

SMARTCATs

2nd General Meeting

&

Workshop on Smart Energy Carriers in Industry

Lisbon, 14-16 November - 2016

Istituto Superior Tecnico de Lisboa hosts the 2nd Annual General Meeting of the Smart Energy Carriers and Technologies COST Action (SMARTCATS- CM1404, www.smartcats.eu) on November 14-16, 2016. The meeting includes a workshop on needs and perspectives of SECs utilization in industrial applications.

The energy scenario has required the redefinition of the concept of the fuel as Smart Energy Carrier enlarging it to a much wider class of compounds. On the other hand, carriers to energy conversion technologies, from small/domestic scale to large power conversion systems as well as to engines, have to provide practical answers to satisfy the energy needs.

The primary aim of this COST Action is to create a Europe-wide network of world leading academic and research institutions and key industries to promote the use of SECs on a large scale in order to increase fuel flexibility and carbon efficiency of energy production and to support distributed energy generation strategies, with the development and the optimization of advanced and emerging combustion technologies.

During the annual Action General Meeting, Action participants meet for sharing and discussing the latest knowledge gained on the conversion and use of SECs, 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.

Chair: Mara de Joannon
IRC-CNR , Italy
dejoannon@irc.cnr.it

Vice-Chair: George Skevis
CPERI /CERTH, Greece
gskevis@cperi.certh.gr

Science officer: Dr Lucia Forzi
COST Association, Belgium

Admin. officer: Ms Svetlana Voinova
COST Association, Belgium

Industrial Advisory Committee:
Fabian Mauss, BTU Cottbus, Germany,
Chair
Helen Brocklehurst, Rolls Royce, UK
Claudia Esarte, Repsol, Spain

STSM Program Manager:
Iliyana Naydenova
Technical University of Sofia, Bulgaria

Early Stage Researcher & Gender
Balance Advisory Committee:
Terese Lovas, Norwegian University of
Science and Technology, Norway

Website and Dissemination Manager:
Raffaele Ragucci, IRC-CNR , Italy

Grant Holder:
Istituto di Ricerche sulla Combustione –
CNR, Italy
Legal representative: Riccardo Chirone
Financial representative: Vincenzo
Scognamiglio
Manager: Antonella Napolitano

Local Organizer:
Mario Costa, mcosta@tecnico.ulisboa.pt
Miriam Rabaçal
Rita Maia
IST -Lisbon - Portugal

MEETING AT A GLANCE

Monday November 14th		Tuesday November 15th		Wednesday November 16th	
8:30 9:45	Registration				
9:45 10:00	Welcome	9:00 10:30	Workgroup 1 <i>Oral presentations - first part</i>	9:00 10:30	Workgroup 3 <i>Oral presentations</i>
10:00 12:30	Workshop on SECs in Industry - first part	10:30 11:00	coffee break & poster exhibition	10:30 10:45	coffee break
12:30 13:30	lunch break	11:00 12:15	Workgroup 1 <i>Oral presentations - second part</i>	10:45 13:00	Workgroup 4 <i>Oral presentations</i>
13:30 14:00	Workshop on SECs in Industry - second part	12:15 13:30	poster exhibition & lunch break	13:00 14:00	lunch break
14:00 15:30	Workgroup 5 <i>Oral presentations - first part</i>	13:30 15:30	Workgroup 2 <i>Oral presentations</i>	14:00 16:00	Data Exchange: towards a community standard
15:30 15:45	coffee break	15:30 15:45	coffee break	16:00	Meeting Closure
15:45 17:00	Workgroup 5 <i>Oral presentations - second part</i>	15:45 18:00	Management Committee Meeting		
		19:00	Networking event		

Working Group leaders/vice:

WG1:
F. Battin-Leclerc, IRL P-CNRS , France / O. Herbinet, IRL P-CNRS , France

WG2:
M.U. Alzueta, University of Zaragoza, Spain / M. Abian, CSIC, Spain

WG3:
S. Voss, TU Bergakademie Freiberg, Germany / T. Kasper, Universitaet Duisburg, Germany

WG4:
E.S. Blurock, Blurock Consulting AB, Sweden / S. Dooley, University of Limerick, Ireland

WG5:
A. Parente, Université Libre de Bruxelles, Belgium / P. Sabia, IRC-CNR, Italy

PROGRAM

9:45 - 10:00	Welcome
Workshop on Smart Energy Carriers in Industry <i>Chairs: F. Mauss - BTU Cottbus and H. Brocklenhurst - Rolls Royce</i>	
November 14 th , 2016 - Auditorium	
10:00 - 10:30	Empiric and Kinetic Model Advances of Industrial Applications of Heating and Diesel Fuels J. Delgado <i>Technology Center of Repsol, Móstoles (Madrid), Spain</i>
10:30 - 11:00	Gas Turbine Fuel Flexibility C. Romano, A. Zucca <i>Nuovo Pignone Tecnologie srl – GE Oil & Gas, Florence - Italy</i>
11:00 - 11:30	Ignition Delay Time is not Enough: Modeling Engine Knock in Gas Engines H. Levinsky, V.M. van Essen, S.Gersen, G.E.H. van Dijk <i>DNV GL Oil&Gas, Groningen, The Netherlands</i>
11:30 - 12:00	A simplified CFD approach for the simulation of industrial flameless burners with capacities from 10 to 1000 kW E. Cresci <i>WVS Warmeprozessestechnik GmbH, Germany</i>
12:00 - 12:30	Development of flameless combustor for an inverted Brayton cycle microturbine used in residential microCHP M. Delanaye¹, A. Giraldo¹, R. Nacereddine¹, M. Rouabah¹, V. Fortunato², A. Parente² <i>MITS SA, Liège, Belgium; Free University of Brussels, Aero-thermo-Mechanical department, Brussels, Belgium</i>
12:30 - 13:30	Lunch Break
13:30 - 14:00	Matching SMEs and Talented Researchers! The H2020 SME Innovation Associate D. Sanopoulos <i>National Coordinator of the Greek EURAXESS Service Network NCP MSCA, CERTH, Greece</i>

SMARTCATs 2nd General Meeting - Workgroup 5 - Part 1 <i>Chairs: A. Parente - ULB and P. Sabia - IRC/CNR</i>	
November 14 th , 2016 - Auditorium	
14:00 - 14:15	"VADEMECOM: VALIDation driven DEVELOPMENT of Modern and Efficient COMBUSTion technologies". An ERC granted project A. Parente <i>Aero-Thermo-Mechanical Department, Université Libre de Bruxelles, Brussels, Belgium</i>
14:15 - 14:30	A Steady State Model of Agricultural Waste Pyrolysis M. Trninic, A. Jovovic, D. Stojiljkovic, N. Manic <i>University of Belgrade, Faculty of Mechanical Engineering, Belgrade - Serbia</i>
14:30 - 14:45	Uncertainty Quantification of Chemical Kinetics for MILD Combustion M. Fürst^{1,2}, A. Parente¹ <i>¹Aero-Thermo-Mechanical Department, Université Libre de Bruxelles, Brussels, Belgium ²Vrije Universiteit Brussel, Combustion and Robust Optimization Group (BURN), Bruxelles, Belgium</i>
14:45 - 15:00	Design And Demonstration of a Gas-Solid Vortex Reactor for the Fast Pyrolysis of Lignocellulosic Biomass K. Van Geem, A. Gonzalez-Quiroga, H. Carstensen, G.B. Marin <i>Laboratory for Chemical Technology, Ghent University, Technologiepark-Zwijnaarde, Belgium</i>
15:00 - 15:15	Experimental Investigation on Emissions and Stability of Combustion Processes with High Level of Internal Recirculation G. Sorrentino, P. Bozza, P. Sabia, R. Ragucci, M. de Joannon <i>Institute of Research on Combustion (IRC)-CNR, Naples, Italy</i>
15:15 - 15:30	Analysis of a 20 kW Flameless Furnace Fired by Natural Gas M. Ferrarotti¹, E. Cresci², D. Lupant³, A. Parente¹ <i>¹Service d'Aero-Thermo-Mecanique, Université libre de Bruxelles, Bruxelles, Belgium ²WVS Warmeprozessestechnik GmbH, Renningen, Germany ³Service de thermique et de combustion, Université de Mons, Mons, Belgium</i>
15:30 - 15:45	Coffee Break

SMARTCATs 2nd General Meeting - Workgroup 5 - Part 2

Chairs: A. Parente - ULB and P. Sabia - IRC/CNR

November 14th, 2016 - Auditorium

15:45 - 16:00	<p>Woody Residues Torrefied and Pelletized at the Small Scale: a New Energy Carrier as a Replacement for Fossil Fuels</p> <p>J. Michel¹, M. McCormick¹, C. Tansley²</p> <p>¹University of Applied Sciences Western Switzerland, HEIG-VD, Industrial Bioenergy Systems, Yverdon-les-Bains, Switzerland ²Granit Technologies SA, Orbe, Switzerland</p>
16:00 - 16:15	<p>Emissions and Performance of Diesel – NG Dual Fuel Engine Operated with Stoichiometric Mixture</p> <p>J. Vávra, M. Takáts, I. Bortel, Z. Syrovátka</p> <p>Vehicle Center of Sustainable Mobility, Faculty of Mechanical Engineering, Czech Technical University in Prague</p>
16:15 - 16:30	<p>Combustion and Emission Analyses of Tire Pyrolysis Oil in a Common Rail Diesel Engine</p> <p>T. Katrašnik, U. Ž. Baškovič, R. Vihar, T. Seljak¹</p> <p>University of Ljubljana, Faculty of Mechanical Engineering, Ljubljana, Slovenia</p>
16:30 - 16:45	<p>Numerical and Experimental Study of a MILD Combustor</p> <p>A. Abou-Taouk</p> <p>Cleanergy AB, Gothenburg, Sweden Chalmers University of Technology, Gothenburg, Sweden</p>
16:45 - 17:00	<p>Diesel Injector Cavitation and Jet Effects on the Combustion Chamber Turbulence Field</p> <p>C. Chasos</p> <p>Frederick University, Nicosia - Cyprus</p>

SMARTCATs 2nd General Meeting - Workgroup 1 - part 1

Chairs: F. Battin-Leclerc - CNRS and K. Van Geem - Ghent University

November 15th, 2016 - Auditorium

9:00 - 9:15	<p>The Reactions of Atomic Oxygen with Unsaturated C4-Hydrocarbons</p> <p>N. Balucani¹, A. Caracciolo¹, G. Vanuzzo¹, P. Casavecchia¹, D. Stranges², C. Cavallotti³</p> <p>¹Dipartimento di Chimica, Biologia e Biotecnologie, Università degli Studi di Perugia ²Dipartimento di Chimica, Università degli Studi La Sapienza di Roma ³Dipartimento di Chimica, Materiali e Ingegneria Chimica "Giulio Natta", Politecnico di Milano</p>
9:15 - 9:30	<p>Formation of C5 Species from Iso-butene</p> <p>L. León, A. Nawdiyal, L. Seidel, F. Mauss</p> <p>Thermodynamics and Thermal Process Engineering, Brandenburg University of Technology, Germany</p>
9:30 - 9:45	<p>Unravelling the Role of Cyclopentadiene and Hexadiene in the Formation of Aromatics</p> <p>K. Van Geem¹, F. Vermeire¹, R. De Bruycker¹, H. Carstensen¹, G.B. Marin¹, O. Herbine², F. Battin-Leclerc², S.S. Mershan³, W.H. Green³</p> <p>¹Laboratory for Chemical Technology, Ghent University, Technologiepark-Zwijnaarde, Belgium; ²Laboratoire Réactions et Génie des Procédés, CNRS, Université de Lorraine, Nancy, France ³Department of Chemical Engineering, Massachusetts Institute of Technology, USA</p>
9:45 - 10:00	<p>Experimental Investigation of Laminar Hydrocarbon/Hydrogen Flames at Elevated Pressures</p> <p>M. Christensen, J. Gao, C. Brackmann, E.J. K. Nilsson</p> <p>Combustion Physics, Lund University, Lund, Sweden</p>
10:00 - 10:15	<p>Critical Issues of Chemical Kinetics in Diluted Combustion Processes</p> <p>P. Sabia, M. Lubrano Lavadera, R. Ragucci, M. de Joannon</p> <p>Institute of Research on Combustion (IRC)-CNR, Naples, Italy</p>
10:15 - 10:30	<p>Laminar Burning Velocity of Diacety/Air Flames. Further Assessment of Combustion Chemistry of Ketene</p> <p>A. Konnov, M. Christensen</p> <p>Division of Combustion Physics, Department of Physics, Lund University, Lund, Sweden</p>

SMARTCATs 2 nd General Meeting - Workgroup 1 - part 2 Chairs: F. Battin-Leclerc - CNRS and K. Van Geem - Ghent University	
November 15 th , 2016 - Auditorium	
10:30 - 11:00	Coffee Break & Poster Exhibition
11:00 - 11:15	Impact of the Presence of Potassium in Cellulose Under Slow and Fast Pyrolysis Conditions A.I. Ferreiro¹, M. Rabaçal¹, M. Costa¹, P. Giudicianni², C.M. Grotola², R. Ragucci² ¹ IDMEC, Mechanical Engineering Department, Instituto Superior Técnico, Universidade de Lisboa ² Institute of Research on Combustion (IRC)-CNR, Naples, Italy
11:15 - 11:30	Kinetic Investigation of the Homogenous Partial Oxidation of CH ₄ /C ₂ H ₅ OH and CH ₄ /n-C ₇ H ₁₆ Mixtures D. Kaczmarek, T. Kasper, B. Atakan Thermodynamics, University of Duisburg-Essen, Duisburg - Germany
11:30 - 11:45	A Modeling and Experimental Study of Laminar Premixed C ₄ -Fames - Iso-butanol Blended with 1,3-Butadiene M. Braun-Unkhoff¹, T. Methling¹, N. Hansen², K. Moshhammer², B. Yang³ ¹ Institute of Combustion Technology, German Aerospace Center (DLR) ² Combustion Research Facility, Sandia National Laboratories, Livermore ³ Center for Combustion Energy, Dept. of Thermal Engineering, Tsinghua University, Beijing
11:45 - 12:00	Revisiting 1-Hexene Low-temperature Oxidation F. Battin-Leclerc¹, X. Meng², A. Rodriguez¹, O. Herbinet¹ ¹ CNRS, Université de Lorraine, Nancy, France ² State Key Laboratory of Engines, Tianjin University
12:00 - 12:15	Trying to Understand the Mechanism of Combustion in Innovative Biofuels: Modelling the case of Oxydized Tetrahydrofuranes A. Gil¹, O. Herbinet², P. Westmoreland³, F. Battin-Leclerc² ¹ Universidade de Lisboa, Portugal ² CNRS, Université de Lorraine, Nancy, France ³ North Carolina State University, USA
12:15 - 13:30	Poster Exhibition & Lunch break

SMARTCATs 2 nd General Meeting - Workgroup 2 - part 1 Chairs: M.U. Alzueta - University of Zaragoza and M. Costa - IST	
November 15 th , 2016 - Auditorium	
13:30 - 13:45	Experimental and Modeling Study of the Soot Formation Process in Very Low Sooting Low Pressure Methane Flames P. Desgroux, A. Faccinnetto, X. Mercier, T. Mouton, A. El Bakali, D.A. Karkar, C. Betrancourt Physical chemistry of Combustion Processes and of the Atmosphere (PC2A), University of Lille Sciences and Technology
13:45 - 14:00	Contribution of Alternate Poly Aromatic Hydrocarbon (PAH) Production Routes in Transportation Fuels Combustion M. Keita¹, A. Nicolle¹, A. El Bakali², P. Desgroux² ¹ Institut Carnot IFPEN Transports Energie, France ² Laboratoire de Physico-Chimie des Processus de Combustion et de l'Atmosphère (PC2A), Université de Lille
14:00 - 14:15	Surface Composition and Reactive Oxygen Species (ROS) Generation: Evaluation of Health Risks of Soot Nanoparticles Based on Quantitative Interfacial Composition M. J. Rossi¹; M.S. Salgado Muñoz², J.-J. Sauvain¹, A. Tapia², M.P. Martín², M. Lapuerta², J. Rodriguez-Fernández², B. Cabañas², O. Popovitcheva³ ¹ Institut Romand de Santé au Travail (IST), Université de Lausanne, Switzerland ² Departamento de Química Física, Universidad de Castilla La Mancha (UCLM), Spain ³ Institute of Nuclear Physics, Moscow State University, Russia
14:15 - 14:30	Impact of Methyl Butanoate Oxidation on NO Formation in Low Pressure Flames N. Lamoureux, M. D. Sylla, P. Desgroux, L. Gasnot Physical chemistry of Combustion Processes and of the Atmosphere (PC2A), University of Lille Sciences and Technology

SMARTCATs 2 nd General Meeting - Workgroup 2 - part 2	
Chairs: M.U. Alzueta - University of Zaragoza and M. Costa - IST	
November 15 th , 2016 - Auditorium	
14:30 - 14:45	<p>Impact of Calcium and Potassium on Single Particle Ignition Behaviour of Biomass Fuels</p> <p>M. Abián¹, M.U. Alzueta¹, A. Carvalho², M. Rabaçal², M. Costa²</p> <p>¹ Aragón Institute of Engineering Research (I3A), University of Zaragoza, Spain ² IDMEC, Mechanical Engineering Department, Instituto Superior Técnico, Universidade de Lisboa, Lisboa, Portugal</p>
14:45 - 15:00	<p>On the Kinetics of Thermal NO Formation</p> <p>T. Turányi, N.A. Buczkó, T. Varga, I.Gy. Zsély</p> <p>Institute of Chemistry, Eötvös Loránd University (ELTE), Budapest, Hungary</p>
15:00 - 15:15	<p>Emissions of Polycyclic Aromatic Hydrocarbons (PAH) During Biomass Combustion in a Drop Tube Furnace</p> <p>J.M. Colom¹, U. Fernandes¹, M. Costa¹, F. Viteri², M.U. Alzueta²</p> <p>¹ IDMEC, Mechanical Engineering Department, Instituto Superior Técnico, Universidade de Lisboa, Lisboa, Portugal ² Aragón Institute of Engineering Research, Dept. of Chemical and Environmental Engineering, University of Zaragoza, Zaragoza, Spain</p>
15:15 - 15:30	<p>Preparation of C₂H₂ Soot Samples for Cytotoxicity Analysis</p> <p>E. Royo¹, M. Conturso², Á. Millera¹, R. Bilbao¹, M.U. Alzueta¹, M. Sirignano², A. D'Anna²</p> <p>¹ Aragón Institute of Engineering Research, Dept. of Chemical and Environmental Engineering, University of Zaragoza, Zaragoza, Spain ² Università degli Studi di Napoli Federico II, Napoli-Italy</p>
15:30 - 15:45	Coffee Break
15:45 - 18:00	Management Committee Meeting
19:00	Networking Event

SMARTCATs 2 nd General Meeting - Workgroup 3	
Chairs: S. Voss - TU Bergakademie Freiberg and T. Kasper - Univ. Duisburg	
November 16 th , 2016 - Auditorium	
9:00 - 9:15	<p>Laser-based and Molecular Beam Sampling Diagnostics for Studies of Combustion Synthesis: from Nanomaterials Fabrication to Syngas Production</p> <p>I. Rahinov¹, A. Pilipody¹, M. Poliak¹, A. Fomin¹, S. Cheskis¹, S. Kluge², P. Fjodorow², L. Deng², H. Wiggers², I. Wlokas², V. Alexeev³, A. Konnov³, V. Tsionsky⁴, C. Schultz¹</p> <p>¹ School of Chemistry, Tel Aviv University ² IVG, Inst. for Combustion and Gas Dynamics, Duisburg-Essen, Germany ³ Division of Combustion Physics, Lund University ⁴ Department of Natural Sciences, The Open University of Israel, Raanana, Israel</p>
9:15 - 9:30	<p>Exploring the Performances of Graphene-like Layers as Chemiresistive Sensing Material for Volatile Organic Compounds (VOCs) Detection</p> <p>V. Gargiulo¹, B. Alfano², E. Massera², M. L. Miglietta², T. Polichetti², G. Di Francia², R. Di Capua³, C. Schiattarella⁴, M. Alfè¹, M. Vorokhta⁵</p> <p>¹ Institute for Research on Combustion (IRC)-CNR, Naples, Italy ² ENEA C.R. Portici, Naples, Italy ³ CNR-SPIN UOS Naples, Italy ⁴ Università di Napoli "Federico II", Italy ⁵ Charles University, Prague, Czech Republic</p>
9:30 - 9:45	<p>Diagnostic of High-temperature Flows Using Ultrasensitive Cavity Ring-down Spectroscopy</p> <p>R. Georges¹, N. Suas-David², A. Benidar², V.N. Kulkarni³, S. Kassi⁴</p> <p>¹ Department of Chemistry, University of Missouri - USA ² Institut de Physique de Rennes, Université de Rennes ³ Indian Institute of Technology Guwahati- India ⁴ Lab. Interdisciplinaire de Physique, Université Grenoble Alpes, CNRS, France</p>
9:45 - 10:00	<p>Experimental Investigation of OH* Chemiluminescence Intensities in Premixed Natural and Producer Gas Flame</p> <p>N. Striugas¹, R. Navakas¹, A. Džiugys¹, A. Saliamonas¹</p> <p>Lithuanian Energy Institute, Lab. of Combustion Processes, Kaunas, Lithuania</p>
10:00 - 10:15	<p>Uncertainties in Species Concentrations Measured by Molecular Beam Mass Spectrometry</p> <p>K. Moshhammer¹, R.X. Fernandes¹</p> <p>Physikalische-Technische Bundesanstalt, Braunschweig, Germany</p>

SMARTCATs 2 nd General Meeting - Workgroup 3	
Chairs: S. Voss - TU Bergakademie Freiberg and T. Kasper - Univ. Duisburg	
November 16 th , 2016 - Auditorium	
10:15 - 10:30	<p>A Comparative Study on the Oxidation of Gaseous and Liquid fuels in a Swirl-stabilized Flame via Chemiluminescence Measurements</p> <p>Z. Malliotakis¹, C. Banyon², H.J. Curran², M. Founti¹, C. Keramiotis¹, G. Vourliotakis¹, P. Koutmos³, G. Paterakis³, K. Soufflas³, F. Mauss⁴, J.J. Rodriguez⁴, G. Skevis⁵</p> <p>¹ School of Mechanical Engineering National Technical University of Athens, Greece ² Combustion Chemistry Center, National University of Ireland, Galway, Ireland ³ Department of Mechanical Engineering and Aeronautics, University of Patras, Greece ⁴ Thermodynamics of Reactive Systems, Brandenburg TU Cottbus, Germany ⁵ Aerosol & Particle Technology Laboratory, CPERI/CERTH, Thessaloniki, Greece</p>
10:30 - 10:45	Coffee Break

SMARTCATs 2 nd General Meeting - Workgroup 4	
Chairs: E.S. Blurock - Bullock Consulting and S. Dooley, University of Limerick	
November 16 th , 2016 - Auditorium	
10:45 - 11:00	<p>PCA & Kriging For Surrogate Models</p> <p>G. Aversano¹, O. Gicquel², A. Parente¹</p> <p>¹ Université Libre de Bruxelles, Brussels, Belgium ² CentraleSupélec, Châtenay-Malabry, France</p>
11:00 - 11:15	<p>Problems of the "Averaged" Least-squares Optimization Identified with the B2B-DC Consistency Analysis of PrlMe</p> <p>N. A. Slavinskaya¹, A. Mirzayeva¹, W. Li¹, M. Frenklach²</p> <p>¹ Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR), German Aerospace Center, Institute of Combustion Technology, Germany</p>
11:15 - 11:30	<p>Towards a fully automated system to develop, validate and evaluate combustion kinetic mechanisms</p> <p>M. Pelucchi¹, A. Rigamonti¹, B. Pernici¹, A. Frassoldati², T. Faravelli²</p> <p>¹ "DEIB" - Politecnico di Milano, Milano, Italy ² DCMIC "G. Natta" - Politecnico di Milano, Milano - Italy</p>

SMARTCATs 2 nd General Meeting - Workgroup 4	
Chairs: E.S. Blurock - Bullock Consulting and S. Dooley, University of Limerick	
November 16 th , 2016 - Auditorium	
11:30 - 11:45	<p>Investigation of the Effect of Correlated Uncertain Rate Parameters on a Model of Syngas Combustion Using a Generalized HDMR method</p> <p>T. Turányi¹, É. Valkó², T. Varga¹, A.S. Tomlin³, Á. Busai¹</p> <p>¹ Institute of Chemistry, Eötvös Loránd University (ELTE), Budapest, Hungary ² MTA-ELTE Research Group on Complex Chemical Systems, Budapest, Hungary ³ School of Chemical and Process Engineering, University of Leeds, UK</p>
11:45 - 12:00	<p>An Open Science Cloud for Molecular Science Services</p> <p>A. Laganà¹, G. Vitillaro², C. Marti¹, L. Pacifici¹</p> <p>¹ Dipartimento di Chimica, Biologia e Biotecnologie, Università di Perugia ² ISTM - C.N.R., Perugia</p>
12:00 - 12:15	<p>Controllability and Reachability of Reactions</p> <p>D.A. Drexler¹, J. Tóth², E. Virágh²</p> <p>¹ Óbuda University, Budapest - Hungary ² Budapest University of Technology and Economics - Hungary</p>
12:15 - 12:30	<p>ChemConnect2016: Interconnected Network of Combustion Data</p> <p>E.S. Blurock</p> <p>Blurock Consulting AB, Sweden</p>
12:30 - 12:45	<p>Reduced Chemical Kinetic Mechanism for PRFs</p> <p>H.S. Soyhan¹, V. Demirtas², G. Coskun¹, U. Demir¹</p> <p>¹ Department of Mechanical Engineering, Sakarya University, Sakarya-Turkey; ² Institute of Natural Sciences, Sakarya University Sakarya-Turkey</p>
12:45 - 13:00	<p>Global Uncertainty and Sensitivity Analysis of a Reduced Chemical Kinetic Mechanism of a Gasoline, n-butanol Blend in a High Pressure Rapid Compression Machine</p> <p>E. Agbro, A.S. Tomlin</p> <p>School of Chemical and Process Engineering, University of Leeds, UK</p>
13:00 - 14:00	lunch break

SMARTCATs 2 nd General Meeting - Data Exchange: Toward a Community Standard	
November 16 th , 2016 - Auditorium	
	Short (5 mins) presentations of perspectives on data transfer and standards
	<p><i>E.S. Blurock</i> <i>Blurock Consulting AB, Sweden</i></p> <p><i>A. Laganà</i> <i>Dipartimento di Chimica, Biologia e Biotecnologie, Università di Perugia</i></p> <p><i>N. A. Slavinskaya</i> <i>Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR), Germany</i></p> <p><i>I. G. Zsely</i> <i>Institute of Chemistry, Eötvös Loránd University (ELTE), Budapest, Hungary</i></p> <p><i>H.J. Curran</i> <i>Combustion Chemistry Center, National University of Ireland, Galway, Ireland</i></p> <p><i>M. Pelucchi,</i> <i>"DEIB"- Politecnico di Milano, Milano, Italy</i></p> <p><i>A. Matrisciano</i> <i>LOGE AB, Sweden</i></p>
14:00 - 14:45	<p>Open Discussion</p> <p><i>The general focus of the discussion will be towards generating a document with regard to data transfer and exchange within the combustion community. The goal is to produce a concrete document from the SMARTCATS community outlining our perspective.</i></p> <p><i>The primary focus of this particular discussion will be:</i></p> <p>1. <i>Defining a set of roles (data user, data generator, software/database provider, ...)</i></p> <p><i>For each role/perspective catalog a prioritised set of requirements, expectations and desires</i></p> <p>2. <i>Cataloging current and proposed efforts (within the community and external) with regard to data (formats, projects, databases, discussions,...)</i></p> <p><i>How can these be incorporated or exploited for our community.</i></p>
14:45 - 16:00	
16:00	Meeting closure

SMARTCATs 2 nd General Meeting - Poster session	
November 15 th , 2016 - Foyer	
P 1	<p>Methane Oxidation over Doped Nickel Catalysts under Reforming Conditions: A DFT Study</p> <p><i>I. Papadimitriou, G. Skevis, A.G. Konstandopoulos</i></p> <p><i>CPERI/CERTH, Thessaloniki, Greece</i></p>
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