

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




Gas-phase Reaction Kinetics of Biofuels Oxygenated Molecules



Agenda

Monday, April 23 rd		
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 Chair: F. Battin-Leclerc</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>Session 1</p> <p>Shock-tube measurements and model development</p> <p>Chairs: G. Vanhove, O. Herbinet</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 1. <i>Physico-Chemical Fundamentals of Combustion, RWTH Aachen University, Germany</i> 2. <i>School of Chemistry, Combustion Chemistry Centre & Ryan Institute, National University of Ireland, Galway, Ireland</i></p>	1-2

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

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

Session 4 Biofuels frontiers in engine applications <i>Chairs: K.A. Heufer, S. Peukert</i>		
17:00 – 17:15	<p>A Comprehensive Approach to the Detailed Kinetic Mechanism of the Blending Behavior of Oxygenated Fuels for Transportation</p> <p><u>M. Mehl</u>^{1,2}, S.W. Wagon¹, K. Zhang¹, G. Kukkadapu¹, C.K. Westbrook¹, W.J. Pitz¹, M. McNenly¹, R. Whitesides¹</p> <p style="margin-left: 40px;">1. Lawrence Livermore National Laboratory, Livermore, USA 2. Department of Chemistry, Materials and Chemical Engineering “G. Natta”, Politecnico di Milano, Italy</p>	1-15
17:15 – 17:30	<p>A study of the kinetics influencing the propensity of n-butanol and its blends with a gasoline surrogate to knocking combustion</p> <p><u>A. S. Tomlin</u>¹, I. Gorbatenko^{1,2}, M. Lawes², D. Bradley²</p> <p style="margin-left: 40px;">1. School of Chemical and Process Engineering, University of Leeds 2. School of Mechanical Engineering, University of Leeds</p>	1-16
17:30 – 17:45	<p>Understanding and Measuring Sub-23 nm Particle Emissions from Direct Injection Engines</p> <p>E. Papaioannou¹, D. Zarvalis¹, <u>E. Daskalos</u>¹, A. Melas¹, D. Deloglou¹, N. Vlachos¹, A.G. Konstandopoulos^{1,2}</p> <p style="margin-left: 40px;">1. Aerosol & Particle Technology Laboratory, CERTH/CPERI, Thessaloniki, Greece 2. Department of Chemical Engineering, Aristotle University, Thessaloniki, Greece</p>	1-17
17:45 – 18:00	<p>Ignition kinetics of 2,5-dimethyltetrahydrofuran in engine-relevant conditions</p> <p>Y. Fenard^{1,2}, H. Song¹, H. Minwegen², P. Parab², C. Sampaio Mergulhão¹, K. A. Heufer², <u>G. Vanhove</u>¹</p> <p style="margin-left: 40px;">1. University of Lille, CNRS, France 2. Physico-Chemical Fundamentals of Combustion, RWTH Aachen, Germany</p>	1-18
20:30 – 22:30	Networking event	

Tuesday, April 24th

9:00 – 9:45	Keynote <i>Chair: A. D'Anna</i> Chemistry Matters: Advanced Biofuels for Internal Combustion Engines Prof. Heinz Pitsch <i>Institute for Combustion Technology, RWTH Aachen, Germany</i>	
Session 5 Theoretical studies on biofuels kinetics <i>Chairs: L.S. Tran, G. Sorrentino</i>		
9:45 – 10:00	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 <i>1. University of Lille, CNRS, France</i> <i>2. Centro de Química e Bioquímica, Faculdade de Ciências da Universidade de Lisboa, Portugal</i> <i>3. Laboratory for Chemical Technology, Ghent University, Belgium</i> <i>4. Department of Chemical & Biomolecular Engineering, North Carolina State University, Raleigh, NC, USA</i> <i>5. Laboratoire Réactions et Génie des Procédés, CNRS, Univ. Lorraine, Nancy, France</i>	2-1
10:00 – 10:15	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 <i>1. Dipartimento di Chimica, Biologia e Biotecnologie, Università di Perugia, 06123 Perugia, Italy</i> <i>2. Department of Chemistry and Biochemistry, Montana State University, Bozeman, Montana 59717, USA</i>	2-2
10:15 – 10:30	Automation of rate constant calculation for biofuels: status and perspectives C. Cavallotti¹, M. Pelucchi¹, Y. Georgievskii², S.J. Klippenstein² <i>1. Department of Chemistry, Materials and Chemical Engineering "G. Natta", Politecnico di Milano, Italy</i> <i>2. Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL, USA</i>	2-3
10:30 – 11:15	Coffee break & Posters	

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

12:30 – 12:45	<p>How the position of the ester function can modify the combustion of biodiesel</p> <p>G. Dayma^{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>I. Weber, 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><i>1. Laboratoire Réactions et Génie des Procédés, CNRS-Université de Lorraine, Nancy, France.</i></p> <p><i>2. Aragón Institute of Engineering Research (I3A). Department of Chemical and Environmental Engineering. University of Zaragoza. Spain</i></p> <p><i>3. Université Lille, CNRS, PC2A-PhysicoChimie des Processus de Combustion et de l'Atmosphère, France.</i></p> <p><i>4. Department of Chemistry, Materials and Chemical Engineering "G. Natta", Politecnico di Milano, Italy.</i></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><i>1. Istituto di Ricerche sulla Combustione – C.N.R. – Napoli, Italy</i></p> <p><i>2. Università Federico II – Napoli, Italy</i></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><i>1. Istituto di Ricerche sulla Combustione – C.N.R. – Napoli, Italy</i></p> <p><i>2. Università Federico II – Napoli, Italy</i></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. <i>Laboratory of Heterogeneous Mixtures and Combustion Systems, Thermal Engineering Section, School of Mechanical Engineering, National Technical University of Athens, Greece.</i></p> <p>2. <i>Aerosol & Particle Technology Laboratory, Chemical Process & Energy Resources Institute, Centre for Research & Technology Hellas, Thessaloniki, Greece.</i></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. <i>Aerosol & Particle Technology Lab., Chemical Process & Energy Resources Inst., Centre for Research & Technology Hellas (APTL/CPERI/CERTH), Thessaloniki, Greece</i></p> <p>2. <i>Department of Chemical and Life Science Engineering, Virginia Commonwealth University, Richmond, VA, USA</i></p> <p>3. <i>Institute of Applied Biosciences, Centre for Research & Technology Hellas (INAB/CERTH), Themi, Greece</i></p> <p>4. <i>Department of Chemical Engineering, Aristotle Univ. of Thessaloniki (AUTH), Thessaloniki, Greece</i></p>
P-9	<p>Ignition delay time measurements of the oxidation of cyclopentanone N. Lokachari, H. Curran</p> <p><i>Combustion chemistry centre (C³) and The Ryan Institute, National University of Ireland, Galway, Ireland</i></p>
P-10	<p>Shock-tube studies on pyrolysis reactions of dimethoxymethane L. Golka¹, I. Weber¹, K. Wegner¹, M. Olzmann¹</p> <p><i>Institute for Physical Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany</i></p>
P-11	<p>OH-reaction Kinetics and Photochemistry of Biomass-derived Cyclic Ethers A. Illés, E. Gombos, M. Nagy, S. Dóbé</p> <p><i>Green Chemistry Research Group, Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences, Budapest, Hungary</i></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. <i>Department of Electronics, Information and Bioengineering, Politecnico di Milano, Italy.</i></p> <p>2. <i>Department of Chemistry, Materials and Chemical Engineering "G. Natta", Politecnico di Milano, Italy.</i></p>

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

P-21

A newly designed cooking burner using Biofuels by modelling Gas-phase Reaction Kinetics

M. Hacı¹, Z. Kahraman¹, H.S. Soyhan^{2,3}

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