

International Bunsen Discussion Meeting

Chemistry and Diagnostics for Clean Combustion

Program

Wednesday, June 21

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| | 8:00 – 9:00 | Registration |
| | 9:00 – 9:15 | Welcome addresses by Prof. Gerhard Sagerer (Rector) and Prof. Gernot Akemann (ZiF) Meeting opening by Prof. K. Kohse-Höinghaus |
| Session 1: Cleaner combustion systems: Understanding needs and details Chairs: <i>Marcus Aldén and Nicole Labbe</i> | 9:15 – 10:00 | Hai Wang, Stanford University, USA: <i>Ten questions concerning mechanisms and models of soot formation</i> |
| | 10:00 – 10:30 | Philippe Dagaut, CNRS Orléans, France: <i>Low-temperature chemical kinetics of alternative and conventional fuels oxidation</i> |
| | 10:30 – 11:00 | <i>Coffee break</i> |
| | 11:00 – 11:30 | Howard Levinsky, Groningen, The Netherlands: <i>Why can't we just burn hydrogen?</i> |
| | 11:30 – 12:00 | Pascale Desgroux, University of Lille, France: <i>About the formation of (some) pollutants in combustion processes</i> |
| | 12:00 – 12:15 | Henning Bockhorn, KIT, Karlsruhe, Germany: <i>Reactivity of diesel soot particles: Why is soot not alike soot</i> |
| | 12:15 – 12:30 | Nils Hansen, Sandia National Labs., USA: <i>New tools for flame diagnostics: Microwaves and X-rays</i> |
| | | 12:30 – 14:00 |
| Session 2: Combustion applications: Impact and reduction of emissions Chairs: <i>Christof Schulz and Michael Burke</i> | 14:00 – 14:45 | Greg Smallwood, National Research Council, Canada: <i>Black carbon: Measurement challenges for climate and health impact mitigation</i> |
| | 14:45 – 15:15 | Heinz Pitsch, RWTH Aachen University, Germany: <i>Autoignition chemistry and model reduction</i> |
| | 15:15 – 15:45 | Terese Løvås, NTNU Trondheim, Norway: <i>Biofuels from thermal conversion of bio-mass, a multi-scale problem</i> |
| | 15:45 – 16:15 | <i>Coffee break and Conference Photo</i> |
| | 16:15 – 16:45 | <ol style="list-style-type: none"> 1. Nancy Faßheber, P14 2. Feng Zhang, P59 3. Yu Song, P45 4. Zhandong Wang, P54 5. Isabelle Weber, P55 |
| | 16:45 – 17:15 | Franz Winter, Technical University Vienna, Austria: <i>Waste combustion and gasification: Implications and challenges</i> |
| | 17:15 – 18:30 | Free time for discussions and networking |
| | 18:30 – 21:00 | Posters & Snacks |

Thursday, June 22

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| Session 3: Chemistry for cleaner combustion: Fuels, mechanisms, and aftertreatment <i>Chairs: Mara de Joannon and Kai Moshammer</i> | 9:15 – 10:00 | Fei Qi, Shanghai Jiao Tong University, PR China: <i>Advanced synchrotron-based combustion diagnostics</i> |
| | 10:00 – 10:30 | Tiziano Faravelli, Politecnico di Milano, Italy: <i>Modeling the lab experiments of sooting flames</i> |
| | 10:30 – 11:00 | <i>Coffee break</i> |
| | 11:00 – 11:30 | Yiguang Ju, Princeton University, USA: <i>Experiments and models of low temperature combustion of alternative fuels</i> |
| | 11:30 – 12:00 | John Mantzaras, Paul Scherrer Institute, Switzerland: <i>Experiments and models for catalytic combustion</i> |
| | 12:00 – 12:15 | Patrick Nau, DLR Stuttgart, Germany: <i>IR absorption spectroscopy for temperature and concentration measurements in a gasifier</i> |
| | 12:15 – 12:30 | Kai Banke, University of Duisburg-Essen, Germany: <i>Combined production of power and syngas in an internal combustion engine</i> |
| | 12:30 – 14:00 | <i>Lunch</i> |
| Session 4: Physics: Tools and techniques <i>Chairs: Katharina Kohse-Höinghaus and Gaetano Magnotti</i> | 14:00 – 14:45 | Mark Linne, University of Edinburgh, UK: <i>Diagnostics for dense sprays in support of predictive models</i> |
| | 14:45 – 15:15 | Tina Kasper, University of Duisburg-Essen, Germany: <i>Diagnostics for combustion and nanoparticle formation</i> |
| | 15:15 – 15:45 | Kristina Eisen, University of Bremen, Germany: <i>Multi-quantity diagnostics for an efficient process design?</i> |
| | 15:45 – 16:15 | <i>Coffee break</i> |
| | 16:15 – 16:45 | <ol style="list-style-type: none"> 1. Isabelle Graf, P20 2. María Abián, P01 3. Ghobad Bagheri, P03 4. Nerijus Striūgas, P47 5. Daniel Felsmann, P15 6. Sebastian Kluge, P29 |
| | 16:45 – 17:15 | Wolfgang Meier, DLR Stuttgart, Germany: <i>Multi-species diagnostics at high pressure for gas turbine combustion</i> |
| | 17:15 – 18:30 | Free time for discussions and networking |
| | 18:30 – 22:00 | Conference Dinner followed by guided Evening Nature Walk in "Teutoburger Wald" forest area |

Friday, June 23

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| Session 5: Discussions | 9:00 – 10:00 | Panel discussion on future needs Panelists: Hai Wang, Tina Kasper, Howard Levinsky, Fei Qi Moderators: Andreas Brockhinke and Katharina Kohse-Höinghaus |
| | 10:00 – 10:30 | <i>Coffee break</i> |
| | 10:30 – 11:30 | Breakout discussions <i>Are there good fuels? Informed choices towards a future fuel portfolio.</i> Chairs: Fokion Egolfopoulos and Bin Yang Reporters: Thomas Bierkandt and Lena Ruwe ----- <i>Cleaning up? Research needs for emission reduction and aftertreatment.</i> Chairs: Nathalie Lamoureux and Joaquin Camacho Reporters: Corina Janzer and Georgios Kelesidis ----- <i>Too many reactions? Chemistry requirements for modeling real applications.</i> Chairs: Tiziano Faravelli and Yiguang Ju Reporters: Luc-Sy Tran and Yuyang Li ----- <i>Beyond 4D? Diagnostics targets, tools, and expectations.</i> Chairs: Jay Jeffries and Wolfgang Meier Reporters: Torsten Endres and Subith Vasu ----- <i>Useful combustion knowledge? Opportunities for transfer to/from other fields.</i> Chairs: Bill Roberts and Burak Atakan Reporters: Yasin Karakaya and Zhen-Yu Tian |
| | 11:30 – 12:30 | Plenary discussion <i>Moderated by Christof Schulz and Mara de Joannon</i> |
| | 12:30 | Meeting adjourn |
| | 12:30 – 14:00 | <i>Lunch</i> |

Posters

- P01: María Abián, Fausto Viteri, Ángela Millera, Rafael Bilbao, María U. Alzueta:
Role of SO₂ and H₂S on the formation of PAH and soot from C₂H₄ pyrolysis
- P02: R. Hegner, M. Werler, R. Schießl, U. Maas, B. Atakan:
Chemical energy storage with piston engines? Theory and experiment
- P03: G. Bagheri, E. Ranzi, M. Pelucchi, M. Lubrano Lavadera, P. Sabia, M. de Joannon, T. Faravelli:
Instability and oscillation in methane MILD combustion diluted with N₂/CO₂/H₂O
- P04: Florian J. Bauer, Franz J.T. Huber, Stefan Will:
Assessment of heat transfer mechanisms for modelling Laser-Induced Incandescence
- P05: Christopher Betrancourt, Fengshan Liu, Pascale Desgroux, Xavier Mercier, Alessandro Faccinetto, Maurin Salamanca, Lena Ruwe, Katharina Kohse-Höinghaus, Daniel Emmrich, André Beyer, Armin Gölzhäuser, Torsten Tritscher:
Comparison of LII, HIM and 1nm-SMPS measurements of incipient soot particle sizes in flat premixed n-butane sooting and nucleation flames
- P06: Thomas Bierkandt, Patrick Hemberger, Patrick Oßwald, Markus Köhler, Tina Kasper:
Investigation of anisole combustion in laminar premixed low-pressure flames
- P07: Michael P. Burke:
Combustion across scales: Uncertainty quantification and non-equilibrium kinetics
- P08: Joaquin Camacho:
Soot particle electrical mobility size distributions extending to 1 nm
- P09: L. Shi, S. Görs, T. Endres, E. Akyildiz, T. Dreier, J.B. Jeffries, B. Witzel, E.V. Klapdor, C. Schulz:
Laser-absorption CO detection at 4.56 µm in the exhaust plume of a full-scale gas turbine burner
- P10: Julia Eble, Johannes Kiecherer, Matthias Olzmann:
The complexity of ignition phenomena in diethyl ether/air mixtures
- P11: Fokion N. Egolfopoulos:
Some recent findings in legacy experimental and modeling approaches in laminar flame studies
- P12: Torsten Endres, Thorsten Benzler, Thomas Baranowski, Thomas Dreier, Christof Schulz:
Toluene fluorescence model for combustion-relevant environmental conditions
- P13: Luming Fan, Oindrila Manna, Cheng Tung Chong, Simone Hochgreb:
Effects of droplet size and concentration on the laminar flame speed of ethanol droplet/methane mixture
- P14: Nancy Faßheber, Nathalie Lamoureux, Yasuyuki Sakai, Gernot Friedrichs:
The reaction NCN + H₂: Rate constant measurements, theoretical modeling, and influence on prompt-NO formation
- P15: Daniel Felsmann, Martina Baroncelli, Heinz Pitsch:
Investigation of coal combustion under oxy-fuel conditions using experimental and numerical methods
- P16: A. Eremin, H. Jander, H. Böhm, S. Peukert, M. Fikri, C. Schulz:
The influence of hydrogen on the initial steps of soot formation

- P17: Benoit Fond, Christopher Abram, Frank Beyrau:
Recent developments in fluid thermometry using thermographic phosphors
- P18: Yi Gao:
Combustion temperature determination utilizing CARS technique
- P19: J. Trabold, S.M. Walther, C. Becker, A. Johchi, B. Böhm, A. Dreizler, D. Geyer:
Flame structures of turbulent premixed methane and alcohol flames inferred from 2D OH-PLIF
- P20: Isabelle Graf, Andreas Brockhinke:
A semi-empirical model for the temperature profile in 1D low-pressure flames
- P21: J. Herzler, Y. Sakai, M. Fikri, C. Schulz:
Experimental and theoretical study of DEE and DEE/PRF95 ignition
- P22: Corina Janzer, Michael Rößler, Amin Velji, Thomas Koch, Matthias Olzmann:
Modeling study of NO₂ formation in the combustion of n-heptane
- P23: Jay B. Jeffries, David F. Davidson, Ronald K. Hanson:
Advances in infrared laser absorption sensing for combustion gases
- P24: Bo Jiang, Dong Liu,:
Nanostructure and oxidation reactivity of nascent soot particles in 2,5-dimethylfuran/n-heptane flames
- P25: Hanfeng Jin, Eike Bräuer, Julia Pieper, Lena Ruwe, Christian Hemken, Luc-Sy Tran, Katharina Kohse-Höinghaus:
Chemical interaction of dual-fuel mixtures in low-temperature oxidation, comparing n-pentane/dimethyl ether and n-pentane/ethanol
- P26: Dennis Kaczmarek, Fikri Sen, Tina Kasper, Burak Atakan:
The effect of dimethylether and ethanol on the homogenous partial oxidation of methane
- P27: Y. Karakaya, A. Dittmann, T. Kasper:
Decomposition of tetramethylsilane in laminar premixed low-pressure flames
- P28: Georgios A. Kelesidis, Eirini Goudeli, Sotiris E. Pratsinis:
Soot mobility size and effective density
- P29: S. Kluge, H. Wiggers, C. Schulz:
MBMS of clusters and nanoparticles during gas phase synthesis
- P30: Nathalie Lamoureux, Xavier Mercier, Pascale Desgroux:
High efficiency of coupling LIF and CRDS for measuring traces species in flames: Case of N-species involved in the prompt-NO formation
- P31: S. Lau, T. Kasper, B. Atakan:
Investigating the flame suppressing behavior of ferrocene as an additive in a premixed ethene/air flame
- P32: Yuyang Li, Xiaoyuan Zhang, Meirong Zeng, Jiabiao Zou, Wei Li, Tianyu Li, Chuangchuang Cao, Yan Zhang, Fei Qi:
Exploration on low temperature oxidation of hydrocarbons and oxygenated hydrocarbons using SVUV-PIMS
- P33: Dong Liu:
Flash-induced ignition of Fe nanoparticles
- P34: Kai Moshhammer, Arnas Lucassen, Sonal Kumar Vallabhuni, Vaibhav Patel:
Investigation of the auto-ignition behavior of different natural gas mixtures containing higher hydrocarbons

- P35: Václav Nevrlý, Zdeněk Zelinger, Michal Dostál, Jan Suchánek, Václav Válek, Petr Bitala, Vít Klečka, Vendula Hanusová, David Štroch, Barbora Baudišová:
Towards revised schemes of C₃O₂ formation in diethyl ether cool flames
- P36: Patrick Oßwald, Friederike Herrmann, Tobias Schripp, Markus Köhler:
Determination and comparison of combustion intermediates from technical alternative jet-fuels
- P37: Warumporn Pejpichestakul, Alessio Frassoldati, Tiziano Faravelli:
Detailed kinetic modeling of soot formation in lightly sooting laminar premixed ethylene flames
- P38: Julia Pieper, Steffen Schmitt, Julia Krüger, Gustavo A. Garcia, Laurent Nahon, Wolfgang Eisfeld, Andreas Brockhinke, Katharina Kohse-Höinghaus:
Isomer selective combustion analysis by double-imaging fixed-photon-energy photoelectron/photoion coincidence (i²PEPICO) spectroscopy
- P39: Mona Lisa Remmers, Raimund Noske, Sadaf Shariati, Dirk Abel, Andreas Brockhinke:
Combustion instabilities: Monitoring and near-instantaneous control with electric fields
- P40: Lena Ruwe, Kai Moshhammer, Nils Hansen, Katharina Kohse-Höinghaus:
Influence of the fuel structure on the combustion chemistry of C₅-fuels
- P41: Maurin Salamanca, Lena Ruwe, Katharina Kohse-Höinghaus:
Effects of the unsaturation degree in methyl esters on the combustion process
- P42: Steffen Schmitt, Isabelle Graf, Bastian Lehrheuer, Maximilian Wick, Jakob Andert, Katharina Kohse-Höinghaus:
Influence of water addition on the combustion chemistry of iso-octane investigating laminar premixed flames
- P43: Thomas Dreier, Torsten Endres, Mustapha Fikri, Simon Görs, Sebastian A. Kaiser, Philipp Niegemann, Christof Schulz, Muhammad A. Shahbaz, Syahar Shawal:
Endoscopic combustion diagnostics: Bridging the gap between application and science
- P44: N.A. Slavinskaya, M. Abbasi, J.H. Starcke, A. Mirzayeva, W. Li, J. Oreluk, A. Hegde, A. Packard, M. Frenklach, G. Gerasimov, O. Shatalov:
Development of an UQ-predictive consistent chemical reaction model
- P45: Yu Song, Oliver Herbinet, Frédérique Battin-Leclerc, Marco Lubrano Lavadera, Pino Sabia, Mara de Joannon, Tiziano Faravelli:
Temperature oscillation of methane oxidation in a jet stirred reactor
- P46: Giancarlo Sorrentino, Pino Sabia, Mara de Joannon, Pio Bozza, Raffaele Ragucci:
Sustainability of MILD combustion in a cyclonic burner. Influence of thermal power
- P47: Nerijus Striūgas, Marius Sadeckas:
Investigation of flame chemiluminescence during combustion of single biomass particle
- P48: Alex Dubem Tagbo, Alba Dieguez-Alonso:
Assessment of a slow pyrolysis reactor using the Artificial Neural Network
- P49: Bo Tian, Cen Zhang, Simone Hochgreb:
Concept of laser-based in-situ measurements of TiO₂ particles in hydrocarbon flames
- P50: Bing-Yin Wang, Yue-Xi Liu, Jun-Jie Weng, Zhen-Yu Tian:
Investigation of the iso-propylbenzene oxidation with JSR

- P51: Dan Yu, Jun-Jie Weng, Li-Dong Zhang, Zhen-Yu Tian:
Theoretical calculation of rate constants of the reactions of 1,2,4-trimethylbenzene and its derived radicals with H/OH/HO₂
- P52: Luc-Sy Tran, Olivier Herbinet, Yuyang Li, Meirong Zeng, Frédérique Battin-Leclerc, Katharina Kohse-Höinghaus, Fei Qi:
Study of the high-pressure low-temperature oxidation chemistry of n-pentane, diethyl ether, and their mixture
- P53: Owen Pryor, Samuel Barak, Erik Ninnemann, Subith Vasu:
Probing combustion and ignition inside shock tubes using multiple diagnostics
- P54: Zhandong Wang, Denisia M. Popolan-Vaida, Bingjie Chen, Kai Moshhammer, Samah Mohamed, Heng Wang, Salim Sioud, Misjudeen A. Raji, Katharina Kohse-Höinghaus, Nils Hansen, Philippe Dagaut, Stephen R. Leone, S. Mani Sarathy:
Direct observation of multi-functional peroxides in gas-phase oxidation of organic compounds
- P55: Isabelle Weber, Lena Genthner, Philipp Friese, Matthias Olzmann:
Pyrolysis of furan and its methyl-substituted derivatives: A H-ARAS / TOF-MS shock-tube study
- P56: Julia Wullenkord, Meirong Zeng, Isabelle Graf, Katharina Kohse-Höinghaus:
Investigations on fuel-structure-dependent effects of small ether addition in premixed n-heptane and iso-octane flames
- P57: Jiaying Wang, Shuang Li, Bin Yang:
Experimental design methods for combustion kinetic model development
- P58: Hongmiao Wang, Xiaoging You, Mark Blitz, Michael Pilling, Straun H. Robertson:
Obtaining effective rate coefficients to describe the decomposition kinetics of graphene oxyradicals at high temperatures
- P59: Feng Zhang, Can Huang, Bin Yang:
Pressure dependent kinetics of 1,3-butadiene and its impact on soot precursors