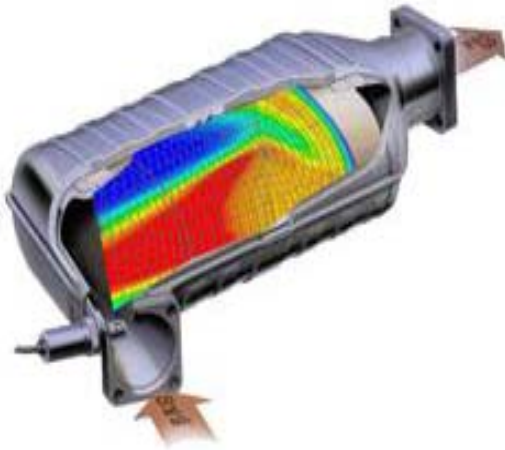


# International Symposium on Modelling of Exhaust Gas After-Treatment



## MODEGAT

14<sup>th</sup>–15<sup>th</sup> September  
2009

Bad

Herrenalb/Karlsruhe  
Germany

## Symposium Program

Preliminary program (status July 21, 2009)

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<b>Sunday, 13.09.2009</b>	
<b>Time</b>	
After 16:00	<b>Arrival</b>
18:30	<b>Dinner</b>
20:00	<b>Dinner (cold food only)</b>
22:00	<b>End of the Day</b>

<b>Monday, 14.09.2009</b>	
<b>Time</b>	
09:00	<b>Tutorial Modeling DOC and DPF</b> G. Koltsakis Laboratory of Applied Thermodynamics Aristotle University Thessaloniki / Greece
10:00	<b>Optimisation of Emission Control Systems Using Computer Modelling</b> M. Ahmadinejad, M. ȚuȚuianu, T. C. Watling Johnson Matthey Technology Centre / UK
10:25	<b>Break</b>
10:55	<b>Simplified reaction modeling of catalytic converters for easier model parameterization</b> D. N. Tsinoglou, M. Weilenmann, A. Karpf, J. Stilli Empa Swiss Federal Laboratories for Materials Testing and Research, Laboratory for Internal Combustion Engines / Switzerland
11:20	<b>Global kinetic modelling of the reaction of soot with NO<sub>x</sub> and O<sub>2</sub> on Fe<sub>2</sub>O<sub>3</sub> catalyst</b> D. Reichert, H. Bockhorn, S. Kureti University of Karlsruhe - Karlsruhe Institute of Technology / Germany
11:45	<b>Modeling of NO<sub>2</sub>-assisted soot conversion and SCR reactions in the combined DPF/SCR filter</b> M. Sokolov <sup>1</sup> , M. Shen <sup>2</sup> <sup>1</sup> Corning Scientific Center, St.Petersburg / Russia <sup>2</sup> Corning Incorporated, Corning NY /USA
12:10	<b>Lunch</b>
13:15	<b>Tutorial Modeling of monolith reactors</b> R. E. Hayes University of Alberta Chemical and Materials Engineering / Canada
14:15	<b>From a detailed 3D model of porous catalytic washcoat to the effective model of entire catalytic monolith</b> P. Kočí <sup>1</sup> , V. Novák <sup>1</sup> , M. Marek <sup>1</sup> , M. Kubíček, F. Štěpánek <sup>1</sup> <sup>1</sup> Department of Chemical Engineering, Institute of Chemical Technology / Czech Republic
14:40	<b>Break</b>
15:10	<b>Computational screening of different catalysts by DFT Modeling of the Reaction Mechanism of Isocyanic Acid Hydrolysis</b> I. Czekaj, O. Kröcher Paul Scherrer Institute / Switzerland
15:35	<b>High throughput screening as a basis for model assisted material optimisation for automotive applications</b>

	A. Sundermann, O. Gerlach hte Aktiengesellschaft / Germany
16:00	<b>Use of latent Variables during the parameter estimation process</b> J. Sjöblom Chalmers University of Technology Department of Chemical and Biological Engineering, Chemical Reaction Engineering / Sweden
16:25	<b>An efficient approach towards predictive kinetic models</b> W. Hauptmann, M. Votsmeier, J. Gieshoff, D.G. Vlachos, A. Drochner, H. Vogel <sup>1</sup> Umicore AG & Co. KG, Hanau <sup>2</sup> University of Delaware Department of Chemical Engineering and Center for Catalytic Science and Technology (CCST) / USA <sup>3</sup> Technische Universität Darmstadt, Ernst-Berl-Institut für Technische und Makromolekulare Chemie / Germany
16:50	<b>Posters</b> <b>Extended Sensitivity Analysis for Targeted Model Improvements</b> J. Sjöblom, Chalmers University of Technology Department of Chemical and Biological Engineering <b>Mathematical modelling of combined DOC, NSRC and (C)DPF system for diesel exhaust aftertreatment</b> M. Schejbal et al., Department of Chemical Engineering Institute of Chemical Technology / Czech Republic J. Štěpánek, P. Kočí and M. Marek, Department of Chemical Engineering Institute of Chemical Technology / Czech Republic M. Kubíček, Department of Mathematics / Czech Republic <b>Evaluation of local diffusion coefficients in porous catalyst</b> V. Novák et al., Institute of Chemical Technology Department of Chemical Engineering / Czech Republic P. Kočí, F. Štěpánek and M. Marek, Institute of Chemical Technology Department of Chemical Engineering / Czech Republic M. Kubíček, Institute of Chemical Technology Department of Mathematics / Czech Republic <b>Simulation of NH<sub>3</sub>-slip Catalysts based on Mapped Elementary Rate Information</b> A. Scheuer et al., Technical University of Darmstadt, Department of Technical Chemistry and Macromolecular Science / Germany A. Drochner and H. Vogel, Technical University of Darmstadt, Department of Technical Chemistry and Macromolecular Science / Germany M. Votsmeier and J. Gieshoff, Umicore AG & Co. KG / Germany <b>Ethanol and acetaldehyde oxidation kinetics on Pt and Pd catalysts for automobile exhaust gas aftertreatment</b> P. Kočí et al., Institute of Chemical Technology Department of Chemical Engineering / Czech Republic J. Štěpánek and M. Marek, Institute of Chemical Technology Department of Chemical Engineering / Czech Republic M. Kubíček, Institute of Chemical Technology Department of Mathematics / Czech Republic T. Maunula and T. Kinnunen, Ecocat Oy / Finland <b>Virtueller Prüfstand (SiL) – Nutzung der Simulation zur Vorentwicklung von Steuergerätefunktionen im Bereich Abgasnachbehandlung</b> S. Dusemund et al., IAV GmbH / Germany K.-J. Langeheinecke, IAV GmbH / Germany R. Bank and H. Harndorf, Universität Rostock / Germany Etc...
18:00	<b>End of first day</b>
19:00	<b>Dinner</b>

<b>Tuesday, 15.09.2009</b>	
<b>Time</b>	
09:00	<b>Tutorial Modeling SCR</b> E. Tronconi Politecnico di Milano Energy Department / Italy
10:00	<b>Development of a SCR System for a Dual Line Exhaust by Using Two- Phase Flow CFD Calculations</b> B. Amon <sup>1</sup> , H. Albert <sup>1</sup> , J.C. Wurzenberger <sup>2</sup> , M. Frobenius <sup>2</sup> <sup>1</sup> Faurecia / Germany <sup>2</sup> AVL / Germany
10:25	<b>Break</b>
10:55	<b>Multiphysics Modeling for Exhaust Gas Treatment</b> H. von Schenk Comsol AB / Sweden
11:20	<b>Object-oriented modelling, dynamic simulation and optimization of heat-integrated exhaust purification systems with ProMoT and DIANA</b> J. Bernnat, M. Rink, U. Tuttlies, G. Eigenberger, U. Nieken University of Stuttgart ICVT / Germany
11:45	<b>Detailed Modeling of Flow-Through Monoliths for Automotive Exhaust Gas Aftertreatment</b> S. Tischer University of Karlsruhe ITCP / Germany
12:10	<b>Lunch</b>
13:15	<b>Tutorial Modeling TWC / NO<sub>x</sub>-storage</b> L. Ollson Chalmers University of Technology Chemical and Biological Engineering / Sweden
14:15	<b>Design of experiments for the calibration of NO<sub>x</sub> storage &amp; reduction catalyst model</b> F. Plát <sup>1</sup> , Š. Bártová <sup>1</sup> , P. Kočí <sup>1</sup> , J. Štěpánek <sup>1</sup> , M. Marek <sup>1</sup> , M. Kubíček <sup>2</sup> <sup>1</sup> Department of Chemical Engineering / Czech Republic <sup>2</sup> Department of Mathematics / Czech Republic
14:40	<b>Focus on the evolution of a Lean NO<sub>x</sub>-Trap model for NO/NO<sub>2</sub> differentiation</b> A. Manigrasso <sup>1,2</sup> , P. Darcy <sup>1</sup> , P. Da Costa <sup>2</sup> <sup>1</sup> Renault SA, Technocentre Renault / France <sup>2</sup> Université Pierre et Marie Curie Laboratoire de Réactivité de Surface / France
15:05	<b>Virtual Integration of Exhaust-Gas After-treatment Devices with complete engine or complete vehicle: modelling approach, challenges &amp; benefits</b> S. Wahiduzzaman, S. Wenzel, C. Armbruster Gamma Technologies GmbH / Germany
15:30	<b>Coffee Break</b>
16:00	<b>End of symposium</b>