

D6.6. Workshop: “Gas-Phase reaction kinetics of oxygenated molecules present in biofuels and bio-oils”

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Project Information

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<u>EXECUTIVE SUMMARY</u>	<u>4</u>
1.1 DESCRIPTION OF THE DELIVERABLE CONTENT AND PURPOSE	4
1.2 BRIEF DESCRIPTION OF THE STATE OF THE ART AND THE INNOVATION BREAKTHROUGHS.....	4
1.3 CORRECTIVE ACTION	4
<u>2 PREPARATION OF THE WORKSHOP</u>	<u>5</u>
2.1 DATE AND LOCATION	5
2.2 COOPERATION WITH THE SMARTCATs INITIATIVE	5
2.3 LOGISTICS	6
2.4 INVITED SPEAKERS	6
2.5 CONFERENCE MATERIAL	6
2.6 WORKSHOP PROMOTION	6
<u>3 WORKSHOP ACTIVITIES.....</u>	<u>7</u>
3.1 OPENING SPEECHES	7
3.2 SCHEDULE ORGANIZATION	7
<u>4 ACHIEVEMENTS.....</u>	<u>15</u>
4.1 GENERAL OUTCOMES.....	15
4.2 IMPROOF OUTCOMES	16
<u>5 CONCLUSIONS</u>	<u>17</u>
<u>6 REFERENCES.....</u>	<u>18</u>

EXECUTIVE SUMMARY

1.1 Description of the deliverable content and purpose

This report describes the activity carried out during the workshop: “Gas-phase Reaction Kinetics of Biofuels Oxygenated Molecules”, as well as its organization procedures. The workshop is part of the Grant Agreement of the IMPROOF project. The project partner in charge of its organization was Politecnico di Milano. The aim of the workshop was to provide an overview of the current research and the most recent advancements in the investigation of the kinetics of oxygenated classes of molecules involved in biofuels pyrolysis and combustion chemistry.

In the first part of this deliverable, the organization measures of the workshop are described in detail. In the second part, the two-days execution of the workshop are illustrated, along with the major achievements of such event.

1.2 Brief description of the state of the art and the innovation breakthroughs

This part is not relevant for this deliverable, being it focused on the preparation and implementation of the workshop.

1.3 Corrective action

The official title of the workshop was slightly changed with respect to the original one: “Gas-Phase reaction kinetics of oxygenated molecules present in biofuels and bio-oils” was modified into “Gas-phase Reaction Kinetics of Biofuels Oxygenated Molecules”. The topic remained unchanged.

Moreover, contrary to the execution date expected in the Grant Agreement, i.e. M32 (May 2019), the Workshop has been anticipated to M19 (April 2018). Such shift was included in the amendment AMD-723706-14, where the deadline of D6.6 was moved to M20.

2 PREPARATION OF THE WORKSHOP

The workshop: “Gas-Phase reaction kinetics of oxygenated molecules present in biofuels and bio-oils” was complementary to the research activity carried out in the IMPROOF WP1. Thus, its organization was coordinated and set up by Politecnico di Milano, in cooperation with CNRS and UGent.

2.1 Date and Location

The dates of the workshop were chosen as functional to the progress of the activity planned in such WP. It was agreed to organize it on April 23rd and 24th, in order to avoid any overlapping with other relevant conferences in Europe, as well as with public holidays in European countries.

Concerning the location, the city of Milan was chosen as venue for three major reasons: (i) it can be easily reached from the rest of Europe at a relatively low cost, (ii) it allows to use the structures of Politecnico di Milano, and (iii) it offers a large availability of hotels and accommodation facilities. Within Politecnico, the “Aula Rogers” with a capacity of 270 people was used for both days [1]. Next to it, two close rooms were available for poster sessions and lunches according to the agenda.



Figure 1. Aula Rogers, Politecnico di Milano. From [1].

2.2 Cooperation with the SMARTCATs initiative

In order to maximize the success of the workshop, the organization was shared with the CM1404 SMARTCATs initiative [2]. This latter is a European COST action [3], aimed at “promoting the use of smart energy carriers on a large scale in order to increase fuel flexibility and carbon efficiency of energy production and to support distributed energy generation strategies.” In particular, several common areas can be identified between Work Package (WP) 1 of the IMPROOF project, and the Working Group (WG) 1 of the SMARTCATs action, targeted at “improving the knowledge on detailed chemistry and thermochemistry for the combustion, pyrolysis, and oxidation of fuels, such as natural gas mixtures” [4]. Sharing such organization has ensured a wider visibility of the workshop itself, especially in the European academic and research institutions (29 European countries are currently part of SMARTCATs action).

2.3 Logistics

Politecnico di Milano dealt with the logistics of the event, which was free of charge for all the participants. Participants were asked to submit a one-page abstract of their contributions, indicating their preference for oral or poster presentation. Students were offered assistance in the lodging reservation, and a list of hotels recommended by Politecnico di Milano, with special rates for such events was provided to the participants via the SMARTCATs webpage [5].

Buffet lunches and coffee breaks (one in the morning, one in the afternoon) were offered next to the meeting room. Finally, a networking event was scheduled during the evening of April, 23rd at “Ristorante ‘Da Berti’” (Via Francesco Algarotti, 20, 20124 Milano MI).

2.4 Invited speakers

Beside the individual contributions of the Workshop participants, three distinguished speakers from both academic and industrial contexts were invited to provide keynote lectures on topics related to the workshop itself.

- On Monday, 23rd Prof. Eliseo Ranzi (Politecnico di Milano, Italy) opened the workshop with a presentation on “Detailed kinetics of vanillin as reference component of pyrolysis bio-oil”
- On Monday, 23rd Dr. Roger Cracknell (Shell Global Solutions, UK) presented a work on “Ethanol and other bio-oxygenates: their role in high octane fuels”
- Finally, on Tuesday, 24th Prof. Heinz Pitsch (Institute for Combustion Technology, RWTH Aachen, Germany) opened the second day of the workshop with a lecture titled “Chemistry Matters: Advanced Biofuels for Internal Combustion Engines”

2.5 Conference material

In order to optimize the success of the event, all the participants were provided with a conference package consisting of a cotton conference bag, containing:

- Personal badge and badge holder;
- 1 pen;
- 1 notebook;
- 1 printed version of the workshop agenda (in A5 format);
- 1 USB key, containing the conference abstracts in PDF format.

2.6 Workshop promotion

The maximum possible visibility was ensured to the event: in addition to the partners of the IMPROOF project, informed through the Project Management Officer (Ayming), the event was advertised through several channels:

- Mailing list of the Italian Section of the Combustion Institute
- Mailing list of the French Section of the Combustion Institute
- Mailing list of the SMARTCATs initiative.
- Social networks (Facebook pages of CRECK modeling group and CM1404 SMARTCATs COST Action)

The event was promoted on the IMPROOF website [6], as well as on the SMARTCATs page [5], where the instructions for application were made available.

3 WORKSHOP ACTIVITIES

The event took place the whole day of April, 23rd, and the morning of April, 24th (until lunchtime). After receiving all the registration forms and setting up the final schedule, the official agenda was released on the SMARTCATs website [5].

3.1 Opening speeches

The conference was opened by Prof. Maurizio Masi, head of the Department of Chemistry, Materials and Chemical Engineering “G. Natta” – Politecnico di Milano, welcoming the participants on behalf of the host institution (Figure 2). It was followed by a short introduction of Ing. Stagni, as part of the organizing committee, who gave an overview of the workshop logistics and schedule. The opening section was then completed by Dr. Mara de Joannon and Prof. Tiziano Faravelli, on behalf of SMARTCATs and IMPROOF, respectively.



Figure 2. Opening speeches of the Workshop. Upper left: Prof. Masi. Upper right: Ing. Stagni. Lower left: Dr. Mara de Joannon. Lower right: Prof. Faravelli

3.2 Schedule organization

The contributions from the participants were split into 6 sessions, according to their topics. After the welcome address, the activities were opened by the keynote lecture of Prof. Eliseo Ranzi on “Detailed kinetics of vanillin as reference component of pyrolysis bio-oil” (Figure 3). His presentation was chaired by Dr. Battin-Leclerc (CNRS Nancy – France).

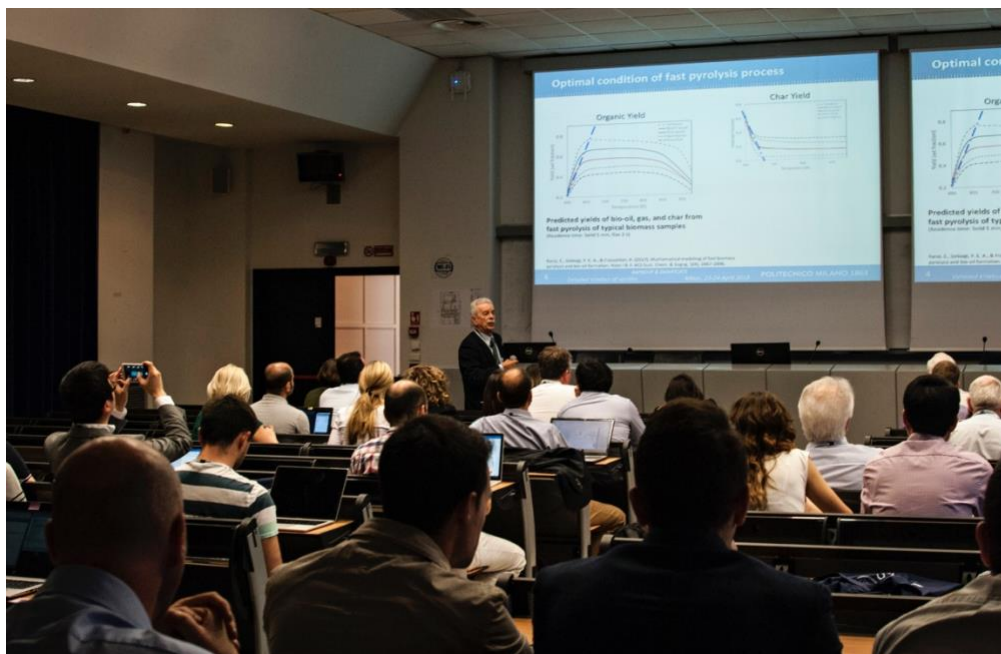


Figure 3. Prof. Ranzi opening lecture

Following Prof. Ranzi's lecture, Session 1 started with “Shock-tube measurements and model development”, chaired by G. Vanhove (Université des Sciences et Technologies de Lille 1 – Lille, France) and O. Herbinet (University of Lorraine – Nancy, France) (Figure 4)

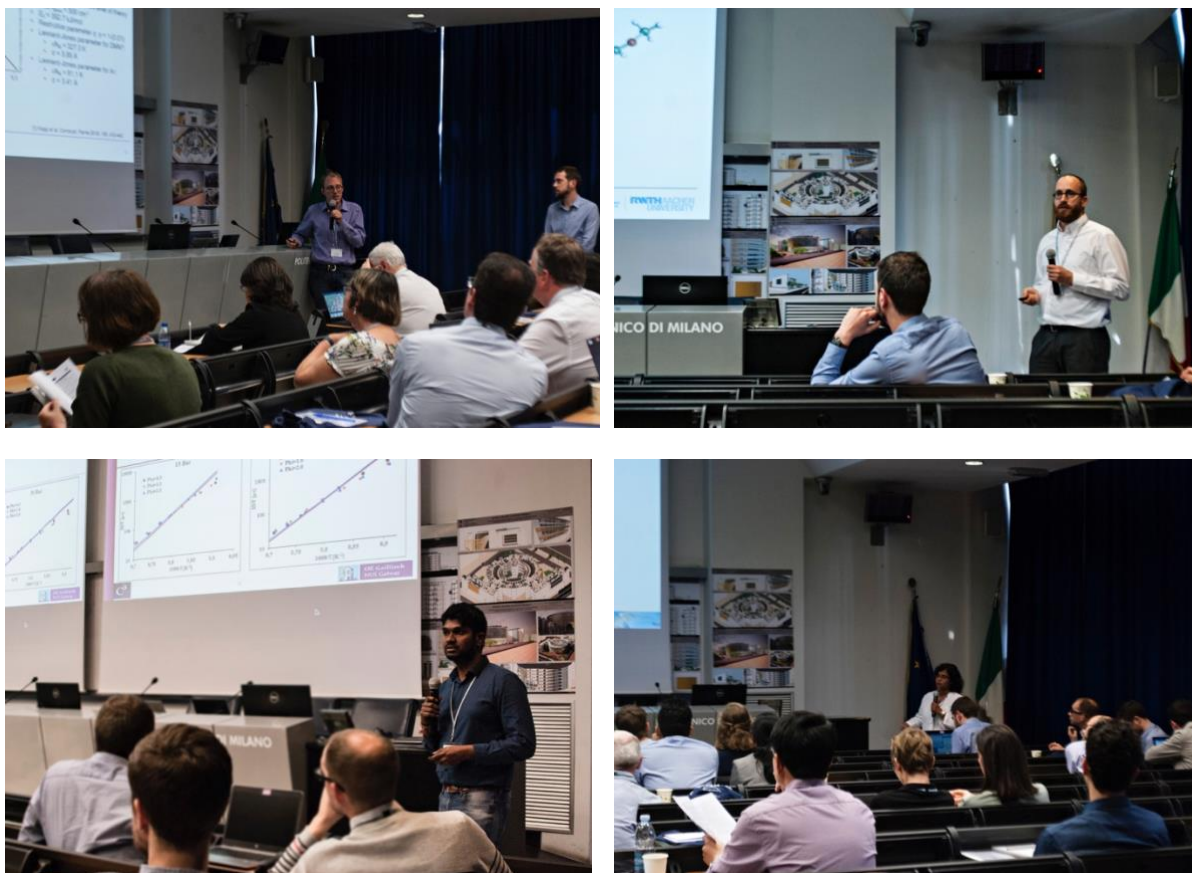


Figure 4. Session 1 presenters.

Session 2 was then focused on “NO_x formation from oxygenated fuels”: it consisted of 5 contributions, and was chaired by Prof. Frassoldati and Prof. Mehl (Politecnico di Milano).



Figure 5. Extract of the presentations from Session 2.



Figure 6. Dr. Cracknell keynote lecture

The afternoon session of day 1 was opened by the second keynote lecture, provided by Dr. Cracknell (Shell Global Solutions, United Kingdom) on “Ethanol and other bio-oxygenates: their role in high octane fuels” (Figure 6).

Session 3 was fully dedicated to the works carried out within the IMPROOF framework, and titled: “Renewable fuels for steam-cracking applications”. It was chaired by Prof. Alberto Cuoci (Politecnico di Milano) and Dr. Pino Sabia (Istituto di Ricerche sulla Combustione – CNR, Naples). In detail, 5 works were presented by:

- Cato Pappijn (Laboratory for Chemical Technology, Ghent University)
- Quentin Cazères (CERFACS, Toulouse)
- Matteo Pelucchi (Politecnico di Milano)
- Sylvain Namysl (CNRS Nancy)
- Stijn Vangaever (Laboratory for Chemical Technology, Ghent University)



Figure 7. Extract of the presentations from Session 3 (IMPROOF)

The first day was finally concluded by Session 4 (Figure 8): “Biofuels frontiers in engine applications”, whose chairs were Prof. A. Heufer (RWTH Aachen University) and Dr. S. Peukert (Universität Duisburg-Essen).



Figure 8. Extract from Session 4.

Day 2 was opened by the last keynote lecture of the workshop delivered by Prof. Pitsch (RWTH Aachen University): “Chemistry Matters: Advanced Biofuels for Internal Combustion Engines” (Figure 9).



Figure 9. Prof. Pitsch keynote lecture

The opening lecture was followed by Session 5 “Theoretical studies on biofuels kinetics” (the shortest one: 3 contributions), where the chairs were Dr. L.S. Tran (Bielefeld University) and Dr. G. Sorrentino (University of Naples “Federico II”).

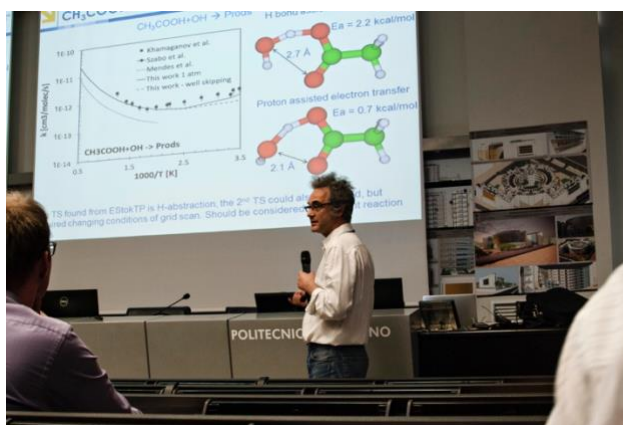


Figure 10. Session 5 presenters

Session 6 (Figure 11) concluded the workshop: “Moving from experiments to kinetic modeling and analysis of oxygenated fuels”, whose chairs were Prof. C. Cavallotti (Politecnico di Milano) and Prof. P. Casavecchia (Universita’ degli Studi di Perugia).

The workshop consisted overall in 28 oral contributions.

In parallel to the oral presentations, poster sessions (Figure 12) were held during lunches and coffee breaks, except for the first coffee break (during which posters were hung). 21 poster contributions were submitted to the workshop, 3 of them were from IMPROOF partners:

- S. Madane (Laboratory for Chemical Technology, Ghent University)
- S.U. Aravindakshan (Laboratory for Chemical Technology, Ghent University)
- Y. Song (CNRS Nancy)

Posters were placed in the meeting room next to “Aula Rogers”, and were grouped by topic.



Figure 11. Extract from Session 6 presenters.

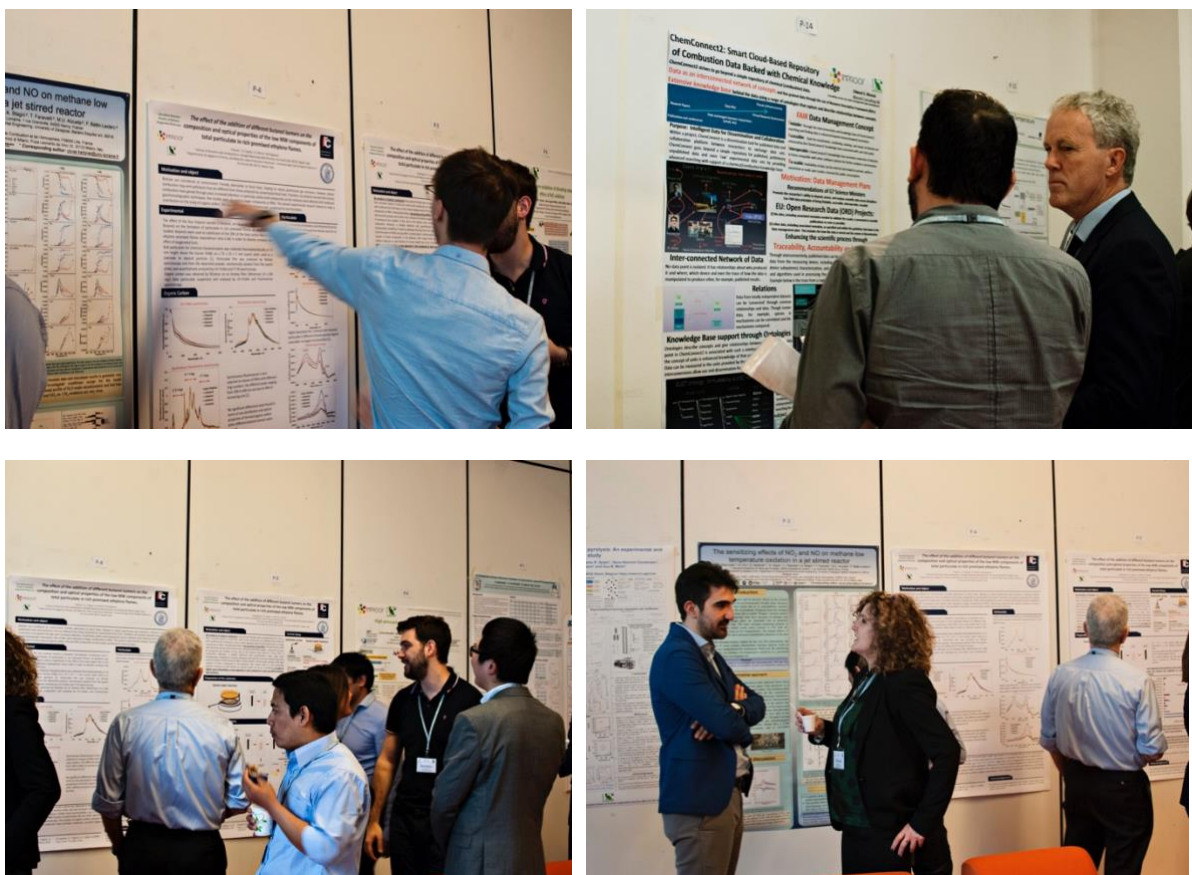


Figure 12. Workshop poster session

4 ACHIEVEMENTS

There are several elements suggesting its successful reception and outcomes of this workshop. This is valid both within and outside the IMPROOF point of view.

4.1 General outcomes

The number of submissions to the workshop was higher than expected: overall, 76 people attended (Figure 13).



Figure 13. Group picture of the workshop participants

The audience was very heterogeneous, under different view points:

- i) Considering the country of origin of the participants' affiliation, 15 different nations were represented:
 - Belgium
 - Bulgaria
 - France
 - Germany
 - Greece
 - Hungary
 - Ireland
 - Italy
 - The Netherlands
 - Serbia
 - Slovenia
 - Spain
 - Sweden
 - Turkey
 - United Kingdom

- ii) Gender balance: 56 male (71.8%) vs 22 female (28.2%) participants. These numbers are in line with the partners composition of the IMPROOF project (currently ~25% female)
- iii) Institution of origin: 26 Universities/Research centers and 7 companies.

4.2 IMPROOF outcomes

Considering the project, 4 universities participated and submitted one or more contributions:

- CERFACS
- Ghent University
- Politecnico di Milano
- CNRS Nancy

4 companies, partners of the project, sent their delegates, too:

- Dow
- AVGI
- Cress BV
- Technip FMC

Overall, 20 participants (out of 76) belonged to IMPROOF partners. The choice of grouping both oral presentations and posters coming from this framework has guaranteed the maximum visibility and dissemination of the results obtained so far.



5 CONCLUSIONS

The present report has described the activity carried out for the preparation and the execution of the Workshop: “Gas-phase Reaction Kinetics of Biofuels Oxygenated Molecules”. The organization of such an event was planned in the Grant Agreement of this project, and was functional to disseminating the research activity currently performed within WP1.

Although initially planned in M32 and anticipated of about 1 year, its organization proceeded without relevant issues. Considering the numbers and typology of attendance, its reception within the EU community was quite large and heterogeneous. Positive outcomes were thus obtained inside and outside the IMPROOF framework. From the project viewpoint, this was a useful occasion to disseminate the results obtained during the first 18 months; from a larger, EU perspective, it was a fruitful opportunity to discuss the state-of-the-art research in terms of bio-fuels and bio-oil combustion among the most relevant academic and industrial institutions in this field.



6 REFERENCES

- [1] Politecnico di Milano. <http://www.polimi.it> (accessed June 2018).
- [2] SMARTCATs - CM1404 COST action. <http://www.smartcats.eu> (accessed June 2018).
- [3] COST - European Cooperation in Science and Technology. <http://www.cost.eu/> (accessed June 2018).
- [4] SMARTCATs Memorandum of Understanding. <http://www.smartcats.eu/wp-content/uploads/2016/06/wg1.pdf> (accessed June 2018).
- [5] SMARTCATs - Gas-phase Reaction Kinetics of Biofuels Oxygenated Molecules. <http://www.smartcats.eu/event/gas-phase-reaction-kinetics-of-biofuels-oxygenated-molecules/> (accessed June 2018).
- [6] IMPROOF website. <https://improof.cerfacs.fr> (accessed June 2018).

April 23 – 24, 2018
Aula Rogers – Politecnico di Milano



Gas-phase Reaction Kinetics of Biofuels Oxygenated Molecules




Agenda

Monday, April 23rd

9:00 – 9:30	Registration	
9:30 – 10:00	<p style="text-align: center;">Welcome address</p> <p>The SMARTCATs challenge Dr. Mara de Joannon <i>Istituto di Ricerche sulla Combustione IRC-CNR, Italy</i></p> <p>IMPROOF: status and perspectives Prof. Tiziano Faravelli <i>Department of Chemistry, Materials and Chemical Engineering “G. Natta”, Politecnico di Milano, Italy</i></p>	
10:00 – 10:30	<p style="text-align: center;">Opening lecture <i>Chair: F. Battin-Leclerc</i></p> <p>Detailed kinetics of vanillin as reference component of pyrolysis bio-oil Prof. Eliseo Ranzi <i>Department of Chemistry, Materials and Chemical Engineering “G. Natta”, Politecnico di Milano, Italy</i></p>	
10:30 – 11:00	Coffee break	
<p style="text-align: center;">Session 1 Shock-tube measurements and model development <i>Chairs: G. Vanhove, O. Herbinet</i></p>		
11:00 – 11:15	<p>Direct measurement of high-temperature rate constants of the thermal decomposition of dimethoxymethane – a shock tube and modeling study S. Peukert, P. Sela, D. Nativel, J. Herzler, M. Fikri, C. Schulz <i>IVG, Institute for Combustion and Gas Dynamics – Reactive Fluids, University of Duisburg-Essen, Germany</i></p>	1-1
11:15 – 11:30	<p>Ignition delay time measurements and detailed kinetic modelling of dimethoxy methane S. Jacobs¹, U. Burke², H. J. Curran², K. A. Heufer¹ <i>1. Physico-Chemical Fundamentals of Combustion, RWTH Aachen University, Germany</i> <i>2. School of Chemistry, Combustion Chemistry Centre & Ryan Institute, National University of Ireland, Galway, Ireland</i></p>	1-2

11:30 – 11:45	An experimental and modelling study on oxidation of ethyl acetate and methyl acetate <u>N. Lokachari</u>, H. Curran <i>Combustion chemistry centre (C3) and The Ryan Institute, National University of Ireland, Galway, Ireland</i>	1-3
11:45 – 12:00	Reaction Kinetics of Ethylene Glycol as a Model Fuel for Pyrolysis Oil <u>T. Kathrotia</u>, C. Naumann, P. Osswald, M. Koehler, U. Riedel <i>Institute of Combustion Technology, German Aerospace Center (DLR), Stuttgart, Germany</i>	1-4
<p style="text-align: center;">Session 2 NO_x formation from oxygenated fuels <i>Chairs: A. Frassoldati, M. Mehl</i></p>		
12:00 – 12:15	Kinetic study of methanol and ethanol oxidation in presence of NO_x <u>K. P. Shrestha</u>¹, L. Seidel², F. Mauss¹ <i>1. Thermodynamics and Thermal Process Engineering, Brandenburg University of Technology, Cottbus, Germany</i> <i>2. LOGE Deutschland GmbH, Cottbus, Germany</i>	1-5
12:15 – 12:30	Influence of bio-cyclic ethers oxidation on nitrogen oxides chemistry <u>L. Giarracca</u>, N. Lamoureux, S. Gosselin, G. Vanhove, L. Gasnot, P. Desgroux <i>University of Lille, CNRS, France</i>	1-6
12:30 – 12:45	A theoretical study of the $CN+C_2H_4$ reaction <u>G. Lendvay</u>¹, N. Balucani², P. Casavecchia² <i>1. Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences, Budapest, Hungary</i> <i>2. Dipartimento di Chimica, Biologia e Biotecnologie, Università degli Studi di Perugia, Italy</i>	1-7
12:45 – 13:00	The effects of NO_x addition on the low-temperature oxidation of n-pentane in a jet stirred reactor <u>L. Marrodán</u>¹, Y. Song², O. Herbinet², M. U. Alzueta¹, F. Battin-Leclerc² <i>1. Aragón Institute of Engineering Research (I3A), Department of Chemical and Environmental Engineering, University of Zaragoza, Spain</i> <i>2. Laboratoire Réactions et Génie des Procédés, CNRS-Université de Lorraine, Nancy, France.</i>	1-8
13:00 – 13:15	Performance of oxygenated biofuels in realistic internal combustion systems <u>T. Seljak</u>¹, T. Katrasnik¹ <i>Faculty of mechanical engineering, University of Ljubljana</i>	1-9
13:15 – 14:30	Lunch & Posters	

14:30 – 15:15	<div>Keynote</div> <div>Chair: G. Skevis</div> <div>Ethanol and other bio-oxygenates: their role in high octane fuels</div> <div>Dr. Roger Cracknell</div> <div>Shell Global Solutions, United Kingdom</div>	
<div>Session 3</div> <div>Renewable fuels for steam-cracking applications</div> <div>Chairs: A. Cuoci, P. Sabia</div> <div></div>		
15:15 – 15:30	<div>Ab initio group additivity model for the free radical reactions of nitrogen-containing compounds</div> <div>C.A.R. Pappijn¹, R. Van de Vijver¹, G.B. Marin¹, M.F. Reyniers¹, K.M. Van Geem¹</div> <div>Laboratory for Chemical Technology, Ghent University, Belgium</div>	1-10
15:30 – 15:45	<div>Reduction of chemical kinetics mechanisms for Large Eddy Simulations of turbulent combustion</div> <div>Q. Cazères¹, P. Pepiot², E. Riber¹, B. Cuenot¹</div> <div>1. CERFACS, Toulouse, France</div> <div>2. Sibley School of Mechanical and Aerospace Engineering, Cornell University, United States</div>	1-11
15:45 – 16:00	<div>Reaction classes characterizing oxygenated fuel combustion: alcohols, aldehydes and carboxylic acids</div> <div>M. Pelucchi¹, S. Namysl², O. Herbinet², F. Battin-Leclerc², T. Faravelli¹</div> <div>1. Department of Chemistry, Materials and Chemical Engineering “G. Natta”, Politecnico di Milano, Italy</div> <div>2. Laboratoire Réactions et Génie des Procédés, CNRS, Université de Lorraine, ENSIC, Nancy, France</div>	1-12
16:00 – 16:15	<div>Experimental investigation of butanoic and pentanoic acids oxidation</div> <div>S. Namysl¹, M. Pelucchi², T. Faravelli², O. Herbinet¹, F. Battin-Leclerc¹</div> <div>1. Laboratoire Réactions et Génie des Procédés, CNRS, Université de Lorraine, ENSIC, Nancy, France</div> <div>2. Department of Chemistry, Materials and Chemical Engineering “G. Natta”, Politecnico di Milano, Italy</div>	1-13
16:15 – 16:30	<div>Computational fluid dynamics-based study of novel technologies in steam cracking furnaces</div> <div>S. Vangaeve¹, G.J. Heynderickx¹, K.M. Van Geem¹, G.B. Marin¹</div> <div>Laboratory for Chemical Technology, Ghent University, Belgium</div>	1-14
16:30 – 17:00	Coffee break & Posters	

Session 4 Biofuels frontiers in engine applications Chairs: K.A. Heufer, S. Peukert		
17:00 – 17:15	A Comprehensive Approach to the Detailed Kinetic Mechanism of the Blending Behavior of Oxygenated Fuels for Transportation M. Mehl^{1,2}, S.W. Wagon¹, K. Zhang¹, G. Kukkadapu¹, C.K. Westbrook¹, W.J. Pitz¹, M. McNenly¹, R. Whitesides¹ 1. Lawrence Livermore National Laboratory, Livermore, USA 2. Department of Chemistry, Materials and Chemical Engineering “G. Natta”, Politecnico di Milano, Italy	1-15
17:15 – 17:30	A study of the kinetics influencing the propensity of n-butanol and its blends with a gasoline surrogate to knocking combustion A. S. Tomlin¹, I. Gorbatenko^{1,2}, M. Lawes², D. Bradley² 1. School of Chemical and Process Engineering, University of Leeds 2. School of Mechanical Engineering, University of Leeds	1-16
17:30 – 17:45	Understanding and Measuring Sub-23 nm Particle Emissions from Direct Injection Engines E. Papaioannou¹, D. Zarvalis¹, E. Daskalos¹, A. Melas¹, D. Deloglou¹, N. Vlachos¹, A.G. Konstandopoulos^{1,2} 1. Aerosol & Particle Technology Laboratory, CERTH/CPERI, Thessaloniki, Greece 2. Department of Chemical Engineering, Aristotle University, Thessaloniki, Greece	1-17
17:45 – 18:00	Ignition kinetics of 2,5-dimethyltetrahydrofuran in engine-relevant conditions Y. Fenard^{1,2}, H. Song¹, H. Minwegen², P. Parab², C. Sampaio Mergulhão¹, K. A. Heufer², G. Vanhove¹ 1. University of Lille, CNRS, France 2. Physico-Chemical Fundamentals of Combustion, RWTH Aachen, Germany	1-18
20:30 – 22:30	Networking event	

Tuesday, April 24th

9:00 – 9:45	<p style="text-align: center;">Keynote Chair: A. D'Anna</p> <p>Chemistry Matters: Advanced Biofuels for Internal Combustion Engines Prof. Heinz Pitsch <i>Institute for Combustion Technology, RWTH Aachen, Germany</i></p>
<p style="text-align: center;">Session 5 Theoretical studies on biofuels kinetics Chairs: L.S. Tran, G. Sorrentino</p>	
9:45 – 10:00	<p>A model of tetrahydrofuran low-temperature oxidation based on theoretically calculated rate constants Y. Fenard¹, A. Gil², G. Vanhove¹, H. Carstensen³, K.M. Van Geem³, P. R. Westmoreland⁴, O. Herbinet⁵, F. Battin Leclerc⁵ 1. University of Lille, CNRS, France 2. Centro de Química e Bioquímica, Faculdade de Ciências da Universidade de Lisboa, Portugal 3. Laboratory for Chemical Technology, Ghent University, Belgium 4. Department of Chemical & Biomolecular Engineering, North Carolina State University, Raleigh, NC, USA 5. Laboratoire Réactions et Génie des Procédés, CNRS, Univ. Lorraine, Nancy, France</p>
10:00 – 10:15	<p>Crossed beam studies of the O(3P,1D) reaction dynamics with benzene and toluene: primary products and branching ratios A. Caracciolo¹, P. Recio Ibañez¹, G. Vanuzzo¹, T. K. Minton², N. Balucani¹, P. Casavecchia¹ 1. Dipartimento di Chimica, Biologia e Biotecnologie, Università di Perugia, 06123 Perugia, Italy 2. Department of Chemistry and Biochemistry, Montana State University, Bozeman, Montana 59717, USA</p>
10:15 – 10:30	<p>Automation of rate constant calculation for biofuels: status and perspectives C. Cavallotti¹, M. Pelucchi¹, Y. Georgievskii², S.J. Klippenstein² 1. Department of Chemistry, Materials and Chemical Engineering "G. Natta", Politecnico di Milano, Italy 2. Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL, USA</p>
10:30 – 11:15	<p style="text-align: center;">Coffee break & Posters</p>

<p align="center">Session 6 Moving from experiments to kinetic modeling and analysis of oxygenated fuels Chairs: C. Cavallotti, P. Casavecchia</p>		
11:15 – 11:30	<p>Oxidation of Energy Carriers With and Without Carbon Content in an Intrinsically Fuel-Flexible Configuration</p> <p><u>P. Sabia</u>¹, G. Sorrentino², P. Bozza¹, M. de Joannon¹, R. Ragucci¹</p> <p>1. Istituto di Ricerche sulla Combustione – C.N.R. – Napoli, Italy 2. Università Federico II – Napoli, Italy</p>	2-4
11:30 – 11:45	<p>Quantitative Measurements of Small Radical Reactions with Molecules of Combustion Interest Investigated through Multiplexed SVUV Photoionization Mass Spectrometry</p> <p><u>J. Bourgalais</u>¹, D. L. Osborn², F. Goulay³, S. D. Le Picard⁴</p> <p>1. Université Versailles St-Quentin, Sorbonne Universités, Guyancourt, France 2. Combustion Research Facility, Sandia National Laboratories, Livermore, California, United States 3. Department of Chemistry, West Virginia University, Morgantown, West Virginia, United States 4. Institut de Physique de Rennes, Département de Physique Moléculaire, Astrophysique de Laboratoire, UMR CNRS 6251, Université de Rennes 1, Campus de Beaulieu, France</p>	2-5
11:45 – 12:00	<p>Modelling oxidation of butanol isomers</p> <p><u>D. Pezo</u>, C. Lou, R. Bilbao, A. Millera, M.U. Alzueta</p> <p>Aragón Institute of Engineering Research (I3A), Department of Chemical and Environmental Engineering, University of Zaragoza, Spain</p>	2-6
12:00 – 12:15	<p>Testing several butanol combustion mechanisms against a large set of experimental data</p> <p><u>M. Bolla</u>, C. Olm, I.G. Zsély, <u>T. Turányi</u></p> <p>Institute of Chemistry, ELTE Eötvös Loránd University</p>	2-7
12:15 – 12:30	<p>Comparative study of the high-pressure low-temperature oxidation of linear five-heavy-atom fuels: diethyl ether vs. n-pentane, and their mixture</p> <p><u>L.S. Tran</u>^{1,2,3}, O. Herbinet², Y. Li⁴, F. Qi⁴, K. Kohse-Höinghaus¹, F. Battin-Leclerc²</p> <p>1. Department of Chemistry, Bielefeld University, Germany 2. Laboratoire Réactions et Génie des Procédés (LRGP), CNRS, Université de Lorraine, Nancy, France 3. University of Lille, CNRS, France 4. School of Mechanical Engineering, Shanghai Jiao Tong University (SJTU), China</p>	2-8

12:30 – 12:45	<p>How the position of the ester function can modify the combustion of biodiesel</p> <p><u>G. Dayma</u>^{1,2}, M. Lailliau¹, S. Thion¹, Z. Serinyel^{1,2}, P. Dagaut¹</p> <p><i>1. CNRS-INSIS, Institut de Combustion, Aérothermique, Réactivité et Environnement 1C, Orléans, France</i></p> <p><i>2. Université d'Orléans, Collegium Sciences et Technologies, France</i></p>	2-9
12:45 – 13:00	<p>Formation of H atoms in the pyrolysis of furan, 2-methylfuran, and 2,5-dimethylfuran: A comparative shock-tube/H-ARAS and modeling study</p> <p><u>I. Weber</u>, P. Friese, L. Genthner, M. Olzmann</p> <p><i>Institute of Physical Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany</i></p>	2-10
13:00 – 14:30	Lunch & Posters	
14:30 – 15:00	Workshop Closure	

Poster session

P-1	<p>On-line detection of heteroatomic compounds in steam cracking effluents</p> <p>S. Madane, R.M. Djokic, P. Mendes, J. Thybaut, K.M. Van Geem</p> <p><i>Laboratory for Chemical Technology, Ghent University, Belgium</i></p>
P-2	<p>Pressure dependence of cyclic compound pyrolysis: An experimental and kinetic modeling study</p> <p>S.U. Aravindakshan, M.V. Khandavilli, M.R. Djokic, H. Carstensen, F.H. Vermeire, K.M. Van Geem, G.B. Marin</p> <p><i>Laboratory for Chemical Technology, Ghent University, Belgium</i></p>
P-3	<p>The sensitizing effects of NO₂ and NO on methane low temperature oxidation in a jet stirred reactor</p> <p>Y. Song¹, L. Marrodán², N. Vin¹, O. Herbinet¹, E. Assaf³, C. Fittschen³, A. Stagni⁴, T. Faravelli⁴, M.U. Alzueta², F. Battin-Leclerc¹</p> <p>1. Laboratoire Réactions et Génie des Procédés, CNRS-Université de Lorraine, Nancy, France. 2. Aragón Institute of Engineering Research (I3A). Department of Chemical and Environmental Engineering. University of Zaragoza. Spain 3. Université Lille, CNRS, PC2A-PhysicoChimie des Processus de Combustion et de l'Atmosphère, France. 4. Department of Chemistry, Materials and Chemical Engineering "G. Natta", Politecnico di Milano, Italy.</p>
P-4	<p>The effect of the addition of different butanol isomers on the composition and optical properties of the low MW components of total particulate in rich premixed ethylene flames.</p> <p>C. Russo¹, A. Ciajolo¹, A. D'Anna², M. Sirignano²</p> <p>1. Istituto di Ricerche sulla Combustione – C.N.R. – Napoli, Italy 2. Università Federico II – Napoli, Italy</p>
P-5	<p>New approach to detect gas phase Oxy-PAHs in biofuel flame</p> <p>M. Sirignano¹, A. Ciajolo², A. D'Anna¹, C. Russo²</p> <p>1. Istituto di Ricerche sulla Combustione – C.N.R. – Napoli, Italy 2. Università Federico II – Napoli, Italy</p>
P-6	<p>High-pressure oxidation of dimethyl ether: the effect of NO addition</p> <p>L. Marrodán, A.J. Arnal, A. Millera, R. Bilbao, M.U. Alzueta</p> <p><i>Aragón Institute of Engineering Research (I3A), Department of Chemical and Environmental Engineering, University of Zaragoza, Spain</i></p>

P-7	<p>A Comparative Study of Benzene Oxidation in Lean-to-Rich Laminar Premixed Flames Z. Malliotakis¹, G. Vourliotakis¹, G. Skevis², M. Founti¹</p> <p>1. Laboratory of Heterogeneous Mixtures and Combustion Systems, Thermal Engineering Section, School of Mechanical Engineering, National Technical University of Athens, Greece. 2. Aerosol & Particle Technology Laboratory, Chemical Process & Energy Resources Institute, Centre for Research & Technology Hellas, Thessaloniki, Greece.</p>
P-8	<p>Cross Evaluating the Effects of a Cerium-Based Diesel Fuel Additive on Exhaust Toxicity with in vitro Air-Liquid Interface Cell Exposure Systems of Different Flow Patterns P.K. Baltzopoulou¹, L.E. Secondo², A. Asimakopoulou¹, D. Deloglou¹, C. Softas¹, S. Petrakis³, L. Chasapidis¹, E. Papaioannou^{1,4}, N.A. Lewinski², A.G. Konstandopoulos^{1,4}</p> <p>1. Aerosol & Particle Technology Lab., Chemical Process & Energy Resources Inst., Centre for Research & Technology Hellas (APTL/CPERI/CERTH), Thessaloniki, Greece 2. Department of Chemical and Life Science Engineering, Virginia Commonwealth University, Richmond, VA, USA 3. Institute of Applied Biosciences, Centre for Research & Technology Hellas (INAB/CERTH), Themi, Greece 4. Department of Chemical Engineering, Aristotle Univ. of Thessaloniki (AUTH), Thessaloniki, Greece</p>
P-9	<p>Ignition delay time measurements of the oxidation of cyclopentanone N. Lokachari, H. Curran</p> <p>Combustion chemistry centre (C³) and The Ryan Institute, National University of Ireland, Galway, Ireland</p>
P-10	<p>Shock-tube studies on pyrolysis reactions of dimethoxymethane L. Golka¹, I. Weber¹, K. Wegner¹, M. Olzmann¹</p> <p>Institute for Physical Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany</p>
P-11	<p>OH-reaction Kinetics and Photochemistry of Biomass-derived Cyclic Ethers A. Illés, E. Gombos, M. Nagy, S. Dóbe</p> <p>Green Chemistry Research Group, Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences, Budapest, Hungary</p>
P-12	<p>Towards an open and automatic framework for data acquisition, data analysis and model development. G. Scalia¹, M. Pelucchi², A. Stagni², T. Faravelli², B. Pernici¹</p> <p>1. Department of Electronics, Information and Bioengineering, Politecnico di Milano, Italy. 2. Department of Chemistry, Materials and Chemical Engineering "G. Natta", Politecnico di Milano, Italy.</p>

P-13	<p>Methane MILD combustion Chemistry</p> <p><u>G. Bagheri</u>^{1,2}, A. Parente², T. Faravelli¹</p> <p>1. Department of Chemistry, Materials and Chemical Engineering “G. Natta”, Politecnico di Milano, Italy.</p> <p>2. Aero-Thermo-Mechanical Laboratory, Ecole Polytechnique de Bruxelles, Université Libre de Bruxelles, Belgium</p>
P-14	<p>ChemConnect2: Smart Cloud-Based Repository of Combustion Data Backed with Chemical Knowledge</p> <p><u>E.S. Blurock</u></p> <p>Blurock Consulting AB, Lund, Sweden</p>
P-15	<p>Kinetic Studies of tert-Butanol under Low Temperature Combustion Conditions</p> <p>S. Sime^{1,2}, K. Greenlees², M. Blitz², <u>A. Tomlin</u>¹, P. Seakins²</p> <p>1. School of Chemical and Process Engineering, University of Leeds, UK</p> <p>2. School of Chemistry, University of Leeds, UK</p>
P-16	<p>A lumped kinetic modeling approach for biomass pyrolysis</p> <p><u>D. Ipsakis</u>¹, E. Heracleous^{1,2}, K. Gkinis¹, S.D. Stefanidis¹, K.G. Kalogiannis¹, A.A. Lappas¹</p> <p>1. Laboratory of Environmental Fuels & Hydrocarbons (LEFH), Chemical Process & Energy Resources Institute/Centre for Research and Technology Hellas (CPERI/CERTH), Thessaloniki, Greece</p> <p>2. School of Science & Technology, International Hellenic University (IHU), Thessaloniki, Greece</p>
P-17	<p>Modeling and simulation of pyrolysis of wheat straw samples</p> <p><u>B. Miljkovic</u>¹, B. Nikolovski²</p> <p>1. Faculty of Technical Sciences, Novi Sad, Serbia</p> <p>2. Faculty of Technology, Novi Sad, Serbia</p>
P-18	<p>Biogas combustion characteristics</p> <p>I. Naydenova, I. Ganev, <u>T. Petrova</u></p> <p>Technical University of Sofia, College of Energy and Electronics, Sofia, Bulgaria</p>
P-19	<p>Using Hotel Generated Food Waste For Biogas Production</p> <p><u>G. Soyhan</u>^{1,2}, O. Batman³</p> <p>1. R&D Technology Department, Sakarya - Turkey</p> <p>2. University of Sakarya, Sakarya - Turkey</p> <p>3. Tourism Faculty, University of Sakarya, Sakarya – Turkey</p>
P-20	<p>Combustion Modeling of Biofuels Oxygenated Molecules by Detailed Kinetic Models</p> <p><u>H.S. Soyhan</u>^{1,2}</p> <p>1. Engineering Faculty, University of Sakarya, Sakarya – Turkey</p> <p>2. R&D Technology Manager, Sakarya - Turkey</p>

P-21	<p data-bbox="337 163 1404 226">A newly designed cooking burner using Biofuels by modelling Gas-phase Reaction Kinetics</p> <p data-bbox="354 237 836 273"><u>M. Hacı</u>¹, Z. Kahraman¹, H.S. Soyhan^{2,3}</p> <ol data-bbox="422 283 1404 420" style="list-style-type: none"> <li data-bbox="422 283 1404 346">1. <i>Oztiryakiler Madeni Esha San. Tic. A.S –R&D Technology Center, Istanbul - Turkey</i> <li data-bbox="422 352 1177 388">2. <i>Engineering Faculty, University of Sakarya, Sakarya – Turkey</i> <li data-bbox="422 394 982 420">3. <i>R&D Technology Manager, Sakarya - Turkey</i>
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