore a crucial issue for improving the safety of nuclear installations.

In this work we develop a method for extrapolating the velocity profile by measuring the variation of the extension in depth of the fresh (or burnt) gas along the tube axis. The method that we propose consists in performing IR-absorption measurements by doping the mixture with trace of alcanes such as methane. Experimental results are then compared to the analytical ones proposed in the literature.

920 - Study on Low Temperature Oxidation with a Separated Cool Flame of n-Heptane in a Micro Flow Reactor with a Controlled Temperature Profile

R. Tatsumi, H. Nakamura, S. Hasegawa, T. Tezuka, K. Maruta

Micro flow reactor with a controlled temperature profile (MFR) is applied as novel methodology for examining low-temperature oxidation of *n*-heptane. In MFR, weak flame can be obtained at very low flow velocity condition, and it has been utilized for examining ignition characteristics of given mixture. Therefore, special attention is paid to weak flames of *n*-heptane/air mixture in MFR in this study. In MFR, there is the stationary temperature profile on the inner surface of reactor tube in the flow direction. Our previous study reported that multiple weak flames for *n*-heptane/air mixtures were observed in MFR. This interprets that general transient multi-stage ignition phenomena can be observed as spatially separated steady three weak flames which correspond to cool, blue and hot flames were conducted in MFR. In the present study, separation of a steady cool flame and species measurements were conducted in MFR.

Using MFR, oxidation process in the stationary temperature gradient can be controlled. Therefore steady cool flame was separated from multiple weak flames and stabilized in MFR by varying temperature gradient.

One-dimensional computations were conducted for the steady separated cool flame to examine key reactions for low temperature oxidations. Radical chain cycle between radical branching reactions which produce ketohydroperoxide and fuel decomposition reaction was found to be important for cool flame formation.



Based on computational results, sampling species were selected. Then species measurements at the exit of MFR were conducted to examine performance of reaction mechanisms (KUCRS mech., LLNL mech. and MFL mech.). There were large discrepancies between experiments and computations so that it was implied that performances of chemical kinetics for low temperature oxidation would be improved by using the species measurements in the present MFR method.

Poster Session I

751 - Ignition Delay Times of Dual-Fuel Mixtures of Silane/Hydrogen at High and Low Temperatures

D. Tropin, A. Fedorov

In paper the ignition delay times dual-fuel mixture of hydrogen / silane / air based on the previously developed model detailed kinetics were calculated. The influence of the concentration of the silane and the temperature of the mixture on the ignition delay times was determined. It was shown that in the temperature range from 800 to 2500 K the addition of a small amount of silane (20%) in the hydrogenair mixture results in a significant decreasing of the ignition delay time of the mixture, while increasing the silane concentration greater than 20% the ignition delay times of hydrogen-air mixture is decreased slightly. In addition, it was found that up to temperatures of 2200 K addition of silane in hydrogen-air mixture leads to a monotonic decrease in ignition delay times as the amount of silane in the mixture increases. However, at temperatures above 2200 K small addition of silane (20%) in the hydrogen-air mixture results in a more significant decreasing of the ignition delay times, compared with mixtures with a large amount of silane.

800 - Study of the Thermal Effects of Microwave Induced Plasma on Premixed Methane-Air Flames

H.Y. Li, Y.C. Chao

In this study, a novel centralized microwave jet burner system is proposed for fundamental studies of the flame-microwave/plasma interaction characteristics and flame enhancement mechanism of the microwave induced plasma flames. At low microwave powers, the flame is influenced only by an electromagnetic field. When power is increased, ionization and eventually breakdown of gas molecules result in a plasma discharge sitting on the top of the electrode. Depending upon the input microwave power, three enhanced stages can be categorized. In first stage "microwave enhanced stage" where microwave energy is low and only the microwave electric field couples to the flame with slight increase in flame speed due to electron heating. As microwave power is increased, a plasma source is initiated and the flame-microwave interaction process turns into the "Thermal enhanced stage". The results indicated that the flame speed were increased on the order of 28 to 49% and the corresponding preheat temperature is ranging from 340 to 390 K. It seems that the observed burning velocity increase can be explained by increase of unburnt gas temperature which means the measured enhancement in burning velocity probably results from simple plasma heating of the unburnt mixtures, and not necessarily from enhancement of a chemical effect. Further increasing the microwave power, the flame reaction zone is directly connected to the plasma region, referred as the "Plasma assisted stage". In this stage, the plasma discharge can ionize methane/air mixture to reactive radicals to further enhance combustion by initiating multiple complex chemical chain reactions.

813 - Outwardly Propagating Spherical Flame with Cellular Instabilities and Laminar Burning Velocities in Methane/Ethylene/Air Premixed Flames.

K.H. Van, H.J. Kim, J. Park, O.B. Kwon, D.K. Lee, S.G. Kim, Y.T. Guahk, D.S. Noh, S.H. Chung Experiments in expanding spherical flame were carried out to investigate unstretched laminar burning velocities by adding ethylene mole fractions of 0.1, 0.2, and 0.3 to methane-air mixtures at room temperature and elevated pressures up to 4 atm. Outwardly propagating premixed spherical flame front was measured by high-speed schlieren images with elevated pressures to acquire laminar burning velocity in methane/ethylene-air premixed flame. Our experimental methodology was validated through comparison of a variety of flame radius ranges from previous experimental studies and three kinds of extrapolation model with numerical ones in methane-air premixed flames on GRI v - 3.0. Based on reliable them, the most reliable detailed reaction mechanism to methane/ethylene-air premixed flame was examined through comparison among GRI v-3.0, USC Mech II, and Wang Mech to evaluate reliable detailed kinetic mechanisms. The results showed that cellular instability was devitalized (enhanced) in increase of ethylene mole fraction with lean case (rich case) at a fixed elevated pressure, whereas it was augmented in increase of pressure at a fixed fuel mole fraction. Effects of ethylene addition and increased pressure on cell formation on the flame surface were

examined though evaluating the Lewis number, flame thickness, and thermal expansion ratio. The cellular instability was enhanced mainly by hydrodynamic instability due to decrease of flame thickness and increase of thermal expiation ratio while the effect of diffusive-thermal instability was minor. The theory applied here accounts for both hydrodynamic and diffusive-thermal effects which is incorporating temperature dependent transport coefficients. The evolution of measured flame propagation speed as a function of flame radius are compared to theoretical one, which shows an excellent agreement. Based on them, also the wrinkling of methane/air with increase of ethylene addition is examined theoretically under increased pressure at various equivalence ratios. Theoretical flame radii which yield the growth rate of small disturbances with a variation of wave numbers, and experimental one defined as the point of transition to cellular flames which are extracted from high-speed schlieren flame imaging, are compared and show excellent consensus.

831 - Combustion Characteristics of Pyrolytic Oil Droplet From Sewage Sludge

G.B. Chen, J.W. Li, H.T. Lin, F.H. Wu, Y.C. Chao

Sewage sludge is a common municipal solid waste and can be utilized as a kind of raw materials for renewable energy. In the work, the pyrolytic oil of sewage sludge is obtained using thermal pyrolysis. The pyrolysis reactions and oxidation reactions of sludge pyrolytic oil are investigated using thermogravimetric analysis. The combustion performance parameters such as the ignition temperature, burnout temperature, flammability index and combustion characteristics index are also calculated and compared with heavy fuel oil to have a better understanding of the combustion properties of sludge pyrolytic oil.

In addition, the suspended droplet experimental system is also used to explore the combustion characteristics of sludge pyrolytic oil and its blends with heavy fuel oil. The pyrolytic oil of sewage sludge is a multi-component fuel and it results in micro-explosion during the heating process. When the droplet is heated at high ambient temperature (600 °C), the flammable mixture forms a flame wrapping around droplets after ignition. The addition of sludge pyrolytic oil in the heavy fuel oil will increase the ignition delay time. However, it enhances the burning rate when compared to the case of pure heavy fuel oil. The fuel combustion characteristics of sludge pyrolytic oil generally follow d^2 -law and it can be approximated with a constant burning rate of $1.62 \text{ mm}^2/s$.

836 - On the Characteristics of Liftoff Heights in Laminar Lifted Flames of Methane in Coflow Jets

N.P. Sapkal, K.H. Van, J. Park, O.B. Kwon, B.J. Lee, S.H. Chung

Lifted flames in laminar co-flow jets of methane diluted with nitrogen have been studied both experimentally and numerically. Characteristics of liftoff heights and flame stabilization in lifted flames were investigated with the effect of fuel nozzle exit velocity, fuel mole fraction and nozzle diameters. Two different liftoff height regimes, decreasing liftoff heights and increasing liftoff heights with increasing the nozzle exit velocities were observed for various nozzle diameters 0.3 mm, 0.8 mm, and 0.95 mm. These flames could be lifted despite the *Sc* number less than unity. The present study is mainly focused on the lifted flame behaviors in decreasing liftoff height regimes with increase of nozzle exit velocities). Results from numerical simulations identified that, buoyancy convection and radiative heat loss played a significant role in such decreasing liftoff height behavior in lifted flames.

839 - A Detailed Numerical Simulation of an Impulsively Started N-Dodecane Lifted Jet Flame at 40 Bar

Y. Minamoto, J.H. Chen

A detailed numerical simulation of an impulsively started n-dodecane-air jet flame under diesel engine relevant conditions has been performed using a DNS code, S3D. Despite the spatial under-resolution by a factor of 3-4, the simulation results exhibit similar trends to that reported in previous numerical and experimental observations for both low- and high-temperature oxidation. The simulation results suggest that intense mixing occurs near the tip of the jet, facilitating the production of relatively intense reactions for both low- and high-temperature ignition. Moreover, the low- and high-temperature ignition processes are spatially entangled and concentrated in localized regions. The competition

between these two ignition processes may be investigated by using highly-resolved direct numerical simulations. After the initiation of high-temperature chemical reactions, the well-known lifted flame with a triple-point is established with additional upstream flame branches related to the low-temperature ignition. This indicates that the insights obtained in previous stabilized lifted flames may also be relevant to the unsteady lifted stabilization process of diesel engine combustion.

875 - Mixed Gaseous Detonation Fabrication of CNTs and CNTs doping with Fe Based Composites

N. Luo, J. Xiang, T. Shen

In this work we firstly report the simple, inexpensive, low-temperature, gaseous and solution gasification new technology for the rapid production of CNTs and the related nanomaterials. Therefore, we designed a series of novel experiments to investigate the condensation and formation of carbon structural nanomaterials in gaseous mixed precursor rapid chemistry reaction, which the gaseous mixture precursor detonation technology roadmap. The detonation technique facilitates the shock wave transient expansion (at ms-molecule reaction level) and nanomaterial growth under extreme chemistry reaction conditions (high temperature, low pressure and rapid chemical reaction) which can help overcome the activation barrier for the chemical bond energy. The experimental results demonstrate that CNTs and CNTs doping with Fe-based nanomaterials can be obtained by detonation of gaseous mixture precursors.

882 - Hybrid RANS/LES Investigation of Precessing Vortex Core (PVC) in a Swirl Premixed Combustor

Z. Mansouri, T. Boushaki

The present study focused on DES computations of isothermal flow fields in premixed vortex burner under unconfined conditions. The burner is operated with air at atmospheric pressure and under high swirl number Sn = 1.05. The multi-block technique is used to generate a structured grid of the vortex burner. The flow fields are characterized using streamline patters colored by axial velocity. The applied DES strategy is useful to capture the averaged flow field with CRZ and ORZ, as well as the specific features of the instantaneous flow filed such as the vortices and the stagnation points in the ISL. PVC is detected in the shear layer of the CRZ. The DES results are found to be in good agreement with experimental data. A phase-angle analysis of the instantaneous flow field show that the PVC further induces unsteady stagnation points. The motion of the stagnation points is linked to the periodic precession of the PVC. The PVC is formed from the contraction to the burner exit and taking on a helical shape. Vectors of the flow fields in two slices across the vortex axis are presented. The circumferential velocity profiles of the vortex centerlines show that the vortex is characterized by the limits of its circumferential velocity u(R) and its corresponding radius R.

889 - Numerical Simulations of Mechanochemical Responses for Confined PBXs Under Low-Velocity Impact

K. Yang, Y. Wu, F. Huang, Z. Zhang

A series of two-dimensional mechanical-chemical simulations were performed to describe the different reaction stages of confined PBX charge undergoing low-velocity impact (~100 m/s). The ratio of length to diameter of the samples are 0.5, 1.0, and 2.0, respectively. An ignition criterion of effective plastic work was employed to predict the ignition response of the PBX charge. A pressure-dependent reaction rate equation was utilized to describe slow burning and its growth to deflagration following ignition. Simulated results show that the incident stress wave reflection from lateral surfaces contributed to the formation of potential ignition regions for cylinder-shaped charges with a length-to-diameter ratio of 2.0. After the ignition, the reaction violence characterized by the reaction rate of the mass fraction increased as impact velocity increased for 150–400 m/s, whereas impact velocity had little influence on the reaction violence for 80–150 m/s.

902 - Phase Transition of RDX Under High Pressure up to 50 GPa

C. Gao, C. Zhang, Z. Sui, Y. Qu, R. Dai, Z. Wang, X. Zheng5, Z. Zhang

Raman spectra of 1, 3, 5-trinitrohexahydro-s-triazine (RDX) are investigated under hydrostatic pressure up to 20 GPa and non-hydrostatic pressure up to 50GPa. Variations of Raman peaks suggest that α -RDX initially transforms to γ -RDX at 2.5 GPa and completes at 4.3 GPa, further to δ -RDX at 18.6 GPa under the hydrostatic pressure. Unlike hydrostatic condition, α -RDX immediately changes to γ -RDX as soon as the pressure reaches 4.6 GPa under non-hydrostatic pressure. γ -RDX further transforms to δ -RDX at 16.9 GPa, less than the transition pressure of 18.6 GPa for the hydrostatic condition. Continuously loading the non-hydrostatic pressure, a new ζ phase was found at about 27.6 GPa based on the appearance of new ring bending vibrations and the NO₂ stretching modes and ζ phase is stable until 43 GPa. This phase transition is reversible after RDX is released back down to ambient pressure.

905 - Temperature Distribution Along a Pulse Detonation Combustor in a Wide Range of Ratios Between the Oxygen-Enriched Heptane-Air Mixture Components

M. Assad, I. Chernukha, O. Penyazkov

The influence of the ratio between the components of the reacting heptane-air-oxygen system on the temperature distribution along a semi-closed detonation combustor operating in the frequency regime was investigated. The temperatures at the six cross-sections found at distances of 20, 140, 240, 340, 490, and 640 mm from the ignitor positioned on the end wall of the prechamber were measured. The fuel equivalence ratio was varied within the range $\phi = 0.95 - 2.57$ The temperature of the walls of the pulse detonation combustor at all the six control points reacted a maximum in the case of burning of a rich fuel mixture with $\phi = 1.75$. Throughout the range of fuel equivalence ratios studied, a minimum temperature was detected in the prechamber in which the fuel components are mixed and the mixture formed is ignited. A maximum temperature was detected in the detonation tube, connected to the prechamber by a conical passage, at distances of 10-14 tube diameters from the ignitor. It shown that a detonation combustion is initiated mainly in the tail part of the detonation tube, and this combustion occurring in the cyclic regime of operation of the combustor substantially influences the temperature distribution along it.

921 - Shock Induced Phase Transition of HMX Considering Initial Temperature Effects

W. Hu, Y. Wu, F. Huang

The purpose of this paper is to develop the crystal plasticity constitutive model to investigate the role of shock induced solid-solid phase transformation on the deformation mechanisms of HMX single crystal, which accounts for nonlinear elasticity, crystalline plasticity and temperature dependent phase transition (β -to- δ phase transition). In this work, the thermal-mechanical-chemical responses of HMX under shock loading with different initial temperatures have been investigated using finite element software ABAQUS. The temperature and phase transition fraction increase with the rising initial temperature effects are also discussed in this paper. The averaged stress and temperature eposes of HMX along wave propagation direction are higher when considering the temperature effects. The responses along different crystal orientation under shock compression are also discussed in this paper. The shock response of β -to- δ phase transition is orientation dependent. The transition fraction is the largest when the shock loading compresses along (010) orientation and the smallest along (100) orientation.

925 - Study of Downward Flame Spread and Fire Risk Evaluation of the Thermoplastic Materials

R. Zong, W. Zhao, C. Liu, X. Liu

This paper focuses its attention on the combustion characteristics and fire risk evaluation on the downward flame spread of polypropylene (PP) and polymethyl methacrylate (PMMA). Many characteristic parameters have been measured under different widths, such as flame spread rate, flame height etc. The influences of widths on flame spread rate have been discussed combined with heat transfer theory. It is shown that the flame spread mode of PP and PMMA are different because of

different pyrolysis mechanism. Due to the comprehensive influences of sample width and flowability, there are some differences in the variation of flame parameters of PP and PMMA. Based on the Analytic Hierarchy Process (AHP), the evaluation of fire risk has been conducted. The flame height, flame spread rate and toxic gas generation rate are selected as the basic evaluation index parameters to establish a comprehensive evaluation model of fire risk. Due to the influence of flowability, the fire risk of PP is greater than PMMA. Results are of great significance to enrich the material fire risk evaluation database.

942 - Oscillatory Combustion Characteristics of Micron-Size Aluminum Powder in Sound Field

J. Li, Y. Wang, N. Wang

In order to understand combustion characteristics of micro-size aluminum particles in sound field, experiment was carried out in a flat burner with a speaker to generate sound. Aluminum particles with diameters of $10 \,\mu\text{m}$, $20 \,\mu\text{m}$ and $30 \,\mu\text{m}$ were used. Effects of particle size on combustion characteristics was studied. The results show that combustion of aluminum particles in the burner can stimulate high-frequency oscillation up to 1350 Hz. With increase of the particle size, sound pressure of the high-frequency oscillation increased from 54 dB to 67 dB. Change of particle size has little effect on the oscillation frequency. With the increase of aluminum particles size, the damping coefficient decreases, burning time of the aluminum particles increases from 1 to 3 ms. According to the sound pressure curve, combustion of micron aluminum powder can be divided into three stages: preheating, burning and attenuation. At the preheating stage, aluminum particles are preheated by the flame. At the burning stage, aluminum. In the moment of alumina hard shell rupture, sound pressure increases rapidly. At the attenuation stage, aluminum droplets react with the surrounding oxygen. The maximum pressure gradient occurs in the combustion stage, and increases with injected aluminum mass, up to $10^4 \, \text{Pa/s}$.

946 - Effects of Ignition Location on Soot and Species Formation Through Tracking Flame Light Emission and Temperature

Y. Wang, Z. Ma, Y. Zhang

The effects of ignition location on soot formation, multiple flame light emission species, and flame temperature evolution in an impinging configuration have been investigated by using a single high-speed camera. Time-dependent spatial evolution of chemiluminescence radicals of CH^* and C_2^* , soot and the intermediate of the soot formation that emitting infrared are simultaneously tracked and quantitatively analysed via image processing techniques. The flame temperature is evaluated using a modified two-colour method to measure the glowing thin silicon carbide fibres positioned in the flow field. It is found that largest amount of soot forms when the flame is ignited at the nozzle than the other locations. If the flame is initiated at the plate centre, the quantity of the soot formation greatly reduces. Wall quenching is observed in all cases at the impinging stage due to the cool plate effect. There is more quenching-induced temperature drop when the flame is ignited at the plate centre.

952 - Structure Evolution of Energetic Material LLM-105 Under High Pressure

Z. Xu, H. Su, X. Zhou, R. Dai, Z. Wang, H. Li, Z. Zhang

Recently, 2,6-diamino-3,5-dinitropyrazine-1-oxide (LLM-105) has been widely studied on its highpressure structure properties both theoretically and experimentally, but no agreement has been reached each other. This works investigate the structure evolution of LLM-105 crystal under high pressure up to 32 GPa by Raman spectroscopy. The results display that there exist two phase transitions occurring at 10 and 17 GPa, respectively. This conclusion is consist with the previous theoretical calculation. With further loading above 17 GPa, the broadening of Raman peaks and the peak shifted to high wavenumber mean that the LLM-105 had a tendency to evolve to amorphous state. Moreover, two different crystal growth directions in the LLM-105 twin crystal are identified by using Raman spectra.

953 - Rise and Fall of Vortex on a Rotating Paper

T. Tsuruda, T. Daitoku, K. Kobayashi

In large-scale fires, fire whirl spreads in a short time. The reports on fire whirls after the Great Kanto Earthquake on September 1, 1923 describe that large fire whirls spread at Hifukusyoato and killed a

large number of evacuees. Fire whirls spread from three directions to the open space. Reports say that fire whirls appeared near the burning area, the rotation directions of fire whirls were not constant, and they traveled in the open space. These observations show that flow vortex and heat source travel as fire whirls. Under most experimental conditions, a fixed heat source is employed. In this study, flame spread in a well-defined circulating flow on a rotating paper disk was examined with video images.

954 - Flame Spread Along a Combustible Slope

T. Tsuruda, K. Hiyama, T. Daitoku

Wild fire consumes combustible above the ground. Its surface may be along a slope. Wild fire seems to spread faster upwards than downwards due to buoyancy-induced flow. Terada carried out a study on flame spread along a slope. He constructed a scaled model with two gauze sheets along an asbestos board. He observed flame spread along the gauze surface from an ignition source. He found that flame spreads only downward direction and flame does not spread upward around the inclined angle of 35 degree. He pointed out that the flow induced by the flame suppresses convective mass transfer of oxygen to the reaction zone of upward spread flame front. In this study, flame spread along slope was examined with a video camera to determine the flame spread with the inclined angle.

955 - Research of the Rocket Engine with Detonation Chamber

M. Kawalec, P. Wolanski

The paper presents results of research devoted to research on rocket engine with detonation combustion chamber. The comparative research was conducted in order to check the advantage of detonation combustion over deflagration. The simplest way to obtain the goal is to test the combustion chamber in a rocket engine.

A working model of a rocket engine running on gaseous propellant was built. Detonation combustion chamber and deflagration combustion chamber tests were conducted and the results were compared analyzing engine specific impulse and pressure registration. The number of waves was determined by means of Fourier analysis.

The research allowed to determine the range of detonation for the mixture of CH_4 and O_2 , the capabilities of throttling of combustion chamber, and the influence of combustion chamber length on specific impulse. It was found out that the system with a detonation combustion chamber has higher specific impulse than the deflagration system.

The research conducted in the Institute of Aviation shows the advantage of detonation combustion over deflagration. Improving specific impulse allows for enhancing rocket engine parameters. It will raise the thrust and lower its temperature.

960 - Investigation of Co-Combustion Characteristics of Pulverized Coal with Miscanthus Floridulus Biochar

H.T. Lin, G.B. Chen, Y.H. Li, Y.C. Chao

As the fadeout of fossil fuels and global warming effects, the use of renewable energy is more and more important. Biomass is a kind of renewable energy and has the advantages of plentiful sources, zero net carbon emission and lower technical threshold. After torrefaction, it can increase grindability of fuel and make the torrefied biomass easier to store and increase the heating value. In this study, miscanthus floridulus is torrefied at 200 °C and then mixed with Australia pulverized coal. The thermogravimetric analysis (TGA) of different biomass blending ratios (BBRs) is performed. It shows that oxidation process is characterized by a two-stage reaction. An increase in BBR leads to decrease ignition temperature and burnout temperature but it will increase combustion characteristic index (S) and reactivity of the fuel. The primary weight loss will shift from the second stage to first stage when BBR=60 wt.%, which means the fuel properties is dominated by biochar. Besides, the blended fuel pellets were combusted in a laboratory scale furnace at 500-700 °C. According to the results, the ignition delay time (t_i) and char combustion time (t_{char}) were reduced, flame length and the rate of weight loss will loss will increase with increasing BBR. The primary reason is that biochar has more volatile substance but less fixed carbon content when compared to pure coal. However, the time required for pellet combustion generally reduced at higher environmental temperature.

966 - Modelling Analysis of Wave Interactions During the Ignition Process of Rotating Detonation Engines

W. Wei, B. Wang

The rotating detonation engines (RDEs) create continuously propagating detonation wave in the annular combustor to achieve the sustained and stable detonation combustion. Although the ignition of RDEs is much simpler and only needed once, the flow field structure is very complex in the ignition process. The interactions among wave structures occur frequently until stable detonation waves form inside the chamber. The possible interactions could lie between detonation wave and shock wave, or combustion wave, or even detonation wave. In this paper the wave interactions are analyzed in onedimension model and then numerically studied. During the process of the interaction between a detonation wave and a shock wave, the pressure of pre-shock rises sharply, while the temperature increases slightly. As the intensity of shock wave increases, the pressure after the detonation wave increases greatly. This induced high pressure would cause the decrease of the inlet mass flow of fresh unburnt gas in the RDE, which may cause the quench of the detonation wave. The interaction between two detonation waves is also studied. The pressure profile and the history of the maximum pressure during the process of the interaction between two detonation waves show that after the interaction of detonation waves, initially the pressure of the wave front increases sharply, which reaches more than 100 atm. Since there is no existence of reactants, both detonation waves extinguish; and then two pressure waves form and decay gradually.

967 - Numerical Simulation of a Single-Mode Sinusoidal Flame Interacting with a Shockwave *W. Wei, B. Wang*

Various research on the instability of multi-fluids with different densities induced by the impaction of shock waves, called Richtmyer-Meshkov instability (RMI), has been conducted to predict the development of the fluid interface and reveal the physical mechanism of the disturbance growth. However, few study has been conducted in chemically reactive fluids in the past decades, especially in regards to the evolution of the shocked interface considering its detailed chemistry. In this paper, a numerical study is performed on the Richtmyer-Meshkov instability of a single-mode sinusoidal interface in chemically reactive fluids. The perturbed flame is initially generated by a premixed combustion of the H₂/O₂ reactive mixture, and then the RMI would be triggered by the incident shock wave introduced from combustion product fluids. The multi-species reactive Navier-Stokes equations are solved using a fifth-order WENO scheme. A detailed chemical reaction mechanism containing of 9 species and 19 steps is adopted. An inert RMI case is firstly simulated under different grid resolutions to validate the present numerical procedures, using the flow parameters in the experiment conducted by Jacobs and Krivets. The reactive cases are studied with different parameters qualitatively and quantitatively to reveal the growth mechanism of disturbance. It is found that the competition of baroclinic effects with the reaction heat release determines the interface evolution. The reaction induction time of shocked unburned fluids decreases and the apparent flame propagation advances if the strength of the incident shock wave increases, thereby leading to a faster chemical reaction. The interface growth will enter the non-linear status earlier as the initial amplitude of the single-mode interface increases. The rollups of mushrooms, representative of unstable flow structures, are accelerated and spatially spread the reaction in the fresh fluids through a stronger incident shock wave. The fast chemical reaction due to the high mixture temperature will consume the unburned fluids in the small-scale structures, where a higher concentration of radical OH is distributed, and the flame will be thickened. The enstrophy is mainly generated on the interface and exhibits increased oscillation, which demonstrates that the impaction of the baroclinic effects of shock wave is greater than that of the dilatation on the increased vorticity.

977 - Physical and Electrical Measurements of Different Metals Used in EBW Detonators

C. Valancius, J. Bainbridge, C. Love, D.R. Richardson

Implementation of the energy density metric has made it possible to better understand the physics of exploding wires. When applying the energy density metric to exploding wire experiments in a porous material bed, results suggest a link between characteristics of wire materials (e.g. their electrical properties during burst and the physical work done by the bursting wire). Previous work has focused

on qualitative comparisons of current and voltage waveforms and the qualitative comparison of schlieren images of wire shocks in air. In these experiments, the wires were all buried in a porous pressing of CL-20 allowing the simultaneous capture of accurate current and voltage to observe the energy density at burst, while simultaneously observing the amount of time the detonator took to produce an output detonation. Observing the time to detonation output in concert with the energy density allows a link to be established between the measured electrical signals and the physical work done by the exploding wire. This research allows a more quantitative link to be established between the electrical energy and the physical energy expended by an exploding wire, allowing for the development of more accurate models and a better understanding of exploding wire physics.

1003 - Numerical Analysis on Liquid JP10 Rotating Detonation Engine

A.K. Hayashi, W. Yoshida, M. Asahara, N. Tsuboi

Liquid-gas two phase detonation has not been studied much because of dealing with different phase and complex dynamics although liquid is actual fuel for aerospace vehicles, boat, car, etc. Recently Dabora et al. reported that cyclodecane of its diameter of 2.6 mm deforms, breakups, evaporates, mixes, and burns after detonation passes its mixture. Cheatham and Kailasanath reported an evaluation of thrust performance of liquid JP10 PDE that specific impulse increases as liquid evaporation rate increases. However there a few work on liquid RDE study. One of the most recent work is presented by Anderson et al. to understand liquid injector performance under the transient atmosphere characteristic of RDE. They showed a strong effect of a passing detonation on liquid atomization. In order to get a stable rotating detonation in RDE when liquid fuel is applied, this study will seek the liquid phase influence on rotating detonation structure.

1018 - Detonation in 3D Annular Chamber with Obstacles and Water Surface on one End

K. Sato, E. Dzieminska, A.K. Hayashi, Y. Tamauchi

Accidents at Hamaoka, the first nuclear power plant, and Fukushima are considered to be due to hydrogen explosion and it was thought that a part of the explosion accidents was caused by detonation. Since the influence of the detonation was not considered by the design of the nuclear power plant, it caused serious damages.

In this study, the relation of flame propagation, obstacles and water surface are investigated by calculating parameters such as overpressure and temperature in case of hydrogen explosion in annularly shaped tank with cylindrical obstacles as a representative example. Therefore, in this study, numerical computations are performed. Also the outbreak energy of the explosion to occur in the container, which had a cylindrical obstacles to confirm the safety in the small capacity apparatus that could exist at a nuclear power plant.

1039 - A Numerical Investigation on Double-Front Detonation in Solid Explosive Mixture with Varying Aluminum Concentration

W. Kim, M. Gwak, J. Yoh

In this study, we deal with an aluminized high explosive including an afterburn of a reactive metal particles (Al particles) in high temperature and pressure states by detonation of high explosive. The research relating to the combustion of Al particles in combustible or reactive gases and in high explosives have been extensively conducted for several decades. In particular, there exist far more test data reported for the gaseous detonation with Al additives than the aluminized high explosives. There have also been numerical studies on the varying Al concentration on the gaseous detonation rather than condensed phase detonation. Specifically, the numerical research for the behavior of Al particles in the gas flow has been conducted with two-phase model based on Eulerian analysis. However, because of the difficulties associated with conducting high explosive tests with Al concentration variation, there exists only a limited experimental data on it and no numerical study has been previously reported in the literature. In this study, the two-phase model (KV model), which was formerly used in the gaseous detonation is redeveloped for understanding the effect of Al concentration on the performance of the aluminized HMX. The concentration of 0~25 % is considered in the KV interaction model for comparison with the post-burn experimental data.

1104 - Numerical Simulation of Rotating Detonation Under Variable Conditions

V. Levin, I. Manuylovich, V. Markov

The problem of rotating detonation initiation and combustion of mixture in a three-dimensional rotating detonation wave confined in the space between two coaxial cylinders is formulated. The model of detonation initiation by energy supply is formulated, and in subsequent numerical experiments the necessary initiator parameters are selected for the formation of rotating detonation. Initiator allows to select the direction of rotation. The system of mixture injection into the combustion chamber is implemented, taking into account the ratio of tank pressure and the static pressure in the combustion chamber near the inlet of the chamber. The series of calculations were carried out, which provided optimal parameters of rotating detonation initiators. A numerical investigation of unsteady flow parameters during rotation of the detonation wave in the combustion chamber is conducted when injecting combustible mixture around its whole end.

It was found that rotating detonation wave is formed in the combustion chamber and the direction of rotation is given by the location of the energy initiator zone relative to the longitudinal solid wall, which disappears (burns) for certain time.

In order to study the behavior of rotating detonation under changing conditions of mixture injection into the combustion chamber, two processes were considered with a linear decrease of the thermodynamic parameters in the tank with a stationary fuel mixture—one with decreasing pressure and constant temperature, and the second – with decreasing temperature and constant pressure. It was found that under time varying stagnation parameters of combustible mixture the rotating detonation wave is formed in the combustion chamber. According to calculations, for variable pressure in the tank the rotating detonation exists until the moment when the total pressure in the tank becomes equal to the critical value. Thus, the existence of minimum critical total pressure at which the detonation does not stop for a long time.

In both cases, the dependencies of gas dynamic parameters were obtained for 11 points inside the combustion chamber and the data were received to construct fields of gas-dynamic parameters at different time moments. Total pressure values were used to calculate the average values for the period of oscillations, required for the determination of total pressure growth compared with the pressure in the tank.

The resulting plots of gas-dynamic parameters' dependence on time show that the process is complicated, periodic and oscillatory. According to calculations, the highs and lows of the static and total pressure at the control points within the combustion chamber substantially change over time in an oscillatory mode.

1136 - A Study of Interaction Between Pressure Waves and Reaction Regions in HCCI Combustion Accompanied by Strong Knocking Based on High-Speed in-Cylinder Visualization and Observation

A. Iijima, K. Takeda, Y. Yoshida, Z. Lin, H. Shoji

In this study, a test engine that allowed the entire combustion chamber to be visualized was operated under conditions giving rise to the formation of strong pressure waves in the combustion chamber. The initiation and development of autoignition in the combustion chamber and the mechanism causing the formation of pressure waves and pressure oscillations were investigated on the basis of high-speed incylinder visualization and observation of combustion and frequency analysis of pressure waves measured in the combustion chamber. The results indicated that under conditions producing strong knocking, a region with a highly brilliant flame forms locally and propagates at high speed to the unburned end zone where areas of unburned mixture autoignite successively. The apparent propagation velocity of autoignition at that time is estimated to be faster than the speed of sound. Presumably, under conditions producing strong pressure waves and pressure oscillations, the interaction of pressure wave fronts and reaction regions induces a state of developing detonation in which rapid combustion occurs.

1137 - Simulation Study on Detonation Propagation Driven by Piston

Z. Lin, J.H. Lee, X. Mi

It's found that there is significant deviation of detonation velocity obtained using real chemistry with that from CJ theory. When the piston move back fast enough relative to the incoming flow, the detonation will always be CJ detonation. It is about 700 m/s of piston relative to flow velocity for the current mixture. When the piston velocity toward the detonation larger than that, the detonation will be overdriven. For the CJ detonation, the flow behind the detonation can also become subsonic, which means the detonation can resist the disturbance in some range. But the real mechanisms lead to this phenomenon hasn't been revealed.

1142 - Sensitivity Study of Solid Fuel Properties and Dynamic Behavior of Pyrolysis in Non-Charring Materials

S. Sabarilal, A. Syed, A. Kumar

The present work examines the fire behaviour of non-charring materials subjected to property variation using an unsteady numerical model. Fuel under study is non-charring thermo plastic PMMA since it is most common polymer studied in fire science. Pyrolysis is the key process in the burning of solid fuels since the rate at which material transforms into a gas phase fuel governs energy release rate in subsequent flames. The influence of various material properties like specimen thickness, absorption coefficient, density specific heat, heat of reaction, on various fire response parameters like MLR and ignition time is analysed. A quantitative assessment was carried out in the form of sensitivity study which highlights the simultaneous effect of thickness and heat flux on the solid fuel properties and was not explored in previous studies. Also, the background of Scaled Energy Balance approach gives better understanding of dynamics of pyrolysis. An amalgamated analysis of both will help us get more insight into various physical processes within pyrolysis and will help in the development of fire-retardant materials with general application in fire safety sciences.

1071 - Experimental Study on Laser Ignition of Low Vulnerability Propellant Based on Nitrocellulose

L. Courty, J.F. Lagrange, P. Gillard, C. Boulnois

Ignition and combustion of a low vulnerability propellant mainly composed of nitrocellulose are studied. Experiments were performed in a cylindrical reactor for different gaseous atmospheres (nitrogen and argon) and different initial pressures between 10 and 70 bars. Ignition is obtained thanks to a laser diode, laser power was varied between 0.66 and 9.95 W. Overpressure, ignition delays and propagation rate are obtained. E50 are also given for different laser powers and gaseous atmospheres. It is found that overpressure are higher in argon than in nitrogen but the effect of gaseous atmosphere on ignition delays is not clear. E50 are strongly decreasing when laser power is increasing.

Poster Session II

777 - Influence of Methane Additions on Self-Ignition of Pulsed Jet of Hydrogen

S. Golovastov, V. Bocharnikov, O. Terekhova

The influence of addition of methane on the self-ignition of a hydrogen jet was studied experimentally for the pulse discharge into an open channel filled with air. During the pulse discharge from a high pressure chamber a shock wave is formed, which heats the surrounding air and a contact surface. The self-ignition of the jet occurred at the contact surface of the jet with air. A mixture of hydrogen with methane was preliminary prepared in a vessel of 40 liters. The initial pressure of the mixture was varied from 3 to 15 MPa. During the discharge of the binary mixture ignition delays were measured relative to the moment of a breaking of the diaphragm. Ignition delays were determined by a photomultiplier tube. The delays were measured for different initial pressures and the methane addition. A molar concentration of the methane addition varied from 5% to 18%. Analysis of the effect of impurities on the thermodynamic parameters of the pulsed jets was carried out.

783 - Double Shock Experiments on PBX Explosive JOB-9003

X. Zhang

One-dimensional plate impact experiments have been performed to study the double shock to detonation transition and Hugoniot state in the HMX-based explosive JOB-9003. The flyer was a combination with sapphire and Kel-F, which could pass two different pressure waves into PBX Explosive JOB-9003 sample after the impact. The particle velocities at interface and different depths in the PBX JOB-9003 sample were measured with Al-based electromagnetic particle velocity gauge technique, thus obtaining particle velocity - time diagram. According to the diagram, the corresponding Hugoniot state can be determined based on the particle velocity and shock wave velocity in the sample. Comparing with the single shock experiments, PBX Explosive JOB-9003 shows desensitization features due to the pre-pressed shock wave, the shock to detonation transition distance is longer than those single shock experiments.

784 - Shock Initiation of Wedge-Shaped Explosive Measured with Smear Camera and Photon Doppler Velocimetry

Y. Gu

Triaminotrinitrobenzene (TATB) is an important insensitive high explosive in conventional weapons due to its safety and high energy. In order to have an insight into the shock initiation performance of a TATB-based insensitive high explosive (IHE), experimental measurements of the particle velocity histories of the TATB-based Explosive using Photon Doppler Velocimetry and shock wave profile of the TATB-based explosive using High Speed Rotating Mirror Smear Camera had been performed. In this paper, we would describe the shock initiation performance of the TATB-based explosive by run-to-detonation distance and the particle velocity history at an initialization shock of about 7.9GPa. The parameters of Hugoniot of unreacted the TATB-based explosive and Pop relationship could be derived with the particle velocity history obtained in this paper

809 - Analysis of the Canonical Turbulent Shock Front

H. Cao, T. Jin, L. Wang, K. Luo, J. Fan

The present work focuses on the effect of turbulence on the shock front, especially the shock front identification and shock curvature statistics. Numerical results show that the shock front can be identified by a representative pressure iso-surface, in consistency with the local minimum dilatation criterion. Kinematically the shock front distortion is closely related to the turbulent velocity fluctuation. By defining the turbulent shock speed as the relative velocity along the shock normal direction between the Lagrangian velocity of the pressure iso-surface and the local fluid velocity on the upstream side, it is found that the mean shock speed is linearly dependent on the local fluid velocity. The physical mechanisms of these interesting features are analyzed.

819 - Experimental Rotating Detonation Engine Behavior Dependence on Detonation Channel Width

M. Fotia, J. Hoke, F. Schauer

Rotating detonation engines have shown promise as a potential avenue to integrate pressure-gain combustion into aerospace propulsion applications. The identification of the driving physical mechanisms in these novel devices that influence both the detonability and attainable propulsive performance are of particular interest. This work seeks to examine the dimensional scaling of the detonation channel while attempting to hold the effect of propellant mixing constant. The successful scaling of rotating detonation engine systems is a key aspect in the future application of pressure-gain combustion technology to aerospace propulsion.

820 - Effects of Flame Instabilities in Hydrogen-Air Explosions

W. Kim, T. Imamura, T. Mogi, R. Dobashi

Experiments have been conducted to examine the flame instabilities on expanding spherical propagation of hydrogen-air flames. The cell formation and development on the surface of hydrogen-air flame were investigated as a function of Pe using image thresholding technique. The cells began to start along the realms of high curvature and propagated across the surface with increasing Pe. The cell size of the flames wrinkled due to diffusional-thermal and hydrodynamic instabilities are measured. It is shown the values of cell size by hydrodynamic instability are greater than that of cells generated by diffusional-thermal instability are characterized. The values of Pe_c increased with increasing f by the stabilization and increase with P_0 by decreasing the flame thickness. Such results Pe_c is promoted by diffusional-thermal as hydrodynamic instabilities. In the present study, the effects of the instabilities on the flame speed are estimated comparing the ratio of increase in the burning velocity decreased with f and increased with P_0 . Our results demonstrate that the cellular flame due to the flame instabilities might cause the increase in the flame speed and thereby lead to the strong blast wave lead to considerable damages generates.

824 - 3D Flame Reconstruction Using Single Camera and Fibers

K. Wang, F. Li, X. Yu

Chemiluminescence measurements are commonly employed in the study of flame geometry and excited species concentrations. Computed tomography of chemiluminescence (CTC) is potential for the three dimensional diagnostics of combustion both on high spatial and temporal resolution. It uses 2D multi-directional projections as inputs incorporated with iterative algorithms to get the 3D distribution. In general, a good simulation of projections processing by charge-couple device (CCD) is important for the reconstruction solution. Bokeh effect out of focus may has an effect on the projections, which is produced by lenses of finite aperture. In order to verify the influence of imaging blurring on 3D-CTC, three different projections models were studied, including Clear-imaging model, Out-of-focus imaging model, Deconvolution model. The results suggest that the model taken the consideration of bokeh effects has the best reconstruction accuracy, but it is time consuming. The projection deconvolution processing can improve reconstruction accuracy without increasing computation time.

829 - Effect of Ambient Oxygen and Temperature on Gaschromic Properties of Pt/WO3 Thin Film Exposed by Hydrogen

K. Yashiki, T. Matsuoka, Y. Nakamura

Hydrogen is received attention as a promising clean fuel for near future. However, it has wider explosion range and lower minimum ignition energy, detection of its leakage is very important task in order to prevent the potential accidents. Platinum-supported tungsten oxide (Pt/WO₃) shows unique feature as sensor of hydrogen gas via "gaschromic reactions". Once it is exposed by the hydrogen, coloration reactions occurs immediately so that the presence (leakage) of hydrogen can be detected easily and quickly by naked eye without any additional devices, which may cause the explosive hazard (e.g. electric circuit). In this study, in order to evaluate for early-hydrogen detection in various ambient conditions, the effects of ambient oxygen and temperature on gaschromic properties of Pt/WO₃ thin

film exposed by hydrogen were investigated. Three kinds of Pt/WO₃ thin films were made by spincoating with sol-gel method over the glass substrate and hydrogen detection test was performed under various ambient conditions of temperature (from room temperature to 333 K) and oxygen concentration (from 8 to 20 %). The structural characterization of the film was confirmed by Scanning Electron Microscope Energy Dispersive X-ray Spectrometry (SEM-EDX) and X-ray Diffractometer (XRD), and it is found that the thickness can be well-controlled by the number of lamination. Through the hydrogen detection test, it is found that the thicker film is preferable for early-hydrogen detection purpose. In addition, detection rate of Pt/WO₃ thin films decreased as increasing ambient oxygen concentration. This result suggests that the present system is preferable to detect hydrogen in lower oxygen ambient condition. As expected, it is confirmed that the detection rate increased as increasing ambient temperature. Through this study it is confirmed that detection feature of Pt/WO₃ thin film exposed by the pure hydrogen is affected not only by the film thickness, but also ambient oxygen concentration and ambient temperature. Because all factors shows similar impact to the coloration rate, it is suggested that they would be competing each other. Further careful study is needed to confirm the precise coloration performance of the Pt/WO₃ thin film. Currently we are upgrading the experimental system to make this possible.

847 - Adjoint-Based Variational Data Assimilation for the Analysis of an Experimental Pulsed Detonation Combustor with a Compact Shock-Focusing Geometry

M. Lemke, J. Gray, J. Reiß, J. Moeck, J. Sesterhenn

Pulsed detonation combustors (PDC) promise higher efficiency compared to isobaric combustors, which are presently used in stationary gas turbines and aero engines. The core idea is to use the thermodynamic advantages of an isochoric cycle. However, in order to directly initiate the detonation, a large amount of energy is required. Therefore, the combustors usually make use of the deflagration-to-detonation transition. In general, the fluid mechanical processes in the chamber are difficult to analyze, due to the inherent measurement restrictions of a detonative flow regime.

The aim of this work is to analyze the experimental data of a PDC with an alternative method of obtaining DDT. Time-resolved pressure measurements serve as the target for an adjoint-based variational data assimilation. An optimal one-dimensional description of the process governed by the reactive Navier–Stokes equations is derived. The parameters of the employed Arrhenius chemistry model and flow parameters are adapted. This is important because once the numerical simulation data match those of the experiment, other quantities, such as velocity and temperature, can be extracted from the numerical solution.

849 - Numerical Modeling on the Flow Characteristic of Catalytic Combustion Over a 2D Cylindrical Bluff Body

C.Y. Wu, C.C. Cheng, Y.S. Lien

In the present study, the flow characteristic of catalytic combustion over a 2D cylindrical bluff body has been numerically studied. Generally, the Von Kármán vortex sheet can be found at the downstream of 2D cylindrical bluff body. The vortex shedding frequency is dominated by the Reynolds number. The conversion ratio can be increased as the gas phase reaction is ignited and sustained in the flow field.

862 - The Model of Detonation Combustion in Liquid Aerosols

O. Girin

Mathematical model of liquid mono-dispersed aerosol detonation is described, which is based on the detailed calculation of the combustible mixture formation and evolution behind detonation front (parent drop atomization kinetics, sprayed mass motion and evaporation with due regard to the dependence on the droplet radii, as well as chemical kinetics). The description of a spray phase formation is based on the concept of high-frequency periodic dispersion from the unstable part of the parent drop surface due to the instability of the gradient flow in conjugated gas-liquid boundary layers.

Equations of combustible mixture motion are composed. The equation of dispersed fuel is supplemented with equation of motion of the droplet-phase continuum coupled with the equation of vapor influx in a spray volume. The equation set is closed by the equations of state of phases.

Assumption is made that the gas components' mixing is much more rapid compared with atomization and vaporization processes, so that the mixing is instantaneous. Modeling the spray multi-velocity medium, we regard the droplet size scale as an independent variable for describing their velocity fields and evaporation rates. We have introduced the transient distribution function of daughter droplets by sizes, as it exactly reflects the entire evolution of droplets resulted from their acceleration and evaporation. Every parent drop is considered as a point source of daughter droplets; in turn, each daughter droplet is a point source of vapor.

The mathematical model is realized for the stoichiometric kerosene–oxygen mixture. Regimes of aerosol burning behind the detonation front are calculated and analyzed. For a given front velocity the equations permit to calculate in one-dimensional plane approximation a flow structure behind the front. The value of self-sustained regime velocity is the eigenvalue of the boundary-value problem for the combustible aerosol flow. The aerosol burning regime is regulated by the ratio of drop atomization time to chemical induction time, which is the governing parameter depending strongly on the shock front velocity D. When D increases, the chemical induction time drops greater than the characteristic time of physical processes, so that chemistry is "waiting" for the physics. Vice versa, when D drops, the chemical induction time raises greater than the characteristic time of physical processes in such a way that the stationary self-sustained regime is possible. The model allows analyzing feasibility of the stationary self-sustained regime in closed form, given the aerosol drop radius and aerosol properties.

878 - Three-Dimensional Supersonic Boundary Layer Separation Induced by Curved Sidewall *G. He, J. Zhou, Y.X. Zhao, Y.L. Zhao*

A three-dimensional supersonic boundary layer separation induced by a curved sidewall is experimentally and numerically studied. The curved sidewall generates a compression wave fan and then focus into a straight shock wave. The results show that all the flow in the inflow boundary layer will be rolled into the separation vortex and the separation flow shows conical symmetry in the far downstream region where the swept shock wave has been formed by the compression wave fan.

897 - Breakdown Ignition of Nonsolvent Ionic Liquid with Double Pulse Laser

N. Itouyama, H. Habu

High energetic ionic liquid is expected as the substitute of conventional liquid propellant for thruster. Based on gas breakdown ignition, we evaluated the ignition ability of ammonium dinitramide (ADN) -based ionic liquid propellant with two methods using double pulse laser. The difference is whether 1st pulse and 2nd pulse pass through same optical axis or not. Our results shows that both methods makes effective gasification and atomization of ionic liquid droplet by 1st pulse irradiation, but 2nd pulse doesn't work as igniter. We considered that this reason arise from combustion limit of product gases.

934 - Numerical Investigation of the Instability of Continuous Detonation Engine

S. Zhang, S. Yao, M. Luan, L. Zhang, J. Wang

A numerical simulation of the continuous detonation engine (CDE) is performed using convergent nozzles for fuel injection. An instability phenomenon of the detonation wave is found and discussed in details. The interaction mechanism between the injection of fresh gas and the detonation waves is revealed. The detonation wave oscillates due to the fuel injection conditions. The oscillation of detonation wave produces a group of weak shock waves, making the flow field very complicated. Some weak shock waves collide with the inlet wall and cause an instant pressure rise, blocking the fuel injection in some locations. As a consequence, the fresh fuel layer presents an irregular shape, which in turn causes the detonation wave oscillating. Furthermore, convergent nozzles are not choked, making the mass flow rate fluctuating, which can aggravate oscillations in the flow field. This irregularity remains in the flow field, so does the instability of the detonation wave which rotates continuously.

951 - Experimental Study on the Explosion Characteristics of Methane-Hydrogen/Air Mixtures *X. Shen, G. Xiu*

Experiments were performed to measure the explosion and combustion parameters of methanehydrogen/air mixtures in a standard 20-L spherical vessel by pressure sensor. The effect of hydrogen addition were carefully analyzed and evaluated. When the hydrogen content is less than 30%, the peaks of the maximum explosion pressures versus methane content are very close due to the similar equivalence ratio and flame expansion ratio of corresponding mixtures. Nevertheless, the peaks of the maximum pressure rise rates versus methane content rise up remarkably with hydrogen content increasing due to the increment of thermal conductivity and laminar flame speed. Besides, with hydrogen addition, both lower and upper flammability limits of methane in the mixture decline prominently. In addition, the laminar flame speed varies similarly to maximum pressure rise rate. And it is predominantly controlled by the total equivalence ratio of the binary fuel blend/air mixture. Overall, the hydrogen addition could significantly enhance the explosion risk and severity of fuel system.

964 - A Study on Burning Velocity Characteristics of Meso-Scale Spherical Laminar Flames for Lean-Hydrogen-Propane Mixtures

M. Nakahara, Y. Maruyama, A. Ishihara, F. Abe, K. Tokunaga

Recently, with the increasing demands on developments not only of micro combustors for power supplies and heat sources of portable/micro-devices, but also of high-thermal efficiency and lowemission SI engines, which need the assured flame kernel development in a flame initiation stage for reducing misfire, understanding burning velocity characteristics for lean-fueled micro/meso-scale flames is important. One important difficulty of lean burning is that the flames are so weak that a stretch of turbulence and/or heat loss can easily cause local extinction leading to weak combustion. One of the lean combustion instability problems can be resolved through addition of hydrogen. The present study is performed to examine experimentally the burning velocity characteristics of meso-scale spherical laminar flames of hydrogen added lean-propane mixtures in the range of flame radius < 5 mm. The mixtures with different equivalence ratios (F=0.5 and 0.8) and hydrogen additional rates ($d_{\rm H}$ =0.0~1.0) are prepared while maintaining the so-called laminar burning velocity SL0 at approximately 25 cm/s, in order to investigate the effect of hydrogen addition on lean-fueled meso-scale laminar flames, where F includes fuel concentration below a flammability limit of propane-air mixtures. The flame radius rf and the burning velocity S_{Ll} of meso-scale flames are obtained by using sequential schlieren images. It was found that S_{L1} at the same r_f and Karlovitz number increases with d_H, regardless of F. The optimal r_f and Karlovitz number with respect to burning velocity appear when $d_{\rm H}$ get as far as approximately 0.8. The SLI at the same rf also tends to meaningfully decrease with the Lewis number and the Markstein number, irrespective of d_H and F.

972 - The Finite Heat Conduction Model of Single Droplet Combustion and its Verification

S. Fei, Y. Qi, Y. Li, M. Wei, G. Guo, Z. Wang

In order to find a reasonable way to take into account the heat conduction at the droplet surface in a steady droplet combustion model, the term describing heat transfer in the classical model is replaced using a finite heat conduction expression, which is obtained by the calculation of a heat conduction process in the droplet. Thus, the finite heat conduction model with respect to the droplet combustion is constructed. The component distribution and the mass burning rate during the combustion process of an isooctane droplet in a certain environmental condition are calculated. The results under corresponding conditions are compared with the previous simulated results and experimental data respectively so as to verify the finite heat conduction model. The results of the verification show that the finite heat conduction model is accurate and correct.

973 - Effect of Additional Diluents on Laminar Burning Velocities and Cellular Instability in Outwardly Propagating Methane/Ethylene-Air Premixed Spherical Flame

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The present work investigated the comparison of laminar flame speeds measured from outwardly propagating spherical flames with diluents (where nitrogen, carbon dioxide, or helium). To study on

them, cylindrical constant volume chamber (CCVC) was used, in that it is excellent experimental facility to measure 1-D flame propagation speed and easily observe the flame configuration. In this study, diluents which were a variety of mixing ratio from 0.1 to 0.5 mole fraction were added to methane/ethylene - air mixture to evaluate effect of unstretched laminar burning velocities and Markstein length with elevated pressure up to 3atm. Experimental results showed that laminar burning velocities significantly decreased with the increase amount of diluents addition to the reactant mixture. In case of diluted carbon dioxide, the propensity for unstretched laminar burning velocity was significantly decreased more than others. Furthermore, the increase of initial pressure reduced not only unstretched laminar burning velocity but also Markstein length. But Markstein length increased with additional diluents ratio. Additionally, the experimentally measured unstretched laminar burning velocities were compared to numerical predictions to obtain a better correlation with experimental value between PREMIX and OPPDIF code based on USC mechanism II. In case of diluted helium, the results showed that flame speeds of PREMIX code had substantial discrepancy with experimental one at equivalence ratio 0.8 and fuel-rich side, because of high conductivity. Although OPPDIF and PREMIX code had small discrepancies at carbon dioxide and nitrogen rather than helium, the predictions of OPPDIF code generally has good agreement with experimental data with diluents. The results showed that cellular instability was devitalized in increase of diluents with diluted carbon dioxide and helium at a fixed elevated pressure, whereas it was augmented in increase of pressure at a fixed fuel mole fraction. Effects of additional diluents and increased pressure on cell formation on the flame surface were examined though evaluating the Lewis number, flame thickness, and thermal expansion ratio.

1010 - Safety Problems of Commercial Cap-Sensitive Emulsion Explosives Turnover in the Territory of the Republic of Kazakhstan

I. Pustovalov, S. Aleshkova, M. Atamanov, E. Aliyev, Z. Mansurov

Insufficient degree of control over the industrial explosives turnover leads to their constantly increasing illegal use for criminal or terrorist purposes. Thus, the actual task is to provide the possibility of labeling (tagging) the industrial explosives in the stage of their production with the secret detection agent, that will allow to identify by technical means the product - as an explosive and to know the trademark of the detected explosive, its manufacturer, and other necessary information. The aim of the research is to reveal in amount of chemicals the most appropriate according to its properties in order for using it as marking substances of the industrial explosives. Determine the principles of data encryption (code of the country of manufacture, the production, the manufacturer, produced batch and the date of manufacture, etc.) in the microcarrier (marking additive). Choose the most accurate and effective physical and chemical methods of identification (analysis) of marked industrial explosives.

1014 - Effects of Discharge Frequency on Ignition Behaviors of DBD for Lean Methane/Air Mixtures

S. Nakaya, X. Gu, T. Kobayashi, S. Iseki, M. Tsue, M. Kono, K. Nakamura

Effects of discharge frequency on the ignition performance of Dielectric Barrier Discharge (DBD) for lean methane/air mixtures were investigated experimentally. Plasma was formed in a combustion chamber with a constant volume, and a spark plug was installed. Firstly, plasma characteristics were investigated at various pressures, and the lifetime of plasma was observed for several frequencies of the current discharge. At 0.1 MPa, low temperature plasma was formed although the thermal plasma seemed to be formed at the higher pressure. At 0.1 MPa and 0.05 MPa, ignition experiments were conducted for lean mixtures. It was found that higher frequencies of the alternate current discharge results in the higher performance with the same discharge counts.

1016 - Flame Propagation and Initiation of Detonation in a Two-Dimensional Annular Channel with Cylindrical Obstacles

H. Sakai, E. Dzieminska, A.K. Hayashi, Y. Tamauchi

This research investigated combustion scenarios with the aim of eventually developing new safety measures for the prevention of explosive accidents, such as the two serious incidents in Japan at the Fukushima and Hamaoka nuclear power plants. Both events are believed to have involved hydrogen

detonations, based on the resulting degree of damage. This study modeled the release of a significant quantity of hydrogen gas followed by an explosion in a two-dimensional annular storage tank in the air-conditioning system of a nuclear reprocessing plant. The objective was to ascertain the effects of obstacles on flame propagation and transition to detonation using numerical calculations. The results obtained with no obstacles and with up to 16 obstacles demonstrate that obstacles render the flame propagation wave approximately 1.2 times slower. However, the presence of obstacles also generates auto-ignition points and shock waves, and the interaction between these shock waves and the propagation wave along the outer wall can contribute energy to the propagation wave. It appears that both auto-ignition and detonation may be more likely when obstacles are present in the channel.

1051 - Comparison of Detailed Mechanisms for the Numerical Simulation of Unsteady Shock-Induced Combustion

P.K. Pavalavanni, J.Y. Choi

Experimental and theoretical studies of Shock-Induced Combustion (SIC) have been extensively reported since 1960's. Numerical simulation of such complex flow was reported and validated by various researchers from as early as 90's. It has regained its interest in the last decade because of its application to aerospace such as in the studies of Oblique Detonation Wave Engine (ODWE), Shock-Induced Combustion Ramjet Engines (SCHRAMJET). Close coupling between gas dynamics and reaction front triggers the chemical instabilities and hence numerical investigation on SIC flows is crucial to understand such complex theoretical phenomena. The combustion flowfield is characterized by the complex coupling and interaction of the shock wave combustion regime and distinctive results depending on the flowfield conditions. Numerical simulation of SIC poses various challenges. Accurate prediction of the induction zone, where the temperature, pressure and density remains almost constant but reactions will progress zone. Another challenge is the selection of numerical schemes. An inaccurate numerical scheme may result in numerical errors which may result in additional release of chemical energy from different reaction rates resulting in "Spurious runaway reactions". One of such is the consideration of detailed reaction mechanisms in the numerical simulation of any reactive flows to obtain accurate a flowfield. Various researchers have used different reaction mechanism in their numerical simulation. In this study, performance of some of the reaction mechanisms, screened based on their usage in SIC flows were compared. A grid dependence study was done for all the reaction mechanisms to analyze the performance of reaction mechanism.

1056 - Roughness Influence on Flame and Detonation Propagation

E. Dzieminska, Y. Hara, M. Morishita

In this study, experiments as well as numerical simulations of flame, detonation, and deflagration-todetonation transition (DDT) were performed to find how surface roughness in micro-scale effects combustion processes and what the smallest roughness that can be a reason for detonation is, which can mean either shorter detonation initiation distance (DID) or induction time. Modeling was done with the two-dimensional channel with boundary conditions of different wall roughness (Ra) from 0 (smooth) to 0.8 μ m, 1.6 μ m, 3.2 μ m, and 1 mm. The numerical results show a process of DDT under all conditions and furthermore, some characteristics of detonation.

Deflagration to detonation transition occurred at about the same time and the same distance under conditions of $Ra = 0 \ \mu m$ (smooth), $Ra = 0.8 \ \mu m$ and $Ra = 1.6 \ \mu m$. It could be confirmed that about 5% shorter induction time and up to 8% shorter DID occurred with $Ra = 3.2 \ \mu m$. And with $Ra = 1 \ m m$ about 12% shorter induction time and up to 15% shorter DID was seen. Thus, the smallest roughness which affects detonation phenomenon should be between $Ra = 1.6 \ \mu m$ and $Ra = 3.2 \ \mu m$. In other words, the micro scale roughness effects are significant in DDT phenomenon. So far the results were only obtained for 0.8 μm rough walls. Calculation model is exactly 10 times smaller than experimental tube and with the same mixture at least we could observe propagating detonation.

1086 - Effect of Swirl Intensity on the Flow and Combustion Characteristics of Pulverized Biomass Flame

A. Elorf, B. Sarh, S.Bostyn, V. Belandria, S. Bonnamy, M. Asbik, F. Tabet, J. Chaoufi, I. Gokalp The aims of this work is to study numerically effect of swirl intensity on the flow behavior and flame characteristics to more clarifying the swirling pulverized biomass flames. Flame stability and combustion gases at each swirl number are analyzed. Four cases with different swirl numbers (Sn) are studied. The numerical approach is based on Reynolds averaged Navier–Stokes (RANS) method. The results presented in this paper concern the influence of swirl number in flow topology, velocity contours, temperature distribution, and species concentrations profiles.

1092 - Impulse Measurement of Small Scale Detonation Tubes Under Direct and Indirect Detonation Initiations

J. He, W. Fan, J. Zheng, Y. Chi

Impulse measurements of millimeter-scale tubes were conducted using a ballistic pendulum. The influences of the system weight was examined. It is concluded that over-weighted pendulum system may affect the results greater than the drag forces created by the wires between the system and the ignitor. The impulses generated by direct and DDT initiation of detonation are the same. Furthermore, it is also hardly affected by different DDT distances at the same mixture contents. When the tube's length to diameter decreases, DDT generated impulse may be possibly larger than that of direct initiation. A visualization of the flame propagation process revealed that the secondary purging of the supersonic gas may contribute a lot to the impulse production.

1123 - Study on Non-Ideal Detonation Behaviour Based on Analog System

Y. Sun, H. Yang, C. Wang

The paper builds the analog system of detonation with loss and the chemical reaction of two step reaction model, wherein an induction zone is followed by an energy and heat release zone. Steady state of detonation wave structures are obtained by analytic method. By changing the value of the sensitivity exponent of reaction rate n and the sensitivity coefficient of loss rate m, we can get the diagrams of steady detonation velocity and the loss coefficient κ under the corresponding parameter and detonation failure of linear boundary, and derive the critical characteristics of detonation failure conditions finally. In view of the above established the analog system of detonation by means of limiting the spread of the disturbance to the upstream, study the stability of the steady state solution under the condition of the ideal and non-ideal (with loss) analog system of detonation and the influence of related parameters on the stability.

The analog system with Arrhenius reaction rate is established. It is bright to change the different control parameters of the analog system to study the one-dimensional detonation instability by direct numerical simulation, after the stability limit, the results show that the oscillation of the pressure of leading shock wave for single-mode condition to the period-doubling bifurcation and entering the chaos instability of the situation finally. At last, analysis of the instability mechanism is essential.

1128 - High Resolution Numerical Simulation of Multi-Phase Hybrid Detonation

C. Wang, Y. Zhao

Investigation on two phase hybrid detonation has a significance for the prevention and control of industrial explosion disaster. Due to the lack of investigation in experiment and theory, numerous detonation phenomena cannot be reasonably explained. Recently, with the development of computer science and numerical method, numerical simulation becomes a key method of studying two phase hybrid detonation. Thus, more and more research of two phase hybrid detonation has been performed by numerical simulation. In this paper, we built the fluid dynamic equations for describing the moving process of gas and solid particles, respectively. By considering the exchange modeling of mass, momentum, energy between two phase to close source term, the governing equations with chemical reaction is built for describing the detonation wave propagation process of gas-solid mixture. In this paper, by using high resolution WENO difference scheme, the governing equations are discretized, and

a parallel code is developed. By using the code, detonation wave propagation law for aluminum powder/air and aluminum powder/ethyne/air are investigated.

1141 - Study of Hypergolic Hybrid Rocket Using Hydrogen Peroxide as Oxidizer

C. Lu, Y. Chou, Y.C. Chao

Hybrid rocket with hypergolic feature is capable of producing reliable rapid ignition and generating thrust without additional ignition device. Hypergolic mechanisms utilized in hybrid rockets also have enormous research potential to develop into throttling and multi-ignition propulsion system and fulfilling the functionality of hybrid rocket propulsion. In this research, the outstanding features of hypergolic ignition are achieved by using high concentration hydrogen peroxide as oxidizer and catalyst was added in fuel grain, a mixture of plastic binder and manganese catalyst for the decomposition of hydrogen peroxide. It is found that as hydrogen peroxide droplets contact with catalytic propellant surface, the exothermic heterogeneous reaction is initiated on the interface and heats up fuel grain surface inducing hypergolic motor ignition. By modifying the oxidizer operating condition and fuel grain configuration, we have successfully ignited the motor within a short period of time (on the order of 100 ms) in hot fire experiments. The results show that the motor starting characteristics can be classified into three characteristic ignition process based on pressure rises shown in Fig.1. From the transparent motor experimental observation, we found that the motor starting characteristics is strongly related with the interaction of hydrogen peroxide droplets and catalytic propellant surface, as liquid oxidizer may induce flooding and splattering phenomenon on propellant surface, leading to hard-start or smooth-start of rocket motor.

1146 - An Overview of PERWAVES: A Sounding Rocket Experiment to Examine Flame Propagation in the Discrete Regime

J. Palecka, S. Goroshin, J. Bergthorson, A. Higgins

An overview of an upcoming microgravity experiment focused on examining the discrete regime of flame propagation in particulate suspensions is presented. The experiment (PERWAVES) will use the microgravity environment onboard the ESA MAXUS 9 sounding rocket to create a suspension of iron particles in a low thermal diffusivity oxygen/xenon mixture. The low diffusivity gaseous medium results in the flame propagation mechanism through the suspension being dominated by the interparticle diffusion time rather than the burn rate of the particles, giving rise to a unique percolation-like regime of propagation. Microgravity is necessary to prevent buoyancy from disrupting the low (approximately 1 cm/s) flame speed. The consequences of this regime for flame propagation dynamics will be reviewed, and the details of the experimental package that will be used to study the flame propagation under microgravity conditions will be defined. Preliminary results obtained in short-duration drop tower tests will be presented as a preview to the results of the PERWAVES experiment.

1153 - The Study of Turbulence Effects in Highly Unstable Detonation Mode

D.R. Cho, J.Y. Choi

Detonation can be classified form weakly to highly unstable mode depending on the mixture composition. In weakly unstable mode, the structure of detonation wave is very regular, smooth and shows the uniform cell size with regular period in the smoked-record. However, in highly-unstable mode, instead of stable and regular movement, the detonation structures have tendency of extremely irregular and wrinkled wave front and cell shapes. Also by the results of Power Spectrum Density (PSD) using Fast Fourier Transform (FFT), the peak points are shown as separated pulse form with stead interval in weakly-unstable mode, whereas irregular interval peak points and unsystematic noise shape in highly-unstable mode. The physical diffusion of viscous effect is important for high grid resolution when the numerical diffusion become negligible. And the cellular structures from the inviscid simulations depend on the grid resolutions. Better grid resolution is required to observe cell structure in highly unstable mode compare to weakly unstable mode in numerical analysis using fixing grid systems. Regardless of many studies done previously there are quite a many unknowns still unresolved and need a systematic investigation. Especially, there was little work on the detailed 3-D numerical analysis is of highly unstable detonation wave front so far, presumed being due to heavy computing cost for the fine grid resolution required to capture the unstable detonation characteristics.



Present study attempts to simulate the highly unstable detonation wave in three-dimension in comparison with an equivalent two-dimensional case.