PROCEEDINGS

CM1404
SMARTCATs

1ST GENERAL MEETING & SMART ENERGY CARRIERS FOR POWER, INDUSTRY AND ENGINES WORKSHOP

CERTH CONFERENCE CENTRE
THESSALONIKI, GREECE
26–28 AUGUST 2015

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CM1404
SMARTCATs

The First Annual Meeting of the SMARTCATs COST Action is held, on August 26–28th, 2015, in the CERTH Conference Centre (www.certh.gr) in Thessaloniki, Greece. Concurrently and as a natural complement to the SMARTCATs meeting a Workshop on 'Smart Energy Carriers for Power, Industry and Engines' is organized. The agendas of the two events have been strongly entangled to help maximize the effective exchange of ideas and respective requirements among industrial and academic participants. To this aim, in the first day of the event, after a short introduction of the Action aims and tools, a Workshop, devoted to the identification of current industrial needs in the field of innovative energy carriers production and utilization, is held. The Workshop concludes with a round-table discussion bringing together academic and industrial representatives. In the following two days a detailed analysis of the European research potential for addressing practical (real) needs is made during dedicated colloquia organized in the framework of the five SMARTCATs Working Groups.

LOCAL ORGANIZER

Aerosol & Particle Technology Laboratory (APTL)
Chemical Process & Energy Resources Institute (CPERI)
Centre for Research & Technology Hellas (CERTH)

LEGAL REPRESENTATIVE

Athanasios G. Konstandopoulos

LOCAL ORGANIZATION COMMITTEE (APTL/CPERI/CERTH)

George Skevis (Chair)
Helen Papaioannou
Dimitrios Zarvalis
Akrivi Asimakopoulou
Athena Moschopoulou

DAY 1: Wednesday 26 August 2015	
08:30 – 09:00	Registration
09:00 – 09:30	Welcome – Introduction to SMARTCATs
09:30 – 10:45	Introduction to Working Groups
10:45 – 11:00	Introduction to STSMs
11:00 – 11:30	COFFEE BREAK
11:30 – 13:15	Smart Energy Carriers for Power, Industry and Energy Workshop
13:15 – 14:15	LUNCH
14:15 – 16:15	Smart Energy Carriers for Power, Industry and Energy Workshop
16:15 – 17:00	COFFEE BREAK
17:00 – 18:00	Round Table Discussion & Conclusions
18:00 – 19:30	Young Researchers Mixer
18:30 – 20:00	MC Meeting
19:00 – 21:00	CHEESE & WINE
DAY 2: Thursday 27 August 2015	
9:00 – 10:45	Working Group 1 – Session I
10:45 – 11:45	COFFEE BREAK
10:45 – 11:45	Working Groups 1 & 2 – Poster Session
11:45 – 13:00	Working Group 1 – Session II
13:00 – 14:00	LUNCH
14:00 – 15:15	Working Group 2
15:15 – 16:30	Working Group 3
16:30 – late	SOCIAL PROGRAM
DAY 3: Friday 28 August 2015	
09:00 – 10:45	Working Group 4
10:45 – 11:45	COFFEE BREAK
10:45 – 11:45	Working Groups 3 & 4 & 5 – Poster Session
11:45 – 13:15	Working Group 5 – Session I
13:15 – 14:15	LUNCH
14:15 – 15:45	Working Group 5 – Session II
15:45 – 16:00	Wrap Up & Closure
16:00 – 17:30	LABS TOUR

Introduction to the COST Action 1404: Chemistry of Smart Energy Carriers and Technologies (SMARTCATs)

The COST Action Chemistry of Smart Energy Carriers and Technologies (SMARTCATs-CM1404, www.smartcats.eu) has the primary aim of creating a Europe-wide network of world leading academic and research institutions and key industries to promote the use of Smart Energy Carriers (SECs) on a large scale in order to increase fuel flexibility and carbon efficiency of energy production and to support distributed energy generation strategies.

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A safe, secure and environmentally-friendly energy supply is among the highest priorities and concerns of contemporary society. Currently, combustion of conventional and alternative fuels accounts for about 80% of total gross energy production in Europe. The greatest challenge that the combustion community has to face in the coming years is the urgent need for maximum fuel flexibility of combustion technologies, the minimization of *greenhouse gas (GHG) emissions* and the adjustment of *distributed energy production*. Fuel flexibility is a prerequisite to exploit a fast changing fuel market and an increasing number of energy carriers available. Mitigation of GHG emissions is a central priority of the EU Framework Programme for Research and Innovation Horizon 2020 and it is clear that a multifaceted approach, encompassing highly efficient low-carbon technologies coupled with medium-term emission containment (e.g. Carbon Capture and Storage/Utilization), will have to be pursued in order to avoid potentially catastrophic climatic consequences. The realization of *a new energy production and distribution system* based on smart grid concepts is often seen as a possible straightforward option for developed countries.

All these factors call for the characterization, specification and proper utilization of new SECs. This category includes conventional and novel energetic molecules from alternative or conventional (re) sources, selected on the basis of their best available production and/or utilization technologies. Accordingly, to be considered 'smart' an energy carrier and related technologies must be energetically and CO_2 efficient and able to provide the most suitable energy mix to exploit varying and locally diverse sources and to satisfy the requirements for eco-compatibility and sustainability. SECs are strong candidates as possible solutions for energy storage, transfer and transformation from renewable (wind, solar, biomass, wastes) and unconventional sources (e.g. shale gas). SECs include a wide range of compounds like aliphatics, oxygenates (alcohols, esters, ethers) as well as olefins, naphthenes and their mixtures with diluents (CO_2 and H_2O). As a consequence, energy conversion systems have to face an increasing variety of smart carriers that change their characteristics depending on the available source. Even though tailor-made fuel technologies are under development, feedstock and fuel processing variability influences fuel properties in a complex and sometimes unpredictable way. To meet these needs, advanced combustion technologies for energy and power generation in the industrial, domestic and transport sectors are required. Such technologies have to be fuel-flexible and able to achieve high efficiencies, often operating under conditions that are significantly different from those of conventional combustion modes. A new knowledge has to be built to make SECs and new combustion technologies usable in an efficient and sustainable way.

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. According to this methodology the SMARTCATs work programme is structured in five Working Groups (WG).

WG1. Smart Energy Carriers gas phase chemistry: from experiments to kinetic models that aims to improve the knowledge on detailed chemistry and thermochemistry for the combustion, pyrolysis, and oxidation of fuels, such as natural gas mixtures (compressed natural gas, liquefied natural gas, syngas natural gas, bio- methane), simple molecules (large normal and iso-paraffins, alcohols, esters, saturated and unsaturated cyclic ethers) that can be present in 1st and 2nd generation biofuels and complex mixtures of molecules actually found in 1st and 2nd generation biofuels or in the proposed surrogates.

WG2. Chemistry for control of by-products in Smart Energy Carrier conversion that aims to increase knowledge on the formation of organic and inorganic combustion by-products. The pollutant tendency of smart energy carriers will be studied by tracing pollutant species typically formed in combustion (carbon monoxide, unburned hydrocarbons (UHC), polycyclic aromatic hydrocarbons (PAH), aldehydes, NOx soot and nano-particles) as well as other classes of pollutants possibly originating from SECs.

WG3. Chemical and optical advanced diagnostics for Smart Energy Carriers conversion monitoring that aims to improve the knowledge on advanced combustion diagnostics, with a strong focus on technology transfer from fundamental to complex systems, and focuses on advanced sampling and chemical analysis diagnostics, laser-based and mass-spectrometric diagnostics in fundamental combustion devices and chemical kinetics experiments, elementary reaction rate measurements, chemical markers for combustion performance characterization, combustion and emission measurements in complex systems (engines, furnaces, household applications, etc).

WG4. Standard definition for data collection and mining toward a virtual chemistry of Smart Energy Carriers that aims towards the identification of the main requirements and tools for the development of databases, software and mathematical tools for data collection and handling as well as chemistry optimization using data mining techniques. Definition of 'crucial' experiments and simulations, uncertainty and sensitivity analysis in combustion modelling will be key issues to be considered.

WG5. Integration of fundamental knowledge towards technology application for Smart Energy Carriers exploitation that is to apply/integrate the knowledge tools developed in WG1-WG4. This will provide optimized ready to use tools and techniques for an effective use of SECs on large scale. The research activities of the WG will be driven by the identification of validation test cases, identified in collaboration with the industrial partners to provide scale-bridging information from the laboratory units to the real applications by means of integration of detailed kinetic mechanisms in large scale numerical simulations, and assessment of the uncertainty related to numerical predictions for their use in new design and regulation.

DAY 1: Wednesday 26 August 2015

08:30 – 09:00	**Registration**
09:00 – 09:30	**Welcome – Introduction to SMARTCATs** M. de Joannon (IRC-CNR, Italy, Chair), G. Skevis (CPERI/CERTH, Greece, Vice Chair)
09:30 – 10:45	**Introduction to Working Groups** **WG1:** F. Battin-Leclerc (LRGP-CNRS, France) O. Herbinet (LRGP-CNRS, France) **WG2:** M. U. Alzueta (University of Zaragoza, Spain) M. Abian (Spanish National Research Council – CSIC, Spain) **WG3:** S. Voss (TU Bergakademie Freiberg, Germany) T. Kasper (Universitaet Duisburg-Essen, Germany) **WG4:** E.S. Blurock (REACTION, Lund, Sweden) S. Dooley (University of Limerick, Ireland) **WG5:** A. Parente (Université Libre de Bruxelles, Belgium) C. Perlman (LOGE AB, Sweden)
10:45 – 11:00	**Introduction to STSMs** I. Naydenova (Technical University of Sofia, Bulgaria)
11:00 – 11:30	COFFEE BREAK
11:30 – 18:00	**Smart Energy Carriers for Power, Industry and Energy Workshop**
11:30 – 11:45	**Introduction** Fabian Mauss (BTU Cottbus, Germany, Chair of the Industrial Advisory Committee)
11:45 – 12:15	**Lecture 1** **Alternative fuels on the road** Ingemar Magnusson (Volvo GTT – Advanced Technology and Research, Sweden)
12:15 – 12:45	**Lecture 2** **Chemical reaction schemes in industrial CFD – today's applications and future requirements** Michael Bogensperger (AVL, Austria)

12:45 – 13:15	**Lecture 3** Helen Brocklehurst (Rolls Royce plc, UK)
13:15 – 14:15	LUNCH
14:15 – 14:45	**Lecture 4** **Gas turbine burner reactor network construction and application for fast fuel sensitivity analysis** Thommie Nilsson[1], Cathleen Perlman[1], Harry Lehtiniemi[1], Daniel Lörstad[2], Sven-Inge Möller[3], Fabian Mauss[4] 1 Lund Combustion Engineering – LOGE AB, Lund, Sweden 2 Siemens Industrial Turbomachinery AB, Finspång, Sweden 3 Division of Combustion Physics, Lund University, Lund, Sweden 4 Thermodynamics and Thermal Process Engineering, Brandenburg University of Technology Cottbus, Germany
14:45 – 15:15	**Lecture 5** **Fuels science and technology in Repsol** Claudia Esarte (Repsol Technology Center, Spain)
15:15 – 15:45	**Lecture 6** **Modelling new fuels** Tiziano Faravelli (Politecnico di Milano, Italy)
15:45 – 16:15	**Lecture 7** **Fuels decarbonization via upgrading of biomass and bio-based intermediates** Stella Bezergianni (CPERI/CERTH, Greece)
16:15 – 17:00	COFFEE BREAK
17:00 – 18:00	**Round Table Discussion & Conclusions**
18:00 – 19:30	**Young Researchers Mixer** Co-organized with the ECCO-MATE MC ITN project
18:30 – 20:00	**MC Meeting**
19:00 – 21:00	CHEESE & WINE

DAY 2: Thursday 27 August 2015

09:00 – 10:45	**Working Group 1** **Smart energy carriers gas phase chemistry: from experiments to kinetic models** **Session I** Chairs: F. Battin-Leclerc, O. Herbinet
09:00 – 09:15	**Smart carbohydrate energy carriers for custom transportation fuel synthesis** T. Flannelly, M. Howard, G. Capriolo, J.J. Leahy, S. Dooley Department of Chemical and Environmental Sciences, University of Limerick, Ireland
09:15 – 09:30	**A comprehensive experimental and kinetic modelling study of aromatics combustion** Y.Li[1], W. Yuan[2], L. Zhao[2], F. Qi[1] 1 Key Laboratory for Power Machinery and Engineering of MOE, Shanghai Jiao Tong University, China 2 National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, China
09:30 – 09:45	**Kinetic modeling of benzene, toluene and methyl-naphthalene oxidation** N.A. Slavinskaya[1], M. Auyelkhankyzy[2], U. Riedel[1], Z.A. Mansurov[2] 1 Institute of Combustion Technology, German Aerospace Center (DLR), Stuttgart, Germany 2 Institute of Combustion Problems, Almaty, Kazakhstan
09:45 – 10:00	**A comparative study of benzene oxidation in lean-to-rich laminar premixed flames** Z. Malliotakis[1], G. Skevis[2], G. Vourliotakis[1], M.A. Founti[1] 1 Laboratory of Heterogeneous Mixture and Combustion Systems, Thermal Engineering Section, School of Mechanical Engineering, National Technical University of Athens, Greece 2 Aerosol and Particle Technology Laboratory, Chemical Process & Energy Resources Institute, Centre for Research & Technology Hellas, Thessaloniki, Greece

10:00 – 10:15 The influence of butanol blending on the ignition properties of gasoline

L. Roberts[1,2], C. Stead[1,2], A.S. Tomlin[1], E. Agbro[1], D. Bradley[3], M. Lawes[3]

1 Energy Research Institute , School of Chemical and Process Engineering, University of Leeds, Leeds, UK
2 Doctoral Training Centre in Bioenergy, University of Leeds, Leeds, UK
3 School of Mechanical Engineering, University of Leeds, Leeds, UK

10:15 – 10:30 Kinetics of the oxidation and autoignition of oxygenated fuels

Y. Fenard, M. Boumehdi, G. Vanhove

PhysicoChimie des Processus de Combustion et de l'Atmosphère, CNRS/Lille 1, Université Lille 1 Sciences et Technologies, Cité scientifique, Villeneuve d'Ascq Cedex, France.

10:30 – 10:45 Investigation of the low temperature oxidation of hexanal in a jet-stirred reactor

A. Rodriguez, O. Herbinet, F. Battin-Leclerc

Laboratoire Reactions et Genies de Procedes, UMR 7274 CNRS-UL, France

10:45 – 11:45 COFFEE BREAK

10:45 – 11:45 Working Groups 1 & 2 – Poster Session

Kinetic investigation of the reactions of cyclic ethers with hydroxyl radicals

J. Eble, C. Bänsch, M. Olzmann

Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Germany

High pressure combustion kinetics – from elementary reaction steps to global models

R. Fernandes

Physikalisch-Technische Bundesanstalt (PTB), Brunswick, Germany

CO_2 and H_2O role as diluents in combustion chemical kinetics: an open issue

M. de Joannon[1], P. Sabia[1], M.L. Lavadera[2], G. Sorrentino[2], R. Ragucci[1]

1 Istituto di Ricerche sulla Combustione-CNR, Naples, Italy
2 DICMAPI – University Federico II, Naples, Italy

Rate coefficient for the reaction of OH radical with 2-methyltetrahydrofuran

Á. Illés, M. Farkas, E. Gombos, G.L. Zügner, S. Dóbé

Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences, Budapest, Hungary

Modelling combustion: the $O(^3P) + CH_3OH$ reaction

L. Pacifici, F. Talotta, N. Balucani, A. Laganà

Department of Chemistry, Biology and Biotechnologies, University of Perugia, Perugia, Italy

Cyclopentadiene conversion

M. Abìan[1,2], S. Nocito[2], M.U. Alzueta[2]

1 Department of Energy and Environment, Instituto de Carboquímica (ICB), Spanish National Research Council (CSIC), Zaragoza, Spain
2 Aragon Institute of Engineering Research (I3A), Department of Chemical and Environmental Engineering, University of Zaragoza, Zaragoza, Spain

Characterizing ignition behaviour through morphing to generic curves

E.S. Blurock

REACTION, Lund, Sweden

The impact of the dual-fuel ethanol-diesel combustion system on size, number, morphology, and chemical features of the emitted soot

M. Alfè[1], V. Gargiulo[1], G. di Blasio[2], C. Beatrice[2]

1 Istituto di Ricerche sulla Combustione – CNR, Napoli, Italy
2 Istituto Motori – CNR, Napoli, Italy

Modelling of soot formation in diesel sprays using tabulated Conditional Moment Closure

H. Lehtiniemi[1], A. Borg[1], F. Mauss[2]

1 Lund Combustion Engineering - LOGE AB, Lund, Sweden
2 Thermodynamics and Thermal Process Engineering, Brandenburg University of Technology Cottbus, Germany

Improvement of ambient air quality

Y. Georgieva[1], I. Naydenova[2]

1 Directorate General 'Operational Programme Environment', Ministry of Environment and Water of Bulgaria, Sofia, Bulgaria
2 Department of Industrial Power Engineering, College of Energy and Electronics, Technical University of Sofia, Sofia, Bulgaria

A kinetic modelling study of propyne and allene pyrolysis: C1-C6 and PAH hydrocarbon products.

G. Vourliotakis[1], M. Braun-Unkhoff[2], M.A. Founti[1]

1 Laboratory of Heterogeneous Mixtures and Combustion Systems, Thermal Engineering Section, School of Mechanical Engineering, National Technical University of Athens, Athens, Greece

2 Department of Chemical Kinetics, Institute of Combustion Technology, German Aerospace Center, Stuttgart, Germany

11:45 – 13:00	**Working Group 1** **Smart energy carriers gas phase chemistry: from experiments to kinetic models** **Session II** Chairs: F. Battin-Leclerc, O. Herbinet
11:45 – 12:00	**Hydrogen combustion mechanism extended by reactions of excited species** A.A. Konnov Division of Combustion Physics, Department of Physics, Lund University, Lund, Sweden
12:00 – 12:15	**A method for predicting sensitive rate coefficients with high accuracy tested for the $H_2/CO/O_2$-system** T. Methling, M. Braun-Unkhoff, U. Riedel Institut fuer Verbrennungstechnik, German Aerospace Centre (DLR), Stuttgart, Germany
12:15 – 12:30	**The reaction of atomic oxygen with terminal alkenes: the effects of intersystem crossing and the relevance of the formaldehyde production channel** N. Balucani[1], G. Vanuzzo[1], F. Leonori[1], S. Falcinelli[2], R. Bigiarini[1], V. Nevrly[3], D. Stranges[4], C. Cavallotti[5], P. Casavecchia[1] 1 DCBB, Università degli studi di Perugia, Perugia, Italy 2 DICA, Università degli studi di Perugia, Perugia, Italy 3 Faculty of Safety Engineering, Technical University of Ostrava, Czech Republic 4 Dipartimento di Chimica, Università di Roma 'La Sapienza', Italy 5 Dipartimneto di Chimica, Materiali e Ingegneria Chimica 'Giulio Natta', Politecnico di Milano, Milano, Italy

12:30 – 12:45	**Theoretical studies of the dynamics of complex-forming bimolecular reactions** P. Szabó[1], G. Lendvay[1,2], G. Czakó[3] 1 Institute of Chemistry, University of Pannonia, Veszprém, Hungary 2 Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences, Budapest, Hungary 2 Insitute of Chemistry, Eotvos University, Budapest, Hungary
12:45 – 13:00	**An investigation on combustion properties of nitrogen-enriched hydrogen-air mixtures** S. Richter, Th. Kick, M. Braun-Unkhoff, C. Naumann, U. Riedel Institut fur Verbrennungstechnik, German Aerospace Centre (DLR), Stuttgart, Germany
13:00 – 14:00	LUNCH
14:00 – 15:15	**Working Group 2** **Chemistry for control of by-products in smart energy carrier conversion** Chairs: M. Alzueta, M. Abian
14:00 – 14:15	**Experimental and kinetic modelling study of C_2H_2 oxidation at high pressure** J. Gimenez-Lopez[1,2], C.L. Rasmussen[1], M.U. Alzueta[2], Y. Gao[3], P. Marshall[3], P. Glarborg[1] 1 DTU Chemical Engineering, Lyngby, Denmark 2 Department of Chemical and Environmental Engineering, University of Zaragoza, Zaragoza, Spain 3 Department of Chemistry, University of North Texas, Denton, USA
14:15 – 14:30	**Simultaneous analysis of PAH and oxy-PAH by gas-chromatography-mass spectrometry** F. Viteri[1,2], R. Bilbao[1], A. Millera[1], M.U. Alzueta[1] 1 Aragon Institute of Engineering Research, University of Zaragoza, Department of Chemical and Environmental Engineering, Laboratory of Thermochemical Processes 2 Faculty of Engineering Sciences, Tecnológica Equinoccial University, Quito, Ecuador

14:30 – 14:45	**Surface composition of diesel soot using heterogeneous (gas-surface) kinetics of reactive probe gases** A. Tapia[1], S. Salgado-Muñoz[1], P. Martin[1], M. Lapuerta[2], J. Rodriguez-Fernandez[2], M.J. Rossi[1], B. Cabanas[1] 1 Universidad de Castilla La Mancha, Departamento de Quimica Fisica, Faculdad de Ciencia y Tecnolgias Quimicas, Ciudad Real, Spain 2 Universidad de Castilla La Mancha, Grupo de Combustible y Motores, Escuela Tecnica Superior de Ingenieros Industriales, Ciudad Real, Spain 3 Laboratorium fuer Atmosphaerenchemie (LAC), Paul Scherrer Insitute (PSI) Villigen, Switzerland
14:45 – 15:00	**Analysis of HRTEM images of carbonaceous materials to extract quantitative nanostructure properties and correlation with their oxidative behaviour** A. Zygogianni[1], M. Syrigou[1,2], M. Kostoglou[3], A.G. Konstandopoulos[1] 1 Aerosol and Particle Technology Laboratory, Chemical Process & Energy Resources Institute, Centre for Research & Technology Hellas, Thessaloniki, Greece 2 Department of Chemical Engineering, Aristotle University of Thessaloniki, Greece 3 Department of Chemistry, Aristotle University of Thessaloniki, Greece
15:00 – 15:15	**Vanadium catalyzed oxidation of SO_2 to SO_3: Application in two-stroke marine diesel engines.** J.M. Colom[1,2], J.M. Christensen[1], P. Glarborg[1], M.U. Alzueta[2] 1 DTU Chemical Engineering, Lyngby, Denmark 2 Department of Chemical and Environmental Engineering, University of Zaragoza, Spain
15:15 – 16:30	**Working Group 3** **Chemical and optical advanced diagnostics for smart energy carriers conversion monitoring** Chairs: S. Voss, T. Kasper
15:15 – 15:30	**Application of synchrotron-based VUV Photoionization Mass Spectrometry in combustion** F. Qi[1], Z. Zhou[1,2], J. Yang[1,2], Y. Li[1] 1 Key Laboratory for Power Machinery and Engineering of MOE, Shanghai Jiao Tong University, China 2 National Synchrotron Radiation Laboratory, University of Science and Technology of China, China

15:30 – 15:45	**Shock-Tube/TOF – MS studies and kinetic modelling of the pyrolysis of furan derivatives** L. Genthner, M. Olzmann Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Germany
15:45 – 16:00	**Product detection of C(^{3}P) reactions with small hydrocarbons using tunable vacuum ultraviolet synchrotron radiation coupled with time of flight mass spectrometry** J. Bourgalais[1], M. Capron[1], R.K.A. Kailasanathan[2], D.L. Osborn[3], S.D. Le Picard[1], F. Goulay[2] 1 Institut de Physique de Rennes, Universitè de Rennes, Rennes, France 2 Department of Chemistry, West Virginia University, West Virginia, USA 3 Sandia National Laboratories, Livermore, California, USA
16:00 – 16:15	**Fiber Laser Intracavity Absorption Spectroscopy (FLICAS) Thermometry for combustion diagnostics** A. Fomin[1], T. Zavlev[1], I. Rahinov[2], S. Cheskis[1] 1 School of Chemistry, Faculty of Exact Sciences, Tel Aviv University, Tel Aviv, Israel 2 Department of Natural Sciences, The Open University of Israel, Raanana, Israel
16:15 – 16:30	**A comparative study of laminar burning velocities of methane, methanol and ethanol using the Heat Flux method** S. Voss[1], E. Volkov[2], F. Rau[1], V.A. Alekseev[2], A.A. Konnov[2], R. Haas-Wittmüß[3], R.T.E. Hermanns[3], L.P.H. de Goey[4] 1 Institute of Thermal Engineering, TU Bergakademie Freiberg, Freiberg, Germany 2 Division of Combustion Physics, Department of Physics, Lund University, Lund, Sweden 3 OWI Oel-Waerme-Institut GmbH, Affiliated Institute to RWTH Aachen, Herzogenrath, Germany 4 Eindhoven University of Technology, Eindhoven, The Netherlands
16:30 – late	SOCIAL PROGRAM

DAY 3: Friday 28 August 2015

09:00 – 10:45 **Working Group 4**
Standard definition for data collection and mining toward a virtual chemistry of smart energy carriers
Chairs: E.S. Blurock, S. Dooley

09:00 – 09:15 **Enthalpies of formation: validation of ATcT data and a recommendation for best practice in determining the energy density of compounds**
J.M. Simmie
Combustion Chemistry Centre, National University of Ireland, Galway, Ireland

09:15 – 09:30 **Challenges in kinetic optimization**
A. Abou-Taouk[1,2], L-E. Eriksson[2]
1 Cleanergy AB, Sweden
2 Chalmers University of Technology, Gothenburg, Sweden

09:30 – 09:45 **A genetic algorithm-based method for the optimization of reduced kinetics mechanisms**
N. Sikalo[1], O. Hasemann[1], C. Schulz[2,3], A. Kempf[1,3,4], I. Wlokas[1,4]
1 Lehrsthul fur Fluiddynamik, Institute fur Verbrennung und Gasdynamik, Universitaet Duisburg-Essen, Duisburg, Germany
2 Lehrsthul fur Reaktive Fluide, Insitute fur Verbrennung und Gasdynamik, Universitaet Duisburg-Essen, Duisburg, Germany
3 Center for Nanointegration Duisburg-Essen – CENIDE, Duisburg, Germany
4 Center for Computational Sciences and Simulation – CCSS, Universität Duisburg-Essen, Germany

09:45 – 10:00 **Reaction kinetics data in the ReSpecTh information system**
T. Varga[1,2], I. Gy. Zsély[1], T. Turányi[1]
1 Institute of Chemistry, Eotvos University (ELTE), Budapest, Hungary
2 MTA-ELTE Complex Chemical Systems Research Group, Budapest, Hungary

10:00 – 10:15 **The Very Open Data Project: characterizing combustion kinetic data with ontologies and meta-data**
E.S. Blurock
REACTION, Lund, Sweden

10:15 – 10:30 **Emerging methodologies for the co-development of simulations and experiments to reduce uncertainty in data interpretation**
L. Deng[1], N. Sikalo[1], T. Bierkandt[2], T. Kasper[2], I. Wlokas[1,3]
1 IVG, Institute for Combustion and Gas Dynamics-Fluid Dynamics-Essen, Duisburg, Germany
2 Massenspektrometrie in Reaktiven Stromungsprozessen, Institut fur Verbrennung und Gasdynamic, Universitaet Duisburg-Essen, Duisburg, Germany
3 Center for Computational Sciences and Simulation – CCSS, Universität Duisburg-Essen, Germany

10:30 – 10:45 **Predictive chemical kinetics towards new standards for smart energy carriers**
R. Fernandes
Physikalisch-Technische Bundesanstalt (PTB), Brunswick, Germany

10:45 – 11:45 COFFEE BREAK

10:45 – 11:45 **Working Groups 3 & 4 & 5 – Poster Session**

Development of a joint hydrogen and syngas combustion mechanism based on an optimization approach
T. Varga[1,2], C. Olm[1,2], I. Gy. Zsély[1], T. Nagy[3], É. Valkó[1,2], R. Pálvölgyi[1], H.J. Curran[4], T. Turányi[1]
1 Institute of Chemistry, Eotvos University (ELTE), Budapest, Hungary
2 MTA-ELTE Complex Chemical Systems Research Group, Budapest, Hungary
3 Institute of Materials and Environmental Chemistry, RCNS of HAS, Budapest, Hungary
4 Combustion Chemistry Centre, National University of Ireland, Galway, Ireland

Combustion kinetics: experiments, analysis, reduction and use in fundamental and applied numerical investigations
C.E. Frouzakis, Y.M. Wright, K. Boulouchos
Aerothermochemistry and Combustion Systems Laboratory (LAV), Swiss Federal Institute of Technology Zurich (ETHZ), Zurich, Switzerland

Characterization of the water-insoluble fraction isolated from the slow steam pyrolysis of biomasses
V. Gargiulo, M. Alfe', P. Giudicianni, R. Ragucci
Istituto di Ricerche sulla Combustione – CNR, Napoli, Italy

Gaseous products formed during the pyrolysis of biomass in a drop tube furnace: experiments and modelling

A. Ferreiro, U. Fernandes, M. Rabaçal, M. Costa

IDMEC, Mechanical Engineering Department, Instituto Superior Técnico, Universidade de Lisboa, Lisboa, Portugal

Potentiality of mass spectrometry in combustion product analysis

M. Passaro[1,2] , B. Apicella[1], A. Tregrossi[1], A. Ciajolo[1]

1 Istituto di Ricerche sulla Combustione – CNR, Napoli, Italy

2 Chemical Engineering, Materials and Industrial Production Department, University of Naples 'Federico II', Napoli, Italy

Primary experiments with an HCCI engine aimed towards the direct combustion of tar loaded biomass syngas

S. Bhaduri[1], F. Contino[2,3], H. Jeanmart[1]

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Adaptive on-the-fly regression tabulation: beyond ISAT

E.S. Blurock

REACTION, Lund, Sweden

An investigation of the effect of close injections under low levels of CO_2 dilution on a single cylinder optical Diesel engine

M. Founti[1], Y. Hardalupas[2], C. Hong[2], Ch. Keramiotis[1,2], K.G. Ramaswamy[2], N. Soulopoulos[2], A. Taylor[2], D.P. Touloupis[2], G. Vourliotakis[1,2]

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2 Thermofluids Division, Mechanical Engineering Department, Imperial College London

Problems of soot fouling on EGRc: technology and engine conditions dependency

Y. Bravo, C. Larrosa, C. Arnal

Valeo Powertrain Thermal Systems, Zaragoza, Spain

Advanced materials and processes for CO_2 capture and conversion to fuels

G. Pantoleontos, D. Koutsonikolas, G. Skevis, G. Karagiannakis, A.G. Konstandopoulos

Aerosol and Particle Technology Laboratory, Chemical Process & Energy Resources Institute, Centre for Research & Technology Hellas, Thessaloniki, Greece

Methyl esters produced from waste cooking oils by using microwave irradiation method: an experimental and modelling study

V.G. Demir[1], V. Demirtas[2], H.S. Soyhan[3,4]

1 Balikesir University, Department of Mechanical Engineering, Turkey

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Characteristics of investigation of disk stabilized propane flames operated under stratified and vitiated inlet mixture conditions

K. Souflas, G. Paterakis, P. Koutmos

Laboratory of Applied Thermodynamics, Department of Mechanical Engineering and Aeronautics, University of Patras, Greece

11:45 – 13:15 — Working Group 5

Integration of fundamental knowledge towards technology application for smart energy carriers exploitation

Session I

Chairs: A Parente, C.Perlman

11:45 – 12:00

Challenges in industrial implementation of global reaction schemes for simulation of MILD combustion with LCF

P. Wettrell[1], A. Abou-Taouk[1,2]

1 Cleanergy AB, Sweden

2 Chalmers University of Technology, Gothenburg, Sweden

12:00 – 12:15

A cyclonic burner as a test case for combustion systems with high level of dilution and internal recirculation

M. de Joannon[2], G. Sorrentino[1], P. Sabia[2], P Bozza[1], R. Ragucci[2]

1 DICMAPI- University Federico II, Naples, Italy

2 Istituto di Ricerche sulla Combustione-CNR, Naples, Italy

12:15 – 12:30	**Technical feasibility analysis of innovative fuel** T. Seljak, T. Katrašnik University of Ljubljana, Faculty of Mechanical Engineering, Slovenia
12:30– 12:45	**Interpreting abnormal combustion phenomena in spark ignition engines via detailed chemical kinetics modelling** K. Somers[1,2], R.F. Cracknell[2], Y. Zhang[1], H.J. Curran[1] 1 Combustion Chemistry Centre, National University of Ireland, Galway, Ireland 2 Shell Global Solutions, UK
12:45 – 13:00	**Increasing fuel flexibility and carbon efficiency of energy conversion in modern IC engines through advanced CAE technologies** J. Dizy, A. Bhave, G.P. Brownbridge, M.D. Hillman Computational Modelling Cambridge Ltd., CMCL Innovations, Cambridge, UK
13:00 – 13:15	**Numerical and experimental comparison of bio-Fisher-Tropsch fuel and commercial diesel fuel for Euro 5 diesel engine** A. Malik, T. Løvås Norwegian University of Science and Technology, Norway
13:15 – 14:15	LUNCH
14:15 – 15:45	**Working Group 5** **Integration of fundamental knowledge towards technology application for smart energy carriers exploitation** **Session II** Chairs: A Parente, C.Perlman
14:15 – 14:30	**Exploring the iron oxide nanoparticle combustion synthesis in a wide range of operating conditions** A. Pilipody[1], L. Deng[2], A. Fomin[1], V. Tsionsky[1,3], S. Cheskis[1], I. Wlokas[2], I. Rahinov[3] 1 School of Chemistry, Faculty of Exact Sciences, Tel Aviv University, Tel Aviv, Israel 2 IVG, Institute for Combustion and Gas Dynamics –Fluid Dynamics-Essen, Duisburg, Germany 3 Department of Natural Sciences, The Open University of Israel, Raanana, Israel
14:30 – 14:45	**Reduced NO mechanisms validation for a coke oven gas fed flameless furnace** V.Fortunato[1], G. Mosca[2], D. Lupant[2], A. Parente[1] 1 Service d'Aéro-Thermo-Mécanique, Université Libre de Bruxelles, Bruxelles, Belgium 2 Faculté Polytechnique de Mons, Thermal Engineering and Combustion Unit, Mons, Belgium
14:45 – 15:00	**Biomass gasification in presence of CO_2, H_2O or O_2 at high temperature in entrained flow reactor: experiment and modelling** J. Billaud[1], S. Valin[1], M. Peyrot[1], S. Salvador[2] 1 CEA, LITEN/DTBH/SBRT/LTB, Grenoble, France 2 RAPSODEE, UMR-CNRS, France
15:00 – 15:15	**Three-dimensional two-phase flow full simulation of injector flow and Diesel jet injection into a combustion chamber** C.A. Chasos Frederick University, Nicosia, Cyprus
15:15 – 15:30	**Characteristics of lean axisymmetric bluff-body stabilized propane flames under premixed or stratified inlet mixture conditions** G. Paterakis, K. Souflas, E. Dogkas, P. Koutmos Laboratory of Applied Thermodynamics, Department of Mechanical Engineering and Aeronautics, University of Patras, Greece
15:30 – 15:45	**Development of a multi-dimensional flamelet approach and its validation with a finite-rate chemistry simulation** A. Rittler[1], L. Deng[1], I. Wlokas[1,2], A. Kempf[1,2,3] 1 Lehrsthul fur Fluiddynamik, Institute fur Verbrennung und Gasdynamik, Universitaet Duisburg-Essen, Duisburg, Germany 2 Center for Computational Sciences and Simulation – CCSS, Universität Duisburg-Essen, Germany 3 Center for Nanointegration Duisburg-Essen – CENIDE, Duisburg, Germany
15:45 – 16:00	**Wrap Up & Closure**
16:00 – 17:30	LABS TOUR

Author: Fingalo

Thessaloniki

Thessaloniki is a unique city. Founded in 315 BC by King Cassander of Macedonia it has remained a vibrant, cosmopolitan metropolis and a city of art and culture ever since. During the course of the Roman Empire Thessaloniki grew to be an important trade hub located on the Via Egnatia. At the time of the Roman Empire Thessaloniki was also an important center for the spread of Christianity. When the Roman Empire was divided into the tetrarchy, Thessaloniki became the administrative capital of one of the four portions of the Empire under Galerius Maximianus Caesar. Galerius commissioned an imperial palace, a new hippodrome, a triumphal arch and a mausoleum among others, which are still important landmarks of the city.

With the Fall of Rome in 476, Thessaloniki became the second largest city of the Eastern Roman Empire – later the Byzantine Empire. Thessaloniki was considered the second city in the Empire after Constantinople both in terms of wealth and size. In the 14th century the city's population exceeded 100,000 to 150,000, making it larger than London at the time. In the 9th century, the Byzantine Greek missionaries Cyril and Methodius, both natives of the city, invented the Glagolitic alphabet and created the first literary language of the Slavs.

Thessaloniki was captured by the Ottomans in 1430 under the Sultan Murad II. However, the change of sovereignty from the Byzantine to Ottoman Empires did not affect the city's prestige as a major imperial city, manufacturing centre and trading hub. At the same time, it became the new home for many ethnic communities that significantly promoted

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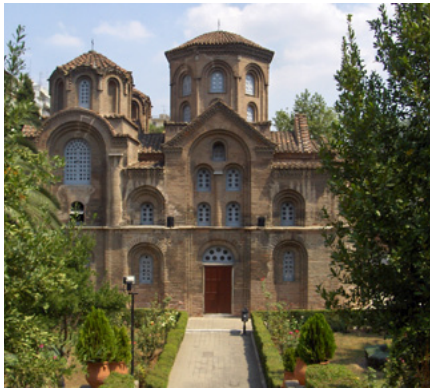
art, culture and architecture. The most important of these communities where the Sephardic Jews, which settled in Thessaloniki in the 15th century. Eventually, the city gained the honorary title of 'Mother of Israel'.

During the 19th century the gradually expanding use of steam and the wide spread of the railways transformed Thessaloniki into the largest industrial center in the Balkans. Huge industrial units were constructed along with a new port. All these led to what the historians called 'California of the East'. The city's population tripled in a time period from 1840 to 1912.

In October 27, 1912 during the first Balkan War the Greek army liberated the city, while in 1917 the city faced what was perhaps its greatest disaster ever, as a huge fire destroyed almost three quarters of the center. Serious efforts were made in order for the city center to be rebuilt like a modern European capital. During the 50's and the 60's the city experienced an unprecedented construction growth that transformed the city center to its present form.

Today, Thessaloniki is a modern metropolis of more than 1,100,000 inhabitants, an important trade and business hub and one of the largest student centers in Southeastern Europe. Thessaloniki was European Capital of Culture in 1997 and the European Youth Capital in 2014. The city's past is kept alive in its aboveground monuments, Roman columns, Paleo-Christian and Byzantine churches, Ottoman mosques and covered markets, synagogues and Jewish markets and magnificent mansions.



Author: Konstantinos Stampoulis

Author: Marsyas

ARCHAEOLOGICAL SITES

The Ancient Forum (dated to the late 2nd or the early 3rd century AD), the palace complex of Galerius Maximianus (4th c. AD), the thermae, the hippodrome, the temples and other monuments.

The Triumphal Arch of Galerius (Kamara), built in AD 305 to commemorate his military successes in the eastern provinces of the Roman Empire.

The Rotunda, an early 4th century building which later was converted into a Christian church.

BYZANTINE SITES

Thessaloniki is justifiably considered an open-air museum of Byzantine art. Wandering through the city, it is worthwhile to see:

The churches of Acheiropoietos (5th century) a three-aisled, timber-roofed basilica, the **Holy Wisdom of God (Hagia Sophia)** (7th century), the **Panaghia (Virgin) Chalkeon** (1028), **Hosios David** (12th century), **St Panteleemon** (late 13th or the early 14th century), a four-columned cross-in-square type, **St Apostoloi** (1310–1314), **Taxiarches** (14th century), **Panagouda** a three-aisled basilica with significant icons, **St Ioannis Prodromos** (Nymphaion), **Vlatadon monastery** a 14th century foundation of which only the katholikon and two cisterns within the precinct survive, and **St Demetrios** (7th century) a splendid basilica dedicated to the patron saint and protector of the city.

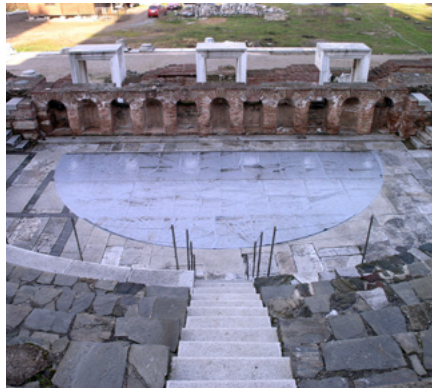
The byzantine walls of the city.

The Heptapyrgion castle, raised in stages, from the early years of the Byzantine Age into the Ottoman period.

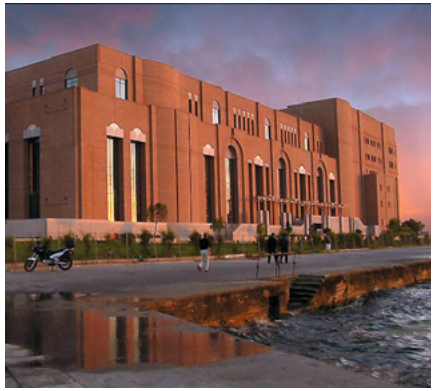
OTTOMAN SITES

The White Tower (15th century), the hallmark of the city.

The Mosques of the Hamza Bey Cami (15th century), the Aladja Imaret Cami (1484) and the Yeni Cami (1902).



Author: Marsyas



Author: Salonica84

Hamams (turkish bathhouses): The Pazar Hamam (15th century), the Pasha Hamam (15th century), Bey Hamam (16th century), Yeni Hamam and the Yahudi Hamam.

THE MODERN CITY

Explore the neighborhoods of the modern city:

The Old City (Ano Polis), in which many notable examples of Ottoman and traditional Macedonian architecture still stand, alongside humble dwellings put up by the refugees who reached Thessaloniki in droves, after the Greek defeat in Asia Minor, in 1922.

The historical quarter of the Ladadika. In recent years, a series of interventions to rehabilitate the urban fabric have helped to enhance the Ladadika as a quarter for leisure pursuits.

The traditional markets: the Modiano, which is housed in a rectangular building of 1922, with pedimented facade and glass roof; the Kapani or Vlalis market; Athonos Square and the 'Louloudadika' (literally flower market).

The central Aristotelous Square, surrounded by monumental buildings and open to the waterfront.

The Thessaloniki Concert Hall. A newly-built, magnificent yet austere, multipurpose venue for cultural and other events.

Archaeological Museum. An exciting tour of the history of ancient Macedonia through important findings dating back to the end of 6th century B.C.

Byzantine Civilization Museum. One of the most important museums of the country, with valuable Byzantine exhibits dating back from the Early Byzantine period to the Turkish occupation. The museum often hosts modern art works and cultural events.

The SMARTCATs Organization

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WORKING GROUPS

WG1: Smart energy carriers gas phase chemistry: from experiments to kinetic models
Leader: Frederique Battin-Leclerc
LRGP-CNRS, France
Vice-Leader: Olivier Herbinet
LRGP-CNRS, France

WG2: Chemistry for control of by-products in smart energy carrier conversion
Leader: Maria U. Alzueta
University of Zaragoza, Spain
Vice-Leader: Maria Abìan
Spanish National Research Council - CSIC, Spain

WG3: Chemical and optical advanced diagnostics for smart energy carriers conversion monitoring
Leader: Stefan Voss
TU Bergakademie Freiberg, Germany
Vice-Leader: Tina Kasper
Universitaet Duisburg-Essen, Germany

WG4: Standard definition for data collection and mining toward a virtual chemistry of smart energy carriers
Leader: Edward S. Blurock
REACTION, Lund, Sweden
Vice-Leader: Stephen Dooley
University of Limerick, Ireland

WG5: Integration of fundamental knowledge towards technology application for smart energy carriers exploitation
Leader: Alessandro Parente
Université Libre de Bruxelles, Belgium
Vice-Leader: Cathleen Perlman
LOGE AB, Sweden

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SMARTCATs

The SMARTCATs COST Action aims to set-up a Europe-wide network of leading academic and research institutions and key industries to promote 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. SMARTCATs is expected to significantly increase the already outstanding level of basic and applied knowledge of the European research institutions and industries in the field of combustion and energy.