Preliminary Program MODEGAT VI - 2019 (2019-08-28)

		Authors	Organization	Title Oral Presentation
Monday, Sep 9, 2019				
09:00-10:00	Plenary	T. V.W. Janssens	Umicore Denmark, Kgs Lyngby., Denmark	Mechanism of the selective catalytic reduction of NOx by ammonia on Cu-CHA
10:00-10:25		N. Usberti, I. Nova, E. Tronconi, R. Koirala, D. Tsinoglou	Politecnico di Milano, Energy Department, Catalysis and Catalytic Processes Laboratory, Italy	NO2 storage and reactivity over Cu-chabazite SCR catalysts
10:25-10:55	Coffee break			
10:55-11:20		M. Bendrich, A. Scheuer, R.E. Hayes, M. Votsmeier	Umicore AG & Co. KG, Hanau, Germany	Model Development and Application over a Cu-CHA Catalyst
11:20-11:55	Key Note	U. Budziankou, M. Börnhorst, C. Kuntz, T. Lauer, O. Deutschmann	Vienna University of Technology, Institute for Powertrains and Automotive Technology	Deposit formation from urea injection: A comprehensive modelling approach
11:55-12:20		C. Lieber, R. Koch, H.-J. Bauer	Karlsruhe Institute of Technology, Institute of Thermal Turbomachinery, Germany	Experimental validation of evaporating urea-water sprays at elevated temperature and pressure
12:20-13:20	Lunch			
13:20-14:20	Plenary	P. Kočí	University of Chemistry and Technology, Prague, Czech Republic	Tutorial Modeling GPF: "Multi-scale modeling of catalytic particulate filters for gasoline engines (GPF)"
14:20-14:45		M. Mitsouridis, G. Koltsakis, Z. Samaras, J. Goodwin, J. Gidney, C. Martin	Aristotle University, Thessaloniki, Greece	GPF modeling supported by size-resolved filtration efficiency measurements
14:45-16:10	Poster Session w/ Coffee			
16:10-16:35		I. Belot, D. Vidal, R. E. Hayes, M. Votsmeier and F. Bertrand	Polytechnique de Montreal, Canada	Numerical study of the impact of washcoat distribution on the overall performance of gasoline particulate filters
16:35-17:00		M. Groisil, S. Loussaief, F. Nicolas, J. Melgar	Siemens Industry Software, Lyon, France	Three-way catalytic converter calibration using optimization algorithm for N2O emission investigation
17:00-17:30	Key Note	S. Schwarz, W.H. Yuan, L. Ruwe, H. Gossler, L. Maier, F. Qi, K. Kohse-Höinghaus, O. Deutschmann	Karlsruhe Institute of Technology, Institute of Technical Chemistry and Polymer Chemistry	Exhaust treatment of natural gas engines
19:00	Conference Dinner with social get-together afterwards on-site			
Tuesday, Sep 10, 2019				
09:00-10:00	Plenary	G. Koltsakis	Aristotle University, Thessaloniki, Greece	Tutorial DPF /SDPF: 'Challenges and model-based solutions in SCR-coated filters applications'
10:00-10:25		T. Watling	Johnson Matthey, UK	Understanding Factors Affecting the Balance Point (and Rate of Balance Point Approach) of a Diesel Particulate Filter: An Analytical Expression for the Balance Point Soot Loading
10:25-11:00	Coffee break			
11:00-11:25		T. Chittipotula, S. Kutschi, A. Natigal and J. C. Wurzenberger	AVL List GmbH, Graz, Austria	Performance of Broken Particulate Filters — A 1D and 3D Simulation Study
11:25-11:50		T. Maunula, M. Tuikka, T. Wolff	Global Catalyst Competence Center Dinex Finland	The reactions and role of ammonia slip catalysts in modern urea-SCR systems
11:50-12:15		I. Cornejo, P. Nikrityuk, R. E. Hayes	University of Alberta, Department of Chemical and Materials Engineering, Canada	Heat and mass transfer inside a monolith: Effect of upstream turbulence and changing thermal properties
12:15-13:30	Lunch			
13:30-14:30	Plenary	L. Lietti	Politecnico di Milano, Milano, Italy	Tutorial Nox Adsorption
14:30-14:55		L.C. Grabow, B. Md. Mushfikur Rahman, U. Menon, A. Gupta, M. P. Harold	University of Houston, Chemical and Biomolecular Engineering, Houston, TX, USA	Nature of Active Sites for Passive NOx Adsorption on Pd-SSZ-13
14:55-15:20		C. März, J. F.-J. Werfel, J. Kühne, F. Inci	IAV GmbH	Approaches for a new generation of fast computing catalyst models
15:20-15:50	Coffee break			
15:50-16:15		W. Wang, E. Bissett, S. Wahiduzzaman	Gamma Technologies, LLC, USA	Hybrid FEM and FDM Approach for Monolithic Catalytic Converters with Pore Diffusion
16:15-16:50	Key Note	M. Bracconi, M. Ambrosetti, F. Franchi, R. Balzarotti, M. Maestri, G. Groppi, E.Tronconi	Politecnico di Milano, Energy Department Milano, Italy	Numerical and experimental study of open cellular structures as innovative supports in environmental catalysis: an application to the selective catalytic reduction of NOx with NH3
16:50-17:30	Farewell coffee			

Poster Programm	Authors	Organization	Title Poster Presentation
	A. Miranda, M. Rodríguez, L.Cadús, D. Borio	PLAPIQUI (UNS/CONICET), Bahía Blanca, Argentina/ INTEQUI (UNSL/CONICET), San Luis, Argentina.	Heat recovery in the catalytic elimination of VOCs under temporary emission patterns
	Y. Bae, J. Hong*	School of Mechanical Engineering, Yonsei University, Seoul, South Korea	Surface reaction characteristics of dry reforming of methane supported by Ni/Al2O3 catalyst at low temperature using an in-situ stagnation flow reactor
	L. F. F. M. Barbosa*, Y. Kaya, M. A. Reddemann, R. Kneer, J. Harmsen	Institute of Heat and Mass Transfer, RWTH Aachen University/ Ford Werke, Research and Innovation Centre Aachen, Germany	Spatially and temporally resolved species measurements in monoliths using Spaci-FTIR
	S. Barth, B. Torkashvand, D. Zengel, M. Casapu, J.-D. Grunwaldt, O. Deutschmann*	Institute for Technical Chemistry and Polymer Chemistry, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany	Determination and validation of the kinetic parameters for a modelling study of Cu-SSZ-13 as pre-turbine DeNOx catalyst
	M. Blažek, M. Václavík, P. Kočí*, M. Svoboda, V. Novák	Department of Chemical Engineering, University of Chemistry and Technology, Prague, Czech Republic/ New Technologies Research Centre, University of West Bohemia, Pilsen, Czech Republic/ Paul Scherrer Institute, Villigen PSI, Switzerland	Microstructure characterization of washcoated catalytic filters
	P. Boutikos, A. Žák, P. Kočí *	Department of Chemical Engineering, University of Chemistry and Technology, Prague, Czech Republic	CO and hydrocarbon light-off inhibition by pre-adsorbed NOx on Pt/CeO2/Al2O3 and Pd/CeO2/Al2O3 diesel oxidation catalysts
	M. Bracconi, M. Ambrosetti, F. Franchi, R. Balzarotti, M. Maestri, G. Groppi and E. Tronconi*	Department of Energy, Politecnico di Milano, Milano, Italy	POCS as potential catalyst supports for environmental applications
	U. Budziankou*, M. Börnhorst*, C. Kuntz, O. Deutschmann, T. Lauer	Institute for Powertrains and Automotive Technology,Vienna University of Technology, Vienna, Austria/ Institute for Chemical Technology and Polymer Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany	Deposit formation from urea injection: A comprehensive modelling approach
	J. Dörnhöfer*, M. Börnhorst, C. Ates, J. Pfeil, M. Wörner, R. Koch, H.-J. Bauer, O. Deutschmann, B. Frohnapfel, T. Koch	Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany	Understanding the Fundamentals of Handling Aqueous Urea Solution for SCR
	M. Eck, O. Deutschmann	Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany	Cyanuric acid hydrolysis studied over titanium dioxide
	R. Greiner *, T. Prill, O. Iliev , B. van Setten, M. Votsmeier	Umicore AG & Co. KG, Hanau, Germany/ TU Darmstadt, Darmstadt, Germany	Tomography based simulation of reactive flow at the micro-scale: Particulate filters with wall integrated catalyst
	J. Han, A. Wang, G. I. Toutizad, H. Härelind, M. Skoglundh, D. Creaser and L. Olsson*	Competence Centre for Catalysis, Chalmers University of Technology, Gothenburg, Sweden	Effect of Zeolite Structure and Copper metal on N2O formation mechanism for NH3-SCR
	R. E. Hayes*, J. P. Mmbaga, A. Donoso-Bravo	Department of Chemical and Materials Engineering, University of Alberta, Edmonton, Alberta, Canada/ Cetaqua, Water Technology Center, Santiago, Chile/ Department of Chemical and Environmental Engineering, Universidad Técnica Federico Santa María, Santiago, Chile	Static Cooling of a Monolith Converter: Influence of Radiation and Natural Convection
	M. Hettel*, E. Daymo, T. Schmidt, O. Deutschmann	Karlsruhe Institute of Technology (KIT), ITCP, Karlsruhe, Germany	CFD-Modeling of Automotive Catalytic Converters
	K. Hong, S. Sutanto, J. Lee, J. Hong*	School of Mechanical Engineering, Yonsei University, Seoul, South Korea	Bimetallic Catalysts for Internal Steam Reforming of Methane at Low-Temperature for High Fuel Utilization of Proton-Conducting Ceramic Fuel Cells
	V. Malashchuk*, C. Steiner, G. Hagen, R. Moos	Department of Functional Materials, University of Bayreuth, Bayreuth, Germany	Simulation model for the radio frequency based state diagnosis of three-way catalytic converters
	I. Vega Mesquida, I. Cornejo , P. Nikrityuk, R. E. Hayes*, M. Votsmeier	Department of Chemical and Materials Engineering, University of Alberta, Edmonton, Canada/ Umicore Automotive Catalysis Division, Research and Development, Hanau, Germany	Modelling pressure drop in particulate filters using different viscous models
	J. Lee, K. Hong, J. Hong*	School of Mechanical Engineering, Yonsei University, Seoul, South Korea	Performance evaluation of Ni-based bimetallic catalysts for dry reforming of methane at low-temperature
	P. Lott, O. Deutschmann*	Karlsruhe Institute of Technology (KIT), ITCP, Karlsruhe, Germany	SpaciPro – A Powerful Operando Technique to Unravel the Mysteries of Exhaust Gas Catalysts
	S. Nasr, N. Semagina, R. E. Hayes*	University of Alberta, Edmonton, Canada	Kinetic modeling of Co3O4- and Pd/Co3O4-catalysed wet lean methane combustion
	J. Němec, P. Kočí*	Department of Chemical Engineering, University of Chemistry and Technology, Prague, Czech Republic	Internal transport limitations in catalytic filter
	R. Pečinka, J. Březina, P. Kočí*	Department of Chemical Engineering, University of Chemistry and Technology, Prague, Czech Republic	Similarities and differences of two-step CO light-off on Pt/Al2O3, Pt/CeO2/Al2O3, Pd/Al2O3 and Pd/CeO2/Al2O3
	M. Plachá, P. Kočí*, M. Isoz, M. Svoboda, E. Price, D. Thompsett	University of Chemistry and Technology, Prague, Czech Republic/ Institute of Thermomechanics, Czech Academy of Sciences, Prague, Czech Republic/ University of West Bohemia, New Technologies Research Centre, Pilsen, Czech Republic/ Johnson Matthey Technology Centre, United Kingdom	Modelling of porous catalytic filters in OpenFOAM
	S. Schwarz*, W.H. Yuan, L. Ruwe, H. Gossler, L. Maier, F. Qi, K. Kohse-Höinghaus, O. Deutschmann	Karlsruhe Institute of Technology (KIT), ITCP, Karlsruhe, Germany	Modelling Homogeneous Gas-Phase Reactions in the Exhaust-Gas tailpipe of Internal Combustion Engines
	D. Schweigert*, B. Damson, H. Lüders, O. Deutschmann	Robert Bosch GmbH, Powertrain Solutions, Advanced Engineering Exhaust Systems/ Karlsruhe Institute of Technology, ITCP	Impact of surface and material properties on spray/wall interaction with urea water solution
	T. Selleri, M. Bracconi, M. Ambrosetti, F. S. Franchi, R. Balzarotti, I. Nova, G. Groppi, E.Tronconi	Department of Energy, Politecnico di Milano, Milano, Italy	Open cellular structures for NOx reduction intensification in automotive applications
	A. Suarez*, L. Olsson, M. Skoglundh, B. Westerberg	Emission Solution Development. SCANIA CV AB/ Department of Chemistry and Chemical Engineering- Chalmers University of Technology	Efficiency in the prediction of After-Treatment Catalytic Systems Modelling. Study Case: Ammonia Adsorption on V-SCR catalyst.
	S. Tischer*, M. Börnhorst, J. Amsler, G. Schoch, O. Deutschmann	IKFT/ ITCP, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany	Thermodynamics and reaction mechanism of urea decomposition
	M. Walander*, J. Sjöblom*, D. Creaser, J. Edvardsson, S. Tamm, B. Lundberg	Mechanics and Maritime Sciences, Chalmers University of Technology/ Chemistry and Chemical Engineering, Chalmers University of Technology/ Johnson Matthey/ Volvo Car Corporation	Parallel 1+1D reactor model for non-uniform, heterogenous catalytic washcoats
	M. Woo, M. E. J. Stettler, M. Rahman, G. Giannopoulos, A. M. Boies*	Centre for Transport Studies, Department of Civil and Environmental Engineering, Imperial College London, London, U.K./ Centre for Sustainable Road Freight, Department of Engineering, University of Cambridge, Cambridge, U.K	Numerical study on modelling and optimisation of a catalytic stripper
	M. Woo, M. E. J. Stettler*	Centre for Transport Studies, Department of Civil and Environmental Engineering, Imperial College London, London, U.K.	A feasibility study of artificial neural networks for modelling catalytic oxidations in a metallic foam reactor
	J. Wurm*, M. Url, F. Woittennek	UMIT – Hall in Tirol/ INNIO Jenbacher GmbH & Co OG	Parameter identification of a control oriented SCR model