CM1404

SMARTCATs

EUROPEAN COOPERATION
IN SCIENCE AND TECHNOLOGY

COST Action 1404

Chemistry of Smart Energy Carriers and Technologies

3rd General Meeting
and
Workshop on SECs in Industry

Prague

October, 25th – 27th - 2017

SCIENTIFIC PROGRAM

J. Heyrovsky Institute
of Physical Chemistry
of the AS CR in Prague

SMARTCATs / CM1404

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Smart Energy Carriers Chemistry and Technologies

COoperation in Science and Technology (COST) is a European framework (www.cost.eu) that aims to create collaboration networks on common research topics, funded by national or international research projects, and to share competences and results in synergistic way.

The idea of SMARTCATs COST Action stems from the need to confront the continuous changes in the prevaling energy scenarios. Even if combustion based energy production will continue to play a major role, an energy production system shift will occur in the near future. The growing volatility of world's economies and politics which has characterized the past decades, in combination with increasing environmental concerns, has strongly affected and modified the fuel portfolio. Moreover, the availability of large amounts of variable renewable electricity (e.g. wind and solar energy), introduced in large amounts into the power system, requires the identification and the efficient use of energy carriers, which are chemical compounds produced as storage from electric energy surplus. On the other hand the spreading of energy production and distribution system based on a smart grid concept imposes the use of locally and diverse available sources.

These scenarios redefine the concept of fuel as smart energy carrier actually enlarging it to a much wider class of compounds. This category can include simple hydrocarbons, natural gas mixtures as well as low calorific value fuels, 1st and 2nd generation biofuels, polymers which can be obtained from wood fatty acid methyl esters, hydro-treated vegetable oils etc.

Carriers-to-energy conversion technologies, from small/domestic scale to large power conversion systems as well as engines, have to provide practical answers to satisfy the energy needs.

SMARTCATs COST Action is a pan-European network of scientists and engineers from academia and industry focused on the study of combustion of a vast palette of energy carriers aiming to the development and optimization of fuel flexible, efficient, advanced and emerging combustion technologies. The main aim is to facilitate the use of the more suitable and (locally) available energy carrier in the best available combustion technologies.

During the annual SMARTCATS General Meeting, Action participants meet for sharing and discussing the latest knowledge gained on the conversion and use of energy carriers, spanning from the development and optimization of kinetic mechanisms for fuel conversion, to pollutants monitoring and control to the advanced diagnostics, from the generation of tools for data collection and mining to the application of smart energy carriers at large scale.

The approach to accomplish this aim is twofold. On the one hand, academic/research organizations will devote strong efforts to bring together fundamental/ advanced numerical and diagnostic tools to improve the understanding of combustion at micro/meso-scale levels.

On the other hand, the exchange between academic and industrial partners will support the optimization of tools developed in the Action exploiting the way that SECs could be utilised at the macro-scale in advanced combustion devices. This interaction will lead to the identification of standards and criteria for the development of internet tools devoted to integration of experimental and numerical physico-chemical combustion data.

Wednesday, October 25th	
9:00 - 9:30	**Welcome Address** prof. Martin Hof, Dr. rer. nat. DSc. *Director, J. Heyrovský Institute of Physical Chemistry* RNDr. Josef Janda *Ministry of Education, Youth and Sports of the CR* *chairs: Z. Zelinger, M. de Joannon*
9:30 - 10:15	**Opening Lecture** *chairs: F. Mauß, R Ragucci* Ammonia Fueled Gas Turbine Power Generation N. Iki *Research Institute for Energy Conservation, Department of Energy and Environment, National Institute of Advanced Industrial Science and Technology, Japan*
10:15 - 10:30	**Coffee Break**
	Workshop **Smart Energy Carriers in Industry** *chairs: G. Skevis, C. Esarte*
10:30 - 11:00	Optically Accessible Test Facilities and Non-intrusive Measurement Techniques for the Investigation of Combustion Processes – Practical Use of Insights in Industrial Product Development and Application K. Hermmann *University of Applied Sciences and Arts Northwestern Switzerland, Switzerland*
11:00 - 11:30	Do we "burn clean"? Realistic Assessment of Effects of New Fuels and Technologies on Harmful Emissions from Combustion Processes Michal Vojtíšek *Czech Technical University in Prague, Czech Republic*
11:30 - 12:00	Laser Induced Breakdown Spectroscopy (LIBS) A Powerful Tool for Analytical Applications in Energy, Metallurgy and Environment S. Couris *University of Patras, Greece*
12:00 - 12:30	Power-to-Gas, -Fuel and -Chemicals via high-temperature electrolysis O. Poszdiech *Sunfire GmbH, Germany*
12:30 - 13:30	**Lunch Break**

Working Group 1 - session 1
Smart energy carriers gas phase chemistry: from experiments to kinetic models
chairs: O. Herbinèt, J. Vavra

13:30 - 13:45	**Experimental and Chemical Kinetic Modeling Study on the Influence of n-Butanol Blending on the Combustion, Autoignition and Knock Properties of Gasoline and its Surrogate in a Spark Ignition Engine** E. Agbro[1], A.S. Tomlin[1], A. Burluka[2], F. Mauss[3], M. Pasternak[3], A. Alfazazi[4], S.M Sarathy[4] *1. University of Leeds, Leeds, UK.* *2. Northumbria University, Newcastle, UK.* *3. Brandenburg University of Technology, Cottbus, Germany.* *4. King Abdullah University of Science and Technology, Thuwal, Saudi Arabia*	**1-1**
13:45 - 14:00	**Investigation of the Effects of n-Butanol Addition to Gasoline and its Surrogate Mixture on the Ignition Delay Times at Different Blending Ratios** I. Gorbatenko[1,2,3], A.S. Tomlin[2], M. Lawes[3] *1. EPSRC CDT in Fluid Dynamics, University of LeedsUK* *2. School of Chemical and Process Engineering, University of Leeds, UK* *3. School of Mechanical Engineering, University of Leeds, UK*	**1-2**
14:00 - 14:15	**A Kinetic Study of the Oscillating Combustion of Hydrogen and Syngas in Well-stirred Reactors** F. De Capitani[1], A. Stagni[1], M. Pelucchi[1], M. de Joannon[2], P. Sabia[2], M. Lubrano Lavadera[2], T. Faravelli[1] *1. Politecnico di Milano, Italy* *2. Istituto di Ricerche sulla Combustione - C.N.R., Napoli, Italy*	**1-3**
14:15 - 14:30	**Ab Initio Study on the Dimerization of Lignol Model Species** H.-H. Carstensen, K. M. Van Geem, M.-F. Reyniers, G.B. Marin *Ghent University, Belgium*	**1-4**
14:30 - 14:45	**Theoretical Studies on the Dynamics of the HO + HBr H2O + Br Reaction** S. Góger[1], G. Lendvay[1,2] *1. University of Pannonia, Veszprém, Hungary* *2. Hungarian Academy of Sciences, Budapest, Hungary*	**1-5**
14:45 - 15:00	**High Temperature Rate Constants of Anisole Decomposition and Ignition Delay Time Measurements of Anisole** B. Shu, J. Herzler, S. Peukert, M. Fikri, C. Schulz *IVG, University of Duisburg-Essen, Germany*	**1-6**
15:00 - 15:15	**Crossed Beam Studies of the O(3P,1D) + Benzene Reaction Dynamics: Primary Products and Branching Ratios** A. Caracciolo[1], G. Vanuzzo[1], T. K. Minton[2], N. Balucani[1], P. Casavecchia[1] *1. Università di Perugia, Italy* *2. Montana State University, Bozeman, Montana, USA*	**1-7**
15:15 - 15:30	**Study of the High-Pressure Low-Oxidation Chemistry of n–Pentane, Diethyl Ether, and their Mixture** O. Herbinet[1], L.S. Tran[1,2], Y. Li[3], F. Battin-Leclerc[1], K. Kohse-Höinghaus[2], F. Qi[3] *1. LRGP - CNRS, Nancy, France* *2. Bielefeld University, Germany* *3. Jiao Tong University, Shanghai, China*	**1-8**

15:30 - 15:45	Laminar Burning Velocities of Methylcyclohexane + Air Flames at Room and Elevated Temperatures S.S. Matveev[1], V.A. Alekseev[2], I.V. Chechet[1], S.G. Matveev[1], A.A. Konnov[2] *1. Samara National Research University, Russia* *2. Lund University, Sweden*	**1-9**
15:45 - 16:00	***Coffee Break***	
	Working Group 1 - session 2 ***Smart energy carriers gas phase chemistry: from experiments to kinetic models*** *chairs: N. Balucani, V. Nevrly*	
16:00 - 16:15	Experimental Investigation of Isothermal and Reacting Flow Topologies Downstream of Axisymmetric Baffle Stabilizers under Different Inlet Mixture Conditions Fuel Topology Strategies G. Paterakis[1], J. Klingmann[2], P. Koutmos[1] *1. University of Patras, Greece* *2. Lund University, Sweden*	**1-10**
16:15 - 16:30	Thermochemical Kinetics for the Lignocellulosic Biofuel, Ethyl Levulinate M.K. Ghosh, S. Dooley *Trinity College, Dublin, Ireland*	**1-11**
16:30 - 16:45	Exploring the Reactivity of C_4–C_6 Linear Alcohols: From Jet Stirred Reactor and Rapid Compression Machine Experiments to Operating Regimes in a HCCI Engine M. Pelucchi[1], S. Namysl[2], M. Bissoli[1], K.P. Somers[3], F. Battin-Leclerc[2], H.J. Curran[3], T. Faravelli[1] *1. Politecnico di Milano, Milan, Italy* *2. LRGP - CNRS, Université de Lorraine, ENSIC, Nancy, France* *3. National University of Ireland, Galway, Ireland*	**1-12**
16:45 - 17:00	Ethanol as Fuel Additive: High-pressure Oxidation of its Mixtures with Acetylene L. Marrodán, M. Fuster, Á. Millera, R. Bilbao, M.U. Alzueta *University of Zaragoza, Spain*	**1-13**
17:00 - 17:15	An Experimental and Detailed Chemical Kinetic Investigation of the Addition of C_2 Oxygenated Species in Rich Ethylene Premixed Flames Z. Malliotakis[1], N. Leplat[2], G. Vourliotakis[1], Ch. Keramiotis[1], G. Skevis[3], M.A. Founti[1], J. Vandooren[2] *1. National Technical University of Athens, Greece* *2. Université Catholique de Louvain, Belgium* *3. CPERI-CERTH, Thessaloniki, Greece*	**1-14**

17:15 - 17:30	Oscillatory Behavior in Simple Hydrocarbons Combustion: on the Influence of the Operating Parameters M. Lubrano Lavadera[1], P. Sabia[1], M de Joannon[1], Y. Song[2], O. Herbinet[2], F. Battin-Leclerc[2], M. Pelucchi[3], A. Stagni[3], T. Faravelli[3] *1. Istituto di Ricerche sulla Combustione - C.N.R., Napoli, Italy* *2. LRGP - CNRS, Université de Lorraine, Nancy, France* *3. Politecnico di Milano, Italy*	**1-15**
17:30 - 17:45	Detailed Kinetic Modeling of Allene Pyrolysis and Combustion M. Auyelkhankyzy[1,2], M. Abbasi[1], N. Slavinskaya[1], Z. Mansurov[2] *1. Institute of Combustion Technology DLR, Stuttgart, Germany* *2. Al-Farabi Kazakh National University, Almaty, Kazakhstan*	**1-16**
17:45 - 18:00	Development and Optimization of H_2/CO-H_2 Reaction Model Using PrIMe A. Mirzayeva[1], N.A. Slavinskaya[1], U. Riedel[1], M. Frenklach[2], A. Packard[2], W. Li[2], J. Oreluk[2], A. Hedge[2] *1. Institute of Combustion Technology DLR, Stuttgart, Germany* *2. University of California, Berkeley, USA*	**1-17**

Thursday, October 26th		
Working Group 1 - session 3 ***Smart energy carriers gas phase chemistry: from experiments to kinetic models*** *chair: O. Herbinèt*		
8:30 - 8:45	Ruthenium Nanoparticles Supported on Nanohydrotalcite: Efficient Heterogeneous Catalyst for the Oxidation of Lignin Model Compounds I.B. Baguc, I.E. Ertas, K. Karakas, M. Celebi, M. Zahmakiran *Yuzuncu Yil University, Van, Turkey*	**1-18**
8:45 - 9:00	A Computational Investigation on the Oxidation of Sulfur N. Sebbar[1], J. W. Bozzelli[2], H. Bockhorn[1], D. Trimis[1] *1. Engler-Bunte-Institut, KIT, Karlsruhe, Germany* *2. Department of Chemical Engineering, NJIT, Newark, USA*	**1-19**
9:00 - 9:15	Skeletal Mechanism Construction by Entropy Production Analysis: Detailed Reaction Mechanisms with Irreversible Reactions L. Acampora[1], M. Kooshkbaghi[2], C.E. Frouzakis[3], F.S. Marra[1] *1. Istituto di Ricerche sulla Combustione - C.N.R., Napoli, Italy* *2. Princeton University, NJ, U.S.A.* *3. Swiss Federal Institute of Technology, Zurich, Switzerland*	**1-20**
9:15 - 9:30	Automated calibration of Thermochemical Models Using MoDS-Kinetics™ Workflow Applied to Biomass Gasification N. Bianco, D. Nurkowski, G.P.E. Brownbridge, A.N. Bhave *CMCL Innovations, Cambridge – UK*	**1-21**
9:30 - 10:00	***Coffee Break and Poster exhibition***	

Working Group 2
Chemistry for control of by-products in smart energy carrier conversion
chair: N. Sebbar, P. Giudicianni

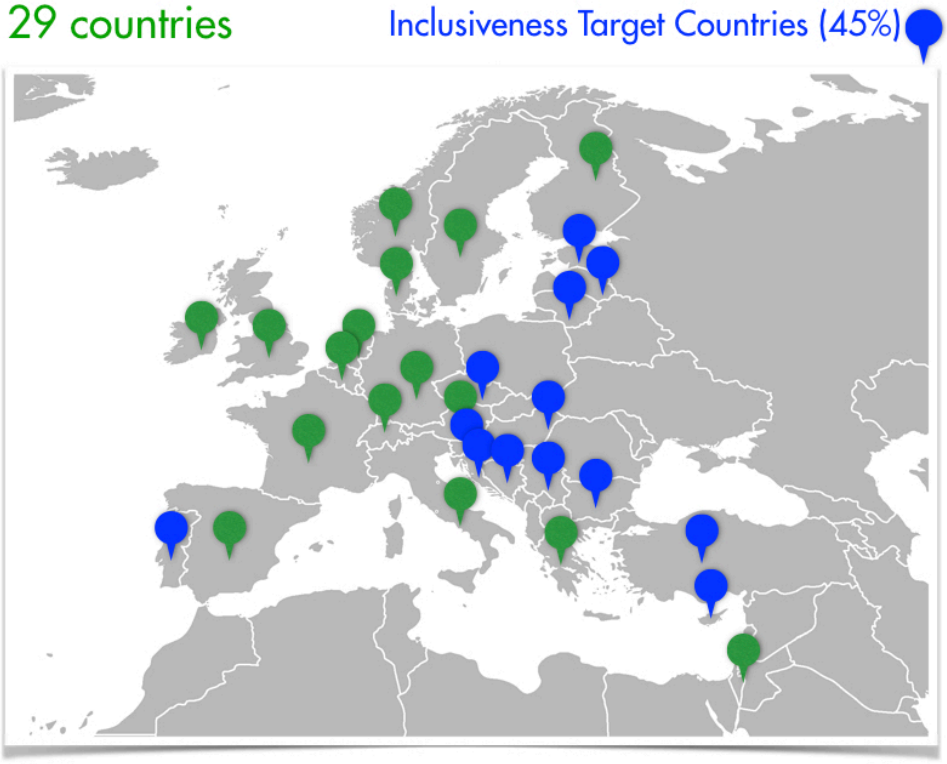
10:00 - 10:15	**Kinetic Modeling for NOx Prediction with Improved Base Chemistry** K.P. Shrestha[1], Lars Seidel[2], Fabian Maußl[1], Thomas Zeuch[3] *1. Brandenburg University of Technology, Cottbus, Germany* *2. Lund Combustion Engineering, LOGE Deutschland GmbH, Cottbus, Germany* *3. Georg-August-Universität, Göttingen, Germany*	**2-1**
10:15 - 10:30	**Investigation of NO Formation in Stoichiometric Premixed Flat $H_2/CH_4/CO/O_2/N_2$ Flames Doped with Benzene** M. Cafiero[1], V. Dias[2], A. Coussement[1], H. Jeanmart[2], A. Parente[1] *1. Université Libre de Bruxelles, Belgium* *2. Université Catholique de Louvain (UCL), Louvain-la-Neuve, Belgium*	**2-2**
10:30 - 10:45	**Research of Na*, K* and Ca* Flame Emission During the Single Biomass Pellet Combustion** M. Sadeckas[1], N. Striūgas[1], M. Costa[2], M. Rabacal[2] *1. Lithuanian Energy Institute, Kaunas, Lithuania* *2. Instituto Superior Tècnico, Lisboa, Portugal*	**2-3**
10:45 - 11:00	**Low-temperature Corrosion Caused by Alkali Phosphate Containing Particulates in Biomass Conversion** E. Vainio, A. Brink, L. Hupa *Åbo Akademi University, Turku, Finland*	**2-4**
11:00 -11:15	**Influence of Heating Oil Formulation on the Combustion and Emissions from Domestic Condensing Boilers** C. Esarte, J. Delgado *Repsol Technology Center, Móstoles (Madrid), Spain*	**2-5**
11:15 - 11:30	**Effects of High Viscosity Biofuels on PM and NOx Emissions of a Micro Gas Turbine** T. Seljak, T. Katrašnik *University of Ljubljana, Slovenia*	**2-6**

Working Group 3
Chemical and optical advanced diagnostics for smart energy carriers conversion monitoring
chairs: Z. Zelinger, B. Stelzner

11:30 - 11:45	**Measurements and Simulations of Iron Nanoparticle and Gas-phase FeO Formation in Boyancy-opposed Nanoparticle Synthesis Reactor** H. Janbazi[1], J. Sellmann[1], S. Kluge[2] , A. Fomin[3], P. Fjodorow[2], A. Pilipodi-Best[4], O. Hasemann[1], S. Cheskis[4], A. Kempf[1], C. Schultz[2], H. Wiggers[2], I. Wlokas[1], I. Rahinov[3] *1. Department of Fluid Dynamics, Institute for Combustion and Gas Dynamics, University of Duisburg-Essen* *2. Department of Reactive Fluids, Institute for Combustion and Gas Dynamics, University of Duisburg-Essen* *3. Department of Natural Sciences, The Open University of Israel* *4. School of Chemistry, Tel Aviv University, Israel*	**3-1**

11:45 - 12:00	Fiber Laser Intracavity Absorption Spectroscopy (FLICAS) for Measurement of Water, CO, and CO2 During Partial Methane Oxidation Y. Sharabi[1], A. Pilipodi Best[1], V. Tsionsky[1], I. Rahinov[2], S. Cheskis[1] *1. School of Chemistry, Tel Aviv University, Israel* *2. The Open University of Israel, Raanana, Israel*	**3-2**
12:00 - 12:15	3D Instantaneous Reconstruction of a Turbulent Industrial Burner Flame Using Computed Tomography of Chemiluminescence (CTC) K. Mohri[1], M. Röder[2], A. Giese[2], A. Al-Halbouni[2], A. Kempf[1] *1. IVG - University of Duisburg-Essen, Germany* *2. Gas- und Wärme-Institut (GWI), Essen, Germany*	**3-3**
12:15 - 12:30	High Resolution Infrared Spectroscopy as Diagnostic Tool for Combustion and Plasma Chemistry Z. Zelinger[1], V. Nevrlý[2,3], E. Grigorová[1,2], P. Bitala[2], M. Dostál[1,2], J. Suchánek[1], P. Kubát[1], P. Engst[1], M. Ferus[1], P. Kubelík[1], S. Civiš[1] *1. J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic* *2. VŠB-Technical University of Ostrava, Czech Republic* *3. Institute of Thermo-mechanics, Czech Academy of Sciences, Prague, Czech Republic*	**3-4**
12:30 - 12:45	Nuclear Magnetic Resonance (NMR) Spectroscopy as a Tool for Functional Group Analysis of Real Fuels A.D. Ure[1], J.E. O'Brien[2], K. Dussan[3], S. Dooley[1] *1. School of Physics, Trinity College, Dublin, Ireland* *2. School of Chemistry, Trinity College, Dublin, Ireland* *3. National University of Ireland Galway, Ireland*	**3-5**
12:45 - 14:00	***Lunch Break and Poster exhibition***	
	Working Group 4 ***Standard definition for data collection and mining toward a virtual chemistry of smart energy carriers*** *chairs: E. Blurock, S. Dooley*	
14:00 - 14:15	Performance of Methane Combustion Mechanisms Based on Shock Tube Ignition Delay Measurements V. Samu, I. Gy. Zsély, T. Varga, R. Pálvölgyi, T. Turányi *ELTE Eötvös Loránd University, Budapest, Hungary*	**4-1**
14:15 - 14:30	Application of the Ideal Gas Law to Determine the Average Molecular Weight of Real Fuel Complex Mixtures J. Touitou, S. Dooley *Trinity College, Dublin, Ireland*	**4-2**
14:30 - 14:45	Uncertainty Assessment of Kinetic Model of Cyclohexane Oxidation, Including PAH formation M. Abbasi, N. Slavinskaya, U. Riedel *Institute of Combustion Technology DLR, Stuttgart, Germany*	**4-3**
14:45- 15:00	ChemConnect2017: Enhancing Combustion Information and Search Through Semantic Relationships E.S. Blurock *Blurock Consulting AB, Lund, Sweden*	**4-4**

15:00 - 15:15	On the new ReSpecTh Kinetics Data Format specification (v2.0) I. Gy. Zsély, C. Olm, T. Varga, Á. Busai, T. Turányi *ELTE Eötvös Loránd University, Budapest, Hungary*	**4.5**
15:15 - 15:45	***Coffee Break and Poster exhibition***	
15:45 - 17:00	***Task Force: Towards efficient data exchange***	
15:45 - 16:15	Towards a Community Standard Data Exchange: An application to Rapid Compression Machine Measurement and Simulation E.S. Blurock[1], S. Dooley[2], M. Pelucchi[3], A. Matrisciano[4], I. Gy. Zsély[5], R. Ragucci[6] *1. Blurock Consulting, Sweden* *2. Trinity College, Dublin, Ireland* *3. Politecnico di Milano, Italy* *4. Lund Combustion Engineering, LOGE Deutschland GmbH, Cottbus, Germany* *5. ELTE Eötvös Loránd University, Budapest, Hungary* *6. Istituto di Ricerche sulla Combustione - C.N.R., Napoli, Italy*	
16:15 - 17:00	***Open Discussion on Task Force Progresses and Perspectives***	
17:00	***Management Committee Meeting***	
20:00	***Networking Event***	



Friday, October 27th

Working Group 5 - Session 1
Integration of fundamental knowledge towards technology application for smart energy carriers exploitation

chairs: A. Parente, P. Sabia

9:00 - 9:15	**Optimization of Chemical Kinetics for Biogas Combustion in MILD conditions** M. Fürst[1,2,3], P. Sabia[4], M. Lubrano Lavadera[4], M. de Joannon[4], A. Frassoldati[3] and A. Parente[1,2] *1. Université Libre de Bruxelles, Brussels, Belgium* *2. Université Libre de Bruxelles - Combustion and Robust Optimization Group (BURN), Bruxelles, Belgium* *3. Istituto di Ricerche sulla Combustione-CNR, Naples, Italy* *4. Politecnico di Milano, Milano, Italy*	5-1
9:15 - 9:30	**Do all Gas Engines Respond the Same Way to Varying Fuel Composition?** V.M. van Essen[1], S.Gersen[1], G.E.H. van Dijk[1], H. Levinsky[1,2] *1. DNV GL Oil&Gas, Groningen, The Netherlands* *2. University of Groningen, Groningen, The Netherlands*	5-2
9:30 - 9:45	**Numerical Investigation of the Delft Jet in Hot-Coflow Burner with EDC Model and Chemistry Reduction in OpenFOAM** Z. Li[1], F. Contino[2], A. Parente[1] *1. Université Libre de Bruxelles, Belgium* *2. Vrije Universiteit Brussel, Belgium*	5-3
9:45 - 10:00	**Optimization of FGM Model for MILD Combustion in a Cyclonic Burner** G. Ceriello[1], G. Sorrentino[1,2], U. Göktolga[3], M. de Joannon[2], P. Sabia[2], J. van Oijen[3], A. Cavaliere[1], P. de Goey[3] *1. Università di Napoli Federico II, Italy* *2. Istituto di Ricerche sulla Combustione - C.N.R., Napoli, Italy* *3. Technical University Eindhoven, The Netherlands*	5-4
10:00 - 10:15	**Optimization of Composition of Methane/syngas Mixtures at Engine-relevant conditions: A NSGA-II Coupled TOPSIS Approach** A. Paykani, C.E. Frouzakis, K. Boulouchos *Swiss Federal Institute of Technology Zurich, Switzerland*	5-5
10:15 - 10:30	**Carbon Sequestration as a Profitable Application of Biomass Pyrolysis Solid Products** V. Gargiulo[1], C. O. Ania[2], A. Gomis-Berenguer[2], P. Giudicianni[1], M. Alfè[1], R. Ragucci[1] *1. Istituto di Ricerche sulla Combustione - C.N.R., Napoli, Italy* *2. CEMHTI, University of Orleans, Orleans, France*	5-6
10:30 - 10:45	**Combustion Dynamics in a Diabatic PSR with Global, Reduced and Detailed Reaction Mechanisms** F.S. Marra, L. Acampora *Istituto di Ricerche sulla Combustione - C.N.R., Napoli, Italy*	5-7
10:45 -11:00	**Coffee Break**	

	Working Group 5 - Session 2 ***Integration of fundamental knowledge towards technology application for smart energy carriers exploitation*** *chairs: A. Parente, P. Sabia*	
11:00 - 11:15	CFD-assisted Process Intensification for Biomass Fast Pyrolysis in Gas-Solid Vortex Reactor Technology S.R. Kulkarni, A.G. Quiroga, P. Perreault, G. Heynderickx, K.M. Van Geem, G. B. Marin *Laboratory for Chemical Technology, Ghent University, Belgium*	**5-8**
11:15 - 11:30	Biomass Burning Emissions and Impacts on Air Quality R. Radic[1], P.Gvero[2] *1. Republic Hydrometeorological Institute, Banja Luka – Bosnia and Herzegovina* *2 University of Banja Luka, Bosnia and Herzegovina*	**5-9**
11:30 - 11:45	Gas Engine with Hydrogen Scavenged Pre-chamber J. Vávra, M. Takáts, Z. Syrovátka, O. Vítek *Czech Technical University in Prague, Czech Republic*	**5-10**
11:45 - 12:00	Emissions and Performance of a Passenger Car Size Diesel Engine Fuelled with HVO-Diesel Fuel Mixtures I. Bortel, J. Vávra, M. Takáts *Czech Technical University in Prague, Czech Republic*	**5-11**
12:00 - 12:15	Natural Gas Injection and Combustion Simulations in a Constant Volume Chamber and a Direct-injection Spark-ignition Engine C. Chasos *Frederick University, Nicosia, Cyprus*	**5-12**
12:15 - 12:30	Chemical/Physical Features of Particles Emitted from an Automotive Modern Dual-fuel Methane-diesel Engine. M. Alfè[1], C. Guido[2], V. Gargiulo[1], P. Napolitano[2], N. Del Giacomo[2], C. Beatrice[2] *1. Istituto di Ricerche sulla Combustione - C.N.R., Napoli, Italy* *2. Istituto Motori - C.N.R., Napoli, Italy*	**5-13**
12:30 - 12:45	Modeling Downdraft Gasification with Use of a Predictive Pyrolysis Model M. Trninić[1], D. Stojiljković[1], N. Manić[1], Ø. Skreiberg[2], L. Wang[2], A. Jovović[1] *1. University of Belgrade, Serbia* *2. SINTEF Energy Research, Trondheim, Norway*	**5-14**
12:45 - 13:00	Experimental and Numerical Characterization of MILD Combustion of Natural Gas in a 20kW Furnace M. Ferrarotti, A. Parente *Université Libre de Bruxelles, Belgium*	**5–15**
13:00 - 14:30	***Farewell meeting and Lunch***	
14:30 - 16:30	***Lab Tour***	

POSTER SESSION Posters will be on display during the whole Thursday	
Laminar Burning Velocities of Rich Ethylene/Air Flames L. van Treek, N. Roth, L. Seidel, F. Mauss *Brandenburg University of Technology, Cottbus, Germany*	**P1–1**
The Interaction of Bluff Body and Swirl Induced Recirculations on the Flow, Mixing and Combustion Performance of Stratified Propane Flames E. Dogkas, P. Koutmos *University of Patras, Greece*	**P1–2**
Pressure-dependent Rate Rules for Intramolecular H-migration Reaction of Hydroperoxyalkylperoxy Radicals in Low Temperature Q. Yao[1], Z.-R. Li[1], X.-Y. Li[2] *1. College of Chemistry, Sichuan University, Chengdu, China* *2. College of Chemical Engineering, Sichuan University, Chengdu, China*	**P1–3**
Modeling for Pyrolysis of Solid Biomass B. Miljković[1], B. Nikolovski[2] *1. Faculty of Technical Sciences, Novi Sad, Serbia* *2. Faculty of Technology, Novi Sad, Serbia*	**P1–4**
A Combined Kinetic and Experimental Approach to Study the Effect of the Ash on Slow Pyrolysis of Xylan A.I. Ferreiro[1], M. Rabaçal[1], M. Costa[1], P. Giudicianni[2], V. Gargiulo[2], M. Alfè[2], R. Ragucci[2] *1. IDMEC, Instituto Superior Técnico, Lisboa, Portugal* *2. Istituto di Ricerche sulla Combustione - C.N.R., Napoli, Italy*	**P1–5**
Update and Validation of Hemicellulose Pyrolysis Kinetic Mechanism P.E. .Debiagi, E. Ranzi, T. Faravelli *Politecnico di Milano, Milano, Italy*	**P1–6**
A Theoretical Kinetic Study of the Reaction of Hydrogen Atoms with 1- and 2-Pentene J. Power[1], C-W.Zhou[2], H.J.Curran[1] *1. National University of Ireland, Galway, Ireland* *2. Beihang University, Beijing, P.R. China*	**P2–1**
An Ab Initio and Kinetic Study of the Reaction of Ḣ-atoms with 1,3-Pentadiene Y. Sun[1], C-W.Zhou[2], H.J.Curran[1] *1. National University of Ireland, Galway, Ireland* *2. Beihang University, Beijing, P.R. China*	**P2–2**
The Characterization of Thin Layers of Particulate Carbon Deposited in Rich Premixed Flames A. Tregrossi[1], B. Apicella[1], A. Ciajolo[1], G. Russo[1], A. D'Anna[2], G. De Falco[2], L. De Stefano[3], M. Iodice[3], I. Rea[3] *1. Istituto di Ricerche sulla Combustione - C.N.R., Napoli, Italy* *2. DICMaPI, Università degli Studi di Napoli "Federico II", Italy* *3. Istituto per la Microelettronica e Microsistemi - CNR, Napoli, Italy*	**P2–3**
Parametric Study of COS and CS_2 Formation from H_2S Conversion in the Presence of CO_2, CO and CH_4 M. Abián, C. Negro, A. Millera, R. Bilbao, M.U. Alzueta *University of Zaragoza, Spain*	**P2–4**

Wavelength Modulation Spectroscopy for Multicomponent Analytics of Biomass Burning Tracers M. Dostál[1,2], V. Válek[1,2], J. Suchánek[1], E. Kristlová[2], P. Roupcová[2], Z. Zelinger[1], V. Nevrlý[2,3], P. Bitala[2], M. Vašinek[4], P. Kubat[1], M. Ferus[1], S. Civiš[1] *1. J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic* *2. VŠB – Technical University of Ostrava, Czech Re-public* *3. Institute of Thermomechanics, Czech Academy of Sciences, Prague - Czech Republic* *4. VŠB – Technical University of Ostrava, Czech Republic*	**P3-1**
Hydroxyl Radical Measurement in Atmospheric Pressure Dimethyl-Ether/Air Laminar Premixed Flat Flame Using Tunable Diode Laser Absorption Spectroscopy V. Nevrlý[1,2], M. Dostál[1,3], P. Bitala[1], Z. Zelinger[3], J. Suchánek[3], V. Válek[1], V. Klečka[1], P. Kubát[3], P. Engst[3], M. Vašinek[4], J. Wild[5] *1. VŠB-Technical University of Ostrava, Czech Republic* *2. Institute of Thermomechanics, Czech Academy of Sciences, Prague, Czech Republic* *3. J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic* *4. VŠB - Technical University of Ostrava, Czech Republic* *5. Faculty of Mathematics and Physics, Charles University in Prague, Czech Republic*	**P3-2**
Comparison of the Performance of Recent Reaction Mechanisms for Describing the Combustion of Hydrogen Doped with Nitrogen Oxides M. Kovács, T. Varga, C. Olm, R. Pálvölgyi, T. Turányi *ELTE Eötvös Loránd University, Budapest, Hungary*	**P4-1**
Using Soy Molasses for Energy Production B. Nikolovski[1], B. Miljković[2], F. Martinović[1], S. Lazić[1] *1. Faculty of Technology, Novi Sad, Serbia* *2. Faculty of Technical Sciences, Novi Sad, Serbia*	**P5–1**
HCCI Engine Powered By Hydrogen And Ammonia Coming From Power-To-Fuel Storage Systems Maxime Pochet[1,2,3], Ida Truedsson[4], Fabrice Foucher[4], Herv´e Jeanmart[1], Francesco Contino[2,3] *1. iMMC, Université catholique de Louvain, Belgium* *2. Vrije Universiteit Brussel, Belgium* *3. BURN Université Libre de Bruxelles, Belgium* *4. Laboratoire PRISME, Université d'Orléans, France*	**P5–2**
Using Innovative-Renewable Energies for Sustainable Tourism G. Soyhan[1,2], Yahya Sevinc[1], Orhan Batman[1] *1.University of Sakarya, Turkey* *2. Team-SAN Co., Teknokent, Sakarya- Turkey*	**P5–3**
Improving Energy Efficiency Systems for Industrial Kitchen Applications M. Haci[1], Z. Kahraman[1], H.S. Soyhan[2,3] *1. R&D Technology Center, Istanbul - Turkey* *2. University of Sakarya, Sakarya – Turkey* *3. Team-SAN Co., Sakarya - Turkey*	**P5–4**
Validation, Reduction and Optimization of Chemical Kinetic Mechanisms for Marine Engine Applications N. Fokas[1], F. Perdikaris[1], D. Kazangas[1], G. Skevis[2], L. Kaiktsis[1] *1. National Technical University of Athens, Athens, Greece* *2. CPERI/CERTH, Thessaloniki, Greece*	**P5–5**

Wednesday
October 25th

8:00 - 9:00	**Registration**
9:00 - 9:30	**Welcome**
9:30 - 10:15	**Opening lecture**
10:15 - 10:30	coffee break
10:30 - 12:30	**Workshop: Smart Energy Carriers in Industry**
12:30 - 13:30	lunch break
13:30 - 15:45	**Workgroup 1/1** *Oral presentations*
15:45 - 16:00	coffee break
16:00 - 18:15	**Workgroup 1/2** *Oral presentations*

Thursday
October 26th

8:30 - 9:30	**Workgroups 1/3** *Oral presentations*
9:30 - 10:00	coffee break & posters
10:00 - 11:30	**Workgroups 2** *Oral presentations*
11:30 - 12:45	**Workgroup 3** *Oral presentations*
12:45 - 14:00	lunch break & posters
14:00 - 15:15	**Workgroup 4** *Oral presentations*
15:15 - 15:45	coffee break & posters
15:45 - 17:00	Task Force: Towards efficient data exchange ***Progresses and Perspectives***
17:00	**Management Committee Meeting**
20:00	**Networking event**

POSTERS

Friday
October 27th

9:00 - 10:30	**Workgroup 5/1** *Oral presentations*
10:30 - 10:45	coffee break
10:45 -13:00	**Workgroup 5/2** *Oral presentations*
13:00 - 14:30	Farewell & Lunch
14:30- 16:30	LAB Tour

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