WORKSHOP

DATA COLLECTION AND MINING TOWARD VIRTUAL CHEMISTRY OF SMART ENERGY CARRIERS

Napoli, April 5-6, 2016
University Federico II

CM1404

SMARTCATs

cost EUROPEAN COOPERATION IN SCIENCE AND TECHNOLOGY

In the framework of the SMARTCATs COST Action (www.smartcats.eu), the Institute of Research on Combustion (CNR) is organizing the Workshop on "Data Collection and Mining toward the Virtual Chemistry of Smart Energy Carriers", related to Action workgroup 4 activities. The Workshop will take place on 5-6 April 2016 at University Federico II of Naples, Scuola Politecnica e delle Scienze di Base, Italy.

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 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.
The Workshop is aimed at collecting qualified opinions, experiences as well as questions and needs for stimulating the discussion on the main requirements and tools for the development of e-infrastructures, databases, software and mathematical tools for data collection and handling as well as chemistry optimization of Smart Energy Carriers.

TIMETABLE

Tuesday 5 April

10:30	12:30	Registration
12:30	13:30	*Get together lunch*
13:30	15:30	Smart Energy Carriers: Modeling, Data and Data analysis
16:10	16:30	*Coffee break*
16:30	18:30	Smart Energy Carriers: Modeling, Data and Data analysis

Wednesday 6 April

9:00	10:45	Databases, Software and Infrastructures
10:45	11:00	*Coffe break*
11:00	13:00	Databases, Software and Infrastructures
13:00	14:00	*Lunch*
14:00	17:00	Databases and systems use cases: presentation and demo session
17:00	18:00	Discussion
19:00		Networking Event

The participation is free upon registration

For further information on workshop and on possible support please contact:
Mara de Joannon, IRC- CNR, Italy - dejoannon@irc.cnr.it
George Skevis, CERTH/CPERI, Greece - gskevis@cperi.certh.gr
Edward Blurock, Blurock Consulting AB, Sweden - edward.blurock@gmail.com
Antonella Napolitano, IRC- CNR - cm1404grantholder@irc.cnr.it

Scuola Politecnica e delle Scienze di Base
Università degli Studi di Napoli Federico II

PROGRAM

Smart Energy Carriers: Modeling, Data and Data analysis	
April 5th, 2016 - Biblioteca"Ferdinando Gasparini"	
13:30 - 13:50	Welcome and opening
13:50 - 14:10	Uncertainty in the experimental products quantification during JSR hydrocarbon gas-phase reactions ***Frédérique Battin-Leclerc*** *Laboratoire Reactions at Genie des Procedes, CNRS - LRGP - Nancy, FRANCE*
14:10 - 14:30	Auto-ignition of Alcohol and Furan based Bio-fuels- Modeling, Experiments and Theory ***Ravi Fernandes*** *Physikalisch-Technische Bundesanstalt Braunschweig - GERMANY*
14:30 - 14:50	Modelling complex liquid transportation fuels: chemical compositions to combustion properties to highly reduced kinetic models ***Stephen Dooley*** *Department of Chemical and Environmental Sciences, University of Limerick - IRELAND*
14:50 - 15:10	Engine combustion modelling with FGM; the need for accurate and detailed chemistry models ***Bart Somers*** *Eindhoven University of Technology- Eindhoven, NETHERLANDS*
15:10 - 15:30	Sources of uncertainty of thermodynamic and reaction kinetic parameters ***Gyorgy Lendvay*** *Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences - Budapest- HUNGARY*
15:30 - 15:50	Investigation and quantification of facility effects in reaction kinetics experiments by simulation ***Irenaeus Wlokas, Lei Deng, Philipp Niegemann, Mustapha Fikri, Tina Kasper, Christof Schulz, Andreas Kempf*** *University of Duisburg-Essen, GERMANY*
15:50 - 16:10	Skeletal mechanism construction and chemistry tabulation: energy production analysis and the relaxation redistribution method ***Mahdi Kooshkbaghi, Christos E. Frouzakis, Ilya Karlin and Konstantinos Boulouchos*** *Swiss Federal Institute of Technology (ETH) - Zurich SWITZERLAND*
16:10 - 16:30	Coffee Break

Smart Energy Carriers: Modeling, Data and Data analysis	
April 5th, 2016 - Biblioteca"Ferdinando Gasparini"	
16:30 - 16:50	Collaboration of experimental data and simulation tools towards the development of predictive models ***Alessandro Parente*** *Université Libre de Bruxelles - Bruxelles, BELGIUM*
16:50 - 17:10	A Mechanism Reduction Method: Necessity analysis ***Hakan Serhad Soyhan, Vedat Demirtaş, Hüseyin Karadeniz, Cem Sorusbay*** *Sakarya Üniversitesi - Sakarya – TURKEY*
17:10 - 17:30	Chemical kinetic schemes to simulate combustion-generated inorganic nanoparticles ***Amit Bhave*, Nicola Bianco*, Michael Hillman*, George Brownbridge*, Jethro Akroyd, Philipp Buerger**, Daniel Nurkowski**, Sebastian Mosbach**, Markus Kraft***** **CMCL Innovations - UK* ***Department of Chemical Engineering and Biotechnology, University of Cambridge - UK*
17:30 - 17:50	Measurement of key values in combustion: The heat flux burner method to determine laminar burning velocities ***Stefan Voss*** *Institute of Thermal Engineering - Freiberg GERMANY*
17:50 - 18:10	Continuation tools as a virtual test bench for chemical reaction mechanisms ***Luigi Acampora, Francesco Saverio Marra*** *Istituto di Ricerche sulla Combustione, CNR - Napoli ITALY*
18:10 - 18:30	Eulerian-Lagrangian spray modelling and computational fluid dynamics simulation and validation framework ***Charalambos Chasos*** *Department of Mechanical Engineering, FREDERICK UNIVERSITY, Nicosia, CYPRUS*

Databases, Software and Infrastructure	
April 6th, 2016 - Aula Scipione Bobbio	
9:00 - 9:15	Introductory Remarks
9:15 - 9:45	US government, Combustion Institute, and related initiatives for data collection and analytics ***Philip Westmoreland*** *Department of Chemical and Biomolecular Engineering, NCSU - UNITED STATES*
9:45 - 10:15	DataCite: Best Practices on Persistent Identifiers for Research Data ***Laura Rueda*** *DataCite, Communications Director – SPAIN*
10:15 - 10:45	Chemical information and data initiatives ***Richard Kidd (remote talk)*** *Publisher, Royal Society of Chemistry, UNITED KINGDOM*
10:45 - 11:00	Coffee Break
11:00 - 11:30	Infrastructure Use Case: ChemConnect: Database within a resource description framework (RDFs) ***Edward Blurock*** *Blurock Consulting AB, SWEDEN*
11:30 - 12:00	How manage Data into the Collaborative Data Infrastructure: a general overview of EUDAT services ***Claudio Cacciari, Giovanni Morelli*** *CINECA - ITALY*
12:00 - 12:30	The SoBigData Infrastructure ***Valerio Grossi*** *CNR - ISTI PISA - KDDLab- ITALY*
12:30 - 13:00	The SUMO-CHEM H2020 proposal, its structure and an example of Smart Energy Carriers ***Antonio Laganà*** *Università degli Studi di Perugia, Dipartimento di Chimica, Biologia e Biotecnologie - ITALY*

Databases and Systems Use Cases: Presentation and Demo Session	
April 6th, 2016 - Aula Scipione Bobbio	
14:00 - 14:45	ReSpecTh: ReSpecTh: a joint reaction kinetics, spectroscopy, and thermochemistry information system ***Tamas Turanyi*** *Chemical Kinetics Laboratory, Institute of Chemistry, Eötvös University - HUNGARY*
14:45 - 15:30	Development of an UQ-Predictive Chemical Reaction Model for Syngas Combustion http://primekinetics.org/ ***N.A. Slavinskaya, J.H.Starcke, M.Abbasi, M. Auyelkhankyzy, U.Riede* W. Li, J. Oreluk, A. Hedge, A. Packard, M. Frenklach***** **German Aerospace Center (DLR), Inst. of Combustion Technology - GERMANY* *** Mechanical Engineering, University of California at Berkeley, USA*
15:30 - 16:15	"CURVE MATCHING" a generalized framework for model comparison with large sets of experiments ***Alessandro Stagni, M. S. Bernardi, M. Pelucchi, L. M. Sangalli, A. Cuoci, A. Frassoldati, P. Secchi, T. Faravelli*** *Dip. di Chimica, Materiali ed Ingegneria Chimica, Politecnico di Milano - ITALY*
16:15 - 17:00	ChemConnect ***Edward Blurock*** *Blurock Consulting AB, SWEDEN*