28th INTERNATIONAL COLLOQUIUM ON THE DYNAMICS OF EXPLOSIONS AND REACTIVE SYSTEMS

JUNE 19 – 24, 2022 NAPLES, ITALY

28th ICDERS Program at a Glance

Time	Sun. (Jun. 19)	Mon. (Jun. 20)	Tue. (Jun. 21)	Wed. (Jun. 22)
8:30–9:00		**Opening ceremony**		
9:00–10:00		**Plenary I**	**Plenary II**	**Plenary III**
10:00–10:10		Break	Break	Break
10:10–10:35		Regular Sessions	Regular Sessions	Regular Sessions
10:35–11:00				
11:00–11:25				
11:25–11:50		Coffee Break & Poster WiP1	Coffee Break & Poster WiP2	Coffee Break
11:50–12:15		Regular Sessions	Regular Sessions	Regular Sessions
12:15–12:40				
12:40–13:05				
13:05–13:30		Lunch	Lunch	
13:30–14:35				Ligth Meal
14:35–15:00		Regular Sessions	Regular Sessions	**Excursion**
15:00–15:25				
15:25–15:50				
15:50–16:15				
16:15–16:40		Coffee Break & Poster WiP1	Coffee Break & Poster WiP2	
16:40–17:05		Regular Sessions	Regular Sessions	
17:05–17:30				
17:30–17:55				
18:00	Welcome Party			
19:30–20:00			Young Researchers' Night	
21:30				

Time	Thu. (Jun. 23)	Fri. (Jun. 24)
09:00–9:25	Regular Sessions	Regular Sessions
9:25–9:50		
9:50–10:15		
10:15–10:40		
10:40–11:05	Coffee Break & Poster WiP3	Coffee Break
11:05–11:30	Regular Sessions	Regular Sessions
11:30–11:55		
11:55–12:20		
12:20–12:45		Farewell Party
12:45–14:15	Lunch	
14:15–14:40	Regular Sessions	
14:40–15:05		
15:05–15:30		
15:30–15:55		
15:55–16:20	Coffee Break & Poster WiP3	
16:20–16:45	Regular Sessions	
16:45–17:10		
17:10–17:35		
18:15–23:00	**Banquet**	

28th ICDERS Program at a Glance

Sun. (Jun. 19)	Start	End	Mon. (Jun. 20)				Tue. (Jun. 21)				Wed. (Jun. 22)			
	8:30	9:00	Opening ceremony											
	9:00	10:00	Plenary I				Plenary II				Plenary III			
	10:00	10:10	Break				Break				Break			
	10:10	11:25	RDE I	Detonation Modelling I	Gas and Dust Explosion I	Chemical Kinetics I	Detonation Modelling II	Detonation Structure II	Stability I	Laminar Flame I	Flame Dynamics & Stability	Dynamics of Reactive Supersonic	Detonation Initiation & limits	Ignition I
	11:25	11:50	Coffee Break & Poster WiP 1				Coffee Break &				Coffee Break			
	11:50	13:05	Gas and Dust Explosion II	Condensed Phase Detonation I	RDE II	Chemical Kinetics II	Laminar Flame II	Detonation Structure III	Detonation Diffraction	Stability II	Pressure-Gain Combustion	Flame Acceleration & DDT II	Detonation Modelling II	Chemical Kinetics V
	13:05													
	13:30	14:35	Lunch				Lunch				Ligth Meal for Excursionists			
	14:35	16:15	IC Engines	Detonation Propagation	RDE III	Chemical Kinetics III	RDE IV	Detonation Structure IV	Multiphase I	Laminar Flame III	Excursion			
	16:15	16:40	Coffee Break & Poster WiP 1				Coffee Break &							
	16:40	17:55	Chemical Kinetics IV	Detonation Structure I	Flame Acceleration & DDT	Explosion Safety I	Multiphase II	Detonation Interface Interaction	RDE V	Laminar Flame IV				
Welcome Party	18:00													
	19:30	20:00					Young Researchers' Night							
		21:30												

Start	End	Thu. (Jun. 23)				Fri. (Jun. 24)			
09:00	10:40	Explosion Safety II	Flame Acceleration & DDT III	Turbulent Flames I	--	Energetic Materials II	Detonation Boundary Interaction	RDE VIII	Multiphase III
10:40	11:05	Coffee Break & Poster WiP 3				Coffee Break			
11:05	12:45	Oblique Detonation	RDE VI	Fire Dynamics	Energetic Materials I	Propulsion Application	RDE IX	--	--
12:45	14:15	Lunch				Farewell Party			
14:15	15:55	Ignition II	Flame Acceleration & DDT IV	RDE VII	Shock Tube I				
15:55	16:20	Coffee Break & Poster WiP 3							
16:20	17:35	Condensed Phase Detonation II	Shock Tube II	Numerical Methods	--				
18:15	23:00	Banquet							

28th INTERNATIONAL COLLOQUIUM ON THE DYNAMICS OF EXPLOSIONS AND REACTIVE SYSTEMS

JUNE 19 – 24, 2022 NAPLES, ITALY

ORGANIZERS

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Ashwin Chinnayya (France), Aslan Kasimov (Russia), Benjamin Akih Kumgeh (USA), Benoit Fiorina (France), Bing Wang (China), Bok Jik Lee (Korea), Huahua Xiao (China), Jack J. Yoh (Korea), Jan Kindracki (Poland), Jiun-Ming Li (Singapore), Josue Melguizo-Gavilanes (France), Kazunori Kuwana (Japan), Ken Matsuoka (Japan), Marc Bellenoue (France), Matei Radulescu (Canada), Matthew Fotia (USA), Ming-Hsun Wu (Taiwan), Mustapha Fikri (Germany), Myles Bohon (Germany), Olivier Mathieu (USA), Peng Dai (China), Regis Bauwens (USA), Remy Mevel (China), Ryan Houim (USA), Shinichi Maeda (Japan), XiaoCheng Mi (Canada), Yuta Sugiyama (Japan)

HONORARY HOST COMMITTEE

Gaetano Continillo (University of Sannio), Emilio Fortunato Campana (CNR – DIITET), Ernesto Salzano (University of Bologna), Mario Commodo (Italian Section of the Combustion Institute)

LOCAL HOST COMMITTEE

Francesco Saverio Marra, CNR – STEMS, Italy

CONFERENCE SECRETARIAT

M.C.M. Congressi

CONTENTS

MESSAGE FROM THE PRESIDENT

On behalf of the Board of the institute for Dynamics of Explosions and Reactive Systems (IDERS), I am delighted to welcome you to the 28th The International Colloquium on the Dynamics of Explosions and Reactive Systems.

The 28th ICDERS is a continuation in the series of biannual international colloquia that have been held throughout the world since 1967. For the first time, the colloquium is being held in Italy, in the beautiful city of Naples.

The 28th ICDERS was initially set to be held in 2021, after the global pandemic due to COVID-19, we had to take the decision to post-pone our gathering to 2022. I would like to express here my deepest thanks to the local organizers chaired by Professor Francesco MARRA for their dedicated work, for their very efficient handling of the Conference amid many changes and uncertainties.

The colloquium would not have been held without the host committee in Naples chaired by Prof. Francesco MARRA and the Program Committee Akiko MATSUO (Chair), Andrea COMANDINI (Co-Chair), Hoi Dick NG (Co-Chair) and Mirko GAMBA (Co-Chair). I would like to express to them my deepest thanks for their wonderful work in organizing the conference that I am sure you will find enjoyable and fruitful. In total, 196 oral presentations and 26 posters, from all over the word, are the focus of our program.

I hope that you will also find the time to enjoy the cultural activities and take the time after the conference to explore Naples and the nice surrounding areas.

Welcome to the 28th ICDERS.

Nabiha Chaumeix
President, IDERS

MESSAGE FROM THE PROGRAM COMMITTEE CHAIRS

ICDERS-2022 is the 28th 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 four researchers representing varying technical areas and geographical locations – Asia, Europe, and North America. The work of the program chairs was expertly supported by 27 members of the program committee, namely, Ashwin Chinnayya, Aslan Kasimov, Benjamin Akih Kumgeh, Benoit Fiorina, Bing Wang, Bok Jik Lee, Huahua Xiao, Jack J. Yoh, Jan Kindracki, Jiun-Ming Li, Josue Melguizo-Gavilanes, Kazunori Kuwana, Ken Matsuoka, Marc Bellenoue, Matei Radulescu, Matthew Fotia, Ming-Hsun Wu, Mustapha Fikri, Myles Bohon, Olivier Mathieu, Peng Dai, Regis Bauwens, Remy Mevel, Ryan Houim, Shinichi Maeda, XiaoCheng Mi, Yuta Sugiyama.

This led to submissions of 250 extended abstracts and 30 abstracts for work in progress posters. All papers were peer reviewed by the program committee. The large number of papers were recommended for oral presentation by the review process, it was decided to organize 4 parallel sessions for oral presentations. Additionally, extended time slots around coffee breaks were reserved for poster presentations with no other parallel sessions.

Three plenary lectures were given reflecting the broad areas of interest to the ICDERS community:

- Jiro Kasahara, Nagoya University, Japan: “Fundamental Research of Detonation Engine and Its Space Flight Experiment Using Sounding Rocket”
- Gaby Ciccarelli, Queen’s University, Canada, “Flame Acceleration and Deflagration-to-Detonation Transition in a Confined Geometry”
- Benoît Fiorina, Université Paris-Saclay, CNRS, Laboratoire EM2C, France: “Including Detailed Chemical Properties in the Modeling of Emerging Turbulent Combustion Systems”

The 28th ICDERS was originally scheduled to be held in 2021, but it has been postponed to June 2022 due to the global expansion of COVID-19. Unfortunately, the COVID-19 disaster continued in 2022 in many parts of the world, and only those in such situations were allowed to participate remotely in the ICDERS. In the late February 2022, the Russian invasion of Ukraine made it difficult to participate in the ICDERS from some areas. The program committee chairs and local organizing committee chair, F. S. Marra met every Wednesday, North America in the morning, Europe in the afternoon, and Japan in the night, in an ongoing effort to properly host the conference. However, even one month before the ICDERS was to be held, the international situation remained unchanged, with the COVID-19 disaster and the invasion of Ukraine. Some presentations of 250 extended abstracts were withdrawn due to various reasons. Finally, about 200 oral presentations were made at the ICDERS including 23 remote presentations from China and other Asian countries. Although the 28th ICDERS has become smaller, we believe that the ICDERS community gets together in the next 29th ICDERS in Korea.

Until now, ICDERS has used the Confmaster as its paper registration system, but this is the first time that the Microsoft CMT system has been adopted. This system is not costly and is mostly stable. We would like to thank ICDERS community for their willingness to accept the new system.

Starting from this edition of ICDERS, a better opportunity is offered to the participants to publish a full version paper of their extended abstract accepted for presentation. The following journals (Shock Waves, Combustion Science and Technology, and Combustion Theory and Modeling) will accept submissions for publication of full-length regular papers of abstract accepted for presentation to the 28th ICDERS Colloquium. The submission will open on March 15, 2022 and will close on July 31, 2022.

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

The program chairs of the 28th ICDERS

Akiko Matsuo, Andrea Comandini, Mirko Gamba, Ng Hoi Dick

MESSAGE FROM THE HOST COMMITTEE CHAIR

On behalf of the Local Committees, you are most welcome to the 28th International Colloquium on the Dynamics and Reactive Systems (ICDERS2019), organized by the Institute for Dynamics of Explosions and Reactive Systems (IDERS), and hosted by CNR, during June 19 – 24, 2022, Napoli, Italy.

No doubt this is an unusual edition. Not only for being the first in this long series, whose first date back to 1967, to be held in Italy, but also, and especially, for being shifted to an even year, 2022, because of the disrupting events of the past years in consequence of the global COVID-19 pandemic. Therefore, something special is about this edition.

On one side it is the occasion for a community to rejoin and feel again the spirit of cooperation and exchange of info and activities necessary to advance in all the specialist fields of science specific to these Colloquia. On the other side, the resurge of antagonist attitudes that pose a threat to the peace we benefitted from for so long time and the sadness for the consequences they pose also on the cooperation in science. It has been an escalation too fast and happening too close to the beginning of the conference, to have had the time to overcome all the obstacles that today make it impossible for some of our colleagues from Russia to participate, despite the effort provided by the local host committee to find alternatives for all the participants still in the impossibility to travel. This effort has at least produced the possibility for most Asian willing to participate and today blocked in their countries to not renounce to present their contribution by presenting them by remote.

The local host committee has a particular thank you to all the participants that have faced the effort and risks to organize their participation in presence. For us has been not easy to insist with you to realize the conference in presence. It could have been much easier to switch to a virtual conference, but it is our convincement that a so long tradition of the ICDERS is because of something, maybe depending on being always at the very front of science and technology development, that cannot be translated into a mere sequence of presentations. We really appreciate your effort in being present in this edition of the ICDERS despite the difficulties. Difficulties that we have tried to overcome at our best, but we had to renounce something. Of course, the choice was to preserve at the best everything needed for the congressional activities. Nevertheless, we hope all participants will enjoy the entire program, including the social events.

The Chair of the local host committee expresses special gratitude to all the people that have practically contributed to the realization of the 28th ICDERS.

First, I like to thank the IDERS, its President Nabiha Chaumeix, and the Board, firstly for having entrusted to me the realization of the 28th ICDERS. Then, during the many months of uncertainties, for the continuous support and for sharing the most difficult decisions.

A special thanks I need to express to Gaetano Continillo, former President of ICDERS, for his support in introducing me to this community and for the substantial help in the organization of the present edition.

The cooperation with the Program Chairs, Akiko Matsuo, Andrea Comandini, Hoi Dick Ng, and Mirko Gamba has been delightful. I think that the team we formed has been formidable.

I am also very grateful to Stefania Acanfora and Lucia Melchiorre, of the Conference Secretariat. Stefania has always, with professionality and patience, looked for solutions and alternatives that could best suit the complex organization of this conference. Lucia has been the irreplaceable reference point for all participants.

A dedicated page has been realized to mention all the sponsors and patronages, but again I have to underline their essential contributions.

I have also to thank some of my colleagues at the hosting institution, the Institute of Science and Technology for Sustainable Energy and Mobility of the National Research Council (CNR – STEMS), who in various ways supported the realization of the conference, especially the team of IT systems.

Finally, I need to thank the other hosting Institutions. The University of Naples Federico II, which is gracefully hosting the conference in their structures, and the University of Sannio, for its substantial contribution.

I wish that all participants could enjoy a fruitful week here in Naples.

Francesco Saverio Marra, CNR-STEMS
Chair of the Local Host Committee, 28th ICDERS

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UNDER THE AUSPICES OF

Prof. Maria Chiara Carrozza

President

Associazione Sezione Italiana del Combustion Institute ASICI

SPONSORS

GOLD	*GOLD*	*SILVER*

GENERAL INFORMATION

CONFERENCE VENUE

School of Engineering, University of Naples Federico II

Address: P.le V. Tecchio 80 - Napoli

REGISTRATION/ INFORMATION DESK AND CONFERENCE SECRETARIAT

Location: School of Engineering 1st floor

Opening time:

June 20th, 2022: from h. 07.30 to 13.00 and from h. 14.30 to 18.30

June 21st, 2022: from h. 08.30 to 13.00 and from 14.30 to 18.00

June 22nd, 2022: from h. 08.30 to 14.00

June 23rd, 2022: from h. 08.30 to 13.00 and from 14.00 to 17.30

June 24th, 2022: from h. 08.30 to 13.00

NAME BADGE

For identification purpose and admission to the conference venue and to social events, badges are expected to be worn at all times during the conference. The strings of badges are color-coded as follows:

- Regular Full Fee – Blue
- Student Registration Full Fee – Red
- Regular Reduced Fee – Orange
- Student Registration Reduced Fee –Yellow
- Accompanying person – Green
- Staff & Volunteer – Yellow

INTERNET

Wireless connection is available at conference venue and the account for login will be provided during the conference.

MEALS

Coffee breaks and lunches will be served according to the program schedule at the School of Engineering, Room “Biblioteca Gasparini” located on the 2nd Floor.

DRESS CODE

Smart casual is suggested for academic sessions. Casual and light wear, hat and comfortable shoes are appropriate for city excursion. T-shirt, short pants, sandals are inappropriate for Banquet and Welcome Party.

CURRENCY EXCHANGE

Most banks provide exchange service for foreign currency and traveler’s checks. Credit cards such as Mastercard, Visa and Amex are accepted in most hotels, shopping centers and restaurants. However, they may not be accepted at small scaled shops or restaurants.

ELECTRICITY

The voltage is 220V in Italy.

TIPS

Tipping is welcome but not mandatory for taxi and restaurants

AIRPORT & FLIGHT

It is advised that you leave the hotel or the conference venue 3 hours in advance for international flights, and 2 hours and a half in advance for domestic flights.

PUBLIC TRANSPORTATIONS

ANM is the main company providing public transport services in Naples. Tickets cannot be bought on board and must be stamped at the beginning of the race.

Almost all bus lines and Metro Line 1 are served by ANM. A 60 minutes ticket valid on all ANM lines costs Euro 1.10.

Ferrovie dello Stato, FS, services Metro Line 2. A different ticket than the ANM ticket is necessary to use Metro Line 2. Alternatively, the so-called integrated ticket, 90 minutes valid on both ANM and FS, costs 1.60 Euro. Tickets can be bought at Stations, several paper shops or Tabacchi shops and also on-line.

The following apps can be used for real time lines info and/or to buy tickets.

NAPLES MOBILITY

moovit

Gira Napoli

TICKETS

UNICO CAMPANIA

Bus transportation

These lines connect the Railway Station (Piazza Garibaldi) to the Conference Venue. Their route covers main central districts.

ANM Bus n° 151

Piazza Garibaldi Main Railway Station
Garibaldi - Circumvesuviana
Via Marina
Marina - Porta Di Massa
Via Depretis - Loggia Dei Pisani
Via Acton - Molo Beverello
Piazza Vittoria
Riviera Di Chiaia
Via Giordano Bruno
Viale Augusto - Piazza San Vitale
Viale Augusto - Via Veniero
Viale Augusto - School of Engineering

EAV

Circumvesuviana Stop
Via Marina
Via Duomo
Via Depretis
Via Acton - Molo Beverello
Piazza Vittoria - Villa Comunale
Riviera Di Chiaia
Viale Augusto
Viale Augusto - School of Engineering

Metro transportation

Lines serving the conference venue are:

L2 (Blue) | Stop: Campi Flegrei

Cumana (Green) | Stop: Mostra

Pre-fixed Taxi rates

	AEROPORTO AIRPORT	VIA PARTENOPE ALBERGHI (San Ferdinando)	MOLO BEVERELLO PORTO / PIAZZA MUNICIPIO	STAZIONE CENTRALE CENTRAL STATION
AGNANO / IPPODROMO	27 €	17 €	17 €	23 €
MERGELLINA / CHIAIA / POSILLIPO	25 €			15 €
CENTRO DIREZIONALE NAPOLI / GIANTURCO	18 €	15 €	13 €	
CITTA' DELLA SCIENZA / BAGNOLI	27 €	15 €		23 €
FUORIGROTTA / STADIO / MOSTRA D'OLTREMARE	25 €	15 €	15 €	18 €
MOLO BEVERELLO / PORTO / PIAZZA MUNICIPIO - *Harbor*	21 €	8 €		13 €
MUSEO CAPODIMONTE - *Capodimonte Museum*	18 €	15 €	13 €	13 €
MUSEO ARCHEOLOGICO NAZIONALE - *National Archaeological Museum*	21 €	13 €	11 €	13 €
MUSEO NAZIONALE FERROVIARIO DI PIETRARSA	23 €	22 €		16 €
MUSEO SAN MARTINO - *San Martino Museum*	25 €	18 €	16 €	16 €
OSPEDALE DEL MARE	21 €		16 €	16 €
STAZIONE CENTRALE - *Central Station*	18 €	15 €	13 €	
TEATRO SAN CARLO - *Opera House San Carlo*	21 €	10 €	9 €	13 €
UNIVERSITA' MONTE SANT'ANGELO	25 €	15 €	17 €	19 €
UNIVERSITA' SAN GIOVANNI A TEDUCCIO	21 €	18 €	16 €	16 €
VIA PARTENOPE / ALBERGHI (San Ferdinando)	25 €		8 €	15 €
ZONA OSPEDALIERA / VOMERO - *Hospital Areas*	21 €	17 €	15 €	16 €
ZTL CENTRO STORICO / CENTRO ANTICO - *Historical Centre*	18 €	10 €	9 €	9 €

You can ask the pre-fixed rate before starting the ride if your route is among those shown in the table.

The direction to the Conference Venue from Railways Station and Airport is "Fuorigrotta/Stadio/Mostra d'Oltremare".

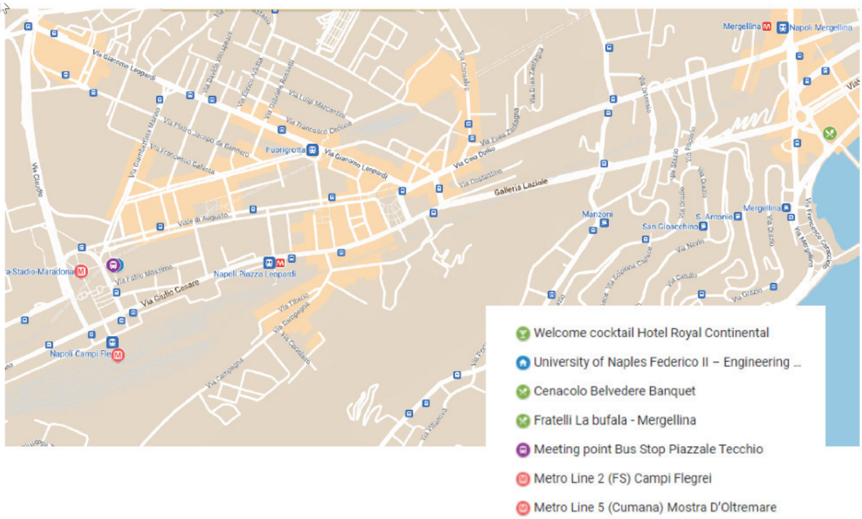
The pre-fixed fare includes all extras:
Night fare, Baggage, Pets, Overcharge, Airport and does not depend on the number of passengers.
Naples motorway toll is not included. Radio taxi call is not included.

If you not use a pre-fixed rate, please ask to the driver to start the Taximeter that will show you the final price plus possible extras.

RADIO TAXI

CONSORTAXI Tel. +39 0812222 - TAXI NAPOLI Tel. +39 0818888 - LA PARTENOPE Tel. +39 0810101 - LA 570 Tel. +39 0815707070

Map of the conference sites:



At the following link, an interactive Google map with the indication of the location of all the conference events is available:

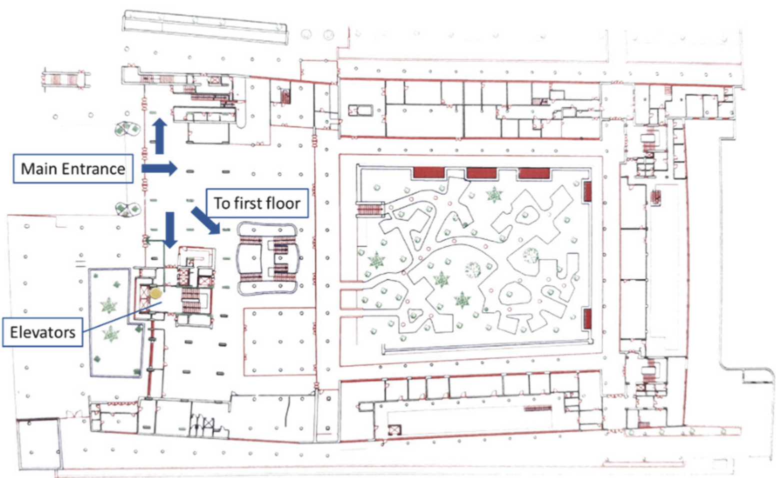
https://www.google.com/maps/d/u/0/edit?mid=1xeWpwPkWGkJu_47Ed-Gg_P4lfd86n1U-&usp=sharing

or use the following qr-code:

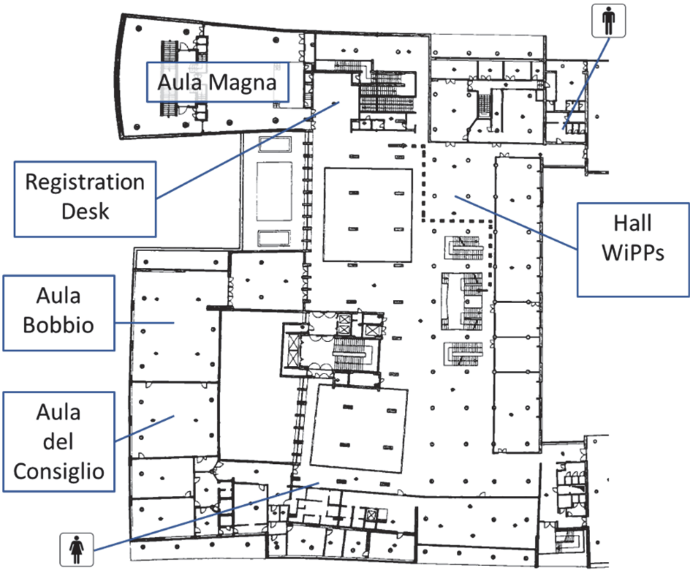
MAPS OF THE CONFERENCE VENUE

Area of the Conference Venue:

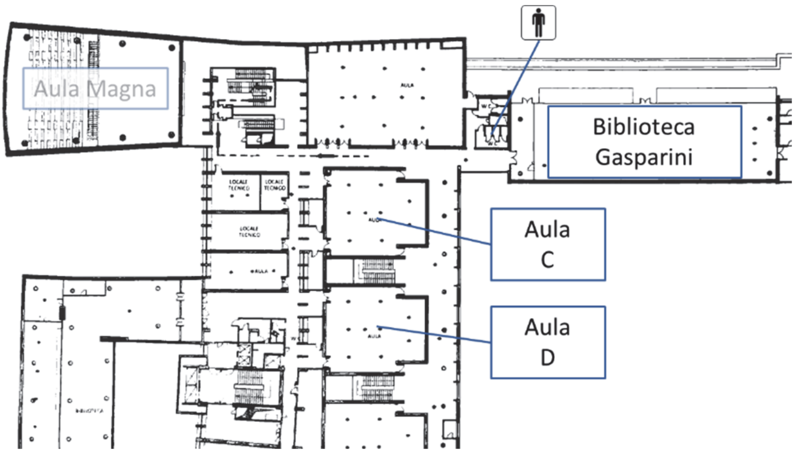
Ground Floor – Main Entrance:



First Floor:



Second Floor:



PRESENTER INSTRUCTIONS

CONTENTS

All of the contents of presentations, including plenary lecture, oral and poster presentations, must be unclassified. The Program Committee and Local Organizing Committee are not responsible for the presented contents. Topics beyond academics are beyond the scope of ICDERS.

ORAL PRESENTATIONS

Presentations should last no longer than 20 minutes to allow 5 minutes for questions and changeover to the next speaker. All screens are in widescreen (16:9) format. Each presenter is strongly encouraged to arrive at the assigned conference room a **minimum of 10 minutes** before the commencement of the session to meet with the session chair.

Each speaker is requested to bring along with them the presentation on a USB pen and to upload the presentation in the room which is assigned to his/her presentation at least **1 hour** before the session starts.

AUDIO-VISUAL EQUIPMENT

Presentation rooms are equipped with projectors for computer-based presentations. Presentations should be prepared in PowerPoint or PDF. Presenters will be provided with a remote controller, with integrated laser pointer, that can be used to advance slides in PowerPoint. Slides with movies (format .MOV or MP4) must be checked for playback on the laptop.

For Mac users: Power Point slides are normally compatible. If you use “Keynote” please take care that the file is converted in PDF.

The use of one’s personal Laptop is not allowed

POSTER SESSIONS

Posters are presented in the Main Foyer in front of the Main Room (Aula Magna). Posters are to be printed at the cost of the author(s) and to be brought already printed (Format A0 Portrait). Each participant for poster presentation will be provided with pins or self-adhesive tape. Posters can be displayed all day of the assigned session. The poster must be removed at the end of the session day. At least one co-author should be available to present the poster during the coffee break time.

VIRTUAL PRESENTATIONS

Those joining the Conference remotely will receive a Zoom Meeting personal link for each session rooms.

When you are an “auditor” please enter the link whenever you wish, and you will be connected with the room of your choice.

When you are “presenter” please make sure to enter the room at least 10 minutes before the start of the session.

In both cases make sure to enter the room with microphone and camera OFF and please turn them on when it is your turn to talk.

To ensure that the presentation can be delivered even in case of connection problems, authors must send to the conference email address:

28icders@stems.cnr.it

an mpeg4 video of the pre-recorded registration of the presentation (with audio and video). The session chair can opt to use this recorder presentation in case of difficulties in having a stable and performant connection.

SOCIAL PROGRAM INFORMATION

WELCOME PARTY

Time: 18:00-20.00, June 19th

Venue: Roof Top Hotel Royal (10th th Floor)

Address: Via Partenope, 38 (seafront district)

Coupon: Full and reduced Delegates and Students fee + Accompanying persons

Transportation will not be provided

YOUNG RESEARCHERS' GET TOGETHER

Time: 19.30 -21.30, June 21th

Venue: Fratelli la Bufala, Mergellina

Address: Via Caracciolo, 10 NAPOLI

Coupon: Students

Transportation will not be provided

Directions: You can easily reach the venue by Metro Line 2 Stop Mergellina. From the Metro station it takes 5 minutes walking distance towards the sea front.

EXCURSION

Time: 14.30-21.30, June 22nd

Depart by bus from: School of Engineering, P.le V. Tecchio 80

A spectacular excursion has been organized for the participants to ICDERS.

The program will include a visit to the Pausilypon Archaeological Site and to the Piscina Mirabilis.

The tour will end with a get together party on a nearby Beach Club.

Pausilypon Archaeological Site

Thanks to the recovery work being done by the Archaeological Sovrintendenza of Naples and Caserta and the contribution of the Comune of Naples, a first nucleus of the huge Pausilypon archaeological site has been permanently reopened to the public.

The fascinating tour begins at the entrance at the end of Coroglio descent, where the magnificant Grotta di Seiano begins. This is a man-made tunnel whose 770 metres run through the tuffaceous hill of Posillipo, connecting the area of Bagnoli and the Flegreaen Fields with the Gaiola deep valley.

This ancient passageway, which was dug out about two thousand years ago and reinforced in the Bourbon period, snakes through the fascinating half-light of the tunnel and then is struck towards the end by the blinding light from side underground passages on the steep coves, which offer a breathtaking view.

Beyond the cavern, we take a path lined with typical Mediterranean vegetation and come to the area of the villa to which Vedio Pollione, a wealthy Roman knight to Ottaviano Agusto, gave a name of Greek derivation, "Pausilypon", or "place which stops all the cares" in order to describe the spell and the beauty of this place called Posillipo.

The villa is adaptable to different circumstances, and was enlarged to satisfy the needs of an imperial residence whose full extent will be discovered only when the Archeological Sovrintendenza will complete the work with the final aim of opening this archeological site of Pausilypon to the public.

There are remarkable archaeological remains in this area - a theatre of splendid structure with 13 rows of seats in the top auditorium and 6 in the middle one, an overall seating capacity of two thousand which exploited the natural slope of the hill, in accordance with the typical technique of Greek amphitheatres. On the opposite side are the remains of the Odeion, the ancient roofed theatre used for recitals of rhetorical poetry and musical performances, which has a small "cavea" or auditorium positioned in front of the large Theatre.

Piscina Mirabilis

The Water Cathedral - Piscina Mirabilis is the largest and most monumental cistern of drinkable water ever built by the ancient Romans. It had the function of supplying water to the numerous ships belonging to the Classis Misenensis of the Roman Navy, once moored in the nearby port of Miseno. The cistern, also known as "the Water Cathedral " for its largeness and majesty, is located in Bauli, the name that the ancient Romans gave to the current city of Bacoli.

The Ancient Cistern - Piscina Mirabilis, partly dug into the tuff, had the capacity of 12,600 cubic meters of water! It was built on a quadrangular plan to obtain four rows of twelve cruciform pillars that divide the interior space into five long and thirteen short naves to support the vault. On the latter it is set the roof terrace paved in terracotta fragments and lime, communicating with the interior by several doors.

Piscina Mirabilis and the Augustan aqueduct of the Serino - Piscina Mirabilis represented the landing and arrival point in Bacoli of the ancient Augustan aqueduct which, from the spring of Serino (AV), located at an altitude of 330 meters and with a journey of 100 kilometers about, brought water to Naples and Campi Flegrei up to the eight meters of Piscina Mirabilis (now at an altitude of 2, due to bradyseism). The Augustan aqueduct was destroyed, between the 4th and 5th century AD. C and Piscina Mirabilis has no longer been used and as a matter of fact it is now emptied of water.

After excursion dinner

Enjoy your dinner at a wonderful beach resort in the spectacular gulf of Miseno.

A music entertainment, "Napoli and beyond", will accompany the evening with musicians Anna Galiano (vocalist), Matteo Dionisio Gulfo (guitar) and Antonio Pignatelli (trumpet).

Time: 19:00-21.30, June 22nd

Venue: Tibidabo Beach Resort

Address: Via Miliscola, 57, Monte di Procida

Coupon: Full Delegate and Student registrations, Accompanying persons

BANQUET

Banquet Time: 19:00-23.00, July 23rd (Buses departure time 18:15)

Venue: Cenacolo Belvedere Carafa

Address: Via Aniello Falcone 122, Napoli

Meeting point: Buses will depart from the School of Engineering at 18.15 and will come back at the same meeting point at about h. 23.00

Coupon: Full Delegate and Full Student registrations, Accompanying persons

During the Banquet the following prizes will be awarded:

R. I. Soloukin Award and ***J. H. S. Lee Young Investigator Award***.

Term charge of Board of Directors Declaration; Site of 29th ICDERS, Host Chair, Program Chair

The venue

formerly known as Palazzo Vandeneynden, and also known as Villa Belvedere, is a monumental villa in Naples, located in the hilly Vomero district.

Villa Belvedere represents a unique example of the oldest history of its neighbourhood, Vomero. It is around this structure, in fact, that the ancient Villaggio del Vomero developed. Over the centuries, there were numerous travellers who became fascinated with it, to the point of immortalizing it in painting, drawings and sketches. The Villa faces the wonderful Gulf of Naples.

FAREWELL PARTY

Time: 12.30 June 24th

Venue: School of Engineering, Biblioteca Gasparini, 2nd floor

Note: *Time of events is subject to change. Please refer to arrangement onsite.*

Monday, June 20th, 2022 (morning sessions)

8:30 9:00	**Opening ceremony and Registrations**			
9:00 10:00	**Plenary Lecture (Aula Magna):** ***Prof. Jiro Kasahara*** *(Nagoya University, Japan)* **Title: Fundamental Research of Detonation Engine and Its Space Flight Experiment Using Sounding Rocket** *Chairs:* ***A. Matsuo and M. Gamba***			
10:00 10:10	Break (Transition to Morning Sessions)			
	Aula Magna (1st Floor)	Aula Bobbio (1st Floor)	Aula C (2nd Floor)	Aula D (2nd Floor)
Topics	**RDE I** *Chair:* ***T. Endo***	**Detonation Modelling I** *Chair:* ***L. Bauwens***	**Gas and Dust Explosion I** *Chair:* ***M. Kuznetsov***	**Chemical Kinetics I** *Chair:* ***M. Fikri***
10:10 10:35	**Preliminary Experimental Study of Propulsive Performance of Hollow Rocket Rotating Detonation Engines with Designed Laval Nozzle** **(137)** *Y. Zhang, J.Z. Ma, J.P. Wang, S. Zhang*	**On the Predicability of Weakly Confined Gaseous Detonations Using the Straight Streamline Approximation** **(191)** *S.A. Lalchandani, M. Radulescu, Z. Hong*	**On the Reactivity of Ethylene/Nitrogen/ Oxygen** **(38)** *G. Pio, S. Renda, V. Palma, E. Salzano*	**Ignition Delay Time and Laminar Flame Speed Measurements of a Li-ion Battery Electrolyte: Ethyl-Methyl-Carbonate** **(46)** *O. Mathieu, Y. Almarzooq, E. Petersen*
10:35 11:00	**Experimental Investigation on the Coal Powder Rotating Detonation Engine** **(247)** *X. Ni, H. Xu, C. Weng, X. Su, B. Xiao, F. Zhang, Y. Luo*	**Numerical Investigation of One-dimensional Pulsating Detonations Using Fickett' s Detonation Analogue with Chain-Branching Kinetics** **(234)** *A. Sow, M.I. Radulescu*	**Characterizing the Reactivity of Large-Scale Dust Explosions** **(114)** *C. R.L. Bauwens, L.R. Boeck, S. Dorofeev*	**Global Quasi-Linearization (GQL) for Model Reduction of Reaction Diffusion Systems** **(68)** *V. Bykov, C.Yu, U. Maas, V. Gol' dshtein*
11:00 11:25	**Numerical Analysis of the Influence of Mixing on Detonation Wave Propagation inside a Rotating Detonation Engine by Using Linear Detonation Channel** **(78)** *F. Wang, T. Mizukaki, S. Matsuyama*	**Characteristic Analysis for 2D Steady Supersonic Reacting Flow: Effect of Confinement on Detonation Flows** **(127)** *M. Short, C. Chiquete*	**Large-Scale Confined Gas and Dust Explosions with Elevated Initial Turbulence** **(108)** *L.R. Boeck, C.R.L Bauwens, S. Dorofeev*	**Ignition delay time measurements of methane/ethane/propane mixtures with addition of ozone** **(178)** *S. Drost, R. Schießl, U. Maas*

11:25 11:50	**Break and Work-In-Progress Posters Session I (Hall of 1th floor)**			
Topics	**Gas and Dust Explosion II** *Chair:* ***C.R. Bauwens***	**Condensed Phase Detonation I** *Chair:* ***M. Short***	**RDE II** *Chair:* ***K. Ahmed***	**Chemical Kinetics II** *Chair:* ***P. Glarborg***
11:50 12:15	**Propagation of Methane Detonation in Coal Dust Suspensions with Different Concentrations** (62) *J. Shi, Y. Xu, W. Ren, H. Zhang*	**Detonation Performance Experiments and Modeling for the High Explosive PETN** **(71)** *E.K. Anderson, C. Chiquete, R. Chicas, S.I. Jackson*	**Simulations of Ethylene-Oxygen Rotating Detonation Waves under Different Local Equivalence Ratio** **(85)** *H. Peng, R. Deiterding*	**Effects of Di(2,2,2-trifluoroethyl) Carbonate on the Ignition Delay Time and Laminar Flame Speed of H2 and CH4** **(258)** *M. Turner, D. Mohr, P. Dievart, L. Catoire, E. Petersen, O. Mathieu*
12:15 12:40	**Gravity Effect on Steady, 1-D Propagation through Dust Clouds** (83) *K. Kuwana, S. Yazaki, W. Kim, T. Mogi, R. Dobashi*	**Detonation Performance Model Calibration and Validation of the HMX-Based High Explosive PBX 9501** **(132)** *C. Chiquete, S.I. Jackson, E.K. Anderson, M. Short, S. Voelkel, Von H. Whitley*	**Three-Dimensional Numerical Investigation on the Effect of Injector Configuration in Rotating Detonation Engine** **(210)** *T. Sada, A. Matsuo, E. Shima, H. Watanabe, A. Kawasaki, K. Matsuoka, J. Kasahara*	**Sensitivity of Reaction-Diffusion Manifolds (REDIM) for Hydrogen Counter-diffusion Flames** **(161)** *U. Maas, V. Bykov*
12:40 13:05	**Expansion Waves Behaviour during Liquified CO2 Depressurization in a Divergent Cross-Section Vessel** **(63)** *O.K. M.Ibrahim, P.M. Hansen, D. Bjerketvedt, K. Vågsæther*	**Towards Finite Rate Chemical Kinetics Modeling of Detonation Afterburn Using the BKW Equation of State** **(142)** *M.P. Clay, B. Taylor, R. Houim*	**Flow Acceleration in an RDRE with Gradual Chamber Constriction** **(22)** *M.C. Ross, J. Burr, A. Batista, C. Lietz*	**Influence of Thermochemistry on Prompt NO formation in Flames** **(10)** *K.P. Shrestha, L. Seidel, B.R. Giri, T. Zeuch, F. Mauss*
13:05 14:35	**Lunch (Biblioteca Gasparini, 2nd Floor)**			

Monday, June 20th, 2022 (afternoon sessions)

	Aula Magna (1st Floor)	Aula Bobbio (1st Floor)	Aula C (2nd Floor)	Aula D (2nd Floor)
Topics	**IC Engines** *Chair:* ***U. Maas***	**Detonation Propagation** *Chair:* ***H.D. Ng***	**RDE III** *Chair:* ***E. Gutmark***	**Chemical Kinetics III** *Chair:* ***O. Mathieu***
14:35 15:00	**0D Laminar Flame Speed Model for Methane Lean Mixture in Dual Fuel Combustion** **(109)** R. De Robbio, E. Mancaruso, B.M. Vaglieco, S. Artham, J. Martín	**Elliptical Experimental Detonation** **(58)** *R. Babin, A. Chinnayya, V. Rodriguez*	**Study of Rotating Detonation Combustor Dynamics During Changes in Operating Mode** **(237)** *J. Shepard, A. Feleo, M. Gamba*	**The Impact of H2 and CO on the NH3 / NO / O2 Chemistry - a Step towards a Predictive Tool for NH3 Oxidation** **(103)** *P. Glarborg, M.U. Alzueta*
15:00 15:25	**Statistics of Flame Topology in Turbulent Spray Flame Water Droplet Interaction** **(26)** R. Concetti, J. Hasslberger, N. Chakraborty, M. Klein	**Study of Imploding Detonations with High-speed Videography and Digital Open-shutter Photography** **(91)** *R.S. Rodriguez A. Higgins, J. Loiseau*	**The Effect of Fuel Partial Premixing on Rotating Detonation Waves** **(111)** *R.F. Burke, T. Rezzag, A.R. Kotler, K. Ahmed*	**Thermal Decomposition-indu-ced Multi-stage Reaction of Diethyl Carbonate Exa-mined by a Micro Flow Reactor with a Controlled Temperature Profile (167)** *K. Kanayama, S. Takahashi, S. Morikura, H. Nakamura, T. Tezuka, K. Maruta*
15:25 15:50	**Effect of Jet Configuration on Knock Characteristics Using a Rapid Compression Machine** **(80)** *W. Liu, Y. Qi, R. Zhang, Q. Zhang, Z. Wang*	**Towards Laser-Induced Fluorescence of Nitric Oxide in Detonation** **(164)** *K.P. Chatelain, S.B. Rojas Chavez, J. Vargas, D.A. Lacoste*	**Numerical Analysis on Pressure Gain of Rotating Detonation Engine Using H2-O2 Gases: Influence of Number of Injector** **(218)** *A.K. Hayashi, K. Yoshidomi, K. Ozawa, N. Tsuboi, H. Kawashima*	**Modeling Soot Formation in LES of Turbulent Flames Using Virtual Chemistry** **(89)** *H. Maldonado Colman, D. Veynante, N. Darabiha, B. Fiorina*
15:50 16:15	**The Effect of the Ignition Energy and Mixture Energy Density on the Detonation Onset in Internal Combustion Engines** **(177)** *H. Xu, C. Weng, C. Yao*	**Multiple-view Imaging of a Small-diameter Detonation Tube at 5 MHz** **(40)** *L. Thomas, F. Schauer, D. Cyrol, B. Sell*	**Initiation Dynamics of Rotating Detonation Engines using C2H4-O2 Mixtures** **(227)** *S.F. Connolly-Boutin, M. Ghali, R. Gilot, J. Loiseau, A. Higgins, C.B. Kiyanda*	**Large Eddy Simulation of a Multi-Regime Burner Using Virtual Chemistry** **(90)** *T.P. Luu, B. Fiorina, N. Darabiha*

16:15 16:40	**Break and Work-In-Progress Posters Session I (Hall of 1th floor)**			
Topics	**Chemical Kinetics IV** *Chair:* ***B. Fiorina***	**Detonation Structure I** *Chair:* ***R. Zitoun***	**Flame Acceleration & DDT I** *Chair:* ***S. Dorofeev***	**Explosion Safety I** *Chair:* ***E. Salzano***
16:40 17:05	**Community Analysis of Bifurcation Maps of Diluted Hydrogen Combustion in WSFRs** **(129)** *J. He, Y. Li, L. Ji, L. Acampora, F.S. Marra*	**Cell Structure and Global Heat Release in 2D and 3D JP10-Air Detonations in Narrow Channels** **(186)** *P.A. Meagher, X. Shi, X. Zhao, S.S. Dammati, A. Poludnenko, H. Wang*	**DDT Run-up Distance Measured by Visualization of an Obstructed Tube** **(256)** *S. Shervin Hashemi Mehr, G. Ciccarelli*	**The Bologna LPG BLEVE** **(197)** *G. Cocchi*
17:05 17:30	**Validation of the Reaction-Diffusion Manifolds (REDIMs) Reduced Chemistry for the Non-premixed CH_4 Counter-flow Diffusion Flames under MILD Condition** **(208)** *Y. Sun*	**Towards the Converged Von Neuman Peak Pressure using Fine Scale Simulation of Detonation Cell Structure** **(200)** *J. Ryu, M. Niyasdeen, J.Y. Choi*	**Visualization of Deflagration-to-detonation Transition in a Channel with Rough Wall** **(163)** *S. Maeda, M. Irokawa, D. Taneichi, T. Obara*	**Numerical Simulation of the effects of a muffler on shock sound mitigation** **(50)** *A. Sethu Venkataraman, E. Oran*
17:30 17:55	**Oscillatory Combustion Kinetic Analysis and Reduction through Functional Weight Coefficient** **(126)** *S. Liang, L. Ji, D. Zhao*	**Predictability of $H_2/O_2/Ar/He$ Detonations in Thin Channels: New Experiments and Improvements in the Quasi-two-dimensional Mode** **(175)** *F. Zangene, A. Sow, M. Radulescu*	**Plasma-assisted Deflagration to Detonation Transition of Dimethyl Ether in a Microchannel** **(235)** *M. Vorenkamp, T. Chen, S. Steinmetz, C. Kliewer, A. Starikovskiy, Y. Ju*	**Experimental study on turbulent flame speed of H_2-CO/air mixtures relevant to late phase accident scenario** **(173)** *A. Desclaux, M. Idir, A. Comandini, A. Bleyer, A. Bentaib, N. Chaumeix*
17:55	**Adjourn**			

Work in Progress Posters Session I

(274) Preliminary investigations of the detonation-bow shock interaction: a pictorial essay
A.S. Venkataraman, E.S. Oran

(287) The comparison of Favre average procedure for the gaseous detonation from Eulerian and Lagrangian point of view
H. Watanabe, A. Matsuo, A. Chinnayya, N. Itouyama, A. Kawasaki, K. Matsuoka, J. Kasahara

(283) Numerical investigation of deflagration to detonation transition in smooth pipes
T. Alzer, L. Engelmann, M. Sens, A. Kempf, I. Wlokas

(272) Recent Research on Rotating Detonation Engines supplied by liquid propellants at the Łukasiewicz Institute of Aviation
M. Kawalec, P. Wolański, W. Perkowski, A. Bilar

(284) Water-Cooled Rotating Detonation Engine
T. Fukuda, K. Sato, T. Nagao, M. Itoh, E. Dzieminska

(279) Cellular structure of helium detonation as a trigger of sub-Chandrasekhar mass Type Ia supernovae
K. Iwata, K. Maeda

(282) Heat Radiation Losses from Propagating Spherical Flames of Mixtures with Methane, Hydrogen, Carbon Monoxide and Air
A. Roque, A. Hamadi, M. Idir, A. Comandini, N. Chaumeix

(293) Onset of Cellular Instability in Spherically Expanding Flames
M. Turner, E. Petersen

Notes

Tuesday, June 21st, 2022 (morning sessions)				
9:00 10:00	**Plenary Lecture (Aula Magna):** ***Prof. Gaby Ciccarelli*** **(Queen's University, Canada)** **Title: Flame Acceleration and Deflagration-to-Detonation Transition in a Confined Geometry** *Chairs:* ***H.D. Ng and A. Matsuo***			
10:00 10:10	Break (Transition to Morning Sessions)			
	Aula Magna (1st Floor)	Aula Bobbio (1st Floor)	Aula C (2nd Floor)	Aula D (2nd Floor)
Topics	**Detonation Modelling II** *Chair:* ***G. Vignat***	**Detonation Structure II** *Chair:* ***N. Tsuboi***	**Stability I** *Chair:* ***M. Liberman***	**Laminar Flame I** *Chair:* ***Y. Ju***
10:10 10:35	**Uncertainty Quantification for the Real Gas Model of Steady Planar Detonation** **(18)** *Z. Weng, R. Mevel*	**Experimental Analysis of Cellular Detonations: a Discussion on Regularity and Three-dimensional Patterns** **(57)** *V. Monnier, V. Rodriguez, P. Vidal, R. Zitoun*	**Fractal-based RANS Modeling of Darrieus—Landau and Thermal-diffusive Instability Effects on Lean Hydrogen Flames** **(33)** *D. Zivkovic, T. Sattelmayer*	**A Study on the Effect of Ethanol Addition on Laminar Flame Speed of a Four-Component Gasoline Surrogate at Elevated Pressure and Temperature** **(56)** *Y. Almarzooq, E. Petersen, I. Schoegl*
10:35 11:00	**Detonation Propagation in the Inhomogeneous Mixtures with Periodic Reactant Concentration Gradient** **(12)** *Y. Wang, Z. Chen*	**Comparative Analysis of the ZND Detonation Structure in Hydrocarbon Fuels** **(245)** *C. Colby, A. Ghosh, S.S. Dammati, A. Poludnenko*	**Investigation of the Scale Similarity Principle for Subgrid Modelling of the Reactive Richtmyer-Meshkov Instability** **(23)** *M. Bambauer, J. Hasslberger, M. Klein*	**Experimental and Numerical Study on a Gasoline Surrogate Mixture** **(238)** *O. Mghanen, N. Chaumeix, M. Matrat, S. Chevillard, N. Obrecht*
11:00 11:25	**Unified Characteristic Relationships of Hydrogen-Oxygen-Argon Detonation Dynamics in Narrow Channels** **(145)** *Q. Xiao, C. Weng*	**Two-Dimensional Detonations in Ethylene-Air Mixtures with Multi-Step Chemistry** **(230)** *S.S. Dammati, A. Poludnenko*	**Numerical Investigation of Fuel Feed Line Instabilities and its Effects in the Partially Premixed Swirling Flame** **(159)** *J. Nam, J.J. Yoh*	**Chemiluminescence of Spherically Expanding Methane-Air Flames Doped with DMMP** **(140)** *M. Turner, P. Parajuli, W. Kulatilaka, E. Petersen*

11:25 11:50	**Break and Work-In-Progress Posters Session II (Hall of 1th floor)**			
Topics	**Laminar Flame II** *Chair:* ***G. Continillo***	**Detonation Structure III** *Chair:* ***R. Deiterding***	**Detonation Diffraction** *Chair:* ***K. Matsuoka***	**Stability II** *Chair:* ***T. Jaravel***
11:50 12:15	**Combustion Characteristics of Butane in a Meso-scale Burner with Ordered Porous Media** **(255)** *X. Chen, J. Li*	**Detonation Structural Response to Multi-dimensional Confinement** **(217)** *J. Crane, J.T. Lipkowicz, X. Shi, I. Wlokas,A. Kempf, H. Wang*	**Numerical Study on Re-Initiation of Detonation Propagating through Double Slits in a Planar Channel** **(101)** *D. Jun, B.J. Lee*	**Oxygen Enrichment Effect on the Stability of Turbulent Diffusion Biogas Flames** **(213)** *S. Fabbro, M. Tkach, M. Birouk*
12:15 12:40	**Analysis of Chemical-Induced Irreversibility in Premixed Counterflow CH4/CO/Air Flame** **(168)** *C.R. Yu, C.Y. Wu*	**Dynamics and Properties of 2D vs. 3D Ethylene-Air Detonations** **(151)** *S.S. Dammati, A. Poludnenko, R. Xu, X. Shi, H. Wang*	**Simplified Numerical Simulation of Gaseous Quasi-Detonation Diffraction from a Rough Walled Channel** **(192)** *C. Yan, X. Sun, X.C. Mi, H.D. Ng*	**Multiple Steady State Solutions for a Flame Stabilized behind a Highly Conductive Bluff Body** **(11)** *V.N. Kurdyumov, C. Jimenez*
12:40 13:05		**Numerical Analysis on Ammonia / Hydrogen / Air Detonation Using Detailed Chemical Reaction model** **(94)** *G. Inoue, N. Tsuboi, K. Ozawa, A.K. Hayashi*	**Data-driven Modeling of Reflection Point Distance Relevant to Diffracting Detonation Wave by using Machine Learning** **(246)** *A. Kawasaki, H. Hasegawa, H. Sun, H. Watanabe, N. Itouyama, K. Matsuoka, J. Kasahara, A. Matsuo, I. Funaki*	
13:05 14:35	**Lunch (Biblioteca Gasparini, 2nd Floor)**			

Tuesday, June 21st, 2022 (afternoon sessions)

	Aula Magna (1st Floor)	Aula Bobbio (1st Floor)	Aula C (2nd Floor)	Aula D (2nd Floor)
Topics	**RDE IV** *Chair:* ***M. Kawalec***	**Detonation Structure IV** *Chair:* ***M. Radulescu***	**Multiphase I** *Chair:* ***J. Yoh***	**Laminar Flame III** *Chair:* ***H. Wang***
14:35 15:00	**Active Direction Control in Rotating Detonation Combustor** **(104)** *Z. Sheng, M. Cheng, D. Shen, K. Wu, J.P. Wang*	**An Investigation of the Detonation Jetting Phenomenon** **(120)** *R. Hytovick, R.F. Burke, T. Rezzag, K. Ahmed*	**Shock Interaction at Mach 4 of a Water and Fuel Droplet** **(244)** *F. Virot, J.-L. Rullier, D. Hébert*	**Experimental Study of Early-Stage Dynamics of the Ascending and Descending Laminar Hydrogen-Air Flames in Vertical Closed Rectangular Tube** **(183)** *N.B. Anikin, I.A. Kirillov*
15:00 15:25	**Experimental Study on the Aluminum Powder Rotating Detonation Engine** **(190)** *H. Xu, C. Weng, Q. Zheng*	**Forward Jetting Phenomenon in Detonations** **(232)** *P.A. Meagher, X. Shi, J. Crane, X. Zhao, A. Poludnenko, H. Wang*	**High-fidelity Simulations of Liquid-gas Colliding Jets Impacted by a Detonation Wave** **(28)** *R.J. Bielawski, S. Prakash, V. Raman*	**Laminar Burning Velocity and Adiabatic Flame Temperature of Biogas/Air Mixture at various CO2 Concentrations** **(152)** *A. Ghabi, T. Boushaki, P. Escot Boucanegra, E. Robert, B. Sarh*
15:25 15:50	**Numerical Investigation of the Effect of Ozone Addition on Detonation in the Two-dimensional RDE Chamber** **(207)** *R. Tanaka, A. Matsuo, E. Shima, H. Watanabe, A. Kawasaki, K. Matsuoka, J. Kasahara*	**Experimental Research On The Biogas – Oxygen Mixture Detonation Cell Size** **(205)** *S. Siatkowski, K. Wacko, J. Kindracki*	**A Computational Model for Single Iron Particle Combustion in Liquid-Phase Droplets** **(96)** *A. Fujinawa, X.C. Mi, J. Jean-Philippe, J. Bergthorson*	**Flame-Acoustics Interaction of Flames Propagating in a Narrow Duct: Effect of Heat Losses and Lewis Number** **(144)** *C. Jimenez, V.N. Kurdyumov*
15:50 16:15	**Effects of Mixing Level and Temperature of Injection in Rotating Detonative Combustion** **(224)** *C. Wang, K. Yao, H. Teng, Y. Wang, C. Tian*	**On Cellular Multiplicity of Detonations in Confined Channels** **(222)** *X. Shi, P.A. Meagher, J. Crane, S.S. Dammati, X. Zhao, A. Poludnenko, H. Wang*	**On the Critical Conditions for Thermal Runaway of Fine Iron Particles** **(97)** *X.C. Mi, A. Fujinawa, J. Bergthorson*	**Evolution of Acoustic Waves in High-Pressure Compressible Counterflow Diffusion Flames** **(48)** *G. Arumapperuma, M.X. Yao, J.P. Hickey, W. Han*

16:15 16:40	**Break and Work-In-Progress Posters Session II (Hall of 1th floor)**			
Topics	**Multiphase II** *Chair:* ***X.C. Mi***	**Detonation Interface Interaction** *Chair:* ***V. Rodriguez***	**RDE V** *Chair:* ***C. Stevens***	**Laminar Flame IV** *Chair:* ***N. Darabiha***
16:40 17:05	**Mixture Distribution of Solid-Gas-Two-Phase Flow for Gaseous Detonation with Aluminium Particles** **(214)** *R. Shimizu, T. Mizukaki*	**Detonation Propagation in a Layer Laterally Confined by Combustion Products** **(226)** *K. Cheevers, M. Raut, S.A. Lalchandani, Z. Hong, M. Radulescu*	**An Explanatory Model for the Multi-Wave Dynamics in Rotating Detonation Engines** **(70)** *C.R. Whitman, X.C. Mi, A. Higgins, C.B. Kiyanda*	**Early Stages of Flame Dynamics in Tubes and Mechanism of Tulip Flame Formation** **(9)** *M.A. Liberman, C. Qian, C. Wang*
17:05 17:30	**Morphology-independent Measurement of Iron Particle Burn Time** **(270)** *D. Ning, Y. Shoshin, J.A. van Oijen, G. Finotello, L.P.H. de Goey*	**Detonation Propagation in a Semi-confined Mixture with a Diffuse Interface** **(249)** *M. McLoughlin, V. Yousefi Asli, G. Ciccarelli*	**Acceleration of Burned gas to Supersonic in a Throatless Rotating Detonation Engine** **(160)** *K. Nakata, K. Ota, S. Ito, K. Ishihara, K. Goto, N. Itouyama, H. Watanabe, A. Kawasaki, K. Matsuoka, J. Kasahara, A. Matsuo, I. Funaki, K. Higashino, J. Braun, T. Meyer, G. Paniagua*	**CFD Modeling of Pressurized Laminar Coflow (Non-premixed) Diffusion Flames with Water Addition** **(162)** *H, Girodon, D. Dunn-Rankin, Y.C. Chien*
17:30 17:55		**Interaction of Detonation Waves with Turbulent Layers** **(242)** *B. Marjaba, H. Fazal, C.B. Kiyanda*	**Propagation of Gaseous Detonations in High Aspect Ratio Planar Curved Channels** **(13)** *M.L. Fotia, J. Hoke, R.J. Hencel, A. Schumaker*	**A Level-set Transport Equation for Tracking Self-ignition Fronts in Hydrogen-Air Mixture** **(158)** *C. Siddappa, Z. Bouali, V. Robin*
17:55	**Adjourn**			
19:00	**Young Researcher’ s Night**			

Work in Progress Posters Session II

(280) Metal Combustion in Composite Solid Propellants
J.C. Thomas, F.A. Rodriguez, K. Herder, G. Lukasik, W. Kulatilaka, E. Petersen

(281) Comparison of Hand and Resonant Acoustic Mixing of AP/HTPB Propellants
F.A. Rodriguez, J.C. Thomas, A. Hong, E. Petersen

(290) Experimental Study of Gasification of Argan Nut Shell and Olives Pomace. Syngas Flame Characteristics
B. Sarh

(291) Study of the Oxidation and Pyrolysis of Lubricants at High Temperatures
R. Juarez, N. Gutierrez, E.L. Petersen

(269) Investigation of Lower Explosion Limit of Hybrid Mixtures in a 20 L-sphere
V. Heilmann, S. Zakel

(276) Experimental study on the performance of the standardized test method for detonation flame arresters
L. Ruwe, T. Heidermann, M. Kreißig, H. Kant, D. Schmidt, F. Gutte, D. Bartsch, P. Bosse, A. Lucassen

(285) Study of Flammability Domain of H2/CO Mixtures at Conditions Representative of the Late Phase of a Severe Accident in a PWR
L. Vastier, S. Nagaraju, A. Desclaux, A. Comandini, A. Bentaib, N. Chaumeix

(288) Experimental study on expanding spherical flames of H2/CO mixtures at O2 reduced conditions
M. Bouton, O. Mghanen, A. Desclaux, A. Comandini, A. Bentaib, N. Chaumeix

Notes

Wednesday, June 22nd, 2022 (morning sessions)				
9:00 10:00	**Plenary Lecture (Aula Magna): Prof. Benoît Fiorina (Université Paris-Saclay, CNRS, Laboratoire EM2C, France)** **Title: Including Detailed Chemical Properties in the Modeling of Emerging Turbulent Combustion Systems** *Chair:* ***A. Comandini and H.D. Ng***			
10:00 10:10	Break (Transition to Morning Sessions)			
	Aula Magna (1st Floor)	Aula Bobbio (1st Floor)	Aula C (2nd Floor)	Aula D (2nd Floor)
Topics	**Flame Dynamics & Stability** *Chair:* ***U. Riedel***	**Dynamics of Reactive Supersonic Flows** *Chair:* ***V. Raman***	**Detonation Initiation & limits** *Chair:* ***S. Maeda***	**Ignition I** *Chair:* ***M.B. Luong***
10:10 10:35	**Isotope Effect on the Chara-cteristics of the Flame-Ball-to-Deflagration. Transition in Ultra-Lean Hydrogen- and Deuterium-Air Mixtures in Horizontal Hele-Shaw Cell (216)** *I.A. Kirillov, V. Denisenko, V. Plaksin, A. Melikhov*	**Numerical Simulation of Laminar Premixed Hydrogen-Air Flame/Shock Interaction under Low-Pressure Conditions (72)** *E. Yhuel, G. Ribert, P. Domingo*	**Experimental Study on Detonation Wave Initiation by Reflected Blast Wave in Laser Ignition (179)** *T. Sato, K. Matsuoka, A. Kawasaki, N. Itouyama, H. Watanabe, J. Kasahara*	**Experimental and Numerical Study of Autoignition/Deflagration Transition Limit in an optical Rapid Compression Machine (155)** *H. Ossman, C. Strozzi, J. Sotton, M. Bellenoue*
10:35 11:00	**A Tsuji Burner in a Counterflow (264)** *B. Li, A.L. Sanchez, F. Williams*	**Stability Analysis of the Noh Problem for Reactive Shocks (265)** *C. Huete, A. Calvo-Rivera, A.L. Velikovich*	**The Critical Dynamics of Direct Initiation of Spherical Detonations (223)** *R. Hernández Sánchez, B. Denet, P. Clavin*	**Comparison between Laser Ignition and Spark-Plug Ignition of Flowing Propane-Air Mixtures (52)** *K. Eto, Y. Kojima, W. Kim, T. Johzaki, T. Endo*
11:00 11:25	**Scaling Laws for Velocity Dynamics of the Ultra-lean Hydrogen-Air Flames Expanding in Horizontal Cylindrical Hele-Shaw Cell (221)** *P.V. Moskalev, V.P. Denisenko, I.A. Kirillov*	**Numerical Study of Low-Frequency Supersonic Combustion Instability in a Hydrogen-fueled Scramjet Engine (199)** *S.M. Jeong, H.S. Han, E.S. Lee, J.-Y. Choi*	**A Three-step, Three-gamma Model for the Numerical Modeling of the Critical Height of the Propagation of Semi-confined Detonation Waves (59)** *S. Taileb, E. Rougon, V. Robin, V. Rodriguez, S. Lau-Chapdelaine, P. Vidal, J. Melguizo-Gavilanes, A. Chinnayya*	**Numerical Simulation of LOx/CH4 Supercritical Combustion in a non-Homogenous Mixture (84)** *F. Monnier, G. Ribert*

11:25 11:50	**Break**			
Topics	**Pressure-Gain Combustion** *Chair: M. Gamba*	**Flame Acceleration & DDT II** *Chair: J. Hasslberger*	**Detonation Modelling II** *Chair: A. Chinnayya*	**Chemical Kinetics V** *Chair: N. Chaumeix*
11:50 12:15	**Identification of Multiple Combustion Modes in Continuous Detonation Engines (87)** *J.Z. Ma, J.P. Wang*	**Critical Conditions for Flame Acceleration and DDT for Hydrogen-Air Mixtures at Cryogenic Temperatures (259)** *M. Kuznetsov, A. Denkevits, A. Friedrich, A. Veser*	**Shock Dynamics from Quenched Detonations: Diffraction and Gallop Problems (156)** *M.I. Radulescu*	**Improvement of the Global Quasi-Linearisation (GQL) Model Reduction Method (69)** *C. Yu, V. Bykov, U. Maas*
12:15 12:40	**TDLAS for Sensing Pre-vaporized Jet A-1 in Liquid-fuel Pressure Gain Combustion (31)** *P.H. Chang, N. Teo, J.M. Li, X. Huang, C.J. Teo, B.C. Khoo*	**On the Possibility of Non-dimensionalizing DDT Limits and Distances (67)** *V. Rodriguez, V. Monnier, P. Vidal, R. Zitoun*	**A Methodology to Develop Simplified Kinetic Schemes for Detonation Simulations (86)** *F. Veiga-Lopez, A. Chinnayya, J. Melguizo-Gavilanes*	**REDIM Reduced Modeling of Flame-Wall-Interactions of Premixed Natural Gas / Air Systems (172)** *C. Straßacker, U. Maas*
12:40 13:05	**Numerical Study on the Unsteady Rotating Detonation Flow-field Interacted with Turbine Guide Vane (102)** *D. Shen, M. Cheng, K. Wu, Z. Sheng, J.P. Wang*	**A One-dimensional Model for Deflagration-to-detonation Transition of an Elongated Flame (82)** *H. Tofailli, P. Clavin, G. Lodato, L. Vervisch*	**Modelling Detonation Reflection with Nonsteady Shock Change Equation (73)** *D.T. Schoeffler, J. Shepherd*	**Experimental Investigation of the Combustion Properties of a Representative Thermal Runaway Gas from Li-Ion Batteries (47)** *O. Mathieu, M. Turner, D. Mohr, J.C. Thomas, E. Petersen*
13:05 13:30		**An Experimentally Informed 1-D DDT Model for Smooth Narrow Channels (106)** *J. Melguizo-Gavilanes, L. Bauwens*	**Numerical Study of Detonation Propagation through a Gravity-driven Layer of Hydrogen-Oxygen over an Inert Gas (257)** *M. Menezes, S. Lau-Chapdelaine, G. Ciccarelli*	**Experimental and Numeric study on the Inhibition Properties of Novec (225)** *S. Nagaraju, S. Abid, A. Comandini, N. Chaumeix*
13:30	**Light Meal for Excursion**			
14:30 - **Wednesday Excursion**				

Thursday, June 23rd, 2022 (morning sessions)				
	Aula Magna (1st Floor)	Aula Bobbio (1st Floor)	Aula C (2nd Floor)	Aula D (2nd Floor)
Topics	**Explosion Safety II** *Chair:* ***K. Vågsæther***	**Flame Acceleration & DDT III** ***Chair: I.A. Kirillov***	**Turbulent Flames I** *Chair:* ***V. Bykov***	
9:00 9:25	**Shock Transmission from Detonating Mixtures in Open Tubes** **(124)** *J.C. Thomas, F.A. Rodriguez, D. Teitge, L. Kunka, N. Gaddis, Z. Browne, C. Ahumada, T. Balci, S.I. Jackson, E. Petersen, E. Oran*	**Detonability Enhancement by Use of a Nanosecond Plasma** **(219)** *M. Ali Cherif, V. Lafaurie, S. Starikovskaia, P. Vidal*	**Surface Density Function and its Evolution in Homogeneous and Inhomogeneous n-Heptane MILD Combustion** **(64)** *K. Abo-Amsha, N. Chakraborty*	
9:25 9:50	**Influence of Hemicylindrical Obstacle Scale and Length on an Impacting Blast Wave** **(181)** *R.N. Gavart, S. Trélat, M.-O. Sturtzer, N. Chaumeix*	**Thermochemical Aspects of Superknock Development in IC Engines** **(261)** *M.B. Luong, E. Tingas, H.G. Im*	**Flame Self-Interactions in Turbulent Homogeneous-Mixture n-heptane MILD Combustion** **(119)** *K. Abo-Amsha, N. Chakraborty*	
9:50 10:15	**REKO-Fire: New Facility to Investigate Cable Fire Impact on Passive Autocatalytic Recombiners** **(171)** *G. Nobrega, M. Klauck, E.-A. Reinecke, N. Chaumeix, A. Bentaib, L. Maas*	**Effect of Mach number on the Flame Acceleration and Deflagration-to-Detonation Transition** **(42)** *W. Zhao, J. Liang, X. Cai, R. Deiterding, X. Wang*	**Numerical Investigation of the Global Equivalence Ratio Effects on the Dynamic Behavior of Turbulent Swirling Diffusion Flame** **(240)** *S. Chakchak, T. Boushaki, A. Hidouri, M. Chrigui*	
10:15 10:40		**Simulation of Flame Acceleration and Deflagration-to-Detonation Transition in Components of Chemical Plants** **(24)** *C. Wieland, C. Hirsch, T. Sattelmayer, F. Scharf, V. Hoferichter, H.P. Schildberg*	**DNS of Turbulent Spray Flame Water Droplet Interaction Using an Euler-Lagrange-Lagrange Scheme** **(25)** *J. Hasslberger, R. Concetti, N. Chakraborty, M. Klein*	

10:40 11:05	Break and Work-In-Progress Posters Session III (Hall of 1th floor)			
Topics	**Oblique Detonation** *Chair:* ***J.Y. Choi***	**RDE VI** *Chair:* ***K. Ishii***	**Fire Dynamics** *Chair:* ***Y. Chien***	**Energetic Materials I** *Chair:* ***S. Jackson***
11:05 11:30	**The Impact of a Micro-Rounded Bump on the Initiation of Oblique Detonation Waves** **(176)** *C. Yan, G. Bakalis, R. El-Chaar, H. Teng, H.D. Ng*	**Experimental Study of Liquid Propellant Rotating Detonation Combustor** **(170)** *S. Ito, K. Ishihara, K. Yoneyama, K. Goto, N. Itouyama, H. Watanabe, A. Kawasaki, K. Matsuoka, J. Kasahara, A. Matsuo, I. Funaki*	**Statistical Research on Firebrand Behaviour in a Simulated 3D Fire Whirl** **(32)** *Y. Zhang, Y. Zhang*	**Pyroelectric Combustion Rate Characterization of Electrically Controlled Solid Propellants** **(193)** *G. Kanagaraj, J.J. Yoh*
11:30 11:55	**Experimental Study of Stabilized Oblique Detonation Waves** **(93)** *D.A. Rosato, M.R. Thornton, K. Ahmed*	**Temperature and Heat-Flux Measurements in a Thin-Wall RDE** **(37)** *C.A. Stevens*	**Experimental Study of Firebrand Lofting Mechanism in a Fire Whirl Induced Flow Field** **(74)** *Y. Zhang, A. Albadi, Y. Zhang*	**Investigation of Micro- and Nano-Catalytic Additive Effects on Ammonium Perchlorate Combustion** **(125)** *F.A. Rodriguez, J.C. Thomas, T. Sammet, D. Teitge, E. Petersen*
11:55 12:20	**Experimental Observation of Non-uniformly Premixed Oblique Detonation** **(189)** *K. Iwata, N. Hanyu, S. Maeda, T. Obara*	**Self-excited Wave Propagation in a Reflective Shuttling Detonation Combustor** **(21)** *M.J. Ullman, S. Prakash, D.R. Jackson, V. Raman C.D. Slabaugh, J.W. Bennewitz*	**Numerical Prediction of Cables Fire Behaviour Using Non-Metallic Components in Cone Calorimeter** **(262)** *A. Alonso Ipina, M. Lazaro, D. Lazaro, D. Alvear*	**Understanding Thermochemical Aspects of the Magnesium Metal Fuel subjected to Hygrothermal Aging with Varied Oxygen Flow Rates** **(195)** *J. Oh, J.J. Yoh*
12:20 12:45	**Formation and Regulation of Unsteady Detonation Mach Stem in A Confined Space** **(20)** *S. Niu, P. Yang, H. Teng*	**Shock-Droplet Interactions and Reaction of Liquid RP-2 Fuel** **(198)** *J.P. Patten, K. Ahmed, R. Hytovick, R.F. Burke*		**Experimental Evaluation of Plain Metal Additives for Solid-Fuel Propulsion Applications** **(123)** *J.C. Thomas, F.A. Rodriguez, E. Petersen*
12:45 14:15	**Lunch (Biblioteca Gasparini, 2nd Floor)**			

Thursday, June 23rd, 2022 (afternoon sessions)

	Aula Magna (1st Floor)	Aula Bobbio (1st Floor)	Aula C (2nd Floor)	Aula D (2nd Floor)
Topics	**Ignition II** *Chair:* ***C. Strozzi***	**Flame Acceleration & DDT IV** *Chair:* ***J. Melguizo-Gavilanes***	**RDE VII** *Chair:* ***A. Kawasaki***	**Shock Tube I** *Chair:* ***D. Nativel***
14:15 14:40	**A Study on Influences of Hydrogen Addition and Turbulence on Ignition Characteristics of Propane Mixtures** (35) *M. Nakahara, K. Tanimoto, H. Kudo, F. Abe, K. Tokunaga*	**Effect of Flame Front Thermo-Diffusive Instability on Flame Acceleration in a Tube** **(220)** *J.-J.Hok, O. Dounia, O. Vermorel, T. Jaravel*	**Detonations and Thermoacoustic Modes in a Flow through RDC** **(139)** *E.J. Gutmark, V. Anand, J. Betancourt, A. Gaetano, T. Pritschau, R. Wiggins*	**Shock-tube Study of the Ignition of Fuel-rich CH_4/ or Natural Gas/Ozone/Air Mixtures at High Pressure** **(15)** *J. Herzler, M. Fikri, C. Schulz*
14:40 15:05	**Real Gas Effect on Ignition Characteristics in Ideal and Non-ideal Reactors** (17) *Z. Weng, Z. Li, R. Mevel*	**Investigation of Iso-propyl Nitrate as a Detonation Improver** **(184)** *R.A. Mousse, M.A. Burnett, S. Abid, S. de Persis, A. Comandini, M.S. Wooldridge, N. Chaumeix*	**State-to-State Model for Rotating Detonation Combustors** **(243)** *M. Gamba, A. Feleo, J. Shepard, F. Chacon*	**Simultaneous CO and H2O Laser Absorption Measurements of Pentene Isomers in a Shock Tube** **(95)** *C.M. Gregoire, C. Westbrook, O. Mathieu, S.P. Cooper, S. Alturaifi, E. Petersen*
15:05 15:30	**Incompletely Stirred Reactor Network Modeling for the Estimation of Turbulent Non-Premixed Autoignition** **(51)** *S. Iavarone, S. Gkantonas, E. Mastorakos*	**Numerical Study of Multi-dimensional Effects on the Transition to Detonation from Subsonic Self-ignition Waves Propagating at Constant Speed** **(130)** *S. Taileb, E. Rougon, A. Chinnayya, V. Robin*	**Experimental Results for 25-mm and 51-mm RDRE Combustors** **(29)** *C. Knowlen, T. Mundt, M. Kurosaka*	**Probing PAH Formation from Cyclopentene Pyrolysis in a Single-Pulse Shock Tube** **(209)** *L. Carneiro Piton, A. Hamadi, F. Cano, S. Abid, N. Chaumeix, A. Comandini*
15:30 15:55		**The Effect of Buoyancy on Flame Acceleration in Hydrogen-air Mixtures: Experiments in Horizontal and Vertical Tubes** **(194)** *E.V. Bezgodov, S.D. Pasyukov, A.A. Tarakanov, M.V. Nikiforov, Yu.F. Davletchin, V.A. Simonenko, I.A. Kirillov*		**Probing Pyrolytic PAH Chemistry in High-Repetition-rate Shock Tube Coupled to Synchrotron-based Double Imaging Photoelectron/ Photoion Coincidence Spectroscopy** **(233)** *F.E. Cano Ardila, S. Nagaraju, R.S. Tranter, S. Abid, A. Desclaux, A. Roque, N. Chaumeix, A. Comandini*

15:55 16:20	**Break and Work-In-Progress Posters Session III (Hall of 1th floor)**			
Topics	**Condensed Phase Detonation II** Chair: ***C. Chiquete***	**Shock Tube II** Chair: ***J. Herzler***	**Numerical Methods** Chair: ***F. Marra***	
16:20 16:45	**Effect of Microstructure on Detonation Performance of the Insensitive High Explosive PBX 9502** **(60)** *S. Voelkel, E.K. Anderson, M. Short, C. Chiquete, S.I. Jackson*	**The Effect of Oxygenated Species on the Fuel-rich Oxidation of CH4 in the Context of Polygeneration: Extinction, CO-Concentration and Temperature Measurements** **(54)** *D. Nativel, J. Herzler, M. Fikri, C. Schulz*	**Reduced Order Modeling of 2-D Reaction-Diffusion System Based on POD-DEIM and k-means Clustering** **(65)** *E.A. Cutillo,G. Petito, K. Bizon, G. Continillo*	
16:45 17:10	**Using a High Speed Hyperspectral Camera to Measure Gas Temperature And Concentration Profiles Resulting From Detonation of TNT** **(266)** *Gagnon, J.-P. (Boubanga-Tombet S.)*	**Ignition of Lubricating Oils using a Novel Spray Injection Technique in a Shock Tube** **(49)** *S.P. Cooper, E. Petersen*	**Numerical Method Based-cellular Automata for Heat Transfer with Application to the Self-Ignition of Energetic Materials** **(135)** *A. Violet, E. El-Tabach, P. Gillard, M. William-Louis*	
17:10 17:35	**Initiation of Sympathetic Detonation between two Separated PETN charges** **(110)** *D. Murray, A. Vashishtha, D. Lenihan, D. Callaghan, C. Nolan*	**Probing PAH Formation from Heptane Pyrolysis in a Single-pulse Shock Tube** **(180)** *A. Hamadi, F. Cano, L. Carneiro Piton, S. Abid, N. Chaumeix, A. Comandini*		
17:35	**Adjourn**			
18:15	**Banquet**			

Work in Progress Posters Session III

(275) Nitromethane Droplet Breakup and Combustion in a Detonation Environment
S. Briggs, N. Berube, D. Dyson, A. Arakelyan, S. Vasu

(277) Investigation of NH3–H2 mixtures in a plug-flow reactor
L. Ruwe, S. Schmitt, D. Zhu, B. Shu, K. Kohse- Höinghaus, A. Lucassen

(289) An Experimental Study of the Formation of CO During Ethanol Pyrolysis and Dry Reforming with CO2
O. Mathieu, C.M. Gregoire, S.P. Coooper, E. Petersen

(292) Spectroscopic CO and H2O Laser Absorption Measurements: Chemical Kinetics Investigation of Toluene Combustion in a Shock-Tube
C.M. Gregoire, S.P. Cooper, E. Petersen

(294) Experimental Investigation of High-Pressure Oxy-Syngas Combustion with High CO2 Dilution
S.P. Cooper, M. Turner, D. Mohr, O. Mathieu, E. Petersen

(278) A mathematical model for autoignition
J. Harris, C. Please, J. Ockendon

(286) A new generation kinetic model for pyrolytic soot formation
T.I. Viola, L. Carneiro Piton, A. Hamadi, N. Chaumeix, A. Comandini

(271) Probing Fuel-rich oxidation of 1,3-Butadiene at high-temperature using quantum-cascade-laser dual-comb spectroscopy
M. Geiser, R. Rahman, F. Arafin, R. Horvath, S. Vasu

(273) Detonation Tube Setup for Liquid Fuel Droplet in Detonation Wave Experiments
N. Berube, S. Briggs, S. Vasu, A. Arakelyan, D. Dyson

Notes

Friday, June 24th, 2022 (morning sessions)

	Aula Magna (1st Floor)	Aula Bobbio (1st Floor)	Aula C (2nd Floor)	Aula D (2nd Floor)
Topics	**Energetic Materials II** *Chair:* ***J.C. Thomas***	**Detonation Boundary Interaction** *Chair:* ***G. Ciccarelli***	**RDE VIII** *Chair:* ***C. Knowlen***	**Multiphase III** *Chair:* ***A. Matsuo***
9:00 9:25	**Hydrodynamic Characterization of the Aging Induced Performance Degradation of HMX-Based Explosive PBX 9404** **(215)** *S.I. Jackson, C. Chiquete, E.K. Anderson*	**Influences of a Small Step on the Side Wall upon Detonation Propagation** **(66)** *Y. Seki, T. Honda, W. Kim, T. Johzaki, T. Endo*	**Development of an Automatic-Calibrating Small-Scale Thrust Stand for Rotating Detonation Rocket Engines** **(112)** *A.R. Kotler, R.F. Burke, T. Rezzag, K. Ahmed*	**Experimental Investigation of Reacting Fuel Droplets Interactions with Detonation Waves** **(250)** *D. Dyson, A. Arakelyan, N. Berube, S. Briggs, J. Ramirez, E. Ninnemann, K. Thurmond, G. Kim, W. Green,*
9:25 9:50	**A Modeling of Metalized Solid Fuel Surface Combustion** **(196)** *H.S. Choi, S.Y. Han, J.J. Yoh*	**An Immersed-Boundary Projection Method for Studies of Detonation Waves Interacting with Thin Obstacles** **(98)** *X. Lu, H. Yu, C. Pantano, E. Oran*	**Experimental Study of the Miniaturized Cylindrical Rotating Detonation Engine** **(201)** *K. Hattori, K. Ota, K. Ishihara, K. Goto, N. Itouyama, H. Watanabe, A. Kawasaki, K. Matsuoka, J. Kasahara, A. Matsuo, I. Funaki*	**Numerical Study of Multi-Dimensional Liquid-Fuel n-Dodecane/Air Detonations with Complex Chemistry** **(150)** *S.S. Dammati, Y. Kozak, A. Poludnenko*
9:50 10:15	**Laser Ignition of a Low-vulnerability RDX-based Propellant: Influence of the Atmosphere on Ignition and Combustion Properties** **(55)** *S. Delbarre, L. Courty, P. Gillard*	**Experiments of the Tri-arc Non-Circular Rotating Detonation Engine (RDE)** **(202)** *J.H. Lee, E.S. Lee, H.S. Han, J.M. Kim, J.-Y. Choi*	**Investigation of Wave Velocity in a Hybrid Rotating Detonation Engine** **(166)** *M. Assad, O. Penyazkov, I. Chernukho*	**Numerical Analysis on the Breakup of Dilute Water Spray in Gaseous Detonation** **(165)** *H. Watanabe, A. Matsuo, A. Chinnayya, K. Matsuoka, A. Kawasaki, J. Kasahara*
10:15 10:40	**Characterization of High Pressure Electrolytic Decomposition of Hydroxylammonium Nitrate Aqueous Solution using FTIR** **(79)** *M.H. Wu, K.I. Lao, Y.T. Chou*		**Wall Heat Flux Measurements behind a Shock Wave Generated by a Detonation** **(239)** *F. Virot, H. Quintens, B. Boust, J. Sotton, M. Bellenoue*	**Steady and Transient One-dimensional Simulations of Multiphase Dodecane/air Detonations** **(252)** *N.J. Tricard, A. Ghosh, S.S. Dammati, A. Poludnenko, X. Zhao*

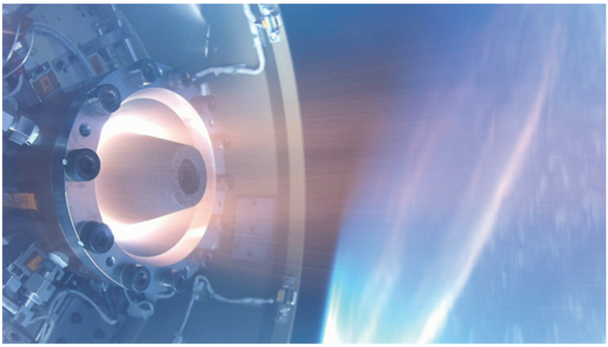
10:40 11:05	**Break**			
Topics	**Propulsion Application** *Chair:* ***G. Ribert***	**RDE IX** *Chair:* ***J. Kasahara***		
11:05 11:30	**Baffled-Tube Ram Accelerator Operation with Methane-Air Propellant** **(45)** *C. Knowlen, B. Leege, J. Correy, C. Smith, A. Higgins*	**Numerical Simulation of the Effect of the Array-hole Injection and Cavity Combustor on the Rotating Detonation Engine Performance** **(88)** *X. He, J. Wang, X. Liu*		
11:30 11:55	**Thermodynamic Analysis of Unsteady Propulsion Systems** **(107)** *R. Fievisohn, C. Stevens*	**Effect of preburn Inhomogeneities on the Detonation Velocity in a Rotating Detonation Rocket Engine** **(148)** *G. Vignat, D. Brouzet, M. Ihme*		
11:55 12:20	**Operation Characteristics of a Disk-Type Rotating Detonation Engine** **(203)** *K. Ishii, K. Ohno, H. Kawana, K. Kawasaki, A.K. Hayashi, N. Tsuboi*	**Study of Fuel-Oxygen Mixing in a Rotating Detonation Engine Cold Analog** **(185)** *M. McLoughlin, S. Gray, G. Ciccarelli*		
12:20	**Adjourn**			
12:30 - **Farewell Party**				

Monday 9:00 – PL1

PL1 Fundamental Research of Detonation Engine and Its Space Flight Experiment Using Sounding Rocket

Jiro Kasahara

The detonation engine generates detonation and compression waves at extremely high frequencies (1–100 kHz) to drastically increase reaction speed, leading to radical reduction of rocket engine weights and high performance by easy generation of thrust. The research group of Nagoya University, Keio University, JAXA/ISAS, and Muroran Institute of technology has successfully demonstrated a detonation engine in space flight. The Detonation Engine System (DES) developed in this study was loaded onto the mission section of the sounding rocket S-520-31 and launched from the JAXA Uchinoura Space Center at 5:30 a.m. on July 27, 2021. After the separation of the first stage rocket, the rotating detonation engine and pulse detonation engine were successfully operated in space, and photo images, pressure, temperature, vibration, position, and attitude data were acquired by telemetry and RATS (Reentry and Recovery Module with Deployable Aeroshell Technology for Sounding Rocket Experiment). The fuel is methane and the oxidizer is oxygen. The success of this space flight demonstration will bring the detonation engine much closer to practical use as a kick motor for deep space exploration, and as a first and second stage engine for rockets.



Monday 10:10 – RDE I

137 Preliminary Experimental Study of Propulsive Performance of Hollow Rocket Rotating Detonation Engines with Designed Laval Nozzle

Zhang, Yunzhen; Ma, John Z.; Wang, Jianping; Zhang, Shujie*

In this paper, we performed a preliminary experimental research about the propulsion performance about the hollow rotating detonation engine (RDE) attached with Laval nozzle. The Laval nozzles we designed have a throat diameter of 30.8 mm and 43 mm. The specific impulse and the c* efficiency which measured the degree of completion of chemical energy releases in combustion chambers were calculated. It is shown that the specific impulse was 0.6-1.0 that of the ideal value. The specific impulse of the hollow RDE increases as the chamber pressure increases. Besides, the c* efficiency of the nozzle with throat diameter of 43 mm is a bit higher than that of 30.8 mm, which might be due to the injecting structure and the coupling of the combustion chamber and the propellant plenum. We also noted that there is a trend that the performance of the detonation is a bit higher than deflagration, which is very encouraging. The study of it is ongoing in our laboratory.

247 Experimental investigation on the coal powder rotating detonation engine

Ni, Xiaodong; Xu, Han; Weng, Chunsheng; Su, Xiaojie; Xiao, Bowen; Zhang, Feng; Luo, Yongchen*

To explore the rotating detonation characteristics of pulverized coal and the effects of the particle size on it, the experiments of coal powder rotating detonation engine were carried out.The experimental results showed that the detonation pressure and detonation velocity can be increased by adding a small amount of porous anthracite powder to the hydrogen-air mixture. When a large amount of porous anthracite powder is added, the detonation pressure continues to rise, but the propagation velocity of detonation wave decreases. For the same porous anthracite, the variation of detonation parameters with particle size is not monotonous. When the hydrogen-air equivalence ratio is 0.7 and the total equivalence ratio is 1.0, the detonation performance of 3 micron porous anthracite is the best. And the average detonation pressure is 1.08 MPa and the propagation frequency is 3990 Hz.

78 Numerical analysis of the influence of mixing on detonation wave propagation inside a rotating detonation engine by using linear detonation channel

Wang, Faming; Mizukaki, Toshiharu; Matsuyama, Shingo*

In the flow field of a rotating detonation engine (RDE), the detonation wave propagates through the reaction with the continuously injected fuel and oxidant mixture. In the previous research using the actual RDE, due to insufficient mixing and other reasons, the detonation wave velocity generated in RDE is usually significantly lower than the characteristic Chapman-Jouguet velocity for corresponding mixture. In this paper, construct a linear detonation channel that simulate the RDE flow field to eliminate the influence of the shape of the combustion chamber and the centrifugal force on the propagation of the detonation wave. The effects of incomplete mixing of fuel and oxidizer mixture on the propagation of detonation waves in the RDE flow field are studied through numerical analysis by using JAXA's in-house code CHARIOT.

191 On the Predicability of Weakly Confined Gaseous Detonations Using the Straight Streamline Approximation

Lalchandani, Sarthak A; Radulescu, Matei; Hong, Zekai*

We evaluate the usefulness of the Straight Streamline Approximation model developed by Watt and co-workers to predict the detonation structure of gaseous detonations, which are weakly - confined by an inert gas. Our calculations are compared to the DNS results obtained by Reynaud, Mi and their co-workers for one-step Arrhenius chemistry. For low activation energy of 10, the model captures the detonation speed dependence on layer thickness very well. The model progressively departs from the numerical results by a factor increasing exponentially with the activation energy. This numerical factor is accounted by the global reduction in the cell-averaged reaction rate computed by Reynaud et al. A rational explanation for this reduction in energy release rate is developed using a model for the distribution of ignition delay behind non-steady shocks in cellular detonations.

234 Numerical Investigation of One-dimensional Pulsating Detonations Using Fickett?s Detonation Analogue with Chain-Branching Kinetics

*Sow , Aliou *; Radulescu, Matei*

The present study aims to investigate the spatiotemporal nonlinear dynamics of detonations in a wide range of reaction time scales away from the neutral stability region. This is addressed by one-dimensional numerical simulations using a Fickett's detonation analogue with a chain-branching kinetics model. A shock-fitting solver is used to reduce the cpu time. Up to almost four thousand simulations have been carried out allowing a detailed investigation of the pulsating dynamics of detonations. For long reaction time scales, the detonation is stable, weakly unstable or quenched. For intermediate reaction time scales, the traditional period-doubling cascade to chaos scenario is observed. For short reaction time scales, the route to chaos is different. The detonation fails prior to reaching the period-2 oscillations. The reignited detonation escapes the even period oscillations in its route to chaos.

127 Characteristic Analysis for 2D Steady Supersonic Reacting Flow: Effect of Confinement on Detonation Flows

Short, Mark; Chiquete, Carlos*

Steady detonation propagation in high explosives is determined by the energy release that occurs within the detonation driving zone (DDZ). This is the subsonic flow region bounded by the detonation shock and sonic flow locus (in a frame traveling with the steadily propagating detonation front). Weak confinement materials were previously thought not to influence the DDZ structure. However, we have recently discovered that information can travel from the material boundary Prandtl-Meyer (PM) fan through the supersonic flow region downstream of the sonic locus, and impact on the sonic locus. Here, we examine the influence that a newly discovered PM expansion wave that emerges at the sonic flow point on the centerline of a 2D planar slab geometry has on the shape of the DDZ. Additionally, we study the effect of geometry on characteristic information flow through the supersonic regime that impacts on the DDZ, contrasting the behavior between 2D planar slab and 2D circular arc geometries.

Monday 10:10 – Gas and Dust Explosion I

38 Experimental and numerical analysis of the laminar burning velocity of oxygen-enriched ethylene mixtures

Pio, Gianmaria; Renda, Simona; Palma, Vincenzo; Salzano, Ernesto*

Ethylene is largely adopted in the chemical industry. It is a key intermediate in combustion modelling, as well. Most of the processes involving this species take place in an oxidative environment. Nonetheless, the reactivity of mixtures containing ethylene, oxygen, and nitrogen are poorly investigated, especially at non-standard conditions. This work is intended to fill the abovementioned gaps utilizing either experimental or numerical analyses. In particular, the heat flux burner was adopted to characterize mixtures of ethylene/oxygen/nitrogen at low temperatures. The collected measurements were compared against numerical estimations resulting from detailed kinetic mechanisms, for the sake of the quantification of the estimation quality. Then, the flammability limits were estimated through the limiting laminar burning velocity theory. Estimated compositions were tested experimentally and compared with flammability limits from the current literature.

114 Characterizing the Reactivity of Large-Scale Dust Explosions

Bauwens, C. Regis L; Boeck, Lorenz R; Dorofeev, Sergey*

Dust explosions can present a severe hazard at any facility where combustible dusts are present. Currently, a parameter referred to as the dust deflagration index is typically used to characterize the reactivity of a specific dust. This parameter, however, only characterizes the reactivity at a single time, typically late in the combustion process. To address this limitation, a new dust-flame combustion model is developed based on a characteristic turbulent burning velocity and a finite reaction time. It was found that this model can reproduce

the overall shape of the experimental rate of pressure rise observed in a wide range of experiments performed in an 8-m^3 vessel. This model can be used to establish equivalency between dust explosion tests performed in different experimental setups and can also provide a basis for future methods of explosion hazard evaluation that considers the level of initial turbulence and the specific materials properties of the dust.

108 Large-Scale Confined Gas and Dust Explosions with Elevated Initial Turbulence

Boeck, Lorenz R; Bauwens, C. Regis L; Dorofeev, Sergey*

Turbulence plays an integral role in the severity of industrial explosions, including explosions of dusts, gases/vapors, and hybrid mixtures. This work examines the dynamics of turbulent gas and dust explosions in an 8-m3 vessel that was equipped with an injection system that creates initial turbulence and injects dust as needed. Under similar levels of turbulence, it was found that propane-air gas explosions produce significantly higher rates of pressure rise than optimal concentrations of cornstarch dust. It was demonstrated that for gas explosions the scaling of initial burning velocity with turbulence differs significantly from the scaling of maximum rate of pressure rise. The appropriate scaling needs to be considered when assessing the hazards of turbulent explosions or designing explosion protection. The results from this work will help inform assessments of explosion risk and explosion protection and provide a basis for future studies on hybrid-mixture explosions.

Monday 10:10 – Chemical Kinetics I

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46 Ignition Delay Time and Laminar Flame Speed Measurements of a Li-ion Battery Electrolyte: Ethyl-Methyl-Carbonate

Mathieu, Olivier; Almarzooq, Yousef; Petersen, Eric*

Electric vehicles use large lithium-ion batteries to store their energy. In such a battery, lithium salt ions move between the anode and the cathode via a liquid electrolyte. The liquid electrolyte is a mixture of various highly flammable organic solvents, linear and cyclic carbonates for the most part.

To better control LIB fires, it is therefore necessary to understand the details of the combustion chemistry of the electrolyte's components. Among these electrolytes, only linear carbonates have been investigated. More specifically, Di-Methyl-carbonate (DMC) and Di-Ethyl-carbonate (DEC) were studied, as they are also considered promising biofuels. In the present study, ignition delay times in a shock tube and laminar flame speeds in a closed vessel were measured for ethyl-methyl carbonate (EMC) for the first time.

68 Global Quasi-Linearization (GQL) for model reduction of reaction diffusion systems

Bykov, Viatcheslav; Yu, Chunkan; Maas, Ulrich; Gol?dshtein, Vladimir*

The Global Quasi-Linearization (GQL) method for model reduction of chemical kinetics is applied to a hydrogen combustion system. The GQL method is based on a characteristic time-scale analysis. It decomposes the homogeneous system dynamics automatically into relatively slow and fast subsystems. The GQL based reduced model for chemical kinetics obtained for auto-ignition problem is applied to premixed flames where additional physical processes i.e. advection and molecular diffusion are taken into account. The paper focuses for illustration on the hydrogen/air system. In this study we show that the fast/slow decomposition of the homogeneous system dynamics is an intrinsic invariant property of the system, which does not even depend on a particular mechanism. A basis of the system decomposition defined for a homogeneous system using a single mechanism can be extended to other mechanisms and accurately describe flame propagation in premixed combustion systems.

178 Ignition delay time measurements of methane/ethane/propane mixtures with addition of ozone

Drost, Simon; Schieál, Robert; Maas, Ulrich*

We investigate the ignition-accelerating effect of ozone on fuel-rich mixtures of natural gas surrogates with diluted oxygen/argon mixtures in a Rapid Compression Machine. Ignition delay times for two natural gas surrogates, namely pure methane and a (90/9/1) methane/ethane/propane mixture were measured, each with and without ozone addition. The investigated conditions are an equivalence ratio of 2, a pressure of 20 bar, and a temperature range from 950 K to 1300 K. In addition to the experimental investigations, detailed chemistry simulations using reaction mechanisms from the literature were carried out in order to assess the ability of these mechanisms to predict the influence of ozone on auto-ignition. We found a discrepancy between the ignition delay times of the experiments and the simulations, and the results can be improved with a revised version of the reaction mechanism.

Monday 11:50 – Gas and Dust Explosion II

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62 Propagation of methane detonation in coal dust suspensions with different concentrations

Shi, Jingtai; Xu, Yong; Ren, Wanxing; Zhang, Huangwei*

Methane/coal dust explosion has been significant hazards in process and mining industries.The concentration and particle size of coal dust have a great influence on the process of methane/coal dust explosion . In this study, two-dimensional methane/coal dustdetonation propagation is studied. The propagation process of gas and coal dust explosions under five different coal dust concentrations is analyzed. Moreover, general features of two-phase and detailed detonation structures are well captured. Detonation process of different coal dust concentrations are analyzed through looking into the evolutions of detonation frontal structure and detonation propagation speed. For the higher concentrations coal dust, the detonation wave first experiences decoupling of the reaction front and shock, and is then re-initiated. The results from this study are of great significance for the study of suppressing methane/coal dust mixed explosion.

83 Gravity effect on steady, 1-D propagation through dust clouds

Kuwana, Kazunori; Yazaki, Shigetoshi; Kim, Wookyung; Mogi, Toshio; Dobashi, Ritsu*

Accurate risk assessment is a key to prevent accidental dust explosions, and insights into combustion characteristics such as propagation speed and extinction limit are essential for quantitative risk assessment. This study presents a continuum dust-explosion model to simulate steady, one-dimensional propagation. Cases of constant density without gravity were first considered, and analytical expressions were obtained to express the propagation velocity as a function of ignition temperature with and without considering heat loss. Basic equations were then numerically solved for cases of variable gas-phase density with gravity. It was found that the propagation velocity increases with an increase in gravity level, and there is a critical gravity level for downward propagation. Propagation is not possible when the absolute value of gravity level exceeds the critical value.

63 Expansion Waves Behaviour during Liquified CO2 Depressurization in a Divergent Cross-Section Vessel

M.Ibrahim, Osama Kabbashi; Hansen, Per Morten; Bjerketvedt, Dag; V†gs‘ther, Knut*

Recent developments in carbon capture and storage have led to an increased concern about the safety of CO_2 transport systems. Hazards that arise from the accidental release of liquid CO_2 include rapid phase change with explosive evaporation and expansion. Therefore, it is essential to study the mechanisms and the dynamics affecting these process developments. This work investigates the phase transition mechanisms during liquified CO_2 depressurization from a double-membrane setup with a high-pressure conical vessel. It provides experimental results and analysis describing divergent cross-section and liquid volume fraction (LVF) effects on expansion waves behaviour. Results indicate a considerable pressure increase at the vessel's bottom after the evaporation wave has passed due to the over-expansion effect. Its peak values were proportional to the increase in LVF. The rarefaction wave velocities were nearly constant. In contrast, they were varied for evaporation wavefront.

Monday 11:50 – Condensed Phase Detonation I

71 Detonation Performance Experiments and Modeling for the High Explosive PETN

Anderson, Eric Karl; Chiquete, Carlos; Chicas, Ritchie; Jackson, Scott I*

PETN is a commonly used high explosive (HE) for detonator, fusing, and booster assemblies. Despite its popularity, detailed detonation performance data is relatively sparse. The large operational density range of PETN requires a significant number of tests to characterize experimentally. Additionally, its short reaction zone requires test assemblies to be very small relative to other common explosives to quantify the effect of confinement and geometry on the explosive performance. In this study, PETN rate sticks and cylinder tests are fielded at the smallest known scales (3-mm HE diameter) at a density of 1.65 g/cc. The resulting data verifies that the flow satisfies continuum measurement at this scale, and analysis yields a Detonation Shock Dynamics (DSD) propagation law and Jones-Wilkens-Lee (JWL) product EOS for programmed burn detonation modeling. This work also provides the first recorded front shape measurements of PETN.

132 Detonation performance model calibration and validation of the HMX-based high explosive PBX 9501

Chiquete, Carlos; Jackson, Scott I; Anderson, Eric Karl; Short, Mark; Voelkel, Stephen; Whitley, Von H.*

Due to the chemical complexity of condensed phase high explosives (HEs), detonation performance models are calibrated to a series of experiments in simplified geometries. These typically include confined and unconfined axisymmetric HE cylinders and/or rectangular cuboids (or “slabs”). In either case, experimental measurements provide information on an HE's unconfined steady-state propagation behavior and wall expansion rates when confined. The fundamental assumption is that detonation performance model parameterizations produced in one geometry, i.e. a copper-confined cylindrical HE charge (CYLEX), can be used to accurately represent the HE behavior in more complex application geometries with a variety of confiner materials. Here, we investigate the predictive capability of such a model for the ideal HMX-based HE PBX 9501 in reference to validation experiments where the geometry and confiner are varied.

142 Towards Finite Rate Chemical Kinetics Modeling of Detonation Afterburn Using the BKW Equation of State

Clay, Matthew P; Taylor, Brian; Houim, Ryan*

High fidelity numerical simulations of high explosive (HE) detonation product afterburn are especially challenging due to the extreme ranges of thermodynamic states and flow scales involved. When modeling high-pressure detonation physics, it is common to use an equation of state (EOS) for the detonation products that does not explicitly account for individual chemical species. With our emphasis on late-time mixing and afterburn, we desire a

model which includes detailed species information and allows finite rate chemical transformations therein. For this we adopt the Becker-Kistiakowsky-Wilson (BKW) EOS, which is an empirical real-gas EOS built upon a multi-species ideal gas mixture, making it well suited for coupling to a finite rate chemical kinetics scheme to model afterburn combustion. We detail important aspects of such a model and show verification tests conducted in the research code HyBurn developed at the University of Florida.

Monday 11:50 – RDE II

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85 Simulations of ethylene-oxygen rotating detonation waves under different local equivalence ratio

Peng, Han; Deiterding, Ralf*

The highly efficient rotating detonation engine (RDE) has been considered as one of the viable replacements for current propulsion and power generation systems that employ constant pressure combustion. In this work, we use the open-source mesh adaptation framework AMROC to simulate the 2-D unwrapped plane of an annular RDE. The multi-component compressible Euler equations are solved within the AMROC-Clawpack finite volume framework. The inviscid flux is evaluated by a hybrid Roe/HLL scheme. A second-order accurate MUSCL-Hancock scheme with Minmod limiter is used for the reconstruction. Strang splitting is adopted for the reactive source term and a simplified ethylene/oxygen reaction mechanism is employed. The effects of a non-uniform local equivalence ratio (ER) on rotating detonation waves are studied. The results show that the number of detonation waves changes at specific local ER. The detonation velocity deficits are also observed when increasing the local ER difference.

210 Three-Dimensional Numerical Investigation on the Effect of Injector Configuration in Rotating Detonation Engine

Sada, Takumi; Matsuo, Akiko; Shima, Eiji; Watanabe, Hiroaki; Kawasaki, Akira; Matsuoka, Ken; Kasahara, Jiro*

To investigate the effects of the injector configuration on the flow characteristics and performance in short rotating detonation combustor, numerical analysis for cylindrical RDEs is performed. The injector located on the bottom or side wall of the combustor. The combustor with 20 mm in diameter of outer wall and 20 mm in length was considered using the stoichiometric hydrogen-air premixed gas. The shape of the propagating high-pressure waves change depending on the injector configurations. However, in all cases, the consumption of fuel to the combustor outlet is observed, and the burned gas was accelerated to the speed of sound. The specific impulse compared to the theoretical value were 102.3% for the injection from the bottom and 95.4% for that from the side wall.

22 Flow Acceleration in an RDRE with Gradual Chamber Constriction

Ross, Mathias C; Burr, Jason; Batista, Armani; Lietz, Christopher*

The addition of a nozzle to a rotating detonation rocket engine (RDRE) impacts the dynamics within the combustion chamber, a relationship that is not fully understood. We present two high fidelity large eddy simulations of gaseous methane-oxygen RDREs: one with a converging-diverging nozzle, and one without. It is found that the classical Mach-area relation prevents supersonic flow from existing in the converging section of an RDRE, in contrast to what is seen in geometries without a nozzle; as such, even a gradual constriction changes the acoustic boundary conditions of the engine. We calculate formation enthalpy change inside the chamber for both simulations and find that the nozzle-less geometry achieves the same level of combustion completeness at a lower average pressure, the sort of detrimental effect that will need to be reduced attempting to leverage the benefits of pressure gain combustion.

Monday 11:50 – Chemical Kinetics II

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258 Effects of Di(2,2,2-trifluoroethyl) Carbonate on the Ignition Delay Time and Laminar Flame Speed of H2 and CH4

*Turner, Mattias; Mohr, Darryl; Dievart, Pascal; Catoire, Laurent; Petersen, Eric; Mathieu, Olivier**

To mitigate the fire hazard of lithium-ion battery, the effect of a specific fire suppressants (di(2,2,2-trifluoroethyl) carbonate (DtFEC)) on combustion properties (Ignition delay time, laminar flame speed) of H2 and CH4 was investigated experimentally.

Even though DtFEC generally inhibited ignition of H2, it also caused a decrease in H2 ignition delay time at high enough temperatures. However, its effectiveness as a fire suppressant is clear in the large decrease in H2 flame speed. For CH4, DtFEC caused CH4 ignition delay time to actually decrease for every tested temperature and equivalence ratio, even though DtFEC also caused decreased flame speed at every tested condition. The results included herein provide much-needed data for validating and improving chemical kinetics mechanisms for the target fire suppressant, of which currently there are none readily available to model these mixtures.

161 Sensitivity of Reaction-Diffusion Manifolds (REDIM) for hydrogen counter-diffusion flames

*Maas, Ulrich ; Bykov, Viatcheslav**

In this study, a mathematical formulation for the calculation of the sensitivity of manifold based simplified chemistry with respect to both elementary reaction rate coefficients and the system gradient estimate is presented for the REDIM manifolds. This allows us to answer how important the system gradient estimate is for the Reaction-Diffusion Manifolds (REDIM) reduced chemistry and how sensitive the reduced scheme is with respect to the kinetic parameters. Based on the governing REDIM evolution equation, the sensitivity equation is derived in form of a linear in-homogeneous partial differential equation system of second order with non-constant coefficients. A hydrogen diluted by nitrogen / air non-premixed combustion system is used as an illustrative example. Moreover, the proposed sensitivity analysis can also be used in other manifold based methods.

10 Influence of Thermochemistry on Prompt NO formation in Flames

Shrestha, Krishna P; Seidel, Lars; Giri, Binod Raj; Zeuch, Thomas; Mauss, Fabian*

In this work, with the exception of NCN, the influence of thermochemistry on prompt NO formation in flames is studied for the first time. Since prompt NO formation is more pronounced under rich conditions, we investigated two fuel-rich methane and acetylene flames. To estimate the sensitivity of the species, we formulated a sensitivity equation based on the maximum NO concentration. We varied the enthalpy of formation of the species by ±1 kJ and ±5 kJ to perform the sensitivity analysis. Our analysis shows that the prompt NO formation is mainly affected by the thermochemistry of NCN, CH, N2, and H species.

Monday 14:35 – IC Engines

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109 0D Laminar Flame Speed Model for Methane Lean Mixture in Dual Fuel Combustion

De Robbio, Roberta; Mancaruso, Ezio; Vaglieco, Bianca Maria; Artham, Sushma; Mart¡n, Jaime*

For decades, the compression ignition engines are widespread in the market because of their reliability and efficiency. But, they have high exhaust emissions of particulate matter and nitric oxides which can be problematic for environment. Dual fuel operation, where gaseous fuels are used with pilot diesel injection, is considered as one efficient solutions to improve exhaust emissions, by substituting part of the diesel with methane forming a premixed charge with air. However, dual fuel combustion is extremely complex to model, since it is characterized by the oxidation of two fuels presenting different features. Indeed, a small amount of diesel, burning in a diffusive flame, starts via a multipoint ignition the propagation of a flame in the air-methane premixed charge. In the present work, a dual-fuel combustion model was built in a commercial software with the aim of simulating the experimental results and investigating the characteristics of methane-diesel combustion.

26 Statistics of flame topology in turbulent spray flame water droplet interaction

Concetti, Riccardo; Hasslberger, Josef; Chakraborty, Nilanjan; Klein, Markus*

The impact of water droplet addition on statistically planar turbulent spray flames has been studied by means of carrier-phase DNS simulations using an Euler-Lagrange-Lagrange scheme. The spray flames considered here are characterized by the coexistence of premixed and diffusive combustion due to mixture inhomogeneity. It has been found by combined measurements of Gauss and mean curvature that the surface topology of reaction progress isosurfaces is dominated by the highly volatile fuel droplets whereas the effect of low-volatility water droplets is rather reflected by the normalized temperature isosurfaces. However, due to the turbulence dampening effect of evaporating droplets, water injection influences the curvature distribution in additional non-trivial ways. The flame topology and curvature have important effects on the flame displacement speed and on the evolution of the surface density function, which are of pivotal importance to well-established combustion modeling concepts.

80 Effect of Jet Configuration on Knock Characteristics Using a Rapid Compression Machine

Liu, Wei; Qi, Yunliang; Zhang, Ridong; Zhang, Qihang; Wang, Zhi*

Jet ignition (JI) method is promising in spark ignition (SI) engines since it holds advantages in burning velocity, thermal efficiency, and combustion stability when compared to SI method. However, knock remains possible under JI. Jet chamber design has vital impacts on burning velocity and jet configuration, thus influences knock characteristics. The design of an optimal jet chamber should give consideration to the interaction between key parameters regarding knock, e.g., residence time, burned mass fraction (BMF), knock intensity. With the change of burning velocity, various BMF and knock intensity might be resulted, bringing in contradictions on whether knock intensity increases with increasing BMF.

In this work, different jet configurations were compared to investigate the effect of jet configuration on knock characteristics on a rapid compression machine (RCM). The impacts of jet configuration were investigated. Relationship between BMF and knock intensity was also discussed.

177 The effect of the ignition energy and mixture energy density on the detonation onset in internal combustion engines

Xu, Han; Weng, Chunsheng; Yao, Chunde*

Self-designed detonation bomb experiments were conducted to explore the detonation onset as well as the knock intensity problem. The experiment was conducted at three typical in-cylinder pressures for representing different mixture energy densities. Spark ignitions with low and high energy were given in each condition, respectively. The in-cylinder combustion process and pressure oscillation process were monitored by the synchronous acquisition of three pressure sensors that were installed in different positions of the chamber. It is found that irrespective of the low or high ignition energy, the super knock as well as the detonation would not occur at the lower pressure, and only mild knock occurs. At the medium pressure, the high ignition energy would result in a detonation wave, while the low ignition energy would not. At the higher pressure, despite the energy of ignition, a detonation wave as well as a super knock would always occur.

58 Elliptical experimental detonation

*Babin, Romane; Chinnayya, Ashwin; Rodriguez, Vincent**

Experimental results of detonation propagation in circular and elliptical tubes have been performed, for three different mixtures, of increasing usual detonation-cell regularity ($2H_2+O_2+N_2$, $2H_2+O_2$, CH_4+2O_2). The ratio of the minor and major axis was one half. Detonation velocity deficits in the circular case have been obtained, as the initial pressure was decreased, from 100 kPa to 12 kPa. The cells were larger in the ellipsis. Even if the detonation velocity could not be measured, we can infer that the reduced radius in the minor axis played a key role in enhancing the losses. The cells seemed to be locked in this axis. An elliptical galloping mode sequence of extinctions and re-ignitions has also been observed in the more unstable case.

91 Study of imploding detonations with high-speed videography and digital open-shutter photography

Rodriguez Rosero, Sebastian; Higgins, Andrew; Loiseau, Jason*

In this work, we revisit the study of the implosion of gaseous detonations. More specifically, with the use of modern visualization techniques such as high-speed videography and open-shutter photography, we have collected results on the stability of convergence and the cellular structure of an imploding detonation. For this experiment, an imploding wave facility was built with a cavity designed to smoothly guide the waves to converge in a test section where a window is located. Video footage of an equimolar acetylene-oxygen detonation was recorded, revealing that the conditions in which the detonation wave enters the cavity are imprinted onto and retained by the converging front. Open-shutter visualization techniques were used to capture the mixture at different initial sub-atmospheric pressures. Ongoing research incorporates the construction of a parameter space for the different factors that influence the converging detonations.

164 Towards laser-induced fluorescence of nitric oxide in detonation

Chatelain, Karl P.; Rojas Chavez, Samir; Vargas, Joao; Lacoste, Deanna*

This study aimed at evaluating the capabilities of the NO-LIF diagnostic for characterizing H_2-air detonation. This objective was achieved in two steps. First, our in-house spectroscopic tool, KAT-LIF, is updated to perform NO-LIF simulations by notably developing a database of NO(A-X) transitions. Second, the validation of KAT-LIF is performed in a laminar CH_4-air flame and H_2-air detonation. The validation results indicate: (i) the simulated NO-LIF intensity evolution in a stoichiometric CH_4-air flame is in agreement with experimental results and other simulation tools (LIFBASE and LIFSim) for different laser excitation wavelengths; (ii) the LIF intensity evolution in a stoichiometric H_2-air detonation is well reproduced. These results evidenced the possibility to use the NO-LIF diagnostic in NO-seeded H_2-air detonation. Also, our simulations revealed that the NO addition does not modify the detonation structure and this quantity can be adjusted to improve signal-to-noise ratio.

40 Multiple-view Imaging of a Small-diameter Detonation Tube at 5 MHz

Thomas, Levi; Schauer, Fred; Cyrol, David; Sell, Brian*

We report here on a novel, yet simple, imaging technique employed on the new, optically accessible, small-diameter detonation tube installed at the Combustion Analysis Optimization Laser (COAL) Lab at the Air Force Institute of Technology (AFIT). A retro-reflecting mirror is placed directly behind and alongside the detonation tube such that reflections from the top and bottom of the passing detonation are imaged in addition to the primary chemiluminescence from the front view. Three simultaneous views of detonations of H_2-O_2 as well as of C_2H_4-O_2 are imaged at 5 MHz using a Shimadzu HPV2 framing camera at varying stoichiometry and dilution with argon. This abstract presents the experimental setup, raw imagery of the triple view detonations as well as enhanced images, and preliminary wave-speed calculations based on both cross-correlation and on a polynomial fitting routine for sub-pixel spatial resolution. Additional analysis and discussion will be presented in the final manuscript.

Monday 14:35 – RDE III

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237 Study of Rotating Detonation Combustor Dynamics During Changes in Operating Mode

Shepard, Joshua; Feleo, Alexander; Gamba, Mirko*

This work seeks to determine the cause(s) of operating mode changes and quantify any system-level indications that may be used to predict when an RDC will depart from or change between modes of pseudo-steady operation. Understanding this phenomena is critical for any device that seeks to utilize an RDE/RDC, as meeting requisite performance parameters and designing appropriate hardware interfaces require predictable operation that can be accounted for in the design phase. Testing was conducted with an axial air inlet design and hydrogen-air mixtures. This study will be conducted through analysis of high-speed pressure measurements obtained during the course of operation and from high-speed videos which captured the chemiluminescence of the wave system(s). The potential benefits of utilizing an RDC are unlikely to

be realized if rapid and repeated transitions between deflagrating, pulsed, and rotating operating modes are not fully understood and able to be avoided or mitigated.

111 The Effect of Fuel Partial Premixing on Rotating Detonation Waves

Burke, Robert F; Rezzag, Taha; Kotler, Adam R; Ahmed, Kareem*

Conventional injection schemes of rotating detonation combustors inject fuel discretely into the combustion channel, thus developing local fuel-rich and fuel-lean mixed regions. In this study, hydrogen and air are premixed in a rotating detonation combustor with parts of the fuel injected into the oxidizer flow at varying amounts. The objective is to investigate the effect of this premixing on the wave dynamics of the combustor. Three premixing schemes are examined. Altogether, these display that there is significant stratification of detonatable mixture without premixing; such that after premixing, the entire annulus becomes more favorable for continuous detonation propagation, evident in a higher detonation wave speed. This result is shown to be independent of the combustor total fuel-air equivalence ratio and the percent of fuel that is premixed into the oxidizer. This research implies that combustor performance could be improved with lean hydrogen premixing in the oxidizer.

218 Numerical Analysis on Pressure Gain of Rotating Detonation Engine Using H2-O2 Gases: Influence of Number of Injector

Hayashi, A. Koichi; Yoshidomi, Keisuke; Ozawa, Kohei; Tsuboi, Nobuyuki; Kawashima, Hideto*

The concept of "Pressure Gain Combustion (PGC)" more probably comes from gas turbine work and is later applied to Pulse Detonation Engine (PDE) study. In 2010 through the present, research moves from PDE to rotating detonation engine (RDE) and PGC concept is applied to RDE. RDE is considered for two applications so far; rocket motor and gas turbine engine.

At this situation RDE turns up and gets attention to the increase of GTE performance by the Humphry cycle of detonation. A cylindrical Combustion chamber without any nozzle will get at most about 60-70% pressure loss (in this case we must count the pressure loss from injection too). The way of calculating PG with detonation base is developed by Paxson. His calculation is to start with combustion chamber RDE.

The objective of the present study is to get a method of calculating PG for any type of RDE numerically, which can be compare with other RDE's PG and to discuss about PG gain and loss.

227 Initiation Dynamics of Rotating Detonation Engines using C2H4-O2 Mixtures

*Connolly-Boutin, Sean Francis; Ghali, Mohammad; Gilot, Ritchard; Loiseau, Jason; Higgins, Andrew; Kiyanda, Charles B**

The transient, initiation dynamics of detonation waves are studied experimentally in a 70 mm diameter throatless, 5.5 mm-high annular rotating detonation engine (RDE) operating on a stoichiometric mixture of C2H4/O2. Two electric initiation systems are employed: a low-energy (10-1000 mJ), automotive-spark based system; and a high-energy (0.25-5 J) capacitive discharge system. Two regimes of initiation have been observed. For low-energy initiation, a roughly 770 microsec period of low chemical activity with no light emission is observed. Following this period, the amount of light emitted by the combustion increases in a single, localized region that travels counter-clockwise. This wave accelerates as the amount of light increases, suggesting a DDT event. For high-energy initiation, a roughly 70 microsec period of inactivity is followed by the sudden appearance of multiple, counter-rotating, bright, combustion waves. These waves undergo periodic collision-reinitiation events.

Monday 14:35 – Chemical Kinetics III

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103 The impact of H_2 and CO on the NH_3 / NO / O_2 chemistry - a step towards a predictive tool for NH_3 oxidation

Glarborg, Peter; Alzueta, Maria Uxue*

Due to the poor ignition and oxidation properties of NH3, its use as a carbon-free fuel typically requires presence of a co-fuel. Downstream of the ignition region in an ammonia-fueled engine or gas turbine, combustibles formed by partial oxidation of the co-fuel are present together with unburned ammonia and trace amounts of nitric oxide, formed in the initial stage. The oxidation of NH3 under these conditions determines the heat release rate as well as the emission levels for NH3, NO and N2O. It is important to develop predictive models for this chemistry for use in design. In the present work, a wide range of experimental studies from the literature on the effect of H2 and/or CO on the NH3 oxidation in the presence of NO is re-interpreted in terms of a detailed chemical kinetic model. The key reactions are identified and the ability of the kinetic models to describe this chemistry is discussed.

167 Thermal Decomposition-induced Multi-stage Reaction of Diethyl Carbonate Examined by a Micro Flow Reactor with a Controlled Temperature Profile

Kanayama, Keisuke; Takahashi, Shintaro; Morikura, Shota; Nakamura, Hisashi; Tezuka, Takuya; Maruta, Kaoru*

Characteristics of oxidation and pyrolysis of diethyl carbonate (DEC) were investigated using a micro flow reactor with a controlled temperature profile. In the oxidation case, CO2 mole fraction showed a two-stage increase: the first increase at low temperatures (Tw,max = 750÷850 K) followed by a plateau (Tw,max = 850÷1000 K), and then the second increase at Tw,max = 1000÷1050 K. Based on the heat release rate profile of DEC/air weak flame, a three-stage reaction appeared. The three-stage reaction consists of thermal decomposition of DEC, oxidation of the decomposition products to CO and oxidation of CO to CO_2. This thermal decomposition-induced multi-stage reaction is distinctive from the ones observed in our past studies on oxidation of n-heptane and dimethyl ether, which were initiated by low-temperature oxidation. The thermal decomposition of DEC at the low temperatures were driven by the existence of ethyl ester group in its molecular structure.

89 Modeling Soot Formation in LES of Turbulent Flames Using Virtual Chemistry

Maldonado Colman, Hernando; Veynante, Denis; Darabiha, Nasser; Fiorina, BenoŒt*

This work introduces a new virtual chemistry methodology to predict soot formation in turbulent reactive flows. The virtual chemistry approach can reproduce relevant flame characteristics, such as laminar flame speed, heat release, and pollutant prediction. In a recent work on laminar flames, new additions have been introduced to include the soot complex phenomena and radiative heat losses. This virtual chemistry model is characterized by its versatility and low CPU cost in simulations, for different combustion regimes and a large range of operating conditions. In the present work, the virtual chemistry model is challenged in a turbulent jet sooting flame from the International Sooting Flame workshop. Large Eddy Simulations (LES) of the 3-D flame configuration were performed using the soot and radiative virtual approaches coupled together with Thickened Flame model. Numerical results are in good agreement with experimental measurements.

90 Large Eddy Simulation of a Multi-Regime Burner Using Virtual Chemistry

Luu, Tan-Phong; Fiorina, BenoŒt; Darabiha, Nasser*

Numerical models must be able to accurately describe the multi-regime flame happening in practical applications. Pollutant formation in particular has been highlighted to be considerably different in multi-regime flames compared to canonical premixed or non-premixed flames. The objective of this work is to challenge an innovative chemistry reduction method called virtual chemistry to the Large Eddy Simulation (LES) of a multi-regime flame configuration. The novel Darmstadt multi-regime burner has been chosen providing a rigorous framework in which simulations can be performed and compared against measurements. The low-Mach YALES2 code using a thickened flame mode for the LES has been employed. Time-averaged experimental and numerical data of axial velocity, temperature and CO mass fraction are compared. Preliminary results show overall good correspondence with experiments near the exit burner, albeit improvement can be expected from a finer mesh and longer time-averaging.

129 Community analysis of bifurcation maps of diluted hydrogen combustion in WSFRs

He, Jiyun; Li, Yue; Ji, Lin; Acampora, Luigi ; Marra, Francesco S.*

This article focuses on the development of an automatic procedure for the inspection of the very complex kinetic mechanisms required to predict accurately the behavior of new generation fuels. By coupling the bifurcation analysis, which identifies the different regimes occurring with a change of the parameters, with algorithms typical of Artificial Intelligence, specifically the Community Analysis, that identify within a large set of individuals (the chemical species) common behavior patterns, we proposed a novel mechanism analysis method that are capable of automatically extract meaningful information for the identification of the key species responsible for the dynamical behavior from the solution maps of a combustion system. Application in a diluted hydrogen combustion system reveal that the recognition of state change are effective based on the heat release rate and the entropy production rate indexes.

208 Validation of the Reaction-diffusion manifolds (REDIMs) reduced chemistry for the non-premixed CH4 counter-flow diffusion flames under MILD condition

*Sun, Yuanxiang **

In this work, Reaction-diffusion manifolds (REDIMs) based simplified chemistry is applied for the numerical simulation of a CH_4/CO_2 versus O_2/CO_2 counter-flow diffusion flame. The REDIM simplified chemistry can be generated easily with little information on the considered flame system. It is shown that the thermo-kinetic quantities can be well predicted by REDIM reduced chemistry for different strain rates until the extinction limit, and although no information for extinction regime needs to be known for the generation of REDIM simplified chemistry, the generated REDIM chemistry can re-produce the extinction limit very well. The extinction strain rate and time histories during extinction processes can be further improved by increasing the dimension of REDIM simplified chemistry to three dimensions, which is the subject of future research.

126 Oscillatory Combustion Kinetic Analysis and Reduction through Functional Weight Coefficient

Liang, Shengyao; Ji, Lin; Zhao, Dan*

In this work, a functional weight analysis method is proposed to analysis the oscillatory combustion mechanism. The inter-species interactions are quantitatively measured by anyanlyzing the data of oscillation so as to recongize the importance of each link. Detailed statistical results in oscillatory MILD combustion mechanism analysis reveal that the weight distributions are often highly heterogenenous, with only limited part of the inter-specise links

dominantly strong. This allow us to easily identify the important process and bulid a skeleton mechaniam for oscillation prediction. In the application in the methane and propane fueled MILD combustion systems, skeleton mechanisms with good prediction ability and reduction efficency are obtained. Besides, the recongnized important reactions agree well with the previous investigations, which further confirms the validity of the method in analyzing the oscillatory combustion mechanism.

Monday 16:40 – Detonation Structure I

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186 Cell Structure and Global Heat Release in 2D and 3D JP10-Air Detonations in Narrow Channels

Meagher, Patrick A; Shi, Xian; Zhao, Xinyu; Dammati, Sai Sandeep; Poludnenko, Alexei; Wang, Hai*

Two-dimensional (2D) and three-dimensional (3D) numerical simulations of jet fuel (JP10)-air detonations in a narrow channel are performed to establish a better understanding of detonation propagation in realistic fuels and boundary conditions. Athena-RFX is employed to solve the Navier-Stokes equations featuring the HyChem model for JP10 combustion. In this study we emphasize the relationship between the detonation cellular structure and global heat release. In 2D, the cellular structure and global burning rate are found to be highly irregular, and instants with global heat release rate at 68% and 155% the CJ heat release rate are evaluated. This irregularity is attributed to periods of quasi-failure and subsequent reignition through transverse detonations. Preliminary results in 3D indicate that the introduction of the third dimension stabilize both the cellular structure and global burning rate.

200 Towards the Converged Von Neuman Peak Pressure using Fine Scale Simulation of Detonation Cell Structure

*Ryu, Jaehoon; Niyasdeen, Mohammed; Choi, Jeong-Yeol**

For this study, a weak condition is purposefully chosen in such a way that making a single detonation cell to propagate in a two-dimensional (2D) channel of unit width. Grid resolution study has also been carried out for a wide range of radial grid spacing (Δy) By considering the finest resolution results in 256 million grid points in 2D simulation, a moving computational window technique is adopted to calculate only the vicinity of detonation wave front where important physics happens. For low resolution cases, numerical fluxes are evaluated by Roe, RoeM, AUSMDV and AUSMPW+ schemes and high resolution was achieved by 3rd-oder MUSCL, 3rd-order WENO, 5th-order WENO and 5th-order oMLP schemes. This paper shows the full details about the comparative performance of each scheme to capture dynamics structure of detonation cell structure including the dynamic maximum value on Von Neumann spike.

175 Predictability of H2/O2/Ar/He detonations in thin channels: new experiments and improvements in the quasi-two-dimensional mode

Zangene, Farzane; Sow , Aliou ; Radulescu, Matei*

The present study is a validation and improvement of the quasi-two-dimensional computational model developed by Xiao and co-workers for detonations propagating in narrow channels. New experiments of the detonation cellular structure in hydrogen-oxygen mixtures with either helium or argon dilution are performed in order to offer a non-ambiguous monitor of the wall losses since only transport properties are affected. In the proposed model for Quasi-2D simulation, an improvement is made to the negative displacement thickness which assumed constant speed flow in the reaction zone. In order to account for the acceleration of the gases in the reaction zone due to heat release. Excellent agreement for both the cellular structures and velocity deficits is obtained when the losses are reduced by a factor of 1.3.

Monday 16:40 – Flame Acceleration & DDT I

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256 DDT run-up distance measured by visualization of an obstructed tube

*Shervin Hashemi Mehr, Shervin; Ciccarelli, Gabriel**

The DDT run-up distance was measured in an acrylic tube filled with orifice plates using self-luminous high-speed video. The initial pressure was varied for mixtures of ethylene-oxygen and hydrogen-oxygen diluted with nitrogen and argon. For higher pressures, where the DDT run-up distance (XDDT) was small, the Silvistrini « CJ velocity (VCJ) correlation predicted the experimentally measured XDDT. For mixtures near the DDT limit, the flame property based correlation was not sufficient. The DDT run-up distance correlated with $X_{DDT}/D=c(d/l)^{-n}$, where l is the detonation cell size and c and n are empirical constants. It is shown that the sensitivity parameter n scales with the mixture activation energy. The data suggest that after the flame reaches «VCJ, there is an induction period before the onset of detonation. A DDT run-up distance correlation is proposed that is the sum of the distance required for the flame to reach «VCJ and the DDT induction distance, that scales with the cell size.

163 Visualization of Deflagration-to-detonation Transition in a Channel with Rough Wall

Maeda, Shinichi; Irokawa, Masahiro; Taneichi, Daiki; Obara, Tetsuro*

Deflagration-to-detonation transition in a channel with rough wall was investigated experimentally. The combustion channel was 486 mm long, 10 by 10 mm cross-section, and the lower or side wall was covered by the knurled stainless-steel plate whose maximum roughness height was 700 micrometers. Time-sequential schlieren and chemiluminescence visualization were conducted to capture the entire DDT process. The observations with and without the knurled plate showed that the flame acceleration could be divided into two stages: the initial stage immediately after ignition, in which the evolution of flame tip velocity was not affected by the surface roughness, and following second stage, in which the flame acceleration was greatly enhanced by the large surface roughness. In the second stage, the promoted chemical reaction was observed on the rough wall, and it formed the protruded flame front which seemed to have significant effect on the second stage of flame acceleration.

235 Plasma-assisted Deflagration to Detonation Transition of Dimethyl Ether in a Microchannel

Vorenkamp, Madeline; Chen, Timothy; Steinmetz, Scott; Kliewer, Christopher; Starikovskiy, Andrey; Ju, Yiguang*

A plasma microchannel is used to experimentally analyze the effect of plasma on deflagration to detonation transition (DDT) in DME:O2:Ar mixtures at atmospheric pressure. Nanosecond dielectric barrier discharges, ns-DBDs, are applied across the length of the microchannel before ignition. A high speed camera is used to trace the time histories of flame front position and velocity and to identify the dynamics and onset of DDT. The results show that plasma discharge can nonlinearly affect the onset time and distance of DDT. A small number of plasma discharge pulses prior to ignition result in reduced DDT onset time and distance by 60% and 40% when compared to the results without pre-excitation by ns discharges, while an increase of plasma discharge pulses results in an extended DDT onset time and distance of 224% and 94%. The present experiments demonstrate the ability to control DDT by using non-equilibrium plasma of transversal DBD for applications in advanced propulsion engines.

Monday 16:40 – Explosion Safety I

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197 The Bologna LPG BLEVE

*Cocchi, Giovanni**

At 1:44 pm of the 6th of August 2018, in the Bologna highway, in Borgo Panigale, a road tanker carrying LPG crashed onto an heavy good vehicle loaded with some tons of waste flammable liquid, that was still for a previous queue, igniting a major fire. Under the simultaneous action of fire and of the internal pressure, the tank collapsed abruptly, releasing the full inventory of LPG and producing a BLEVE. In the work we will expose the findings related to the pool fire that engulfed the LPG truck, the modeling of thermal transient in the tank that led to BLEVE and blast analysis. The work will show that the Bologna BLEVE is an LPG transportation accident whose development was rather typical and that provides a solid benchmark for modeling approaches that had been proposed in the technical literature, making it a valuable - real world-lesson on the forensic investigation and consequence modeling of BLEVE accidents.

50 Numerical Simulation of the effects of a muffler on shock sound mitigation

Sethu Venkataraman, Ashwath; Oran, Elaine*

The upcoming Detonation Research Test Facility (DRTF) consists of a large-scale detonation tube (DT), planned to be 200 m long and 2m in diameter. Unlike other large-scale detonation facilities, the DRTF will be located close to habitation. This means we need to develop sound mitigation strategies to keep the sound intensity within permissible limits. To this end, an idea was proposed to allow the high-pressure flow to expand in a large enclosed chamber, called the muffler, before being released into the atmosphere. This paper describes one step in developing a design for the muffler. Several design configurations are evaluated by numerically solving the two-dimensional (2D) and three-dimensional (3D), unsteady Euler equations. The resulting flow field and its implications for muffler design and discussed.

173 Experimental study on turbulent flame speed of H2-CO/air mixtures relevant to late phase accident scenario

Desclaux, Anthony; Idir, Mahmoud; Comandini, Andrea; Bleyer, Alexandre; BENTAIB, Ahmed; Chaumeix, Nabiha*

The aim of this work is to report new experimental results on the effect of turbulence on the propagation speed of H2-CO/air mixtures for conditions relevant to late phase accident scenario in a nuclear power plant. A spherical vessel has been used to investigate the effect of turbulence intensity on the behavior of H2-CO/air flame speed and the combustion pressure. The binary H2/CO (50/50) in the air content was between 11 and 15 %. The initial turbulence condition was varied from 0.31 to 1.05 m/s. Under non-turbulent conditions, the combustion was incomplete for the leanest mixtures. The turbulent burning speed increases with the turbulence level but the maximum combustion pressure remains constant. The evolution of the normalized turbulent burning speed has shown that the initial turbulence has a greater influence on the leanest conditions. The correlations developed for H2/air mixtures were not able to well reproduce the experimental results obtained for H2-CO mixtures in air.

Tuesday 9:00 – PL2

PL2 – Flame Acceleration and Deflagration to Detonation Transition in a Confined Geometry

Gaby Ciccarelli

Most industrial gaseous explosions involve the rapid acceleration of a flame ignited at a weak energy source. In the worst-case scenario, flame acceleration can lead to deflagration-to-detonation transition (DDT) resulting in catastrophic property damage and fatalities. In a laboratory setting, a channel equipped with obstructions is used to study flame acceleration and DDT. A review of the state-of-the-art in 2008 can be found in Ciccarelli and Dorofeev [1]. Flame acceleration is associated with an increasing volumetric burning rate that is governed by flame area enhancement. Key to flame acceleration is the expansion of the combustion products that leads to flow of the unburned gas ahead of the flame. In the earliest stage of flame acceleration, large-scale laminar flame folding occurs because of the unburned gas flow nonuniformity generated by the obstructions. As the flow velocity ahead of the flame increases, it leads to turbulence in the form of shear layers, boundary layers and larger recirculation zones behind the obstructions. Eventually compressibility effects become important and compression waves form ahead of the flame that eventually coalesce into a strong shock wave. The reflection of this shock off the boundaries produce reflected shock waves that interact with the flame leading to flame instabilities. At this stage, the combustion wave is referred to as a fast-flame, or choked-flame. Under certain conditions DDT occurs, generally because of shock reflection off an obstruction, producing a detonation wave that propagates at a velocity significantly below the Chapman-Jouguet (CJ) value. For a CJ detonation wave the velocity is governed by the mixture energetics, independent of reactivity; in an obstructed channel, the detonation velocity is governed primarily by the mixture reactivity and the boundary conditions. The present talk first provides a general background on detonation waves and outlines the current understanding of flame acceleration and DDT in obstructed channels. The mechanisms controlling flame acceleration, detonation initiation, and detonation propagation are outlined based on recent experimental results. The affect of detonation reaction-zone stability on the DDT run-up distance is discussed.

References

1. G. Ciccarelli and S. Dorofeev, Flame Acceleration and Transition to Detonation in Ducts, Progress in Combustion Science, 34(4): 499-550, 2008.

Tuesday 10:10 – Detonation Modelling II

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18 Uncertainty Quantification for the Real Gas Model of Steady Planar Detonation

*Weng, Z.; Mevel, Remy**

We studied the uncertainty on the induction distance of the steady planar detonation propagating in hydrogen/air mixture at elevated pressure. The real gas effect was incorporated by using the Peng-Robinson equation of state, along with its thermodynamic functions and reaction kinetic law. The uncertainty originates from the molecular attraction and covolume parameters in the real gas model. It was quantified using a Monte Carlo sampling approach. The uncertainty increases linearly with initial pressure and is mainly determined by

the contribution of the species with larger mole fraction weighted molecular attraction and covolume parameters. Compared to the uncertainty caused by the reaction mechanism, the real gas model uncertainty is negligible at low pressure, but becomes of the same order of magnitude at elevated pressure. The reaction model uncertainty still dominates the overall uncertainty of combustion simulation of steady detonation waves.

12 Detonation propagation in the inhomogeneous mixtures with periodic reactant concentration gradient

Wang, Yuan; Chen, Zheng*

One- and two-dimensional simulations are conducted for detonation propagation in a stoichiometric hydrogen/air with periodic sinusoidal or square wave distribution of the reactant concentration. It is found that there is a critical amplitude of the periodic mixture composition distribution, above which the detonation quenches. When the amplitude is below the critical value, detonation quenching and reinitiation occur alternatively in the inhomogeneous mixture. A double period of the leading shock pressure for 1D simulations and a double cellular structure consisting of substructures and a large-scale structure for 2D simulations are observed. The detonation reinitiation process and the formation of the double cellular structure are interpreted. The large-scale cell size is found to be linearly proportional to the wavelength. The averaged detonation speed decreases with both wavelength and amplitude. The unburned fuel left behind the detonation was used to interpret the speed deficit.

145 Unified Characteristic Relationships of Hydrogen-Oxygen-Argon Detonation Dynamics in Narrow Channels

Xiao, Qiang; Weng, Chunsheng*

Real gaseous detonations in narrow channels usually propagate in the presence of significant boundary layers, which notably diverge the flows in the trailing reaction zone and as a result lead to considerable velocity deficits. In order to seek a unified description of the macro-scale dynamics of detonations in narrow channels, the present work adopted the well-posed generalized ZND model with the boundary-layer-induced flow divergence for computing the weakly unstable $H_2/O_2/Ar$ detonation dynamics. Effects of both the characteristic channel width and the argon dilutions on detonation dynamics were demonstrated. Although the typical induction length fails to collapse the non-dimensional velocity-flow divergence relationships, the more realistic induction length, evaluated by considering the presence of losses, was found to be capable of very well unifying the dynamics of $H_2/O_2/Ar$ detonations in narrow channels, being independent of argon dilutions and channel dimensions.

57 Experimental analysis of cellular detonations: a discussion on regularity and three-dimensional patterns

Monnier, Vianney; Rodriguez, Vincent; Vidal, Pierre; Zitoun, Ratiba*

The cellular patterns on the surface of a detonation front in the $2H_2+O_2+2Ar$ mixture are analyzed from experimental head-on and wall soot recordings in square (Q), triangular (T) and round (R) cross-section tubes with the same area. The head-on patterns are irregular in the T and R tubes even when they are regular in the Q tube, and all are irregular regardless of the tube at sufficiently large initial pressures. Paradoxically, all wall patterns are regular even when the head-on patterns are not. The differences in the cell widths measured at walls from one section shape to another increase with decreasing initial pressure. The regular patterns at walls of Q tubes show a continuously-variable phase shift possibly due to long-wavelength and low-amplitude instabilities from ignition or multi-physics wall phenomena. These results question the relevance of the cell width and regularity as usually measured at walls and suggests now describing detonation cells as 3D objects.

245 Comparative Analysis of the ZND Detonation Structure in Hydrocarbon Fuels

Colby, Calvin; Ghosh, Abeetath; Dammati, Sai Sandeep; Poludnenko, Alexei*

A detailed analysis of the ZND solutions for four hydrocarbon fuels (n-dodecane, JP10, JetA2, and ethylene) is presented. These solutions are part of a detailed database of the ZND solutions for a wide range of traditional fuels obtained using state-of-the-art complex multistep chemical kinetics. For each of the fuels examined, we consider a range of equivalence ratios (ϕ = 0.5-1.0), preheat temperatures (T = 300-800 K), and initial pressures (P = 1 bar and 5 bar). The effects of these parameters on the ZND solutions are presented. Several key features of the steady-state detonation solutions are highlighted and discussed in detail, including strong induction zone endothermicity due to the heavy fuel pyrolysis, CO trapping in products, and variation of characteristic induction and exothermic pulse lengths. Finally, implications of these features for the detonation dynamics are discussed.

230 Two-Dimensional Detonations in Ethylene-Air Mixtures with Multi-Step Chemistry

Dammati, Sai Sandeep; Poludnenko, Alexei*

Recent years have seen an increasing interest in the use of ethylene as a fuel for gas-phase detonative combustion due to its high reactivity and excellent detonability. At the same time, to date, detailed numerical simulations describing the dynamics and structure of detonations in ethylene mixtures remain scarce. Here, we perform the first systematic study of detonation properties in ethylene/air mixtures using complex chemical kinetics in 2D channels with adiabatic walls. In particular, we study the near-limit behavior by varying the channel width and equivalence ratio from stoichiometric to lean.

Overall, we observe the formation of highly complex and irregular hierarchical detonation cell structure characteristic of unstable mixtures, which is produced by recurring failure-reignition events and associated formation of transverse detonations. Finally, we find that a minimum channel width is required for stable detonation propagation even in channels with lossless walls.

33 Fractal-based RANS Modeling of Darrieus--Landau and Thermal-diffusive Instability Effects on Lean Hydrogen Flames

Zivkovic, Dario; Sattelmayer, Thomas*

Darrieus-Landau instability is an essential driving mechanism behind the flame acceleration in conditions of low turbulence intensity. Such conditions are particularly relevant for explosion safety. One of the challenges of numerical modeling in that domain lies in large geometric scales of process- and nuclear facilities under consideration. Dealing with large scales severely hinders practical application of models that rely on resolving the flame structure for predicting the flame dynamics. In present work, a new, sub-grid, RANS model is introduced, based on a scale-adaptive, fractal-based closure, aimed at modeling the effects of the Darrieus-Landau and thermal-diffusive instabilities. Model validation was performed using lean hydrogen deflagration experiments at medium and large scales.

23 Investigation of the Scale Similarity Principle for Subgrid Modelling of the Reactive Richtmyer-Meshkov Instability

Bambauer, Maximilian; Hasslberger, Josef; Klein, Markus*

The Richtmyer-Meshkov instability (RMI) can contribute to flame acceleration and detonation in geometrically confined explosions. Direct numerical simulations (DNS) of hydrogen/air shock-flame interactions are performed to calculate the increase of flame wrinkling and integral reaction rate as caused by the reactive RMI. In lower resolved Large Eddy Simulations (LES), it is found that the modelling of the reactive source term can be greatly improved by applying corrections for the unburned gas quantities, the laminar flame speed and the subgrid flame wrinkling. The flame wrinkling can be extracted from the LES-data by applying a test filter, assuming scale similarity in the resolved flame wrinkling and the subgrid scales. The correction terms greatly improve the model prediction of the integral reaction rate, especially after the first and second shock-flame interaction, while larger deviations occur at later times.

159 Numerical Investigation of Fuel Feed Line Instabilities and its Effects in the Partially Premixed Swirling Flame

Nam, Jaehyun; Yoh, Jack J.*

Large eddy simulations (LES) of the partially premixed swirl flame in the model gas turbine combustor are performed. Simulations under acoustically forced and uniform inlet conditions are conducted to find the driving source of instabilities in the fuel feed line. The result shows that a low-frequency instability develops in the fuel feed line due to turbulence and vortices, which resonates with the inlet low-frequency forcing velocity. Flame transfer function (FTF) and related cold-flow transfer function (CTF) results show a noticeable peak of FTF/CTF gain in the low-frequency domain, which is similar to the naturally occurring instability frequency in a stable flow. These observations are in good agreement with previous experimental results. This work suggests that the coupling of fuel feed line instability with external oscillation causes high gain in FTF/CTF, which possibly leads to the development of combustion instability.

Tuesday 10:10 – Laminar Flame I

56 A Study on the Effect of Ethanol Addition on Laminar Flame Speed of a Four-Component Gasoline Surrogate at Elevated Pressure and Temperature

Almarzooq, Yousef; Petersen, Eric; Schoegl, Ingmar*

Laminar flame speeds of a four-component gasoline-surrogate and its mixture with ethanol are investigated using a heated, constant-volume vessel. The baseline fuel for the current study consisted of four components, namely, iso-octane, n-heptane, toluene, and 1-hexene. This baseline fuel was mixed with ethanol at 3 different percentages, 30%, 50%, and 85%. To assess the effect of ethanol addition, the baseline fuel (0% ethanol) was also investigated. Initial temperature of 335, 359, and 408 K and initial pressures of 1 and 3 bar were covered herein. The findings of this study are compared to results in the literature, which show good agreement for E0 but some deviation for the E30 blend. In general, the study showed an increase in laminar flame speed as the ethanol percentage increases in the mixture. Finally, the results are compared to an existing chemical kinetics model.

238 Experimental and numerical study on a gasoline surrogate mixture

Mghanen, Outmane; Chaumeix, Nabiha; Matrat, Mickael; Chevillard, Stephane; Obrecht, Nicolas*

The aim of the present work is to characterize the combustion of a gasoline surrogate mixture constituted of 79.57% mole fraction of Toluene and 20.43% mole fraction of 1-hexene. The first part is an experimental investigation of the the laminar flame speed of the surrogate fuel. The laminar flame speed was measured at an initial pressure of 1 bar and at 2 different initial temperatures of 375 and 475 Kelvin over a wide range of equivalence ratio. A detailed kinetic mechanism, from POLIMI, was used to simulated the flame speed for validation purposes. The mechanism was then used to derive a correlation that expresses

the variation of the laminar flame speed over a wide range of initial pressure and temperatures relevant to gasoline engines.

140 Chemiluminescence of Spherically Expanding Methane-Air Flames Doped with DMMP

Turner, Mattias; Parajuli, Pradeep; Kulatilaka, Waruna; Petersen, Eric*

Chemiluminescence spectra of atmospheric-pressure flames doped with dimethyl methylphosphonate (DMMP) were obtained using spherically expanding flames and compared to spectra obtained from undoped flames. The undoped parent flames were mixtures of methane-air. Spectra were recorded in the wavelength range from 200?800 nm and at three equivalence ratios (ϕ = 0.8, 1.0, 1.2). For all three ϕ, the intensity of the doped flame emission increased relative to the neat flames by over an order of magnitude, but no clear spectral features aside from a broad, featureless continuum could be identified. The observance of a continuum of emission for all the doped flames is attributed to PO2* chemiluminescence and blackbody emission, likely from high-temperature soot particles in the flame (the latter from condensed, phosphorus-containing combustion products). However, a unique, narrow chemiluminescence feature indicative of phosphorus combustion cannot be identified at this time.

Tuesday 11:50 – Laminar Flame II

255 Combustion characteristics of butane in a meso-scale burner with ordered porous media

*Chen, Xinjian; Li, Junwei**

In this study, ordered porous alumina is manufactured via additive manufacturing technology, and combustion characteristics are studied. The flame can be stabilized in the porous media even when the flow velocity is greater than the laminar flame speed. The uniform porous media can improve the wall temperature and the uniformity of the cross-sectional temperature. The enhanced heat transfer and radiant heat loss by the porous media reduce the temperature of the reaction zone, which reduces the NOx content in the exhaust gas, but causes the CO content to rise, and the combustion process needs to be further optimized.

168 Analysis of chemical-induced irreversibility in premixed counterflow CH4/CO/air flame

*Yu, Chien-Ru; Wu, Chih-Yung**

In the present study, the characteristics of chemical-induced irreversibility, as known as exergy loss, are discussed in the room temperature and atmosphere. The irreversibility caused by each chemical reaction can be found. In addition, an empirical formula was concluded. By this formula, the irreversibility caused by the chemical reaction can be evaluated easily. In conclusion, this study hopes to give biomass combustion a more comprehensive understanding and application.

217 Detonation structural response to multi-dimensional confinement

Crane, Jackson; Lipkowicz, Jonathan T.; Shi, Xian; Wlokas, Irenaeus; Kempf, Andreas; Wang, Hai*

3D detonation simulations solving compressible Navier-Stokes equations with detailed chemistry are performed in both square channel and tube geometries. The simulations are compared with each other and with 2D channel simulations and tube experiments of identical mixture and conditions (stoichiometric hydrogen oxygen with 3000 PPMv ozone at 300 K and 15 kPa) with the goal of understanding the effect of confinement on detonation structure. Results show detonation structural features can be dramatically affected by confinement: a highly regular pattern emerges in the square channel, while the tube simulation exhibits a seemingly more chaotic pattern similar to that measured from the tube experiment. Two types of detonation kernels are observed in 3D simulations, a point (or disc in tubes) kernel from 3-4 waves collapsing, and a line kernel from 2 waves collapsing. Analysis of kernel dynamics explain the structural differences observed in different geometries.

151 Dynamics and Properties of 2D vs. 3D Ethylene-Air Detonations

Dammati, Sai Sandeep; Poludnenko, Alexei; Xu, Rui; Shi, Xian; Wang, Hai*

Study of detonation dynamics in hydrocarbon fuels is crucial for the design and development of detonation-based engines, accident prevention in industrial settings, and development of accurate chemistry models. Ethylene is characterized by high reactivity and hence high detonability making it the fuel of choice in many detonation systems. We present the first comparison of ethylene/air detonations modelled using multi-step chemistry in 2D and 3D channels with realistic no-slip, isothermal boundaries. We find that 2D detonations are highly unstable with a complex front structure and a hierarchy of detonation cell sizes, which has been previously found in other unstable mixtures. In contrast, the 3D case does not exhibit such dynamics and is more stable despite wall losses, with cells having much more uniform sizes. Our results indicate that in unstable mixtures, such as ethylene/air, 2D models may not be representative of the actual detonation dynamics in realistic 3D channels.

94 Numerical Analysis on Ammonia / Hydrogen / Air Detonation Using Detailed Chemical Reaction model

Inoue, Go; Tsuboi, Nobuyuki; Ozawa, Kohei; Hayashi, A. Koichi*

In recent years, global warming has become a serious problem, and carbon-free fuels that do not emit carbon dioxide during combustion are attracting attention. Among them, ammonia is expected as a next-generation fuel because

it has excellent transportability and storability. The purpose of this study was to clarify the detonation characteristics of ammonia in order to use it safely as a fuel. Specifically, the effect of co-firing ammonia and hydrogen on the detonation characteristics was evaluated.

As a result of this study, it is found that the decomposition reaction of ammonia is promoted by co-firing with hydrogen. It is also found that the NH2 formation reaction was promoted as the hydrogen mixing ratio was increased, and as a result, the NO production amount was found to decrease.

Tuesday 11:50 – Detonation Diffraction

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101 Numerical Study on Re-Initiation of Detonation Propagating through Double Slits in a Planar Channel

*Jun, Daeyoung; Lee, Bok Jik**

For the safety of flammable gas transports and handling, suppressing the detonation wave is an important demand for the industry related to flammable gas handling. In particular, one way of detonation quenching is diffraction. Sudden expansions during the detonation propagation decrease the temperature and contribute to reducing reaction rates and separating the shock wave and reaction front. In the present study, numerical simulations on a stoichiometric hydrogen-oxygen detonation re-initiation process of planar channels with double slits were performed to examine the diffracted shock-shock re-initiation process in detail. Shock-shock re-initiations were demonstrated by the CFD solution.

192 Simplified Numerical Simulation of Gaseous Quasi-Detonation Diffraction from a Rough Walled Channel

Yan, Chian; Sun, Xuxu; Mi, XiaoCheng; Ng, Hoi Dick*

In this study, two-dimensional numerical simulations using the reactive Euler equations with a two-step induction-reaction chemical kinetics are performed to investigate the propagation and diffraction of quasi-detonation. In the present simplified numerical simulations, the quasi-detonation is generated in a rough-walled channel with relatively small obstacles. The velocity deficit and also a highly irregular cellular pattern for quasi-detonation are observed. For the quasi-detonation diffraction at the sub-critical condition of the CJ detonation case in a smooth channel, despite the additional velocity deficit of the leading detonation front, the increasingly higher inherent cellular instabilities of the quasi-detonation in rough walled geometry appear to promote the transmission or re-initiation of the detonation downstream in the open area.

246 Data-driven Modeling of Reflection Point Distance Relevant to Diffracting Detonation Wave by Using Machine Learning

Kawasaki, Akira*; Hasegawa, Hiroki; Sun, Han; Watanabe, Hiroaki; Itouyama, Noboru; Matsuoka, Ken; Kasahara, Jiro; Matsuo, Akiko; Funaki, Ikkoh

A predictive model of the reflection point distance, which is a characteristic length scale relevant to detonation diffraction, was constructed and evaluated based on an existing experimental dataset for familiar gaseous fuels. The model was a statistical model obtained by a data-driven approach utilizing methods of machine learning, in which the reflection point distance was a function of thermodynamic and chemical parameters of fuel-oxidizer mixtures. A multilayer, totally coupled neural network was particularly chosen as the learning model. As a result, we obtained the following conclusions: The obtained model exhibits a good regression performance; the model well acquired typical dependencies of the reflection point distance on the initial pressure, equivalence ratio, and dilution ratio. The obtained model also exhibits a good prediction performance; the model well predicted reflection point distances unknown for the model. This suggests that the model has been well generalized.

Tuesday 11:50 – Stability II

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213 Oxygen Enrichment Effect on the Stability of Turbulent Diffusion Biogas Flames

*Fabbro, Sean; Tkach, Martin; Birouk, Madjid**

This paper presents an experimental study of oxygen enrichment of a swirling co-airflow on the stability limits of non-premixed biogas flames. Additionally, two distinct swirling methods were tested while keeping same the rest of burner geometry and test conditions. The composition of the biogas is also kept constant at 40% CO_2 and 60% CH_4 by volume. The results showed that the axially swirling co-airflow has much wider stability limits than the tangential. More importantly, oxygen enrichment of the co-airflow is found to significantly improve the stability limits of biogas flames. However, the extent of this improvement is much significant at fuel lean conditions (lower stability limit).

11 Multiple steady state solutions for a flame stabilized behind a highly conductive bluff body

Kurdyumov, Vadim N; Jimenez, Carmen*

We present an investigation of the stabilization of premixed laminar flames by means of an isolated highly conductive bluff-body, a circular cylinder, placed in a uniform flow of a combustible mixture. It is shown that for certain values of the parameters the problem has multiple steady-state solutions. Moreover, we solve the time-dependent equations to check the stability of these solutions and we show that at least two stationary states are stable. One of these solutions corresponds to a relatively cold cylinder and one to a cylinder at high temperature, close to the flame adiabatic temperature.

104 Active Direction Control in Rotating Detonation Combustor

Sheng, Zhaohua; Cheng, Miao; Shen, Dawen; Wu, Kevin; Wang, Jian-Ping*

Directing the detonation wave is necessary for the integration of rotating detonation engine and turbine when applying rotating detonation engine to aero-engine. However, the propagating direction of rotating detonation waves is still uncertain in both experimental tests and numerical simulations. In this research, an active direction control method is presented, which can regulate the direction of rotating detonation wave during engine operating. A 9-species, 19-step hydrogen/air chemical reaction mechanism is used to solve Euler equation with chemical reaction source terms. And three-dimensional numerical simulation of a rotating detonation chamber equipped with a pre-detonator is carried out to demonstrate the direction control method.

190 Experimental study on the aluminum powder rotating detonation engine

Xu, Han; Weng, Chunsheng; Zheng, Quan*

The operation of the Aluminum/Air RDE (rotating detonation engine) is experimentally realized. Conducted at the same equivalence ratio of 1, the detonation characteristics and the propulsion performance of the Aluminum/Air RDE are compared with that of the Hydrogen/Air RDE. It is found that the Aluminum/Air RDE could generate a higher thrust than the Hydrogen/Air RDE; the detonation intensity of the Aluminum/Air is higher than that of the Hydrogen/Air; the detonation velocity of the Aluminum/Air is lower than that of the Hydrogen/Air; the detonation propagation mode of the Aluminum/Air is the same with that of the Hydrogen/Air: single wave mode. The experimental results could provide a feasible solution for the air breathing aluminum powder RDE and establish a foundation for the solid powder RDEs.

207 Numerical Investigation of the Effect of Ozone Addition on Detonation in the Two-dimensional RDE Chamber

Tanaka, Raimu; Matsuo, Akiko; Shima, Eiji; Watanabe, Hiroaki; Kawasaki, Akira; Matsuoka, Ken; Kasahara, Jiro*

To put the Rotating Detonation Engine (RDE) to practical use, the study of the limits and stability of detonation actively researched. Recently, ozone addition is attracting attention as a means of improving the stability of detonation and extending its limits, and the investigation of the ozonated detonation targeting a wide range of unburned mixture conditions and realistic systems are awaited. In this paper, to investigate the effect of ozone on detonation in the RDE chamber, we performed the numerical simulation focus on the circumferentially

deployed 2D RDE chamber. The results suggested that the ozone addition cause the high-pressure region to stay lower on the bottom and ozone has the potential to increase the detonation propagation velocity in the RDE chamber. This indicates that combustion is completed closer to the bottom via the ozone addition, and ozone can be expected to improve the velocity deficits and achieve more stable propagation.

224 Effects of mixing level and temperature of injection in rotating detonative combustion

*Wang, Chun; Yao, Kepeng; Teng, Honghui; Wang, Yang; Tian, Cheng**

Numerical simulations with detailed chemistry are conducted for two-dimensional rotating detonative combustion with separate injection of fuel and oxidant. The influence of stagnation temperature and mixing level of hydrogen and air in the propagation of rotating detonation waves in combustor are investigated. Higher stagnation temperature make rotating detonation wave propagation mode transfers from single wave mode to the multiple wave mode and lower mixing level leads to the disappearance of detonation wave. The coupled effects of stagnation temperature and mixing level are investigated. With the higher stagnation temperature, the RDWs can be reestablished, but the RDWs still disappear if the mixing is too bad.

Tuesday 14:35 – Detonation Structure IV

120 An Investigation of the Detonation Jetting Phenomenon

Hytovick, Rachel; Burke, Robert F; Rezzag, Taha; Ahmed, Kareem*

The current work aims to explore the dynamics of an unsteady detonation front. Transverse waves, mach stems, and triple points are commonly examined as large features responsible for detonation propagation. However, it has become evident that there are local instabilities and features to be considered as well. Among those, lie the detonation jetting phenomenon. Generally referred to as the coalescence of transverse waves, these jets produce local areas with large heat release that significantly contribute to detonation propagation. This experiment examines the localized jetting phenomenon in both gaseous hydrogen and liquid hydrocarbon fuels. The work seeks to attain insight into these largely theoretical instabilities to further understand the jet fuel detonation process via ultra-high-speed optical diagnostics and pressure measurements.

232 Forward Jetting Phenomenon in Detonations

Meagher, Patrick A; Shi, Xian; Crane, Jackson; Zhao, Xinyu; Poludnenko, Alexei; Wang, Hai*

The present study aims to study the jetting phenomenon and its dependence on mixture properties. To this end, we first present a novel approach for creating experimentally viable mixtures where global activation energy can be controlled independently of other mixture parameters, notably the ratio of specific heats γ. Two hydrogen-oxygen mixtures with equivalent global activation energy, but low and high γ values, are designed within this framework. Two-dimensional Navier-Stokes simulations of cellular detonations for the above two cases are performed. Simulations employ detailed thermodynamic, chemical kinetic, and molecular transport models to capture the real physics to the best of current capabilities. We corroborate previous findings using idealized mixtures, with higher γ values reducing the frequency of Mach stem bifurcations. Finally, we show that forward jetting is ubiquitous to all mixtures and suggest a definition independent of Mach stem bifurcation.

205 Experimental Research on The Biogas - Oxygen Mixture Detonation Cell Size

*Siatkowski, Stanislaw; Wacko, Krzysztof; Kindracki, Jan**

Interest in alternative and renewable energy sources has risen significantly in recent years. Biogas is a prime example of a promising, alternative fuel. It is easily storable and as such is a more reliable and stable source of energy than weather dependent solar and wind sources. The authors report experimental results of cell size measurements done for a number of different biogas-oxygen mixtures compositions, equivalence ratios (0.5÷1.5) and initial pressures (0.6÷1.6 bar). The soot foil technique was used to determine the width of the detonation cells. The conducted experiments and subsequent analysis confirm that both the increase in the initial pressure of the mixture or move away from stoichiometric composition is accompanied by a decrease in the detonation cell size. The authors also argue that due to the unstable cellular structure of the detonation, it is insufficient to report only the average cell size.

222 On Cellular Multiplicity of Detonations in Confined Channels

Shi, Xian; Meagher, Patrick A; Crane, Jackson; Dammati, Sai Sandeep; Zhao, Xinyu; Poludnenko, Alexei; Wang, Hai*

Detonation cellular multiplicity was observed in hydrogen/oxygen detonation simulations in two-dimensional narrow channels. Several stable cellular detonations were achieved in simulations of identical mixtures but with different initial conditions. These differing structures are physically possible through variations of local expanding wave dynamics, with larger detonation cells resulting from stronger and longer-lived local expanding waves. This observation challenges the traditional notion of a unique cell size for a given mixture, and indicates that detonation cellular structures are a result of both the mixture properties and the properties of its confining geometry, boundary conditions, and propagation histories. Cellular multiplicity also provides an alternative explanation to cellular regularity, as for any mixture there may exist multiple possible cellular structures which result in cells of varying sizes under the influence of specific boundary conditions.

244 Shock interaction at Mach 4 of a water and fuel droplet

Virot, Florent; Rullier, Jean-Luc; H,bert, David*

Experiments on the interaction between a drop and a shock wave propagating in air at Mach 4 were carried out using a detonation driven shock tube. Water droplet of 430µm to 850µm diameter were tracked over long duration i.e. for times adimensioned by the Rayleigh time up to T=9. Thus, a sequence of high resolution images of the droplet atomization shows the evolution of the surrounding mist until its almost disappearance. Besides, droplet positions and bow shock distances to the droplet can be grouped in dimensionless space. Finally, preliminary tests with a low-vapor fuel were done.

28 High-fidelity Simulations of Liquid-gas Colliding Jets Impacted by a Detonation Wave

Bielawski, Ral J; Prakash, Supraj; Raman, Venkat*

In order to use detonation-based propulsion devices, it is necessary to understand the role of detonations interacting with liquid droplets. In particular, the reaction structure introduced by this multiphase system will determine the detonation propagation characteristics and strength. Due to the presence of multiple phases and extreme pressure/temperature conditions, numerical simulations remain the best approach to gaining fundamental insight. Here, detailed simulations of a rocket-propellant oxygen liquid-jet/gaseous-oxidizer-jet system interacting with a detonation wave are conducted. The focus here is to conduct injection-focused simulations with the goal of understanding detonation propagation over spatially inhomogeneous fuel-air mixtures. A single injection element of a model RDE configuration is used here. The impact of the detonation wave characteristics that impinge on the droplet-laden flow is studied.

96 A Computational Model for Single Iron Particle Combustion in Liquid-Phase

Fujinawa, Aki; Mi, XiaoCheng; Jean-Philyppe, Joel; Bergthorson, Jeffrey*

The current work presents a quantitative model for the liquid-phase combustion of a single fine iron particle. A zero-dimensional numerical model is developed based on the assumption of fast internal kinetics, such that the combustion rate is limited by the rate of external oxygen (O2) transport. The model considers a mixed droplet of liquid-phase iron (Fe) and liquid-phase wüstite (FeO). The gas-phase transport of O2 and evaporated Fe and FeO, governed by diffusion and Stefan flow transport, is resolved with a nonlinear solver. The outward gas-phase Fe and FeO consume inwards transported oxygen to stoichiometrically oxidize into FeO and magnetite (Fe3O4), and the remaining oxygen that reaches the particle surface is entirely consumed to form liquid-phase FeO. The time

history of simulated particle temperature is compared against experimental results in ambient air. Possible sources of error are discussed.

97 On the Critical Conditions for Thermal Runaway of Fine Iron Particles

Mi, XiaoCheng; Fujinawa, Aki; Bergthorson, Jeffrey*

Ignition of iron particles in an oxidizing environment marks the onset of a self-sustained combustion. The objective of the current study is to quantitatively examine the ignition characteristics of fine iron particles (i.e., 1- to 100-micron-sized) governed by the kinetics of solid-phase iron oxidation. The oxidation rates are inversely proportional to the thickness of the oxide layer (i.e., following a parabolic rate law) and calibrated using the experimentally measured growth of iron-oxide layers over time. Unsteady ignition analysis has been performed to probe the dependence of the critical gas temperature required to trigger a thermal runaway (namely, the ignition temperature) on particle size, inert gas species, and the collective heating effect in a suspension of particles.

Tuesday 14:35 – Laminar Flame III

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183 Experimental Study of Early-Stage Dynamics of the Ascending and Descending Laminar Hydrogen-Air Flames in Vertical Closed Rectangular Tube

Anikin, Nikolay B; Kirillov, Igor A*

The upward ultra-lean hydrogen-air flames were studied in a vertical rectangular tube using high fidelity schlieren video system under normal temperature and pressure at MUT facility. In order to close a gap in the ultra-lean flame classification a systematic recording of the complete changes of combustion appearance in response to gradual changes in mixture stoichiometry (from 4 to 16 vol.% H_2, with an increment down to 0.2 vol.% H_2 nearby some equivalence ratios) was made. Three basic morphological patterns of the ultra-lean quasi-isobaric hydrogen-air combustion – “raspberry-like”, “vortex-like”, “cellular (or wrinkled)”, and one transient pattern – “mushroom-like” - have been delineated. Each of the detected flame morphotype exists and is stably reproduced within the appropriate concentration limits.

152 Laminar Burning Velocity and Adiabatic Flame Temperature of Biogas/Air Mixture at various CO_2 Concentrations

Ghabi, Ahlem; Boushaki, Toufik; Escot Boucanegra, Pablo ; Robert, Eric; SARH, Brahim*

This paper reports some results about characteristics of methane (CH_4)-carbon dioxide (CO_2)-air combustion. Laminar burning velocities have been numerically calculated using CANTERA software by one-dimensional steady code with several chemical kinetic mechanisms as GRI-Mech3.0, San Diego, Blanquart et al and Aramco 1.3, and compared to some experimental results from the literature. The laminar burning velocity and the adiabatic temperature of CH_4-CO_2/Air combustion were calculated with CO_2 concentration ranging from 0 to 50 percent in the mixture. The equivalence ratio was varied from 0.4 to 1.4, the initial pressure was set at 1 bar, and the temperature was set to 300 K. Results show that calculations with Blanquart et al mechanism show the best agreement with results from the literature and that the CO_2 addition in biogas mixture leads to a decrease of laminar burning velocity and flame temperature.

144 Flame-Acoustics Interaction of Flames Propagating in a Narrow Duct: Effect of Heat Losses and Lewis Number

Jimenez, Carmen; Kurdyumov, Vadim N*

We study numerically the effect of the wall thermal properties and the Lewis number on the flame-acoustics interaction, for flames propagating from the open to the closed end of a narrow planar channel. We know from previous studies that symmetric and non-symmetric flames present different responses to acoustic forcing. Results of the present study show that heat losses and the Lewis number affect the shape of the flame, and as a consequence the flame-acoustics interaction: increasing the heat losses tends to make the flames symmetric, but very low Lewis numbers result in non-symmetric shapes.

48 Evolution of Acoustic Waves in High-Pressure Compressible Counterflow Diffusion Flames

Arumapperuma, Geveen; Yao, Matthew X; Hickey, Jean-Pierre; Han, Wang*

This study numerically investigates acoustics in a hydrogen-air counterflow diffusion flame at high pressure conditions. A fully compressible reacting flow solver is employed to simulate the flame under a temporally and spatially evolving pressure field. Under the assumption of fully reflecting boundary conditions, for all tested pressures (1-60 bar) a growth in the acoustics can be observed, where the acoustic perturbations grow with time indicating a coupling between the heat release rate and the acoustic field. The growth rate of the acoustics is found to be significantly larger at 5 bar than at 1 bar. However, above 5 bar, the growth rate saturates, where the growth rate of the acoustics marginally increase with pressure. Spectral analysis showed the pressure perturbations on the fuel side to be more periodic compared to the oxidizer side. The periodicity is found to reduce as the pressure increased where more complex acoustics with multiple frequencies start to develop.

Tuesday 16:40 – Multiphase II

214 Mixture Distribution of Solid-Gas-Two-Phase Flow for Gaseous Detonation with Aluminum particles

Shimizu, Ryunosuke; Mizukaki, Toshiharu*

If a detonation wave can be generated using metal particles as fuel in a carbon dioxide atmosphere, it can be developed into a propulsion device that can operate even in an atmosphere containing carbon dioxide as a main component such as Mars. In this study, the effect of ethylene as an additive on reducing the DDT length of aluminum-oxygen mixture detonation was investigated as a preliminary experiment of detonation generation using aluminum-carbon dioxide. When ethylene was added to a mixture of aluminum and oxygen at a ratio of 50%, the DDT distance became shorter than 250 mm. When the aluminum particle size decreased, the peak pressure decreased because of condensation. Based on the experimental results, the experimental section was extended, and an apparatus to disperse the particles was planned for the experimental setup. The experimental results using the improved experimental system will be reported at the conference.

270 Morphology-Independent Measurement of Iron Particle Burn Time

Ning, Daoguan; Shoshin, Yuri; Van Oijen, Jeroen A.; Finotello, Giulia; de Goey, Philip*

Iron powders is one of promising energy carriers for the “metal fuel cycle”, in which metal powder is combusted and the produced oxides are reduced back to iron using clean energy. In order to successfully apply metal powders as alternative clean fuels, fundamental properties of single particles need to be studied. One of the important parameter of single particle combustion is the particle burn time, which can be used to evaluate the combustion regime (diffusion-controlled v.s. kinetic-controlled) and validate numerical models. The morphology of iron particles used in different experiments may vary significantly (see Fig.2), which leads to a large uncertainty in the measured burn time as a function of the initial particle diameter. Therefore, morphology-independent measurement of iron particle burn time is required. In this work, an experimental method is proposed to measure the morphology-independent particle burn time of iron particles.

Tuesday 16:40 – Detonation Interface Interaction

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226 Detonation Propagation in a Layer Laterally Confined by Combustion Products

Cheevers, Kevin; Raut, Mihir; Lalchandani, Sarthak A; Hong, Zekai; Radulescu, Matei*

The structure of detonations as found in Rotating Detonation Engines (RDE) consists of a detonation propagating through a thin layer of reactive gas, weakly confined by combustion products from previous cycles. The current study proposes a novel experimental method to visualize the structure of a detonation propagating through a thin reactive channel weakly confined by its own products, analogous to an RDE. A flame is initiated in the centre of a long rectangular cross-sectioned shock tube, which propagates faster towards the extremities of the shock tube due to preferential convection. The flattening flame then forms a thin reactive channel of unburnt gas at the bottom of the tube, through which a detonation initiated at a tube extremity will propagate. High-speed direct luminescence visualization and Schlieren visualization is used to study the evolution of the system.

249 Detonation propagation in a semi-confined mixture with a diffuse interface

*McLoughlin, Michael; Yousefi Asli, Vahid; Ciccarelli, Gabriel**

An experimental study was carried out to investigate detonation propagation in a buoyancy driven layer of hydrogen-oxygen over an inert gas. The layer was generated in a 12.7 mm wide horizontal channel by opening a sliding door that initially separated the hydrogen-oxygen from either argon or nitrogen. A CJ detonation interacted with the layer at different stages in the layer development. Schlieren video and soot foils were used to measure the extent of detonation propagation through the layer. It was shown that detonation propagation through the layer is self-limiting due to over-mixing at the layer leading edge driven by mass transport of the surrounding inert gas. Inert gas dilution of the layer, predicted by 3D simulations including viscosity and multicomponent mass diffusion effects, was used to show that the detonation failure criterion proposed by Bauwens-Dorofeev successfully predicts the extent of detonation propagation in the layer.

242 Interaction of Detonation Waves with Turbulent Layers

*Marjaba, Bernard; Fazal, Hania; Kiyanda, Charles B**

A turbulent reactive mixture is achieved in a square cross-section detonation tube. The extent of turbulence is controlled through the injection process and the dynamics of a detonation wave, travelling through the turbulent medium, is observed by high-speed schlieren videography. The pre-detonation pressure is varied, and it is found that at low pressures (and thus comparatively larger cells), the turbulence enhances the wave's propagation. At higher pressures, however (and thus at comparatively smaller cells), the turbulence has a detrimental effect on the propagation of the wave and acts as a further loss, ultimately creating a larger velocity decrement. Further, the effect of turbulence is short-lived for detonations propagating in low-pressure medium, whereas its effect survives well outside the expected turbulent region for higher pre-detonation pressures. The mixture will be varied in order to examine the effect of turbulence in stable vs. unstable mixtures.

Tuesday 16:40 – RDE V

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70 An Explanatory Model for the Multi-Wave Dynamics in Rotating Detonation Engines

Whitman, Charles R; Mi, XiaoCheng; Higgins, Andrew; Kiyanda, Charles*

A series of numerical simulations of the Rotating Detonation Engine (RDE) were performed, varying the engine perimeter and plenum temperature. These simulations were used to identify the mode of operation - the presence of one or more co-rotating waves, counter-rotating waves, or failure to sustain a detonation. In order to explain the observations, an explanatory model is developed. The model consists of two criteria. The induction time criterion predicts that a given co-rotating mode will be unachievable if the time between passages of a detonation wave is greater than the time taken by an injected fluid element to complete its induction period. The critical-layer thickness criterion predicts that a given co-rotating mode will likewise be unachievable if the time between detonation wave passages is shorter than the time taken for the column of injected fluid to surpass the critical-layer thickness. The predictions are presented and compared with the result of the simulations.

160 Acceleration of Burned Gas to Supersonic in a Throat-less Rotating Detonation Engine

Nakata, Kotaro; Ota, Kosei; Ito, Shiro; Ishihara, Kazuki; Goto, Keisuke; Itouyama, Noboru; Watanabe, Hiroaki; Kawasaki, Akira; Matsuoka, Ken; Kasahara, Jiro; Matsuo, Akiko; Funaki, Ikkoh; Higashino, Kazuyuki; Braun, James; Meyer, Terrence; Paniagua, Guillermo*

Acceleration of the subsonic gas without converging section via heat addition was focused on in this study. Detonation combustion with a short combustion completion distance was applied to investigate the possibility of acceleration. An RDE with an inlet diameter of 20 mm, an axial length of 70 or 35 mm, and a diverging angle of 5 or 10 deg was designed and tested. In addition to the pressure and thrust measurement, normal-speed imaging for the exhaust plume was conducted. The results suggested that the exhaust flow of the RDEs was supersonic for a 70-mm type. The speed of the exhaust flow of a 35-mm type was estimated to be above Mach 1. This result indicates the validity of the quasi-1-D flow model presented in the previous study. Furthermore, the supersonic exhaust with a larger Mach number from a 10-deg type suggested that the diverging angle of the channel has a limited effect on the length of the heat release region in the range from 5 to 10 deg.

13 Propagation of Gaseous Detonations in High Aspect Ratio Planar Curved Channels

Fotia, Matthew L; Hoke, John; Hencel, Regan J; Schumaker, Alex*

Propagation of gaseous detonations through a planar curved channel has practical engineering applications including the study of fundamental combustion initiation, investigating failure mechanisms that prevent stable propagation of detonations, and aiding in the design of rotating detonation engines (RDEs). The lack of laboratory experiments on a scale relevant to an air breathing rotating detonation combustor provide an opportunity for this work to further the general understanding of these configurations. Presented is the relationship between the inner/outer radii and the reactant mixture. The goal of this work is to outline the geometric requirements and detonation cell scales that promote a stable propagating detonation wave, with minimal velocity deficit and/or no extinction of the wave as it transits the test section. Successful design of a detonation driven combustor is dependent on understanding how the detonation wave and the geometry of the combustor interact with one another.

Tuesday 16:40 – Laminar Flame IV

9 Early Stages of Flame Dynamics in Tubes and Mechanism of Tulip Flame Formation

Liberman, Michael A.; Qian, Chengeng; Wang, Cheng*

The dynamics of flames propagating in tubes and the formation of a tulip flame was investigated for closed and semi-open tubes by solving the fully compressible reactive Navier-Stokes equations with a one-step Arrhenius model for H2/air and CH4/air mixtures. The development of tulip hydrogen/air flame obtained in simulations with a one-step model was compared with simulations using a detailed chemical model. It is shown that the inversion of the flame front and the onset of the tulip flame occurs due to rarefaction waves generated by the decelerating flame when its surface is reduced due to extinguishing of the rear parts of the flame skirt at the sidewalls. The rarefaction waves reduce velocities in the unburned gas flow and cause the inversion of the flame front. The formation of a tulip flame is a pure gas-dynamical phenomenon, where which in agreement with the recent experimental studies does not involve the flame instabilities, or vortex motion.

162 CFD Modeling of Pressurized Laminar Coflow (Non-Premixed) Diffusion Flames with Water Addition

Girodon, Hugo; Dunn-Rankin, Derek; Chien, Yu-Chien*

This research aims to examine the effect of water vapor addition to pressurized flames by computation. It is a continuation of a series of experiments and numerical simulations focused on the addition of very high levels of water vapor to the fuel of diffusion flames. The motivation of this research is to understand the limitation especially the uncertainty regarding the role of water as a diluent. The current work extends the prior research and study on the effect of water addition to the fuel side of a laminar coflow diffusion flame under different pressures, and identifies whether water addition changes chemical reactions. The current results show that the peak temperature of the water diluted flames reduces and the flames even lift with water concentration increase. The pressure influence is to elongate the flame and thin the reaction zone. In general, the flame responds more to water addition than to pressure, and the flame behaves similarly with water addition at all pressures.

158 A Level-Set Transport Equation for Tracking Self-Ignition Fronts in Hydrogen-Air Mixture

*Siddappa, Chethan; Bouali, Zakaria; Robin, Vincent**

The increase of the use of hydrogen in association with conventional fuels in combustion systems may lead to unexpected physical mechanisms as self-ignition front propagation. The self-ignition and flame propagation interactions taking place in these highly heterogeneous mixtures may be responsible for local flame accelerations or even for the destruction of the practical device. The objective of this work is to develop and validate a new model dealing with transitions from self-ignition to laminar flame propagation. This abstract focuses on the validation using DNS of the most original proposition of this strategy: a level-set transport equation to track the propagation of self-ignition fronts. Eventually, the results highlight the relevance of the level-set approach proposed to track the self-ignition fronts in the presence of a significant diffusion process. The resulting field also yields a clear identification of the transition between self-ignition and laminar flame propagation.

Wednesday 9:00 – PL3

PL3 Including Detailed Chemical Properties in the Modeling of Emerging Turbulent Combustion Systems

Benoît Fiorina

Hydrocarbon combustion, involved in more than 90% of the worldwide primary energy consumption, produces most anthropogenic CO2 emissions [1]. Electrification will not entirely replace combustion in the short term for two main reasons: first, batteries exhibit an energy density about 50-100 lower than hydrocarbon fuels. Combustion will, therefore, still be required to power long-distance transport vehicles, such as boats, trucks, or aircraft. Second, many industrial sectors, such as steel, cement, glass, and aluminum, require high temperature (more than 500°C) heat sources that can hardly be delivered without a combustion process.

Developing and optimizing new energy systems that integrate carbon-neutral fuels such as biofuels, efuel, hydrogen or ammonia constitutes a relevant energy scenario to limit global warming. However, sustainable fuels still produce pollutants, in particular NOx. To reduce pollutant emissions, the strategy of combustion engineers is to decrease the temperature of flames by increasing the air-to-fuel ratio. The problem with lean flames is that they are prone to instabilities and extinction, thus causing essential safety issues and mechanical damage [2]. The challenge is to ensure flame stability and minimize pollutant formation by possibly implementing new adapted devices. Combustion engineers need reliable numerical tools for designing future combustion chambers. Advanced modeling of combustion phenomena is required for optimizing the injection system, the combustion chamber geometry, the wall heat transfers but also the pollutant formation. Simulations are also needed to challenge solutions to stabilize low-temperature flames.

The scientific challenges are to model the complex interactions between combustion chemistry and the turbulence of the flow at an affordable computational cost, compatible with industrial constraints [3]. The first difficulty is that the kinetics of combustion involves hundreds of chemical species that react through thousands of elementary reactions. To save computing time, the detailed mechanisms that describe this complex chemistry are reduced before being used in CFD codes. The second issue is related to the modeling of the turbulence / chemistry coupling which is not fully resolved in simulations.

This presentation aims to establish a brief state-of-the-art of both kinetic reduction methods and turbulent combustion models suitable for simulating emerging combustion technologies. The discussion focuses on large eddy simulation (LES) formalism, especially relevant to capture unsteady interactions between chemistry and turbulence. As an illustrative example, the presentation will end by showing recent simulations of plasma-assisted combustion, an emerging solution to enhance low-temperature flames. The importance of complex chemistry effects on flame stabilization mechanisms are highlighted.

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Wednesday 10:10 – Flame Dynamics & Stability

216 Isotope Effect on the Characteristics of the Flame-Ball-to-Deflagration Transition in Ultra-Lean Hydrogen- and Deuterium-Air Mixtures in Horizontal Hele-Shaw Cell

Kirillov, Igor A; Denisenko, Valery; Plaksin, Vadim; Melikhov, Anatoly*

It was experimentally revealed in horizontal Hele-Shaw cell that the Flame-Ball-to-Deflagration-Transition (FBDT) characteristics in deuterium-air gas mixtures are simbat to the hydrogen-air characteristics with appropriate regular bias on stoichiometry scale. Observed shift in the critical values of initial H_2 and D_2 concentrations is similar to the shift of the concentration limits for downward propagation of the hydrogen and deuterium deflagration flames, revealed by Koroll and Kumar. The following FBDT characteristics were recorded and measured. Qualitative characteristics - 1) macroscopic morphotypes of the ultra-lean flames, 2) microscopic elementary building constituents - drifting flame balls, 3) critical morphological phenomena, governing the mechanism of the FBDT. Quantitative ones: 1) concentration ranges for morphotypes and constituents, 2) dependencies of the fractal dimension of the product-reagents interface and combustion incompleteness upon initial stoichiometry.

264 A Tsuji Burner in a Counterflow

Li, Brandon; Sanchez, Antonio L; Williams, Forman*

This paper addresses the aerodynamics of a new type of Tsuji burner involving a cylindrical porous fuel injector of radius a placed at the center of a planar air counterflow configuration with strain rate A_∞, with specific attention given to flows with large values of the Reynolds number $A_\infty a^2/\nu$, where ν represents the air kinematic viscosity. For cases in which the fuel-injection velocity U_i is comparable to the characteristic counterflow velocity A_∞ a, the boundary layer is blown off from the cylinder surface, so that the flame is embedded in the thin twin mixing layers that form about the stream surfaces separating the outer air stream from the fuel stream.

221 Scaling Laws for Velocity Dynamics of the Ultra-Lean Hydrogen-Air Flames Expanding in Horizontal Cylindrical Hele-Shaw Cell

Moskalev, Pavel V; Denisenko, Valery; Kirillov, Igor A*

Using the method of frame-by-frame difference projection, we investigated the dynamics of ultra-lean hydrogen-air flames expanding in a horizontal cylindrical Hele-Shaw cell. To quantitatively estimate the dependencies of the averaged flame front velocities on time and the initial flame front velocity on the stoichiometry of the initial hydrogen-air mixture, we proposed two scaling laws. The first law of time scaling uniformly approximates the dependence of the trajectory of the flame front in hydrogen-air mixtures with an initial hydrogen concentration exceeding a certain critical value. The second law of stoichiometric scaling approximates the dependence of the maximum initial velocities of the flame front on the initial hydrogen concentration. The uniform

scaling laws for two topologically different morphotypes of an ultra-lean hydrogen flame can be interpreted as evidence of the self-similarity nature of the Flame-Ball-to-Deflagration-Transition phenomenon.

72 Numerical Simulation of Laminar Premixed Hydrogen-Air Flame/Shock Interaction under Low-Pressure Conditions

Yhuel, Emilie; Ribert, Guillaume; Domingo, Pascale*

Within the framework of the use of hydrogen as an energy vector, a study relating to the numerical simulation of the propagation of a laminar flame in a channel and interacting with a normal shockwave is proposed. A lean hydrogen/air flame propagates from the closed end of a two-dimensional channel and faces an incoming shockwave travelling at a Mach number $M_s = 1.4$. The high speed of the shock pushes the flame towards the back wall, and the reflected wave splits the flame into two parts, one progressing again toward the fresh gases make using of the velocity deficit in the top and bottom boundary layers and the other reorganising itself at the back of the channel displaying significant Richtmyer-Meshkov instabilities.

265 Stability analysis of the Noh problem for reactive shocks

Calvo-Rivera, Andr,s; huete, Cesar; Velikovich, Alexander L.*

The studies of shock compression of condensed media and shock-front stability started simultaneously in the 1940s within nuclear weapons projects. Notwithstanding the impressive progress made in both fields since then, the fundamental shock-front instability theoretically discovered by D'yakov (1954) and Kontorovich (1957) (DK) in the USSR still challenges our understanding of shock compression. DK predicted non-decaying oscillations of an isolated planar shock front, accompanied by spontaneous acoustic emission. This subtle effect is only possible under strict constraints on the equation of state and shock strength resulting in a specific shape of the Hugoniot curve. It took 20 years since the DK discovery to find realistic shock-compression conditions for its manifestation (in copper, Bushman, 1976) and many more years till its first numerical demonstration (in van der Waals fluid, Bates & Montgomery, 2000). We revisit this problem by extending the analysis to reactive shocks.

199 Numerical Study of Low-frequency Supersonic Combustion Instability in a Hydrogen-fueled Scramjet Engine

*Jeong, Seung-Min; Han, Hyung-Seok Han; Lee, Eun-Sung; Choi, Jeong-Yeol**

Numerical simulation of direct-connect supersonic combustor is carried out to investigate the mechanism and dynamic feature of combustion instability in a scramjet engine using hybrid RANS/LES numerical approach. The obtained numerical analysis results were analyzed by the modal decomposition method to find dynamic characteristics of combustion instability. The results exhibited that low-frequency combustion instability which has the order of 100 Hz frequency range. This dynamic behavior which has the order of “ms” period showed a dynamic coupling/decoupling process of heat release by combustion, and a formation/traveling of shock waves that interact with the boundary layer.

Wednesday 10:10 – Detonation Initiation & limits

179 Experimental Study on Detonation Wave Initiation by Reflected Blast Wave in Laser Ignition

Sato, Tomoyuki; Matsuoka, Ken; Kawasaki, Akira; Itouyama, Noboru; Watanabe, Hiroaki; Kasahara, Jiro*

Using ethylene-oxygen mixtures, laser ignition experiments were conducted with two types of reflection walls and an elliptic cavity. From the schlieren visualization of the flowfield, in the case of vertical and horizontal reflection walls, it was clarified that the blast wave creates a high pressure/temperature region after reflection on the wall. The expansion waves behind the leading and the reflected blast wave, as well as the decay of the leading blast wave, which is due to its three-dimensional expansion, are considered to lower the unburned gas pressure. As for the elliptic cavity, blast wave reflections and shock-shock interaction was observed. From the pressure profile after the intersection, it was clarified that the displacement of the ignition point resulted in the difference between the reflected blast waves propagation form and the displacement of the pressure peak.

223 Critical Dynamics of Direct Initiation of Spherical Detonations

Hern ndez S nchez, Ra£l; Denet, Bruno; Clavin, Paul*

The asymptotic limit of small heat release is investigated in the context of the critical dynamics of detonation direct initiation. The analysis, limited to spherical geometry, includes unsteadiness, curvature effects, and the gradient of the burnt-gas flow. Numerical integration of the hyperbolic equation governing the dynamics provides the basis of the study. The critical trajectories “detonation velocity vs radius” are characterized by a decay well below the CJ velocity at a small radius followed by a re-acceleration process back to a CJ detonation. The key mechanism is identified as the slowdown produced as soon as the sonic point reaches the exit of the reaction zone. Under this condition, the time delay of the nonlinear response of the front to the rarefaction-wave-induced decay increases significantly. Detonation fails if the decay rate is strong enough to prevent the sonic point to catch the exit of the reaction zone.

59 A Three-Step, Three-Gamma Model for The Numerical Modeling of the Critical Height of The Propagation of Semi-Confined Detonation Waves

*Taileb, Said; Rougon, Emmeline; Robin, Vincent; Rodriguez, Vincent; Lau-Chapdelaine, Shem; Vidal, Pierre; Melguizo-Gavilanes, Josue; Chinnayya, Ashwin**

The determination of the critical height of the detonation propagation in a semi-confined environment depends on the chemical modeling. The calibration of the induction times of reduced models against the reference detailed chemistry is not sufficient to obtain the quenching limit. Slight modifications of an initial three-step chain branching model are proposed, in order to take into account (i) thermodynamic variations of the molecular weight and polytropic coefficient and (ii) the reaction length of the ideal ZND model. Preliminary results showed that these two additions help to decrease the critical height towards the reference one.

Wednesday 10:10 – Ignition I

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155 Experimental and Numerical Study of Autoignition/Deflagration Transition Limit in an optical Rapid Compression Machine

Ossman, Hicham; Strozzi, Camille; Sotton, Julien; Bellenoue, Marc*

This works investigates the transition limit between auto-ignition front and deflagration in hot and premixed conditions. In particular, the objective is to analyze the sensitivity of the combustion regime to the temperature gradient, mixture composition and thermodynamical conditions, which is first analyzed numerically. The results are then experimentally validated in an optical RCM, fitted with a flat piston and a multi-zone heating system. Temperature gradient after compression is measured in the hot core region using two thin wire thermocouples of about 7.6 μm diameter. The chemiluminescence records confirm that the dynamics of autoignition fronts is strongly dependent on (i) the mixture composition and the thermodynamical conditions, and (ii) on thermal gradients in the unburned mixture. In particular, the authors evidence experimental conditions for which a steeper gradient leads to a transition from autoignition to deflagration.

52 Comparison between Laser Ignition and Spark-Plug Ignition of Flowing Propane-Air Mixtures

Eto, Kosuke; Kojima, Yusaku; Kim, Wookyung; Johzaki, Tomoyuki; Endo, Takuma*

Laser ignition and spark-plug ignition were experimentally compared in the pipe flows of pre-mixed propane-air mixtures, where the mole fraction of propane was varied within 2.3-4.0% and the flow speed was varied within 0-88 m/s, corresponding to the Reynolds number up to 115,000. In the laser ignition, a Nd:YAG laser of 12-ns pulse duration and 1064-nm wavelength was used, while in the spark-plug ignition, a spark plug of 1.6-ms discharge duration was used. In both ignition methods, the deposited energy was approximately 25 mJ. For examining the ignition and burning properties, the self-emission images were observed using a high-speed camera. It was found that the ignition ability of the laser-induced breakdown was superior to that of the spark-plug-induced breakdown, although the properties of the fully-developed flames were independent of the ignition methods. In addition, it was found that the ignition success rate is governed by the turbulent Damk”hler number of first species.

84 Numerical Simulation of LOx/CH4 Supercritical Combustion in a non-Homogenous Mixture

*Monnier, Florian; Ribert, Guillaume**

To ensure a correct description of the combustion process in a liquid rocket engine (LRE), validated chemistry is required as well as adequate thermochemistry and transport properties suitable for high-pressure conditions. In the present study, a reduced chemistry is evaluated with success on a O2-CH4 non-homogeneous mixture. Such a situation is closer to the cases encountered in real LRE where the methane is injected separately from the oxygen by means of a coaxial injector. When firing such mixtures, triple flames appear separating the methane blob from the surrounding oxygen. The behavior of the reduced scheme is compared with the results obtained using the detailed kinetic from which it was created. A very good agreement is observed on a configuration where multi-blob of methane interact with oxygen in a turbulent environment.

Wednesday 11:50 – Pressure-Gain Combustion

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87 Identification of Multiple Combustion Modes in Continuous Detonation Engines

Ma, John Z.; Wang, Jian-Ping*

Several Continuous Detonation Engines (CDEs) were designed, and nearly 300 effective experimental tests were carried out in order to quickly and accurately identify the combustion modes. The operating modes were assessed based on pressure measurements in the combustor annulus and verified with high-speed video of the natural flame luminosity from the aft end of the Continuous Detonation Combustor (CDC). Seven different combustion modes are found, and the typical characteristics of dynamic pressure curves are further summarized. These combustion modes include deflagration, DDT process, coexistence of strong and weak detonations, coexistence of detonation with deflagration, double-single wave transition, single-double wave transition, and stable detonation. It will have important reference value for the study of unstable combustion process in CDEs.

31 TDLAS for Sensing Pre-vaporized Jet A-1 in Liquid-fuel Pressure Gain Combustion

Chang, Po-Hsiung; Teo, Nathanael; Li, Jiun-Ming; Huang, Xin; Teo, Chiang Juay; Khoo , B. C.*

A liquid-fuel pressure gain combustion incorporated the pre-vaporization method has been successfully established. With the help of TDLAS techniques, the vapor-phase equivalence ratio and the airflow rate exceeding 0.66 and 0.156 kg/s, respectively, were found as the critical conditions for the onset of detonation. It is difficult to obtain the detonation combustion when the oxygen concentration in the oxidizer was reduced to 15%.

102 Numerical Study on the Unsteady Rotating Detonation Flow-Field Interacted with Turbine Guide Vane

Shen, Dawen; Cheng, Miao; Wu, Kevin; Sheng, Zhaohua; Wang, Jianping*

Attempts of the effective integration of turbomachinery with rotating detonation engine (RDE) have been made. However, strong fluctuations of RDE exhaust flow pose significant challenges to the downstream turbines, then an RDE equipped with turbine guide vane (TGV) is proposed to handle this. In this paper, the flow-field generated by the integration of RDE with three kinds of TGV configurations is numerically simulated. A novel shock wave system termed rake-type shock envelope is obtained in every case integrated with TGVs. Additionally, influence of the vanes with different inclination angles on flow angle, fluctuation, and total pressure during one period is compared. Results show that TGV plays a vital role in alleviating flow-field unsteadiness and conditioning flow. The intensity of rotating detonation wave and shock development among TGV passages are considered as the main factors resulting in the difference of total pressure loss in every TGV configuration.

Wednesday 11:50 – Flame Acceleration & DDT II

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259 Critical Conditions for Flame Acceleration and DDT for Hydrogen-Air Mixtures at Cryogenic Temperatures

Kuznetsov, Mike; Denkevits, Andrey; Friedrich, Andreas; Veser, Anke*

A series of more than 200 experiments with hydrogen-air mixtures at cryogenic temperatures have been performed. A wide range of hydrogen concentrations from 8 to 60%H2 in the shock tube of the length of 5 m and 50 mm id was tested at cryogenic temperatures from 80 to 130K at ambient pressure. Flame propagation regimes were investigated for all hydrogen compositions in a tube with blockage ratios (BR) 0, 0.3 and 0.6 as a function of initial temperature. A critical expansion ratio for an effective flame acceleration to the speed of sound was experimentally found at cryogenic temperatures. The detonability criterion for smooth and obstructed channels was used to evaluate the detonation cell sizes at cryogenic temperatures as well. It was experimentally found that the maximum combustion pressure was several times higher compared to ambient temperature and the run-up-distance to detonation was several times shorter independent of lower chemical reactivity at cryogenic conditions.

67 On the possibility of non-dimensionalizing DDT limits and distances

Rodriguez, Vincent; Monnier, Vianney; Vidal, Pierre; Zitoun, Ratiba*

This experimental analysis proposes a non-dimensionalization of the limits and distances of deflagration-to-detonation transitions (DDT) ignited by jets of hot gases. The jets were obtained from the impact of a CJ detonation on a multi-perforated plate and distributed over the cross section of a square tube. Observable characteristics parameters were used, namely the CJ cell width, the thickness of the plates, the number and diameter of the holes in the plates. The DDT distances well correlate with the non-dimensional number for the relative effects of surface re-ignition formed by the interaction of the jets coming out of the holes. The DDT limits are found independent of the non-dimensional number for the relative effects of the surface-dissipation phenomena in the holes. The results are independent of the cell regularity - from soot recordings at walls - of the investigated mixtures, so this regularity may not always be relevant for interpreting deflagration and detonation dynamics.

82 A One-dimensional Model for Deflagration-to-detonation Transition of an Elongated Flame

Tofaili, Hassan; Clavin, Paul; Lodato, Guido; Vervisch, Luc*

Recent advances in the theoretical modelling of DDT for elongated flames in tubes are presented. A laminar flame starting from the closed end of a tube is considered, and a double-feedback mechanism for DDT of such a flame is proposed, in which compression heating by the lead shock is augmented by an effective piston acceleration due to the back-flow of burnt gas into the flame tip. After simplifying the problem into a one-dimensional flame supported by an accelerating piston, it is shown that a self-similar solution for the flow exhibits a turning point at which the flame acceleration diverges. Further analysis beyond self-similarity reveals the formation of a shockwave on the flame at the turning point. Such a shock formation is a good candidate to blow up the inner structure of the flame and produce the transition to a detonation.

106 An Experimentally Informed 1-D DDT Model for Smooth Narrow Channels

Melguizo-Gavilanes, Josue; Bauwens, Luc*

The flame front position as a function of time, x_f vs. t, can be very accurately determined in optically accessible channels or tubes equipped with photodiodes. These x-t diagrams arguably contain the combined effect of momentum and energy losses during flame acceleration and detonation onset known to play a role in narrow channels. However, measuring the spatial and temporal variations in pressure, temperature and species concentrations in the gas is not trivial. In this work, a gas dynamical model in which experimental x_f-t diagrams are used together with the 1-D reactive Euler equations to investigate the gas dynamics ahead of an accelerating flame in a simple way. The role of the late stages of flame acceleration in forming a significantly stronger secondary precursor shock very close to the flame front was elucidated.

156 Shock Dynamics from Quenched Detonations: Diffraction and Gallop Problems

*Radulescu, Matei**

Analytical models are presented for the shock dynamics resulting from detonation quenching. The first is the classical problem of detonation diffraction at a corner. The second is the dynamics of galloping detonations. In both cases, the dynamics result from the shock change equations, relating the shock dynamics (speed, acceleration and curvature) to one partial derivative evaluated behind the shock. For diffracting detonations, the quasi-steady rear piston support by the detonation products are modeled by neglecting the particle speed variation with time. For 1D galloping detonations modelled by inert shock decays punctuated by instantaneous ""kicks"" of energy release, limit cycles are approximated by constant particle speed gradients, since these are preserved upon instantaneous kicks. In both cases, results are found in very good agreement with simulations and experiments.

86 A Methodology to Develop Simplified Kinetic Schemes for Detonation Simulations

Veiga-Lopez, Fernando; Chinnayya, Ashwin; Melguizo-Gavilanes, Josue*

A methodology to develop more predictive simplified kinetics schemes (1-step / 3-step chain-branching) is presented in which *D-k* curves obtained with detailed kinetics are used as the fitting target aiming to capture the turning point of the curve k_{crit}.

This was motivated by the similar trend observed between the k_{crit} values and the critical reactive layer heights for detonation propagation under yielding confinement, h_{crit}, determined by Taileb et al. (CNF 218, 2020) in which simplified kinetics fitted with conventional methods were used. Both updated schemes satisfactorily reproduce the target *D-k* curves and are currently being used to recompute revised h_{crit} values.

73 Modeling Detonation Reflection with Nonsteady Shock Change Equation

Schoeffler, Donner T; Shepherd, Joseph*

Upon colliding with an end wall, a detonation reflects a shock wave, which travels through the nonsteady and nonuniform flow that trailed the detonation wave. Prediction of the shock wave's trajectory requires considering both the variation in upstream and downstream parameters. The problem is treated with an extension to the shock change equation that considers a general nonuniform and nonsteady upstream flow. This extension is derived and applied to the problem of detonation reflection, formulating the reflected shock trajectory as an initial value problem. For an example set of initial conditions, the equation is integrated, and the results are compared with a CFD simulation of the same problem. Agreement between results illustrates the model's ability for predicting the reflected shock wave trajectory in one dimension for a general mixture and equation of state.

257 Numerical Study of Detonation Propagation Through a Gravity-Driven Layer Of Hydrogen-Oxygen Over an Inert Gas

Menezes, Myron; Lau-Chapdelaine, Shem; Ciccarelli, Gabriel*

An important aspect of explosion safety is predicting detonation propagation in a combustible cloud that forms following an accidental release. When buoyancy is important, as is the case with light or heavy fuels, such clouds take the form of a stratified layer bounded by a single solid wall.

This study simulates experiments carried out in a narrow channel where a detonation wave propagates through a gravity-driven stratified layer of hydrogen-oxygen above an inert gas with a diffuse interface. The objective of this study is to study detonation failure, specifically the detonation failure at the leading-edge of the layer observed in the experiment that is not predicted by the Bauwens and Dorofeev cell size gradient failure criteria.

Wednesday 11:50 – Chemical Kinetics V

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69 Improvement of the Global Quasi-Linearisation (GQL) Model Reduction Method

Yu, Chunkan; Bykov, Viatcheslav; Maas, Ulrich*

Manifolds based model reduction approaches have been developed extensively in the past. The problem of efficient implementation of these manifolds, however, remains challenging and not yet generically solved especially for those having relatively high dimension. The current study deals with this problem and shows how we can improve the performance of the reduced model integration by increasing the order of the approximation. As an example the Global Quasi-Linearisation (GQL) is used to simplify the chemical kinetics. The proposed method can improve significantly the accuracy and performance of the reduced model. The method is based on the first order correction of the manifold equation. It can be generically implemented in the GQL numerical implementation, but also in other low-dimensional model representations. In order to illustrate the proposed method and to show improved performance a benchmark model of the hydrogen-air ignition problem of combustion is considered.

172 REDIM Reduced Modeling of Flame-Wall-Interactions of Premixed Natural Gas / Air Systems

Straáacker, Christina; Maas, Ulrich*

In this work, the Reaction-Diffusion Manifold (REDIM) method, a method for model reduction, is applied to a premixed natural gas-air system with Flame-

Wall-Interactions (FWI). In this way it is demonstrated that the REDIM method is not restricted to single-component fuels. In order to provide an accurate reduced kinetic model, a detailed model for the diffusive processes including thermal diffusion is applied. The REDIM is constructed and validated by comparing results of detailed and reduced kinetics. It is shown that the reduced kinetics reproduce the results of the FWI very accurately. This leads to the conclusion, that the suggested reduced model can be used to accurately describe the Flame-Wall-Interactions.

47 Experimental Investigation of the Combustion Properties of a Representative Thermal Runaway Gas from Li-Ion Batteries

Mathieu, Olivier; Turner, Mattias; Mohr, Darryl; Thomas, James C; Petersen, Eric*

Lithium-Ion batteries are used in most electronic devices and in electric vehicles (EV). In case of severe collision, the battery of an EV can be crushed or penetrated which can lead to a short circuit and to a thermal runaway. Flammable gases are then created, which can lead to a fire. Thermal runaway gases (TRG) from Li-ion batteries have been characterized in many studies, but their combustion properties have never been investigated at the fundamental combustion level.

In the present study, we assembled the detailed composition of the vent gases from the literature and a final mixture composed of H_2, CH_4, C_2H_4, C_2H_6, C_3H_8, CO, and CO_2 was determined from forty compositions. While these fuels have been studied extensively individually, such a complex mixture of these gases was never investigated before. Ignition delay times and laminar flame speeds were measured in a shock tube and in a closed vessel, respectively. Models were compared with the data for assessment.

225 Experimental and Numeric Study on the Inhibition Properties of Novec

Nagaraju, Sharath; Abid, Said; Comandini, Andrea; Chaumeix, Nabiha*

An investigation into the flame inhibition properties of Novec in stoichiometric propane/air mixture has been experimentally carried out in a cylindrical vessel, NC2V, at ICARE-CNRS. The results showed that a minimum of 9.3% of Novec is required to completely inhibit the stoichiometric propane/air mixture. Numerical simulation was also carried out for a larger domain of propane/air equivalence ratio and Novec concentration to explore the dynamics of the propane flame in presence of Novec.

Thursday 9:00 – Explosion Safety II

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124 Shock Transmission from Detonating Mixtures in Open Tubes

Thomas, James C; Rodriguez, Felix A; Teitge, David; Kunka, Logan; Gaddis, Nathan; Browne, Zachary; Ahumada, Cassio; Balci, Tarik; Jackson, Scott I; Petersen, Eric; Oran, Elaine*

Transmission of a shock wave from a steady-state detonation inside of a tube into an open atmosphere is an engineering problem relevant to many applications ranging from fundamental research experiments to pulse-detonation engines. Texas A&M University (TAMU) is currently developing an open-ended detonation tube (ID~2 m, L~200 m) for large-scale experimentation purposes including studying low-reactive fuel mixtures where the detonation dynamics are not geometrically constrained. Accordingly, we were motivated to gain a better fundamental understanding of the conditions outside of the open end of the tube when steady-state detonation waves propagate from it and into the surrounding atmosphere. Three lab-scale detonation tubes were designed and built to evaluate the underlying physical phenomena and potential scaling problems associated with these conditions, ultimately leading to the prediction of large-scale facility behavior.

181 Influence of Hemicylindrical Obstacle Scale and Length on an Impacting Blast Wave

Gavart, Raphael N; Trélat, Sophie; Sturtzer, Michel-Olivier; Chaumeix, Nabiha*

The aim of the present paper is to provide an experimental study on the characterization of blast waves initiated by a solid explosive and the interaction with a rigid obstacle (hemicylinder). The coupling between several pressure transducers along the path of the blast wave and a high-speed imaging (BOS) allows (i) the measurement of the overpressure at different locations and (ii) the characterization of the blast wave inception, propagation, and reflection on the hemicylinder. The scaling effect has been addressed by performing experiments located at two different facilities: (i) scale A at the IRSN facilities and (ii) a larger scale, scale 2A, at the ISL facilities.

171 REKO-Fire: New Facility to Investigate Cable Fire Impact on Passive Autocatalytic Recombiners

Nobrega, Gabriela; Klauck, Michael; Reinecke, Ernst-Arndt ; Chaumeix, Nabiha; Bentaib, Ahmed; Maas, Ludovic*

Fires in nuclear power plants (NPPs) represent a significant risk to nuclear safety. Cable fires may occur not only at any time in the course of a severe accident but may also be the initiating event of a severe accident sequence. The effect of cable fire products inside the containment and their interaction with the catalyst surfaces of passive autocatalytic recombiners (PARs) is of significant relevance for safety analyses in order to assess the hydrogen explosion mitigation efficiency under these conditions.

The newly built REKO-Fire facility combines a flow tube reactor for catalyst investigation with a steady-state tube furnace for the constant generation of cable fire products at varying combustion conditions. The installation has been used to investigate the effect of combustion products obtained from flame-retardant power cables under three different fire conditions on the start-up of Pd-based catalysts for hydrogen recombination.

219 Detonability Enhancement by Use of a Nanosecond Plasma

Ali Cherif, Mhedine; Lafaurie, Victor; Starikovskaia, Svetlana; Vidal, Pierre*

This work shows that a non-equilibrium, nanosecond plasma enhances the detonability of a gas mixture at moderate initial pressure. Two parameters were investigated: (i) the length for deflagration-detonation transition (DDT) and (ii) the detonation cell width. Experiments were carried out in H2:O2-based mixtures for initial pressures 120-800 mbar. ICCD imaging, back current shunts, soot plates and schlieren imaging were used to characterize plasma and the combustion waves. The experiments brought out differences in the DDT process between a classical spark plug and a developed multi-channel nanosecond plasma igniter. Differences in ignition of the mixture, flame speed and evolution, in particular shorter DDT lengths, were analyzed. The action of a nanosecond plasma ahead of a detonation front reduces was found to significantly the detonation cell width in the region where the plasma was applied. The effect of the plasma is instantaneous in the timescale of the detonation processes.

261 Thermochemical Aspects of Superknock Development in IC Engines

Luong, Minh Bau; Tingas, Efstathios-Al; Im, Hong G.*

This study elucidates the thermochemical characteristics of a developing ignition process by performing computational singular perturbation (CSP) and tangential stretching rate (TSR) analysis. The relative contribution of chemical kinetics, diffusion, and convection on the progression of superknock development is identified. It is found that in addition to the dominant contribution of chemical kinetics, the contribution of transport in triggering the developing detonation transition (DDT) is non-negligible, i.e., ranging approximately from 10% to 50% in the preheat zone where the DDT occurs

42 Effect of Mach number on the flame acceleration and deflagration-to-detonation transition

Zhao, Wandong; Liang, Jianhan; Cai, Xiaodong; Diterding, Ralf; Wang, Xinxin*

The flame acceleration and deflagration-to-detonation transition that occurred in the supersonic and subsonic mixtures were studied using two-dimensional Naiver-Stokes equations with a detailed chemical reaction mechanism and adaptive mech refinement technology. A classical hot spot-based DDT mechanism is formed in the supersonic mixture. Whereas, the onset of detonation ignited by pressure build-up at the leading edge of the flame front is obtained in the combustion chamber with the subsonic mixture. It is found that the run-up time and distance of the DDT in the subsonic mixture are much higher than that in the supersonic mixture.

24 Simulation of Flame Acceleration and Deflagration-to-Detonation Transition in Components of Chemical Plants

Wieland, Christoph; Hirsch, Christoph; Sattelmayer, Thomas; Scharf, Florian; Hoferichter, Vera; Schildberg, Hans-Peter*

Risk analysis is a central aspect of plant design in the chemical and process industry as potentially hazardous mixtures are involved in the production. Comprehensive analysis must always consider a huge variety of accident scenarios that could lead to a DDT. The wide variety of mixtures, geometries and process conditions does not allow for an experimental investigation. Therefore, a hybrid pressure-/density-based solver is presented which is capable of simulating flame acceleration and DDT of H2/O2/N2 and C2H4/O2/N2 mixtures in smooth pipes and spheres. Short calculation runtimes are achieved by using under-resolved grids. As a consequence, essential physical phenomena have to be modelled. Smooth pipes and a 20 l sphere were considered for validation. Therefore, two different types of flame propagation: quasi 1-D propagation in the smooth pipes and 3-D propagation in the sphere could be considered, where good agreement is achieved in general.

Thursday 9:00 – Turbulent Flames I

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64 Surface Density Function and its Evolution in Homogeneous and Inhomogeneous n-heptane MILD Combustion

Abo-Amsha, Khalil; Chakraborty, Nilanjan*

Moderate or Intense Low-Oxygen Dilution (MILD) combustion is a novel combustion concept with potential to simultaneously improve thermal efficiency and reduce emissions. This paper focuses on the mean behaviour of the Surface Density Function (SDF=magnitude of the reaction progress variable gradient) and its evolution for exhaust gas recirculation (EGR) type, homogeneous and inhomogeneous mixture n-heptane combustion under MILD conditions using Direct Numerical Simulations (DNS) with reduced chemical mechanism. Two oxygen concentration have been considered here for the homogeneous mixture case, namely, 3.0% and 4.5%. The mean values of the SDF in turbulent MILD combustion cases are found to be smaller compared to the corresponding laminar flame cases. Moreover, the effect of mixture inhomogeneity was negligible on SDF for the parameters considered here. It is found that increasing the dilution factor gives rise to slightly thinner reaction zone.

119 Flame Self-Interactions in Turbulent Homogeneous-Mixture n-heptane MILD Combustion

Abo-Amsha, Khalil; Chakraborty, Nilanjan*

Moderate or Intense Low-oxygen Dilution (MILD) combustion has been demonstrated to have the potential to achieve both high energy efficiency and ultra-low emissions. This paper adopts the critical point theory to investigate the effect of turbulence intensity and dilution level on Flame-Self Interactions (FSI) in turbulent, homogeneous mixture, n-heptane MILD combustion using Direct Numerical Simulations (DNS) with reduced chemical mechanism. The local flame geometry has also been categorised using the mean and Gauss curvatures. It was found that increasing the turbulence intensity has led to enhanced FSI frequency and resulted in higher mean curvature levels, while increasing the dilution factor caused a reduction in the frequency of FSI events towards the burned gas side, but produced higher levels of mean and Gauss curvatures.

240 Numerical Investigation of The Global Equivalence Ratio Effects on the Dynamic Behavior of Turbulent Swirling Diffusion Flame

Chakchak, Sawssen; Boushaki, Toufik; Hidouri, Ammar; Chrigui, Mouldi*

The present work investigates numerically the influence of global equivalence ratio under lean, stoichiometric and rich conditions on the dynamic behavior of non-premixing swirling flame provided by a swirl coaxial burner. Fuel is injected radially through eight holes in the central tube. The simulations are performed using the ANSYS-Fluent CFD code. Reynolds averaged Navier-Stokes (RANS) is used to capture the turbulence and the eddy dissipation combustion model (EDM) to resolve the turbulence/chemistry interaction. The results of mean axial and tangential velocities and turbulent kinetic energy for various equivalence ratios (0.5, 0.8, 1, 1.2, 1.3) at two different positions (Z=10mm and Z=60mm) are presented. The decrease of equivalence ratio affects the Central Recirculation Zone and leads to an important increase in the maximum value of mean axial velocity by around 50%. Decreasing the global equivalence ratio increases the TKE and hence increases the velocities fluctuations.

25 DNS of Turbulent Spray Flame Water Droplet Interaction Using an Euler-Lagrange-Lagrange Scheme

Hasslberger, Josef; Concetti, Riccardo; Chakraborty, Nilanjan; Klein, Markus*

Carrier-phase DNS based on a novel Euler-Lagrange-Lagrange scheme has been used to study the impact of water droplet addition on statistically planar turbulent flames. It has been shown earlier that the main effect on key flame characteristics, such as flame speed and flame thickness, is due to the heat sink associated to evaporating water droplets. However, water droplet addition influences spray combustion in a more intricate way than premixed combustion. Despite the steam-related dilution effect, the spray flame burns under fuel-richer conditions, i.e. higher gaseous equivalence ratio, at identical overall equivalence ratio (gaseous + liquid). Due to the non-linear influence of droplet size on the evaporation law, considerable differences have been observed for water droplet sizes of 4% (moderate effect) and 2% (strong effect) of the unstretched laminar thermal flame thickness at identical overall water loading.

Thursday 11:05 – Oblique Detonation

176 The Impact of a Micro-Rounded Bump on the Initiation of Oblique Detonation Waves

*Yan, Chian; Bakalis, Georgios; Chaar, Richard El; Teng, Honghui; Ng, Hoi Dick**

In this study, the effect of a micro-obstacle on the wedge-induced initiation of oblique detonation wave is studied via simplified two-dimensional numerical simulations. For focusing mainly on gas dynamics, the reactive Euler equations with a one-step Arrhenius kinetic model are adopted for the reactive flow. The governing equations are solved numerically using a 2nd order finite volume scheme and computations are carried out using the Graphics Processing Units (GPUs) computing technology. A parametric study is carried out to explore the effects of the micro-bump on the type of oblique shock-to-oblique detonation transition, as well as its potential in promoting the oblique detonation initiation by reducing the initiation length for practical applications, are investigated and discussed.

93 Experimental Study of Stabilized Oblique Detonation Waves

Rosato, Daniel A; Thornton, Mason R; Ahmed, Kareem*

This paper details the experimental study completed using the HyperReact facility that has shown evidence for the initiation and stabilization of an Oblique Detonation Wave (ODW) in a continuous flow facility. A ramp was placed in a pre-heated, high-enthalpy, supersonic flow of hydrogen and air to create the needed conditions for the ODW. A quasi-stable reaction was observed wherein the detonation front went through a cycle of being over- and under-driven, but remaining in the region above the ramp. Tests were conducted at multiple pressures, temperatures, and mixture equivalence ratios, which have shown multiple regimes of reaction behaviors within this facility. The stable reaction occurs at the highest pressure and temperature conditions tested in this study.

189 Experimental Observation of Non-uniformly Premixed Oblique Detonation

Iwata, Kazuya; Hanyu, Naoki; Maeda, Shinichi; Obara, Tetsuro*

Morphologies of detonation in non-uniform mixture have been attracting increasing attention since it is likely to be seen in most actual situations including explosive accidents and the application in aerospace vehicles. Experimental observation was first attempted against non-uniformly premixed oblique detonation wave (ODW), which is beneficial for analyzing the theoretical features for its steadiness in a body-fixed frame. ODW was successful in every strength of concentration gradient in this study which was controlled by the waiting time after fuel injection. Local wave angles most agreed with those of Chapman-Jouguet (C-J) detonation, and a little deviation observed was quantitatively explained by the curvature effect. Furthermore, some critical features including Straw-Hat structure and local quenching appeared, which was attributed to critical curvature radius instead of non-dimensional sphere diameter that is a critical parameter in uniform mixture.

20 Formation and Regulation of Unsteady Detonation Mach Stem in A Confined Space

Shuzhen, Niu; Pengfei, Yang; Honghui, Teng*

Detonation-based engines have attracted increasing attentions owning to pressure-gain combustion. Using an oblique detonation wave (ODW), the oblique detonation engine is suitable for hypersonic propulsion system. For the engine's combustor, detonation wave may interact with the solid surface and the appearance of an unstable Mach stem is a huge challenge for the operation of combustion system. In this study, considering the geometric complexity of a combustor, the effects of inflow Mach number variation on the wave systems and the regulation law of ODW Mach reflection in a confined combustor is explored. Simulated results shows that a slight increase in inflow Mach number can suppress the upstream movement of Mach stem at the early stage of detonation instability. As the Mach stem moves upstream, it is increasingly hard to restabilize the ODW. A series of pressure waves are originated from the interaction point, which is the main factor of Mach stem's instability.

Thursday 11:05 – RDE VI

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170 Experimental Study of Liquid Propellant Rotating Detonation Combustor

Ito, Shiro; Ishihara, Kazuki; Yoneyama, Kentaro; Goto, Keisuke; Itouyama, Noboru; Watanabe, Hiroaki; Kawasaki, Akira; Matsuoka, Ken; Kasahara, Jiro; Matsuo, Akiko; Funaki, Ikkoh*

Combustion tests were conducted using gaseous ethylene and liquid oxygen in a cylindrical rotating detonation engine with a diameter of 20 mm and a combustor length of 210 mm. A high-speed camera captures high-luminescence areas rotating along the combustion chamber wall, with a propagation velocity of 1383 ± 80 m/s. This indicates that rotating detonation occurred in the combustion test.

The thrust measured by the load cell was in good agreement with the two types of theoretical thrust. One was calculated based on the pressure and momentum exchange, and thus the agreement validated the thrust measurement. The other was computed based on the equilibrium calculation and the assumption that the exhaust velocity was sonic. Thus the agreement suggested that the liquid oxygen reacts completely and that the thrust performance of cylindrical RDCs using liquid propellants can be predicted by the same method as used for the conventional constant pressure combustion rocket engines.

37 Temperature and Heat-Flux Measurements in a Thin-Wall RDE

*Stevens, Christopher A**

Thermal management remains one of the more difficult challenges facing the development of practical Rotating Detonation Engines. Data on the heat transfer environment within an RDE remains limited, and published results so far have focused on cold wall or transient heat transfer. In this work, a thin-walled, stainless steel RDE was constructed to fill in some to the gap. The RDE was operated on a hydrogen/air mixture at independently controlled flowrate and equivalence ratio. Measurements of the temperature and heat flux were obtained via thermocouples and infra-red imaging. The measured heat fluxes were smaller compared to cooled walls while the temperatures are predictably higher. The results of this work imply that hotter channel walls are preferred in RDEs so long as the chance of failure remains low.

21 Self-excited Wave Propagation in a Reflective Shuttling Detonation Combustor

Ullman, Michael J; Prakash, Supraj; Jackson, Deborah R; Raman, Venkat; Slabaugh, Carson D; Bennewitz, John W*

Detonation combustors have gained attention in recent years for the higher thermal efficiencies they offer over conventional combustion systems. However, the effects of inflow conditions, fuel-oxidizer mixing, and other boundary conditions on these systems are not well understood. To provide increased optical accessibility and better understand the wave dynamics within RDEs, a reflective shuttling detonation combustor (RSDC) with an open-closed combustor configuration is studied. Two inflow conditions are studied numerically, and comparisons are made to similar experimental configurations. The results show the emergence of two unique wave modes: the first consisting of bi-directional weak detonations, and the second consisting of strong detonations with a directional preference towards the open end of the combustion chamber. The peak wave speeds were lower than the CJ speeds for both cases, likely due to insufficient reactant mixing and interactions with counter-propagating waves.

198 Shock-Droplet Interactions and Reaction of Liquid RP-2 Fuel

Patten, John P; Ahmed, Kareem; Hytovick, Rachel; Burke, Robert F*

This experiment attempts to characterize and describe the effect of shock waves and detonation waves interacting with liquid fuel columns and droplets of RP-2; demonstrating the influence that liquid fuel has on different reacting flow regimes. It was determined that liquid RP-2 reacts more favorably as the shock Mach number is increased; ignition can occur in Mach numbers as low as 1.7, allowing detonation waves to be sustained. This research will help to advance

RDEs and other liquid-fed detonation-based propulsion methods by enabling detonation waves to be more easily sustained.

32 Statistical research on firebrand behaviour in a simulated 3D fire whirl

Zhang, Yuchen; Zhang, Yang*

The firebrands lofted by flow field is a vital mechanism of long-distance fire spread in the forest fire. Although many previous researches have been investigated the transportation of firebrands under the convective plume, few focused on the impact of fire whirl. The existence of a fire whirl will largely increase the maximum spotting distance, while researchers know little about its detailed physics. In this paper, a 3D fire whirl has been created by FDS, in order to study the effect of aerodynamic lift in the lofting mechanism of firebrands in fire whirl. By tracking each firebrand's trajectories, a relationship between the inclined angle to the maximum reachable height has been established. The trajectories that considered and ignored the impact of aerodynamic lift demonstrated that the aerodynamic lift's impact on the trajectories is significant. It suggests that the aerodynamic lift should be included in the prediction of firebrand lofting to improve the accuracy.

74 Experimental Study of Firebrand Lofting Mechanism in a Fire Whirl Induced Flow Field

Zhang, Yuchen; Albadi, Ahmed; Zhang, Yang*

This study aims to develop a new understanding of firebrands? lofting mechanism, which has taken the aerodynamic lift into account. A statistical approach of measuring the percentage of different paper lofting patterns has been introduced to evaluate the probabilistic behaviours of firebrand lofting. Samples of various aspect ratios and cross-sectional areas have been tested with and without the fire whirl. The experiment results have shown a noticeable increase in the percentage of the flying and floating samples with the existence of fire whirl. A simple analysis has shown that the aerodynamic lift should not be neglected. A quantitative analysis of the lift effect and drag effect has been introduced. In the calculation, the additional effect after introducing the aerodynamic lift fit the experimental results of fire whirl contribution.

262 Numerical Prediction of Cables Fire Behaviour Using Non-Metallic Components in Cone Calorimeter

Alonso, Alain A; Lazaro, Mariano; Lazaro, David; Alvear, Daniel*

The way to increase the fire performance of cables can lead to a trial and error process. In order to skip the process and obtain some evidences of the fire behaviour, the researches have been executing bench scale tests (Cone calorimetric-CC). However, the execution of these tests to develop new cables

requires the design and construction of the whole cable. It could represent time-consuming issue. To overcome this limitation, computational models represent a powerful tool, and they are widely employed in fire engineering area. This work proposes the characterization of the cable materials separately (sheath and insulation), applying the inverse modelling, and then replicate the results of CC tests of two multipolar cables. Testing pieces of cable before fabricate them allow manufactures to discard low efficiency materials. Basis on the results, the developed methodology has been proved helpful for modelling CC tests of complete cable.

Thursday 11:05 – Energetic Materials I

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193 Pyroelectric Combustion Rate Characterization of Electrically Controlled Solid Propellants

*Kanagaraj, Gnanaprakash; Yoh, Jack J.**

Solid rocket propellants that demonstrate variable combustion rates are highly desirable in various propulsion applications. Electrically controlled solid propellants (ECSPs) are one such kind that ignite and combust only when external electric power is applied. In this study, pyroelectric combustion rates of metallized ECSP containing 5% tungsten (W) were obtained and compared with those of the non-metallized propellant. Pyroelectric combustion images of these ECSPs showed this process in detail. Overall burn time was less and the combustion zone appeared more luminous for metallized ECSP relative to the baseline case. Lower voltage rise time for metallized ECSP implied that their ionic conductivity was higher. Pyroelectric combustion rates of both ECSPs increased with increase in the initial voltage. However, addition of W to ECSPs enhanced (60%) their combustion rates significantly only at low voltages (<200 V), whereas this effect was negligible at high voltages (>300 V).

125 Investigation of Micro- and Nano-Catalytic Additive Effects on Ammonium Perchlorate Combustion

Rodriguez, Felix A; Thomas, James C; Sammet, Tom; Teitge, David; Petersen, Eric*

AP pellets were manufactured with micro- and nano-iron oxide (Fe_2O_3) and micro- and nano-titanium oxide (TiO_2) at several mass loadings (0-3% by mass) and were burned from 3.45-34.5 MPa (500-5,000 psi) in a constant-volume strand bomb. Microscopy characterization was completed for both additives and representative pellet samples. The incorporation of 1% micro-Fe_2O_3 yielded the highest burning rate among all formulations herein within the investigated pressure range. All micro-additive formulations investigated increased the burning rate at pressures ranging from roughly 13.45- 17.24 MPa (1,950-2,500 psi) and 4.50-8.60 MPa (650-1,250 psi) for micro-TiO_2 and micro-Fe_2O_3, respectively; and these effects were dependent on the catalyst mass loading.

The nano-formulations increased the burning rate at pressures greater than 11.27 (1,620 psi) and 8.27 MPa (1,200 psi) for nano-TiO_2 and nano-Fe_2O_3, respectively.

195 Understanding Thermochemical Aspects of the Magnesium Metal Fuel Subjected to Hygrothermal Aging with Varied Oxygen Flow Rates

Oh, Juyoung; Yoh, Jack J.*

For transition towards low-carbon systems to resolve the fossil fuel-related environmental concerns, researches on metal fuels, which can generate heat energy without CO_2 formation, have been produced recently. The current study focused on Mg and performed thermochemical analysis to investigate the aging effects on thermal properties as well as combustion efficiency. The aged Mg commonly showed reactivity degradation. Also, a kinetic analysis combining statistical information on the activation energy for Mg was newly provided. Firstly, hygrothermally aged Mg showed decreasing trend of activation energy in the O_2-lean condition by the creation of hydroxides as aging products. However, thermally aged Mg effectively reacted at the O_2-rich condition due to the formation of more oxides. Thus, the observed results revealed that changes in reaction paths and degraded thermochemical characteristics can occur upon the exposure of Mg to moisture.

123 Experimental Evaluation of Plain Metal Additives for Solid-Fuel Propulsion Applications

Thomas, James C; Rodriguez, Felix A; Petersen, Eric*

Hybrid rocket engines (HREs) have unique advantages in comparison to pure solid or liquid propellants, but several drawbacks have hindered their widespread adoption. Inclusion of energetic additives can increase fuel regression as well as improve performance (specific impulse or density specific impulse). The current study aimed to evaluate alternative, potential metallic additives for use in HREs and SFRJs alongside standard aluminum and boron particles. This objective was completed through an in-depth theoretical performance analysis focused on HRE applications followed by a series of ballistic experiments completed on a lab-scale HRE. Theoretical analyses and ballistic results indicate Zirconium metal is superior to standard aluminum- or boron-based additives. In addition, this study has directly correlated combustor residence time to the combustion efficiency in HREs or SFRJs.

Thursday 14:15 – Ignition II

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35 A Study on Influences of Hydrogen addition and Turbulence on Ignition Characteristics of Propane Mixtures

Nakahara, Masaya; Tanimoto, Kodai; Kudo, Hisanobu; Abe, Fumiaki; Tokunaga, Kenichi*

This study is performed to investigate the effect of hydrogen addition on properties of ignition and flame-kernel development in both quiescence and isotropic and homogeneous turbulence, in order to examine the improvement of ignition and combustion caused by hydrogen addition to propane mixtures in a high-intensity turbulence field. The mixtures with different equivalence ratios (0.5~1.4) and hydrogen additional rates are used while maintaining the laminar burning velocity (25 or 15 cm/s). First, in quiescence, the influence of hydrogen addition on the minimum ignition energy (MIE) as well as the burning velocity characteristics of meso-scale outwardly propagating spherical flames is examined in a constant volume vessel. Then, the influence of turbulence on MIE is examined over a wide range of turbulence intensity (~1.79m/s). This study also focuses on assessing the presence of MIE transition by using the turbulent Karlovitz number based on the burning velocity of meso-scale flames.

17 Real Gas Effect on Ignition Characteristics in Ideal and Non-ideal Reactors

*Weng, Z.; Li, Zongtai; Mevel, Remy**

We studied the real gas effect on the ignition characteristics in ideal and non-ideal reactors with one-step irreversible reaction. The real gas effect, characterized by the finite molecular volume, was described with the Noble-Abel equation of state. The non-ideal pressure variation in shock tube (ST) and rapid compression machine (RCM) were accurately reproduced with a linear function and a logarithmic function, respectively. In all cases, the real gas effect promotes ignition. In ST, the non-ideal process couples with the real gas effect to further reduce the ignition delay-time. On the contrary, in RCM, the expansion caused by heat loss diminishes the real gas effect. The heat capacity ratio becomes important when the non-ideal pressure change is strong. In practice, the non-ideal effect has larger impact on ignition for longer test time. However, the real gas effect becomes the dominant factor when the dimensionless covolume parameter reaches 0.1 or above.

51 Incompletely Stirred Reactor Network Modeling for the Estimation of Turbulent Non-Premixed Autoignition

Iavarone, Salvatore; Gkantonas, Savvas; Mastorakos, Epaminondas*

Autoignition in turbulent reactive flows is a problem of great importance and practical interest. The understanding of the complex interactions between turbulence, micro-mixing and chemistry, leading to autoignition, is crucial to the design of several combustion devices, especially when highly reactive fuels are used. In this work, an Imperfectly Stirred Reactor Network (ISRN) approach is employed to predict the autoignition of hydrogen in a turbulent co-flow of preheated air. The ISRN equations are solved in post-processing on top of a well-resolved inert flow LES of the axisymmetric hydrogen plume. The effects of non-adiabatic conditions and differential diffusion on the prediction of autoignition lengths are studied. The results show that the approach can well capture the autoignition behaviour of hydrogen and that the autoignition location is sensitive not only to the inlet air temperature but also to the average wall temperature and the presence of differential diffusion.

220 Effect of Flame Front Thermo-Diffusive Instability on Flame Acceleration in a Tube

Hok, Jean-Jacques; Dounia, Omar; Vermorel, Olivier; Jaravel, Thomas*

Numerical simulations of lean hydrogen-air explosion scenarios in tubes are considered. The competing effects of two acceleration mechanisms are investigated: finger-flame effects and flame front thermo-diffusive instabilities. While the former effect is observed for any flame ignited in a tube, the latter is specific to subunity-Lewis number mixtures which include lean hydrogen-air mixtures. Two chemistries are considered, the only difference being transport properties: a unity-Lewis number scheme which is free of thermo-diffusive phenomena, and a ""realistic""-Lewis number scheme which is subject to instabilities. By carrying out simulations in 3 tubes of different radii and comparing both cases with a theoretical finger-flame propagation, it is shown that unity-Lewis number cases show a good agreement with theory, whereas realistic-Lewis number simulations go faster due to additional wrinkling by the instabilities. Besides, this effect is dependent on the tube radius.

184 Investigation of Iso-Propyl Nitrate as a Detonation Improver

Mousse Rayaleh, Ayan; Burnett, Miles A; Abid, Said; de Persis, Stephanie; Comandini, Andrea; Wooldridge, Margaret S; Chaumeix, Nabiha*

This study aims at studying the sensitizing effect achieved by the addition of IPN on propane in the presence of oxygen and the dilution with nitrogen in the framework of Pulsed Detonation Engine (PDE) applications. It consists of studying the shock-to detonation-transition (SDT) process in a 78 mm diameter tube in order to reduce the distance and transition time. The shock to detonation transition is monitored via 22 fast shock and pressure transducers. The stoechiometric C_3H_8/O_2 and $C_3H_8/O_2/N_2$ were studied at 2 differents initial pressure, 6.7 kPA and 13.3 kPa. The addition of IPN proved to be very efficient in increasing the sensitivity of propane mixtures. Detonation cell size were measured for non-diluted mixture.

130 Numerical Study of Multi-Dimensional Effects on the Transition to Detonation From Subsonic Self-Ignition Waves Propagating at Constant Speed

*Taileb, Said; Rougon, Emmeline; Chinnayya, Ashwin; Robin, Vincent**

This paper describes the initiation of a cellular detonation structure from initial subsonic spontaneous ignition waves. The originality of the numerical simulations lies in the carefully defined initial condition: a constant gradient of induction times, inducing a constant spontaneous wave velocity. The initially very low speed of the reactive front produces weak compression waves that have negligible effects on the fresh gases conditions. Thus, the self-ignition front propagating in 1-D space cannot induce any transition. However, their multi-dimensional counterpart exhibits a combination of hydrodynamic effects leading to localized flow accelerations, hot spot generation and eventually transition to detonation. Therefore, these results highlight the key mechanisms behind the early development of a cellular detonation structure.

194 The Effect of Buoyancy on Flame Acceleration in Hydrogen-Air Mixtures: Experiments in Horizontal and Vertical Tubes

Bezgodov, Evgenii; Simonenko, Vadim; Kirillov, Igor*

Accidents at large-scale production facilities or hydrogen storages can result in the release of large amounts of pure hydrogen. When mixing with air, hydrogen generates explosive mixtures, which can lead to significant damage to infrastructure or injure the staff of the facility. One of the important tasks of improving safety is to clarify the limit of self-propagating deflagration combustion, capable of transition to fast flames. The work gives the results of the first experiments on the BM-T facility designed to determine the acceleration limits of flames from slow to fast flames in homogeneous hydrogen-air mixtures for horizontal and vertical tube orientations. A decrease in acceleration limit was revealed in the vertical tube. This indicates the influence of gravitation force on flame acceleration process, which is likely to be considered when adjusting the existing criteria and flame acceleration limits.

Thursday 14:15 – RDE VII

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139 Detonations and Thermoacoustic Modes in a Flow through RDC

Gutmark, Ephraim J; Anand, Vijay; Betancourt, Jorge; Gaetano, Alec; Pritschau, Tyler; Wiggins, Rachel*

Rotating detonation combustors (RDC) can operate in stable detonative mode with single or multiple waves or in deflagrative thermoacoustic modes, depending on the air and fuel flow rates. A flow through RDC was studied using ethylene and air. The tests utilized azimuthally distributed high frequency response pressure transducers to track the evolution of the rotating combustion waves and determine the operating mode. High-speed imaging taken from the back side of the combustor was used to visualize the internal combustion dynamics. The pressure transducers and high-speed imaging complemented each other and provided information for the identification of the operating modes of RDCs. Spectral proper orthogonal decomposition (SPOD) analysis and a spaciotemporal analysis of the high-speed video were applied to determine the operative modes and the deflagration to detonation process present for

different combinations of air flow rates and equivalence ratios of the flow through RDC.

243 State-to-State Model for Rotating Detonation Combustors

Gamba, Mirko; Feleo, Alexander; Shepard, Joshua; Chacon, Fabian*

This work presents a model for predicting the performance of rotating detonation combustors (RDCs). The model is based on a (thermodynamic) state-to-state description of the flow evolution in the RDC connected by elementary processes. The model is intrinsically a lump-state model, and it may provide only a global and qualitative insight into the performance of RDCs and its dependence on operating details which may be useful for engineering evaluations. The goal of this work is to develop the model, demonstrate its use for parametric studies on hypothetical systems and apply the model against operations RDCs to attempt its validation.

29 Experimental Results for 25-mm and 51-mm RDRE Combustors

Knowlen, Carl; Mundt, Tyler; Kurosaka, Mitsuru*

The RDRE program at the UW is investigating the influence of annulus radii on combustor operating characteristics. To facilitate isolation of all but radius of curvature effects, the annular gap was kept constant at 5 mm in combustors having either 25-mm or 51-mm O.D. The injectors were scaled so that their net injector-to-gap area ratio was constant at AR = 0.11. Geometric scaling was investigated with experiments having the same range of mass flux (80 $kg/s/m^2$ to 500 $kg/s/m^2$) and equivalence ratio ($0.25<ER<2.5$) of gaseous CH4-O2 propellant. Results showed that at any mass flux where stable 2-wave operation was established in the 51-mm-RDRE, stable 1-wave operation would occur in the 25-mm-RDRE. Stable 1-wave operation was established in the 51-mm-RDRE at mass fluxes of 240 $kg/s/m^2$ and below. Under these conditions, however, a counter-rotating wave appeared in the 25-mm-RDRE while it operated with a single dominant wave.

Thursday 14:15 – Shock Tube I

15 Shock-tube Study of the Ignition of Fuel-Rich CH4/ or Natural Gas/Ozone/Air Mixtures at High Pressure

Herzler, Jurgen; Fikri, Mustapha; Schulz, Christof*

The influence of ozone on the ignition delay times of methane and natural gas was determined in a high-pressure shock tube at fuel-rich conditions (equivalence ratio of 2) and pressures of about 30 bar. The measured ignition delay times agree very well with simulations using the AramcoMech 3.0 (Zhou et al., Combust. Flame 197 (2018): 423) complemented by ozone reactions of Zhao et al. (Combust. Flame 173 (2016): 187). A strong decrease of the ignition delay times was observed for temperatures below 1100 K. The influence of 600 ppm ozone was similar to the influence of 7000 ppm of other additives (n-heptane, dimethyl ether, diethyl ether, dimethoxymethane). The results are important to develop and optimize polygeneration concepts in an ICE and show that relative expensive additives like ethers can be replaced by on-line produced ozone at lower costs. Further ignition delay and product measurement studies at an equivalence ratio of 10 with ozone as additive will be performed.

95 Simultaneous CO and H2O Laser Absorption Measurements of Pentene Isomers in a Shock Tube

Gregoire, Claire M; Westbrook, Charles; Mathieu, Olivier; Cooper, Sean P; Alturaifi, Sulaiman; Petersen, Eric*

Treatment of the full group of C5 olefins is presented with new measurements on 1-pentene, 2-pentene, and 3-Methyl-1-Butene combined with published data obtained in similar conditions on 2-Methyl-2-Butene from Alturaifi et al. and 2-Methyl-1-Butene from Gregoire et al. This extensive experimental database contains carbon monoxide and water time-history profiles. The oxidation of the five pentene isomers was carried out at three equivalence ratios in mixtures diluted in 99.5% Helium-Argon. The experiments were performed for temperatures ranging from 1400 to 1900 K near atmospheric pressure. A unique comparison of the complete set of C5 pentene isomers permits the understanding of the C=C double bond position and branching impacts on combustion properties. Numerical predictions using up to 6 models available in the literature were performed. An error score function shows that Dong et al. and Gregoire et al. performed the best and are accurate within 13% accuracy overall for all isomers.

209 Probing PAH Formation from Cyclopentene Pyrolysis in a Single-Pulse Shock Tube

CARNEIRO PITON, Leticia; Hamadi, Alaa; Cano, Fabian; ABID, SAID; CHAUMEIX, Nabiha; Comandini, Andrea*

The pyrolysis of cyclopentene (CYC5H8) and CYC5H8+acetylene is studied in a shock-tube coupled to gas chromatography/mass spectrometry techniques under highly argon-diluted conditions with the goal of providing new experimental information about the polycyclic aromatic hydrocarbon (PAH) formation from cyclic C5 species. Experiments are carried out at a residence time of 4 ms, a pressure of 20 bar, and temperatures from 940 to 1650 K. An ongoing detailed PAH kinetic model is updated to successfully capture the fuel decomposition, the formation of small hydrocarbons, and main PAH products. CYC5H8 mainly decomposes into linear pentadiene and cyclopentadiene. In all the datasets, small hydrocarbons mainly come from the consumption of pentadiene, and the channels leading to PAHs basically originate from reactions of cyclopentadienyl radical with other intermediates and resonantly stabilized radicals. The comparison between experimental and simulated results data is overall satisfying.

233 Probing Pyrolytic PAH Chemistry in High-Repetition-Rate Shock Tube Coupled to Synchrotron-Based Double Imaging Photoelectron/Photoion Coincidence Spectroscopy

Cano Ardila, Fabian E; Nagaraju, Sharath; Tranter, Robert S; Abid, Said; Desclaux, Anthony; Roque, Anthony; Chaumeix, Nabiha; Comandini, Andrea*

The first pyrolytic study on aromatic chemistry performed with the HRRST/i2PEPICO techniques is presented, illustrating the capabilities of such techniques on the PAH formation chemistry that cannot be achieved with regular analytic studies. In this work, are reported the decomposition of 0.1% toluene in argon at a T5 and P5 of 1488 K and 7.6 bar. Two different series of experiments have been performed: (i) pulsed mode (reflected shock time identified) with more than 100 000 runs at an ionization level of 10 eV and (ii) continuous mode with more than 40 000 runs at an ionization level of 8.5 eV. Well defined MS and the evolution of the species profiles during the pyrolysis of toluene have been obtained (from light species up to 5-member rings). In the continuous mode, PES was obtained for some PAHs which allowed the identification of isomers which could not have been done without i2PEPICO. This work also exemplifies the need of high repetition rate shock tubes to perform such studies

Thursday 16:20 – Condensed Phase Detonation II

60 Effect of Microstructure on Detonation Performance of the Insensitive High Explosive PBX 9502

Voelkel, Stephen; Anderson, Eric Karl; Short, Mark; Chiquete, Carlos; Jackson, Scott I*

We investigate the detonation performance of virgin and recycled lots of PBX 9502. PBX 9502 is polymer-bonded high explosive (HE) with 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) as the HE crystal bound with KEL F-800 or FK-800, a co-polymer of chloro-trifluoro-ethylene and vinylidene-fluoride. PBX 9502 consists of 95 wt.\% TATB with 5 wt.\% KEL-F 800 (FK 800), Recycled lots of PBX 9502 generally have a higher percentage of finer TATB particles compared to virgin lots. We describe new detonation performance characterization rate-stick and cylinder expansion tests on two virgin and two recycled lots. Modeling of both the detonation timing and detonation products equation of state shows that the metal push capabilities are very similar between the virgin and recycled lots, but that detonations in virgin lots, on average, run slower than those in recycled lots. We surmise that this is due to a slower rate of reaction in virgin lots associated with the larger TATB particle sizes.

266 Using a High Speed Hyperspectral Camera to Measure Gas Temperature And Concentration Profiles Resulting From Detonation of TNT

*Gagnon, Jean-Philippe**

The measurement of physical properties of expanding gases in the infrared region following a high-explosive detonation requires cameras having both high framerate and fine spectral resolution. To achieve this goal, a Telops MW Fast-M350 high-speed broad-band camera and a Hyper-Cam-MWE hyperspectral camera were used to capture such energetic, fast-changing events. Moreover, an accurate gas model is required to adequately explain and quantify the rapidly-evolving events based on properly-interpreted gas emissivity signatures. The constrained detonations took place in a closed explosion chamber at ADD (Agency for Defense Development)'s facility. They consisted of ~ 100 g of TNT or C4 explosives, initiated by a small amount of Booster Comp. A5 (8 g) and DXC-56 (1.25 g). The method is thus able to extract gas (CO2, H2O, CO, HCl, NO) temperatures and concentrations as a function of time from the initial explosion.

110 Initiation of Sympathetic Detonation between two Separated PETN charges

Murray, Desmond; Vashishtha, Ashish; Lenihan, Donncha; Callaghan, Dean ; Nolan, Cathal*

This study is motivated to understand sympathetic detonation by modelling and simulating it and establishing the models to estimate the required donor charge to dispose of the given munition. The experiments are carried out for two separated bare charges of fixed masses, composed of plastic explosive such as Pentaerythritol tetranitrate (PETN). The 2D numerical simulations are carried out for the same and modelling parameters are adjusted to achieve the behaviour of sympathetic detonation similar to the results obtained from experiments. The main objectives of this study are: 1) Model sympathetic detonation of two separated PETN charges using open-source solver blastFOAM, 2) Perform a parametric numerical study to accurately model sympathetic detonating of PETN charges as observed in experiments 3) Develop an understanding of the dynamics of shockwaves, which leads to sympathetic detonation of an acceptor charge, based on different charge sizes and the gap between acceptor and donor.

Thursday 16:20 – Shock Tube II

54 The Effect of Oxygenated Species on the Fuel-Rich Oxidation of Ch4 in the Context of Polygeneration: Extinction, CO-concentration and Temperature Measurements

Nativel, Damien; Herzler, J rgen; Fikri, Mustapha; Schulz, Christof*

Fuel-rich mixtures of methane, methane/DEE and methane/methanol were studied under oxidative (phi = 5) conditions behind reflected shock waves at ~ 5 bar and in the range of 1484÷1875 K. Pure methane mixtures (10 mol%) were first studied and DEE and methanol were then used as additive (1 mol%). The mixtures were diluted in helium/argon. Time-resolved CO concentration and temperature measurements were obtained using two continuous quantum-cascade lasers to account for temperature variations. The CO concentration was determined from absorption measurements using the highly sensitive P(8), v'' = 0 transition at 4.73 μm. The two fundamental vibrations of CO (v'' = 0, P(8), 4.73 μm and v'' = 1, R(21), 4.56 μm) were selected for ratiometric temperature measurements. In addition, extinction measurements were performed using a He-Ne laser to measure soot inception times and the resulting optical density at 633 nm. The results were compared with simulations based on detailed kinetics mechanisms.

49 Ignition of Lubricating Oils using a Novel Spray Injection Technique in a Shock Tube

Cooper, Sean P; Petersen, Eric*

Lubricant ignition is a highly undesirable event in any mechanical system. Gas turbines in particular require lubrication in high-temperature environments, increasing the possibility of lubricant auto-ignition. Understanding this event and how to prevent it requires a fundamental understanding of the ignition kinetics of these lubricants. To this end, a novel spray technique using an automotive injector in a shock tube was developed. Using this new experiment, ignition of Jet-A and a gas turbine lubricant (Mobil DTE 732) was observed using an OH* chemiluminescence diagnostic at the sidewall location of the shock tube. Comparison of Jet-A results with the literature show good agreement. A combination of an extended shock-tube driver and driver-gas tailoring were utilized to observe ignition for a wide range of temperatures and ignition delay times at near-atmospheric pressures. A clear, two-stage-ignition process was observed for lubricant tests.

180 Probing PAH Formation from Heptane Pyrolysis in a Single-Pulse Shock Tube

Hamadi, Alaa; Cano, Fabian; Carneiro Piton, Leticia; Abid, Said; Chaumeix, Nabiha; Comandini, Andrea*

With the goal of improving our capabilities to model surrogate fuels, in particular in relation to PAH and soot formation, the pyrolysis of n-heptane is studied in a single-pulse shock tube over a broad range of temperatures (900-1700 K) at 20 bar nominal pressure and 4 ms residence time. Three different initial fuel mole fractions were considered, 100, 500, and 2000 ppm of n-heptane in argon. Fuel and intermediate species, including aromatics up to phenanthrene, are measured using gas chromatography and mass spectrometry. An ongoing detailed chemical kinetic model for PAH chemistry has been updated to successfully capture the fuel decomposition, the formation of small hydrocarbons, and the concentration of the main PAH products. Major reaction pathways to PAHs are discussed as well as the role of important intermediate species.

65 Reduced Order Modeling of 2-D Reaction-Diffusion System Based on POD-DEIM and k-means Clustering

Cutillo, Enrico Alberto; Petito, Gianmarco; Bizon, Katarzyna; Continillo, Gaetano*

In this work, the method of Proper Orthogonal Decomposition (POD) is applied to a problem of self-ignition of a coal stockpile, described by two-dimensional reaction-diffusion equations, to create a Reduced Order Model (ROM). To improve the ROM performance, different sampling strategies, clustering and Discrete Empirical Interpolation Model (DEIM) nodes collocation are studied. Various ROMs are compared against each other by drawing the resulting solution diagram as a function of the nondimensional activation energy ? . The POD-DEIM model reproduces the reference Full Order Model (FOM) solutions with high accuracy and much lower computational cost: in fact, combination of DEIM and k-means clustering constructs a global basis for the reproduction of the FOM solution diagram, which reduces up to 1020 times the computational time for the calculation of one solution, and catches all of the bifurcation points found with the FOM, thus showing quantitative and qualitative agreement.

135 Numerical Method Based-Cellular Automata for Heat Transfer with Application to the Self-Ignition of Energetic Materials

Violet, Alix; El-Tabach, Eddy; Gillard, Philippe; William-Louis, Mame*

This study relates to the development of a program based on cellular automata (CA) for the simulation of the combustion in condensed and heterogeneous phase of powdery energetic materials representative of pyrotechnic compositions.

The originality of the CA used in this work is that they take into account the heterogeneity of the pyrotechnic compositions and their random stacking.

The developed program makes it possible to solve the unsteady heat equation numerically in 2D by discretizing the studied field and by involving the surface thermal resistances between each cell. It also takes into account redox reactions thanks to Arrhenius's law.

The program was validated by comparing the results of the CA with experimental tests. The effectiveness of CA was also shown by comparing its results with those of the Frank-Kamenetskii self-ignition model.

215 Hydrodynamic characterization of the aging induced performance degradation of HMX-based explosive PBX 9404

Jackson, Scott I; Chiquete, Carlos; Anderson, Eric Karl*

Deployed explosives generally consist of formulations of several different compounds to achieve specific requirements. During storage, some compounds can chemically interact to reduce their chemical potential energy. Nitrocellulose formulations are of particular concern and much analysis has focused on energy loss of aged PBX 9404 explosive, which contains both HMX and nitrocellulose. This work builds on prior efforts by using modern detonation performance modeling methodologies and higher fidelity calibration processes in a hydrocode framework. Consistent with prior work, linear regression of the modeled energy delivery at relevant fixed specific volumes shows a measurable decrement in explosive energy and Chapman-Jouguet (CJ) pressure with explosive age. While there is uncertainty in the magnitude of the energy loss rate due to the sparse dataset, this analysis confirms degradation of both the explosive energy content and detonation CJ pressure with age.

196 A Modeling of Metalized Solid Fuel Surface Combustion

*Choi, Hong-Suk; Han, SangYeop; Yoh, Jack J.**

We revisit the complex surface burning dynamics of metalized energetic materials where the micro and nano metal particles interact with the oxidizer during a highly complex process that takes place in three specific regions: the outflow region composed of hot product gas with gasified metal particles exposed to the air, the melt layer comprised of reacting particles with oxidizers in condensed phase, and the solid inner layer kept at temperature below melting point of the energetic compound under investigation. We focus on modeling the melt layer by introducing two separate domains. The hot product gas expansion is allowed in one domain while the structurally deforming particles are independently simulated for proper description of the surface burning via using the level sets and the reaction rate law constructed from calorimetry for a target pyrotechnic substance, zirconium potassium perchlorate (ZPP).

55 Laser Ignition of a Low-Vulnerability RDX-based Propellant: Influence of the Atmosphere on Ignition and Combustion Properties

Delbarre, Samuel; Courty, Leo; Gillard, Philippe*

Designed to increase safety of people and property during their different stages of life (storage, transportation, handling), Low-Vulnerability Ammunition (LOVA) can lead to ignition issues during their use. Ignition and combustion characteristics of a LOVA RDX-based gun propellant are experimentally investigated in this paper. The ignition is performed by a laser diode and combustion is studied in a closed-volume reactor for different initial pressures (10 to 60 bar) and laser powers (1.43 to 9.95 W). Present study especially

focuses on the influence of atmosphere nature: new results under synthetic air are compared with results previously obtained under argon and nitrogen. Air appears to be an enhancer for overpressures and propagation rates with this kind of propellant. Higher combustion properties under argon compared with nitrogen had already been noticed. Ignition delays and probabilities, as for them, seem to be more sensitive to laser power than to atmosphere nature.

79 Characterization of High Pressure Electrolytic Decomposition of Hydroxylammonium Nitrate Aqueous Solution using FTIR

Wu, Ming-Hsun; Lao, Kuan Io; Chou, Yu-Ting*

Experiments were conducted to reveal the effects of pressure on electrolysis of 76 wt.% HAN aqueous solution. Electrolytic approach was feasible to ignite HAN even under room pressure. The higher the pressure applied, the more vigorous was the reaction. HAN is so pressure-sensitive that it may undergo various reaction pathway under different initial pressures, bringing out major products of the same species but different intensity.

Friday 9:00 – Detonation Boundary Interaction

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66 Influences of a Small Step on the Side Wall upon Detonation Propagation

Seki, Yoko; Honda, Tomoaki; Kim, Wookyung; Johzaki, Tomoyuki; Endo, Takuma*

The influences of a small obstacle on the side wall upon the detonation cellular pattern were studied, where forward-facing steps and slopes, and backward-facing steps and slopes were used, and their height was in the same order of magnitude as the detonation cell width. The forward-facing steps and slopes created negligibly small influences. However, the backward-facing steps created influences of the enlargement of the cellular pattern and subsequent re-initiation phenomenon followed by finer cellular pattern, which relaxed to the cellular pattern of the steady detonation downstream about ten times the distance between the step and the re-initiation position. In the cases of the backward-facing slopes, the influences by the 40-degree slope were similar to those by the backward-facing steps. However, the influences by the 20-degree slope were qualitatively different, where the cellular pattern did not disappear and the detonation continued to propagate.

98 An Immersed-Boundary Projection Method for Studies of Detonation Waves Interacting with Thin Obstacles

Lu, Xiaoyi; Yu, Hang; Pantano, Carlos; Oran, Elaine*

Numerical simulations on Cartesian grids for supersonic flows interacting with solid structures routinely use cut-cell methods or sharp-interface immersed boundary methods (IBM). Both are capable of modeling complex geometries of either rigid or elastic bodies. However, there are difficulties in treating thin obstacles. In contrast, direct forcing IBM based on a projection method, where singular forces are computed implicitly on immersed surfaces, is well-suited. A new IBM of this category has been recently developed for compressible viscous flow simulations of parachute systems. This method allows any well-posed boundary conditions imposed on arbitrarily irregular and thin obstacles, including Dirichlet-type slip, non-slip, isothermal wall conditions, and Neumann-type heat flux conditions. The present work implements this method with a shock-capturing scheme for reactive Euler equations and performs a preliminary study on detonation waves interacting with thin obstacles.

202 Experiments of the Tri-arc Non-Circular Rotating Detonation Engine (RDE)

*Lee, Eun Sung; Han, Hyung-Seok; Kim, Jung-Min; Lee, Jae-Hyuk; Choi, Jeong-Yeol**

RDE is a combustor where the compression effect by the detonation wave provides the thermodynamic cycle efficiency to generate enough useful work to be called an "engine". However, no rotating parts such as compressor and turbine are required in a "rotating" detonation engine, but only the detonation wave is moving around a closed channel. Thus, no geometrical constraint of circular configuration is imposed except the closed channel. Non-circular geometrical flexibility would be useful for the design of a propulsion system that could be installed into the airframe designed for optimum stealth characteristics or aerodynamic performance. The present work will further discuss the recent experimental results on the characteristics of detonation propagation in non-circular 'Tri-Arc' RDE.

Friday 9:00 – RDE VIII

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112 Development of an Automatic-Calibrating Small-Scale Thrust Stand for Rotating Detonation Rocket Engines

Kotler, Adam R; Burke, Robert F; Rezzag, Taha; Ahmed, Kareem*

The Rotating Detonation Engine has been seen as the next step for rocket propulsion applications with the advent of the Rotating Detonation Rocket Engine, an engine configuration developed by the Air Force Research Laboratory. In an effort to flight-test this engine and provide a dataset to train detonation-based simulation, the Rotating Detonation Rocket Engine has been tested in a collaborative effort including the University of Central Florida. For this testing, a thrust stand was developed to obtain the key thrust and impulse data necessary for advancing the engine to flight readiness. This thrust stand utilized the small-scale of the Rotating Detonation Rocket Engine to motivate an axial-loading measurement approach and the integration of an automatic-calibration subassembly, altogether which allows for incredibly accurate thrust measurements from an engine. Results using this thrust stand have been validated with identical engine configurations at other research laboratories.

201 Experimental Study of the Miniaturized Cylindrical Rotating Detonation Engine

Hattori, Karin; Ota, Kosei; Ishihara, Kazuki; Goto, Keisuke; Itouyama, Noboru; Watanabe, Hiroaki; Kawasaki, Akira; Matsuoka, Ken; Kasahara, Jiro; Matsuo, Akiko; Funaki, Ikkoh*

A small combustor with an inner diameter of 16mm and a different bottom shape was fabricated, and the combustion cross-sectional area considering the boundary layer at the outlet surface was measured from the appearance during combustion. As a result, there was no difference in combustion due to the shape of the bottom, and the ratio of the cross-sectional area of combustion to the cross-sectional area of the combustor was 0.75~0.85. The cross-sectional area of combustion including the thickness of the boundary layer was substituted into the theoretical values of combustion pressure and thrust, and the validity was confirmed with the ratio of that was 0.8.

166 Investigation of Wave Velocity in a Hybrid Rotating Detonation Engine

Assad, Mohamad; Penyazkov, Oleg; Chernukho, Ivan*

In this work, a new scheme of a jet engine using the detonation principle of fuel combustion is proposed - a hybrid detonation engine (HDE) which is a symbiosis of a turbojet engine and a detonation module operating on liquid fuel (jet fuel, heptane, etc.). The features of propagation of the combustion wave in the detonation module are investigated. It is shown that with a pulsed supply of jet fuel, air and oxygen, the wave velocity reaches 1200 m/s. A continuous flow of air with a pulsed supply of jet fuel and oxygen leads to wave acceleration up to 1800 m/s, while the thrust of the HDE increases by almost 25%.

239 Wall Heat Flux Measurements behind a Shock Wave Generated by a Detonation

Virot, Florent; Quintens, Hugo; Boust, Bastien; Sotton, Julien; Bellenoue, Marc*

A detonation driven shock tube is used for studying the influence of the shock velocity on the wall heat flux generated during its propagation. Stoichiometric H_2/O_2 driver initial pressure is varied from 50kPa to 100kPa to generate a shock between Mach 2 and Mach 3 in air initially at atmospheric conditions. Postprocessing temperature of type-E eroding surface thermocouples gives wall heat flux peaks from 3 to 19 MW/m2.

Friday 9:00 – Multiphase III

250 Experimental Investigation of Reacting Fuel Droplets Interactions with Detonation Waves

*Dyson, Daniel; Arakelyan, Artem; Berube, Nicolas; Briggs, Sydney M; Ramirez, Jonnathan; Ninnemann, Erik; Thurmond, Kyle; Kim, Gihun; Green, William; Udaykumar, H.S.; Menon, Suresh; Vasu, Subith**

The current study investigated the effects of a sustained detonation wave on an isopropanol droplet in a detonation tube environment. The detonation waves were initiated using a methane-oxygen mixture. Two sets of high-speed images were recorded for detonation waves traveling through mixtures with equivalence ratios of 1.0 and 0.9 at a frame rate of 340,000 fps and 900,000 fps, respectively. The initial temperature and pressure in the detonation tube were 293 K and 760 torr, respectively. The results show that the displacement, deformation, and disintegration of the isopropanol droplets are comparable to previous studies investigating the interaction of shock waves on water droplets and on liquid fuel droplets. This may imply that the droplet disintegration process may be largely independent of the presence of combustion.

150 Numerical Study of Multi-Dimensional Liquid-Fuel n-Dodecane/Air Detonations with Complex Chemistry

Dammati, Sai Sandeep; Kozak, Yoram; Poludnenko, Alexei*

Understanding liquid-fuel detonations is critical in a variety of practical systems, e.g., novel detonation-based engines or vapor-cloud based industrial explosions. The presence of a liquid spray introduces physical effects not present in gas-phase systems such as droplet-gas interactions, droplet break-up, and evaporative cooling. Here we present a two-dimensional simulation of a spray detonation in a n-dodecane/air mixture. The simulation is carried out in a Eulerian-Lagrangian framework and for the first-time it uses realistic 24-species chemical kinetics along with the detailed models for droplet drag, heat transfer, and evaporation. In contrast with a gas-phase case, a liquid-fuel detonation has much larger induction and exothermic lengths primarily due to relatively slow droplet evaporation. This results in a more stable detonation propagation and larger resulting cell size. We also discuss directions to improve the realism of numerical modeling of detonations in liquid sprays.

165 Numerical Analysis on the Breakup of Dilute Water Spray in Gaseous Detonation

Watanabe, Hiroaki; Matsuo, Akiko; Chinnayya, Ashwin; Matsuoka, Ken; Kawasaki, Akira; Kasahara, Jiro*

The 2D numerical simulations based on an Eulerian-Lagrangian method were conducted to model a gaseous detonation laden with polydisperse water droplets (WDs). The premixed mixture was a stoichiometric hydrogen oxygen slightly diluted with nitrogen mixture at low pressure. The behavior of polydisperse WDs behind the leading shock front was analyzed. The distribution in droplet diameter was regularized by breakup process behind the leading

shock front, and the polydispersity in the final droplet diameter came from the cellular instabilities and the degree of the change in the dynamic pressure during the breakup process, depending on the initial droplet diameter. In addition, the outcome of the breakup process was deviated from the estimation based on the post-shock condition. Indeed, the average relative dynamic pressure between the front and the point where the breakup completes should be used for the better estimation as Dabora et al. (Proc. Combust. Inst. 12 (1969) 19-26) suggested.

252 Steady and Transient One-Dimensional Simulations of Multiphase Dodecane/Air Detonations

Tricard, Nicolas J; Ghosh, Abeetath; Dammati, Sai Sandeep; Poludnenko, Alexei; Zhao, Xinyu*

Two independent models of 1-D spray detonations have been developed in this study. One offers steady-state, computationally inexpensive analysis of detonations with ZND-type structure under a variety of conditions. Another offers transient modeling with accurate molecular diffusion and viscous effects. The two models are run with equivalence ratios of 1.0 and 0.7, and appropriate comparisons are made. Post-shock temperature, pressure, density, velocity, fuel mass fraction, and heat release rates match well for 10- and 20-micron droplets, even with differing droplet heating and vaporization models. The steady-state model cannot capture the pulsation that is associated with the 5-micron droplets at equivalence ratio 0.7 in the transient simulation. Future work includes matching the models between the two solvers and studying the detonation limits under lossy conditions.

Friday 11:05 – Propulsion Application

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45 Baffled-Tube Ram Accelerator Operation with Methane-Air Propellant

Knowlen, Carl; Leege, Brian; Correy, John; Smith, Chase; Higgins, Andrew*

The baffled-tube ram accelerator (BTRA) is a device for accelerating axisymmetric projectiles through a tube utilizing gaseous combustible mixtures. Continuous BTRA operation with axisymmetric projectiles was demonstrated from 700 m/s to 1350 m/s (Mach 2.0 to 3.8) in CH_4 / O_2-enriched air propellant. The minimum entrance velocity was determined to be 700 m/s, which is 2.4% greater than the theoretical minimum in baffle chambers having an effective chamber-to-bore area ratio of 2.22. With polycarbonate projectiles, the thrust decreased with increasing Mach number more than predicted by theory in 4-m-long BTRA experiments. These experiments have shown that the BTRA operates effectively and reliably over a relatively wide range of conditions. The results of experiments with methane-air propellant utilizing flat-faced baffles in a 38-mm-bore test apparatus are presented.

107 Thermodynamic Analysis of Unsteady Propulsion Systems

Fievisohn, Robert T; Stevens, Christopher A*

Unsteady detonative propulsion devices have the potential to increase thermodynamic efficiency over steady deflagrative devices. The basis of any study concerning these propulsion systems generally starts with a thermodynamic analysis. Paxson and Kaemming developed a control mass/volume approach to correctly conserve energy when analyzing a constant volume combustion cycle. This work extends these ideas to an idealized detonation cycle. Another goal is to develop a better understanding of how the unsteady, quasi one-dimensional Euler equations are used in the analysis of unsteady propulsion devices. An often over-looked term relevant to the ideal expansion of combustion products during a blowdown process is introduced. By carefully applying the correct form of the mass, momentum, and energy equations, new insights are developed in the thermodynamic analysis of unsteady propulsion devices. These insights lead to new questions and research topics for future work.

203 Operation Characteristics of a Disk-Type Rotating Detonation Engine

Ishii, Kazuhiro; Ohno, Kanta; Kawana, Haruhiro; Kawasaki, Kazuma; Hayashi, A. Koichi; Tsuboi, Nobuyuki*

In the present work, the behavior of rotating detonation waves in the disk-type rotating detonation engine with constant chamber area was experimentally studied for various total mass flow rates and a wide variety of equivalence ratios of hydrogen-air mixtures. From the visualization, the rotating detonation wave was found to propagate near the outer wall of the combustion chamber, regardless of the wave mode. In the present test conditions, single and double wave modes are observed, depending on the equivalence ratio of the mixture. The pressure gain was evaluated from the chamber static pressure measured with the CTAP technique. Although the present DRDE configuration provided the negative pressure gain in all the test conditions, it was found that the single wave mode was superior to the double wave mode in terms of the pressure gain.

Friday 11:05 – RDE IX

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88 Numerical Simulation of the Effect of the Array-hole Injection and Cavity Combustor on the Rotating Detonation Engine Performance

He, Xiaojian; Wang, Jianping; Liu, Xiangyang*

The subject of this paper is to use the discrete fuel injection model to simulate the discontinuous distribution of reactants in rotating detonation engine experiments, and the cavity combustor is also utilized in simulation to get a deeper insight about the performance of the cavity RDE. Four kinds of injection patterns are employed with inlet-area ratio 44.5%, 49.8%, 54.7% and 100%, and four RDE models of different cavity depths are employed. In case_C1h1 to case_C1h4, we can draw the conclusion that the array-hole injection pattern is the dominant factor that leads to the multi-DWC modes, and when the array-hole count increases, the DWC is getting close to 1. As the inlet-area ratios increases, the Fsp increase rate of model C4 is the highest initially, and later on it becomes the slowest, resulting in the lowest Fsp finally which is significantly less than that of cavity combustor, indicating the promising advantages of cavity RDE over traditional RDE in propulsive performance.

148 Effect of Preburn Inhomogeneities on the Detonation Velocity in a Rotating Detonation Rocket Engine

Vignat, Guillaume; Brouzet, Davy; Ihme, Matthias*

The Air Force Research Laboratory Rotating Detonation Rocket Engine is a modular laboratory-scale engine used to study oxygen-methane pressure gain combustion for space propulsion applications. In the present study, a large eddy simulation of this device is performed using a fully compressible solver on an unstructured hybrid mesh and using a multi-species finite rate chemistry model with a analytically reduced chemical scheme. The result reported show that there are vitiated pockets in the flow and that the velocity of detonation waves is low compared to the Chapman Jouguet value. To better understand the underlying reason for this discrepancy, a post-processing is developed to extract the local velocity of the wave and a local analysis of the wave velocity is performed by examining quantities on the upstream and downstream side of the shock. It turns out that the detonations are weak in the present simulation, and that the wave propagate mostly as a shock wave in burnt products.

185 Study of Fuel-Oxygen Mixing in a Rotating Detonation Engine Cold Analog

*McLoughlin, Michael; Gray, Scott; Ciccarelli, Gabriel**

The paper presents the results from an experimental study of detonation propagation through a combustible layer of hydrogen-oxygen in a 13 mm wide channel. The layer was generated by non-premixed injection of hydrogen and oxygen into the channel initially filled with argon at 1 atm. Schlieren video and soot foils were used to characterize detonation propagation. Simultaneous soot foils on both windows show that the detonation is asymmetric across the channel width. Numerical simulations of the gas injection system were carried out to predict the hydrogen-oxygen-argon mixing in the channel. The simulations showed that the higher momentum oxygen jet produces a hydrogen-oxygen wall jet on the window that cell structure was observed in the experiment. The results are directly applicable to mixing issues that can affect detonation propagation in RDEs.

Monday 11:25 and 16:15 – WiP Posters Session I

274 Preliminary investigations of the detonation-bow shock interaction: a pictorial essay

Sethu Venkataraman, Ashwath; S. Oran, Elaine*

AMRFCT is a newly developed multidimensional compressible fluid dynamics model optimized for solving the Euler and Navier-Stokes equations. The code combines a fully unsplit flux-corrected transport algorithm (FCT) to solve the reactive-flow conservation equations with a calibrated Chemical-Diffusive Model for the reaction source term. The effects of obstacles are included by coupling a cut-cell flux redistribution method with AMRFCT. We describe two-dimensional inviscid simulations performed with AMRFCT to study the interactions of high-speed objects with shocks and detonations for energetic gaseous mixtures. We describe how a detonation interacts with the shock structure generated by supersonic flow over two obstacles: a triangular prism and a circle. Various physical phenomena including detonation diffraction, energy deposition by shocks, change in cellular structure and flow expansion over obstacles are combined to develop a physical picture of the detonation-bow shock interaction.

287 The comparison of Favre average procedure for the gaseous detonation from Eulerian and Lagrangian point of view

Watanabe, Hiroaki; Matsuo, Akiko; Chinnayya, Ashwin; Itouyama, Noboru; Kawasaki, Akira; Matsuoka, Ken; Kasahara, Jiro*

Statistical approach is useful to analyze the results of unsteady multidimensional structures of detonation waves. In the previous Favre average procedures (Radulescu et al. (JFM 2007), Sow et al. (JFM 2014)), instantaneous 1D profiles were extracted from straight lines parallel to the propagation direction. However, the gaseous trajectories are not straight (Sow et al. (PROCI 2021)). Therefore, the average procedure from this Eulerian point of view needs to be compared with the Lagrangian one. Numerical 2D simulations with particle tracking were conducted. Although slight differences among the mean profiles could be observed near the front from the different averaging processes, the distribution of the chemical species was almost the same regardless of the instability of the mixtures tested. This means that the Eulerian Favre average procedure gives the mean structure of the gaseous detonation with a reasonable accuracy.

283 Numerical investigation of deflagration to detonation transition in smooth pipes

*Alzer, Tom; Engelmann, Linus; Sens, Marvin; Kempf, Andreas; Wlokas, Irenaeus**

The transition from deflagration to detonation (DDT) is a process highly relevant to the safe design of devices and facilities in chemical engineering. The DDT is difficult to predict, particularly in unconfined spaces and in smooth pipes and the numerical scheme must cover a wide range of Mach-numbers for this transient process. We present 2D and 1D simulations of DDT in H2/O2 mixtures. In an attempt to separate the effects which determine the onset of detonation, inviscid and viscous solutions were investigated for a large set of grid resolutions. From the results, a description of the flame acceleration is presented alongside a detailed description of the DDT. Besides, an attempt is made to describe the thermodynamics associated with the DDT using the *p,v*- and the *h,s*-diagram. The presented results give already a hint on the computational and model requirements required for a reliable prediction of the DDT in smooth pipes.

272 Recent Research on Rotating Detonation Engines supplied by liquid propellants at the Łukasiewicz - Institute of Aviation

Kawalec, Michał; Wolański, Piotr; Perkowski, Witold; Bilar, Adam*

The use of gaseous propellants to power Rotating Detonation Engines (RDE) is widely tested in many research centers around the world. Nevertheless, the use of liquid fuels is more promising from the point of view of aviation and space propulsion. This article describes the research of the rotating detonation process using mixtures based on liquid fuels. The results of the research on an air-breathing kerosene fueled combustion chamber are presented (a stable rotating detonation process was obtained without the use of any special admixtures). The use of rocket RDE allows to design lighter and smaller engines with lower pressures in the supply system. The development of liquid-propellants rocket RDE allowed to conduct the world's first successful rocket flight powered by RDE- only.

284 Water-Cooled Rotating Detonation Engine

*Fukuda, Takayuki; Sato, Kohei; Nagao, Takahisa; Itoh, Mitsunori; Dzieminska, Edyta**

In recent years, propulsion systems using detonation have been studied all over the world. Among them, rotating detonation engine (RDE) has the advantages of a simple structure and only one initiation compared with other types (i.e. pulse detonation engine). The purpose of this study is to contribute to the applied research of RDE by enabling long-time and stable operation, which is one of the problems to be solved nowadays. The detonation temperature is much higher than the heatproof temperature of the combustor, so it would melt the construction is a shot time without a proper cooling system. Therefore, by using a cooling system, the combustor is brought to lower temperatures guaranteeing a longer operation time. In this study, a water-cooled RDE was tested experimentally. A high-speed camera was used to record the state of detonation, a thermocouple to monitor the temperature of the cooling water, and a load cell to observe the thrust of the combustor.

279 Cellular structure of helium detonation as a trigger of sub-Chandrasekhar mass Type Ia supernovae

Iwata, Kazuya; Maeda, Keiichi*

Astrophysical detonation in Type Ia supernovae has been addressed in the context of near-Chandrasekhar mass explosion in which detonation of carbon/oxygen is initiated in the core of a white dwarf. On the other hand, sub-Chandrasekhar mass explosion is driven by double-detonation, in which accretion stream from the companion star induces thermonuclear runaway in the helium-rich layer on the surface of the white dwarf, and helium detonation thereby initiated ignites the core detonation via converging shock. To assess the probability of ignition, propagation in the surface layer, and subsequent initiation of the core detonation, its cellular dynamics takes an important role as it does in terrestrial detonable systems.

In this study, 2D numerical simulation was conducted employing alpha-chain nuclear reaction networks. In the conference, we will discuss the cell width and the irregularity of the cellular structure depending on the initial temperature/density, and the initial composition.

282 Heat Radiation Losses from Propagating Spherical Flames of Mixtures With Methane, Hydrogen, Carbon Monoxide and Air

Roque, Anthony; Hamadi, Alaa; Idir, Mahmoud; Comandini, Andrea; Chaumeix, Nabiha*

The propagating spherical flame or spherical expanding flame (SEF) method is specified for many authors as the most convenient to determine the laminar flame speed and the Markstein length. However, this method presents many shortcomings, such as spark ignition, confinement, radiation losses, compression effects of unburned gases and products, among others. In this study, the radiation-induced uncertainty is under analysis using numerical and experimental data. Currently in the literature, the radiation effect on the flame speed determination was studied numerically. This is the first time that experimental data is exploited to quantify the level of radiation losses. Mixtures of methane (CH_4), carbon monoxide (CO), and hydrogen (H_2) under different initial pressures and temperatures were considered.

293 Onset of Cellular Instability in Spherically Expanding Flames

Turner, Mattias; Petersen, Eric*

Laminar flame stability relies on multiple stabilizing and destabilizing phenomena, dependent on many properties of the gas mixture and the flame which largely must be predicted from thermodynamic and chemical kinetic modeling. Critical Peclet numbers have been extracted from 10-atm spherically expanding flame experiments over a range of high Lewis numbers (1.5 to 2.4). Test mixtures were comprised of stoichiometric oxy-syngas diluted in high levels of CO2 and He. The onset of instability is shown to be strongly correlated with the Lewis number. The leading theoretical model overpredicts the critical Peclet number by 13-83%. Ongoing work addresses deviations of the model predictions from the experimental results in terms of conflicting formulations of flame thickness and inaccurate mixture property predictions, like global activation energy, due to gaps in kinetics modeling.

Tuesday 11:25 and 16:15 – WiP Posters Session II

280 Metal Combustion in Composite Solid Propellants

Thomas, James C; Rodriguez, Felix A; Herder, Kristen; Lukasik, Gavin; Kulatilaka, Waruna; Petersen, Eric*

Metal fuels, such as Al, B, and Fe can improve performance of solid propellants. In the current study, composite AP/HTPB propellant strands and AP/HTPB/AP laminate samples were loaded with these energetic metal fuels were burned in an optically accessible strand bomb over a pressure range of 500?2,500 psia (3.45?17.2 MPa) and at 500 psia (3.45 MPa), respectively. Metal loadings were optimized for maximum performance using NASA's Chemical Equilibrium with Applications (CEA) code. Combustion processes were monitored with a high-magnification imaging system having a 3.83-μm/pixel resolution. Burning rates were recorded for composite strand samples, while burning rates, particle agglomeration size, and particle velocities were tracked for laminate propellant samples. Comparisons are provided between the burning rates, particle ejections, and particle aggregation on the surface of composite and laminate propellants manufactured and tested in the same facility.

281 Comparison of Hand and Resonant Acoustic Mixing of AP/HTPB Propellants

Rodriguez, Felix A; Thomas, James C; Hong, Alvin; Petersen, Eric*

Composite solid propellants can be mixed by a variety of techniques. Recent R&D efforts have considered resonant acoustic mixing (RAM) strategies for improved homogeneity, reduced complexity, and faster mixing capabilities. In the current study, a standard high-performance propellant formulation was mixed by standard laboratory techniques (i.e., hand mixed) and RAM to allow for direct comparison of these methods. Propellant samples were burned in a constant-volume, optically accessible strand burner at pressures between 3.45?20.7 MPa. Propellant microstructures were evaluated with scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS) techniques. Implementation of RAM yielded a significant increase in the propellant burning rate (~25%) in comparison to the standard hand-mixing strategy. The observed performance improvement in the RAM formulation was attributed to improved catalyst/oxidizer contact, yielding improved catalysis during propellant combustion.

290 Experimental Study of Gasification of Argan Nut Shell and Olives Pomace. Syngas Flame Characteristics

*Sarh, Brahim**

The main objective of this research is to investigate the gasification in a downdraft gasifier of argan nut shell and olive pomace biomass. The syngas obtained is conveyed to a coaxial burner placed in a boiler. The flame obtained is a syngas/air diffusion flame. Thermocouples Type-K and S were used for recording temperature profiles at different parts of the gasifier. The syngas composition was measured by a gas analyzer. Physicochemical characterizations of biomass were checked through ultimate and proximate analyses as well as energy content measurement. A calorimetric bomb was used to measure the HHV. In this work, we will compare the performance of biomasses as fuels for gasification to reveal the influences of reactor temperature and equivalence ratio on syngas composition. Equilibrium modeling was used to predict the gasification process in the downdraft gasifier.

291 Study of the Oxidation and Pyrolysis of Lubricants at High Temperatures

Juarez , Raquel; Gutierrez, Noble; Petersen, Eric L.*

When exposed to overly high temperatures, lubricating oils undergo oxidation and pyrolysis processes that lead to the formation of solid deposits. It is also suspected that degraded oil is more susceptible to undesirable ignition at high temperatures. Since information about the degradation process is scarce, particularly regarding pyrolysis, a test rig was constructed to study lubricant degradation at high temperatures. It consists of a flow loop with a heated section through which the oil flows, degrades over time, and forms deposits. A deposit induction time may be determined using surface and bulk oil temperature measurements. Oil samples may be removed periodically to study changes in its composition and properties (including ignition delay time). Initial data obtained that show degradation of the oil and formation of solid deposits is included. Future testing will include analyzing the oil and deposit composition over time to study the chemical kinetics of lubricant degradation.

269 Investigation of Lower Explosion Limit of Hybrid Mixtures in a 20 L-sphere

Heilmann, Vanessa; Zakel, Sabine*

A hybrid mixture is a multi-phase system of fuel vapor with air and dust. Such mixtures are encountered during industrial processes, e.g. in the pharmaceutical industries. To assess the safety risks, it is necessary to know about the behavior of the flammable substances and their safety characteristics. Previous studies provided evidence that hybrid mixtures may have a wider explosion range and the effects of explosions may be more severe. Thus, information on safety characteristics of hybrid mixtures is crucial. In the present study, the standard 20 L-sphere, was added with a vapor injection. However, first results of measuring the lower explosion limit for hybrid mixtures revealed a scattering of the explosion pressures. Pure dusts are shown similar results. The scattering of these parameters might be caused by the inhomogeneous dust distribution around the igniter. The dust is blown into the vessel and caused a high turbulence. An adaption on hybrid mixtures has to be investigated.

276 Experimental study on the performance of the standardized test method for detonation flame arresters

Ruwe, Lena; Heidermann, Thomas; Kreiáig, Michael; Kant, Hanjo; Schmidt, Dirk; Gutte, Frank; Bartsch, Dirk; Bosse, Philip; Lucassen, Arnas*

Flame arresters are autonomous protection systems and are among the constructive explosion protection measures that limit the effects of an explosion.

In this study, the performance of the standardized test method regulated in the DIN EN ISO 16852 standard for in-line flame arresters for stable and unstable detonations, which is mainly designed for atmospheric conditions, is examined. In an interlaboratory comparison, experiments are performed for different pressures before ignition and explosion groups according to the standardized test method. The experimental data is analyzed in detail to further optimize the test method and to thus achieve an improved reproducibility of detonation tests at high pressures, especially regarding the deflagration to detonation transition.

Based on these results, an improved test method for detonation flame arresters will be developed, which will ensure better reproducibility as well as applicability under non-atmospheric conditions.

285 Study of Flammability Domain of H2/CO Mixtures at Conditions Representative of the Late Phase of a Severe Accident in a PWR

Vastier, Laura; Nagaraju, Sharath; Desclaux, Anthony; Comandini, Andrea; BENTAIB, Ahmed; Chaumeix, Nabiha*

The aim of this work is to study the ignition energy and oxygen starvation effect on the H_2/CO flammability domain, for conditions representative of the late phase of a severe accident in nuclear power plants. The experiments are performed in a spherical bomb with central ignition. The flammability limits are determined based on visual and pressure criteria by using high-speed camera and high frequency pressure sensor. The experiments were conducted at 1 bar and ambient temperature. The ignition energy was fixed at 1.6 and 265 mJ, the O_2/N_2 ratio was fixed to 0.264 and 0.11. The results show the strong impact of the O_2 starvation which leads to a narrower flammability domain.

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288 Experimental study on expanding spherical flames of H2/CO mixtures at O2 reduced conditions

Bouton, Maxime; MGHANEN, Outmane; Desclaux, Anthony; Comandini, Andrea; BENTAIB, Ahmed; Chaumeix, Nabiha*

In the framework of H2 risk in nuclear power plants, the late phase sequence corresponding to the ex-vessel phase of the accident CO can also be released in the atmosphere leading to the formation of mixtures containing H2 and CO. Moreover, O2 is also depleted leading to a lower O2/N2 ratio than air. In this work, we study expanding flames of H2/CO mixtures in O2 depleted in quiescent and well-controlled initial turbulence. The laminar and turbulent flame speeds are obtained for a large set of initial conditions in terms of fuel content, turbulence intensity for O2 depleted air. The study has been conducted in the BS-III facility dedicated to expanding spherical flames. The facility is coupled to a Z-Schlieren imaging system with a high-speed camera, Phantom V1610, a high frequency pressure transducer to monitor the combustion overpressure during the flame propagation. These new data are needed by the CFD codes used in the analysis of risk assessment in nuclear power plants.

Thursday 10:40 and 15:55 – WiP Posters Session III

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275 Nitromethane Droplet Breakup and Combustion in a Detonation Environment

Briggs, Sydney M; Berube, Nicolas; Dyson, Daniel; Arakelyan, Artem; Vasu, Subith*

A detonation tube is used to produce detonation waves (DW) that propagate to the location of fuel droplet introduction in a novel study. The nitromethane (NM) fuel droplets are introduced into the test section of the detonation tube with a nominal size of about 2 mm. A high-speed camera is used to record video and images of the deformation and breakup process of the NM droplet due to the DW which moves in the Mach 6-7 range. The DW propagates into a mixture of methane and oxygen and the Weber number from the impact was found to be approximately 120.2(10^3). A preliminary analysis shows that the NM droplet appears to experience a catastrophic breakup mode characterized by Rayleigh-Taylor (RT) or Shear-Induced Entrainment (SIE) instability, or some combination of both, on the droplet surface, noted by the wave-like structure on the leading edge of the drop. It is expected that any leftover oxygen after the combustion of the methane-oxygen mixture will react with the fuel droplet.

277 Investigation of NH3?H2 mixtures in a plug-flow reactor

Ruwe, Lena; Schmitt, Steffen; Zhu, Denghao; Shu, Bo; Kohse-H”inghaus, Katharina; Lucassen, Arnas*

Ammonia (NH3) is a promising fuel as it is carbon free and easier to store and transport than hydrogen (H2). However, an ignition enhancer such as H2 might be needed for technical applications due the rather poor ignition properties of NH3.

In this study, different mixtures of NH3 and H2 were investigated in a plug-flow reactor at nearly ambient pressure (970 mbar). Temperature-dependent mole fraction profiles of main species and intermediates were obtained in a temperature range between 650 Ä1200 K using electron ionization molecular-beam mass spectrometry (EI-MBMS). Fuel-lean conditions (ϕ=0.6) were chosen for all mixtures as these are more likely in technical applications. Special attention was devoted to the possible formation of nitrogen oxides as these emissions would be very harmful to health and environment. Tunable diode laser absorption spectroscopy (TDLAS) has therefore been adapted to the plug-flow reactor as additional analysis method to determine NO concentrations.

289 An Experimental Study of the Formation of CO During Ethanol Pyrolysis and Dry Reforming with CO2

Mathieu, Olivier; Gregoire, Claire M; Cooper, Sean P; Petersen, Eric*

Beside their historical role in transportation, piston engines can be used as a chemical reactor to efficiently produce valuable chemicals. High pressures and temperatures can be generated in a short time during the compression stroke, and the fast temperature quench of the expansion stroke can allow preserving a target species under a nonequilibrium state, where optimal yield and efficiency is reached. Targeted chemicals are syngas, C2H2, C2H4, CH3OH, and CH2O. Those chemicals can be used to produce energy, for chemical energy storage, or employed directly in many industries. To obtain these products with net negative CO2 emissions, the dry reforming of ethanol, a very common biofuel, and CO2 was investigated experimentally in a shock tube by following the formation of CO with a laser absorption setup. Results were compared to modern detailed kinetics mechanisms, and this comparison shows that no model can accurately predict the data over the entire range of conditions investigated.

292 Spectroscopic CO and H2O Laser Absorption Measurements: Chemical Kinetics Investigation of Toluene Combustion in a Shock-Tube

Gregoire, Claire M; Cooper, Sean P; Petersen, Eric*

Toluene oxidation was investigated behind reflected shock wave using spectroscopic laser diagnostics to simultaneously measure carbon monoxide (CO) and water (H2O) time-history profiles. CO and H2O time-histories are unique in the available database for toluene speciation as only a total of five H-atom profiles can be found in the literature and were carried for pyrolysis instead. These new experimental measurements can help in validating detailed chemical kinetics mechanisms over highly dilute conditions. The experiments cover three equivalence ratios temperatures ranging from 1433 to 1921 K near atmospheric pressure. The most accurate model from the literature was selected to further understand toluene chemistry. Rate-of-production and sensitivity analyses support that toluene (A1CH3 in the model) decomposes via A1CH3 (+M) = A1CH2 + H (+M) and mostly produces CO and H2O with the following sequences: A1CH3 - A1CH2 - A1CH2O - CH2O - HCO - CO and A1CH3 - A1CH2 - CH3 - H2O, respectively.

294 Experimental Investigation of High-Pressure Oxy-Syngas Combustion with High CO2 Dilution

Cooper, Sean P; Turner, Mattias; Mohr, Darryl; Mathieu, Olivier; Petersen, Eric*

Syngas is a desirable, high-hydrogen fuel source for combustors utilizing the Allam-Fetvedt cycle involving supercritical-CO2 (sCO2). Minimal ignition delay time (IDT) and flame speed data are available with high concentrations of CO2Ignition delay time data were collected for syngas mixtures for pressures of 20 and 40 atm with 85% CO2 mixtures at stoichiometric conditions and H2:CO fuel ratios of 1:1 and 1:4. Laminar flame speed (FS) and burned-gas Markstein length data for H2-CO-O2-CO2-He mixtures from spherically expanding flames were also measured. The experiments were conducted at 10 atm and room temperature for H2:CO ratios ranging from 2:1 to 1:4 and overall CO2 mole fractions from 0 to 30%. CO2 dilution. Chemical kinetic modeling revealed considerable model disagreements for IDTs and slight disagreement for FS with high CO2/CO concentrations. Sensitivity analyses revealed avenues for kinetic modeling improvements using literature reaction rate measurements for CO+HO2 = CO2+OH.

278 A mathematical model for autoignition

Harris, James P; Please, Colin; Ockendon, John*

Knock in car engines is the result of autoignition in the unburnt gas ahead of the spark-ignited flame. This phenomenon has been observed in one-dimensional simulations by Yu and Chen [2015, Combustion and Flame] for the combustion of hydrogen in a chamber of finite length. Starting with a one-dimensional mathematical model for premixed combustion, we use asymptotic analysis to exploit the size of key parameters (such as the dimensionless activation energy) to develop a simplified model of autoignition. This reveals how repeated reflection of acoustic waves can raise the unburnt gas temperature to the critical value required to initiate autoignition. It can also reveal the structure of the resulting very fast autoignition front.

286 A new generation kinetic model for pyrolytic soot formation

Viola, Tullio l; Carneiro Piton, Leticia; Hamadi, Alaa; Chaumeix, Nabiha; Comandini, Andrea*

Despite decades of investigations, soot chemistry still represents a challenge for experimentalists and theoreticians, mainly due to the complexity of the processes involved. The aim of this work is the development of a new kinetic mechanism for soot formation under pyrolytic conditions validated against shock tube experiments.

The kinetic model contains an up-to-date kinetic mechanism for PAH growth coupled to the solid-phase chemistry based on the sectional method, while the kinetic parameters are chosen based on relevant reaction classes. The preliminary validation of the pyrolytic mechanisms will be carried out based on laser-based shock tube data. Numerical comparison will be made with other kinetic mechanisms available in the literature to test the performance and effectiveness of the developed model.

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No. 756785).

271 Probing Fuel-rich oxidation of 1,3-Butadiene at high-temperature using quantum-cascade-laser dual-comb spectroscopy

Geiser, Markus; Rahman, Ramees; Arafin, Farhan; Horvath, Raphael; Vasu, Subith*

1,3-Butadiene is an important intermediate during the pyrolysis of larger hydrocarbons. It is also an important intermediate formed during the combustion of hydroxyl-terminated polybutadiene. The knowledge of the kinetics of high-temperature decomposition of butadiene plays a vital role in developing kinetic models for larger hydrocarbons and propellants. This work demonstrates using quantum-cascade-laser dual-comb spectroscopy to measure butadiene's mole fraction time history at high temperatures. The measurements were conducted behind reflected shock waves in the temperature range of 1100 ÷ 1400 K near 1 atm pressure at an equivalence ratio of 4. 1,3-Butadiene was measured in the spectral range of 1590-1650 cm-1 with a temporal resolution of 4 μs. The butadiene mole fraction time history was obtained utilizing the broadband spectra with an improved signal-to-noise ratio. Results were compared with recent chemical kinetic mechanisms from literature, and the comparisons are presented.

273 Detonation Tube Setup for Liquid Fuel Droplet in Detonation Wave Experiments

Berube, Nicolas; Briggs, Sydney M; Vasu, Subith; Arakelyan, Artem; Dyson, Daniel*

Considerations for a new facility's detonation tube, which will consist of a deflagration to detonation transition section, test section, and dump section. The tube will operate at a max of 150 °C and a brief 100 bar max detonation. The test section will be a 10x10 cm square cross-section, 155 cm long channels bolted and sealed with longitudinal O-rings between plates and lateral O-rings between the flanges and the plate-ends. Ports and windows are all sealed the same. It will have 49 circular ports for PCBs, and ion gauge measurements or for laser measurements through 1.27 cm diameter circular windows. Droplet imaging will occur through four rectangular windows of 20 x 7.6 cm or 20 x 3.8 cm viewing areas, as well as a window in the dump section to view downstream ignition. The longer windows will allow for laser sheet imaging of flow boundaries. Droplet introduction will occur at one of these rectangular ports and will trigger the mixture's ignition when the droplet is in midflight.


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