3rd International Symposium on Modeling of Exhaust-Gas After-Treatment (MODEGAT III)
08th – 10th September 2013, Bad Herrenalb/Karlsruhe, Germany

Program Overview

Sunday, 08.09.2013

17:00-18:30	**Conference check-in**
19:00	**Dinner**

Monday, 09.09.2013

from 08:00	**Conference check-in**
08:45	Welcome
09:00	Tronconi **Tutorial Modeling SCR**
10:00	Boullion
10:25	**Coffee Break**
10:55	Shwan
11:20	Brack
11:45	Montoya
12:10	**Lunch**
13:15	Harold **Modeling and Analysis of Lean NOx Traps and LNT/SCR Dual Function Catalysts**
14:15	Watling
14:40	**Posters with Coffee**
16:00	Kočí
16:25	Grunwaldt
16:50	Andersson, R.
17:15	**End**
19:00	**Dinner** with social get-together afterwards on-site

Tuesday, 10.09.2013

09:00	Konstandopoulos **Tutorial Modeling DPF**
10:00	Bissett
10:25	**Coffee Break**
11:00	Opitz
11:25	Koutoufaris
11:50	Nova
12:15	**Lunch**
13:30	Fisher **Accomplishments and Developing Issues in Vehicle Exhaust Catalysis**
14:30	Rink
14:55	**Coffee Break**
15:25	Hayes
15:50	Adelberg
16:15	Ekström
16:40	**Coffee Farewell**

Symposium Program

	Monday, 09.09.2013
08:45	**Welcome**
	Session SCR chaired by D. Chatterjee
09:00	**Tutorial Modeling SCR** E. Tronconi, Politecnico di Milano, Milano, Italy
10:00	**Software-in-the-Loop in Exhaust Aftertreatment Simulation** E. Bouillon*, M. McMackin, B. Lumpp, E. Trapel, MAN Truck & Bus AG, Nuremberg, Germany M. Tanimou, M. Münzenmay, Robert Bosch GmbH, Stuttgart, Germany
10:25	**Coffee break**
10:55	**Kinetic deactivation model for Fe-BEA as NH3-SCR catalyst** S.Shwan*, L.Olsson, M. Skoglundh, Chalmers University of Technology, Gothenburg, Sweden J.Jansson, Volvo Group Trucks Technology, Gothenburg, Sweden
11:20	**Kinetic modeling of urea decomposition** W. Brack*, B. Heine, F. Birkhold, M. Kruse, Robert Bosch GmbH, Stuttgart, Germany G. Schoch, S. Tischer, O. Deutschmann, Karlsruhe Institute of Technology, Karlsruhe, Germany
11:45	**Development, validation and calibration of a SCR-system to fulfil Euro 4 and Euro 5 emissions limits** O. Montoya*, S. Egger, MBtech Group GmbH & Co. KGaA, Fellbach-Schmiden, Germany
12:10	**Lunch**
	Session NOx chaired by M. Votsmeier
13:15	**Tutorial Modeling and Analysis of Lean NOx Traps and LNT/SCR Dual Function Catalysts** M.P. Harold*, V. Balakotaiah, D. Luss, University of Houston, Houston/TX, USA
14:15	**Comparison of Different Kinetic Models for NOx Storage on a Lean NOx Trap** T.C. Watling*, Johnson Matthey Technology Centre, Reading, UK P.D. Bolton, D. Swallow, Johnson Matthey Emission Control Technologies, Royston, UK
14:40	**Posters with Coffee**
16:00	**Global approximation of NOx reduction selectivity in automotive catalysts based on platinum group metals** P. Kočí*, D. Mráček, M. Marek, Institute of Chemical Technology, Prague, Czech Republic
16:25	**Structural information on catalysts during NOx and CO oxidation as basis for advanced modelling in exhaust-gas aftertreatment** J.-D. Grunwaldt*, A. Gänzler, A. Boubnov, M. Casapu, D.E. Doronkin H. Lichtenberg, H.W.P. de Carvalho, Karlsruhe Institute of Technology, Karlsruhe, Germany A. Frenkel, Yeshiva University, New York/NY, USA
16:50	**On the accuracy of SpaciMS measurements** R. Andersson*, Chalmers University of Technology, Gothenburg, Sweden
17:15	**END of first day's sessions**
19:00	**Dinner** with social get-together afterwards on-site

	Tuesday, 10.09.2013
	Session DPF chaired by R.E. Hayes
09:00	**Tutorial Modeling DPF** A. Konstandopoulos, Aristotle University of Thessaloniki, Thessaloniki, Greece
10:00	**On the Implications of Wall Reynolds Number Dependent Nusselt Number and Friction Factor on the Accuracy of Wall-Flow DPF Modeling** E. Bissett*, W. Wang, J. Brown, S. Wahiduzzaman, Gamma Technologies, Westmont/IL, USA
10:25	**Coffee break**
11:00	**An experimental and simulation study on the cold-start behaviour of gasoline particulate filters** B. Opitz*, A. Drochner, H. Vogel, Technische Universität Darmstadt, Darmstadt, Germany M. Votsmeier, Umicore AG & Co. KG, Hanau, Germany
11:25	**Heat- and mass-transfer induced hysteresis effects during catalyst light-off testing** I. Koutoufaris, Exothermia SA, Pylaia, Greece G. Koltsakis*, Aristotle University of Thessaloniki, Thessaloniki, Greece
11:50	**Comparative study of Standard SCR and NO oxidation to NO2 on Fe- and Cu-promoted zeolites** M.P. Ruggeri, I. Nova, E. Tronconi*, Politecnico di Milano, Milano, Italy
12:15	**Lunch**
	Session TWC/DOC chaired by O. Deutschmann
13:30	**Tutorial Accomplishments and Developing Issues in Vehicle Exhaust Catalysis** G.B. Fisher**,** University of Michigan, Ann Harbor/MI, USA
14:30	**Heat-integrated exhaust purification with minimized cold start emissions for natural gas powered engines** M. Rink*, G. Eigenberger, U. Nieken, University of Stuttgart, Stuttgart, Germany
14:55	**Coffee break**
15:25	**A Case Study in Multiscale Model Reduction:** **The Effect of Cell Density on Catalytic Converter Light-Off** A. Fadic, T.W. Nien, J.P. Mmbaga, R.E. Hayes*, University of Alberta, Edmonton, Canada M. Votsmeier, Umicore AG & Co. KG, Hanau, Germany
15:50	**"Virtual Certification" – Intelligent, model based system integration for the development of commercial vehicle EU6 concepts** S. Adelberg*, F. Schrade, P. Eckert, L. Krämer, IAV GmbH, Berlin, Germany
16:15	**Multidisciplinary Optimization of Emission Control systems for Light-Duty Vehicles** F. Ekström*, Volvo Car Corporation, Gothenburg, Sweden
16:40	**Coffee and farewell**

Underlined: First Author/Presenting Author
Asterisk*: Corresponding Author

Poster Presentations

(in alphabetical order of first author's last name)

Title, Authors (underlined: first/presenting author, asterisk*: corresponding author)

Oxygen storage level based reaction kinetics for three-way catalyst modeling
J. Bickel*, G. Eigenberger, U. Nieken

Correlation of Static Ageing Effects on Automotive Catalysts
L. Blades*, R. Douglas, G. McCullough, A. Woods

Spatially-resolved XAS during NH3-SCR and related reactions over representative Fe- and Cu-zeolite catalysts
D.E. Doronkin*, M. Casapu, T. Günter, O. Müller, R. Frahm, H. Lichtenberg, J.-D. Grunwaldt

Efficient prediction of diffusivity in porous catalytic coating
M. Dudák, P. Kočí*, M. Marek, V. Novák, P. Blanco-García, G. Jones, D. Thompsett

Approximate Pressure Drop and Filtration Efficiency Expressions for Semi-Open Wall-Flow Channels
O. Haralampous*, T. Kontzias

Estimation of Local Aging Effects of Three-Way-Catalysts by Analysis of their Spatial Temperature and CO conversion profiles
C. Hauck*, S. Tischer, L. Maier, O. Deutschmann

Rapid interpolation of precomputed kinetic data employing reduced local Hermite methods
M. Klingenberger*, J. Gieshoff, A. Drochner, H. Vogel, M. Votsmeier

Adsorption investigations of oxygen and NO over Pt-supported catalyst
O. Mihai, D. Creaser, L. Olsson*

Mass Spectroscopic Study of the Oxidation and Reduction of Zirconium Oxide Clusters in the Gas-Phase
K. Miyajima, F. Mafuné*

Dodecane conversion in heavy-duty Diesel oxidation catalyst
D. Mráček, P. Kočí*, M. Marek

Application of Optimisation Techniques to Determine Reaction Kinetic Parameters of Automotive Catalysts.
A. Pedlow*, G. McCullough, A. Goguet

Investigation of cold-start phenomena over a Cu-zeolite NH3-SCR catalysts for Diesel exhaust gas aftertreatment
M.P. Ruggeri, M. Colombo, I. Nova, E. Tronconi*

Embedding complex Three-Way-Catalyst Models for Rapid Control Prototyping in Automotive Applications
S. Schödel*, G. Fischerauer, M. Votsmeier

Modelling of particulate matter transformations and capture efficiency
J. Sjöblom*, H. Ström

CFD characterization of monolithic reactors for kinetic studies
S. Soltani, R. Andersson, B. Andersson*

Detailed kinetic modelling of automotive exhaust NO reduction by CO/H2 over Rh
Q. Su*, Y. Li, L. Xie, B. Ma

Title, Authors (underlined: first/presenting author, asterisk*: corresponding author)

Detailed validation of an auto catalysis model using spatially resolved measurements within the catalyst substrate

J. Stewart*, R. Douglas, A. Goguet, C. Stere

Application of Proper Orthogonal Decomposition Methods in Reactive Pore Diffusion Simulations

M. Ullmann*, J. Seidel, U. Prüfert, O. Ernst, C. Hasse

Kinetic Mechanism Generation via Modified GA and ISAT

Q. Xie*, B. Rogg

Catalysis of electric charges accumulated in subnano-space through strong cluster-substrate interaction

H. Yasumatsu*, N. Fukui