Karlsruhe Institute of Technology

Catalytic combustion: Modeling and Simulation

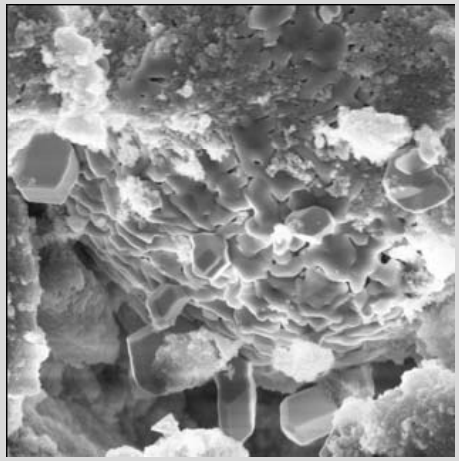
3rd Combustion School, Salvador, Basil, 04.07.2011

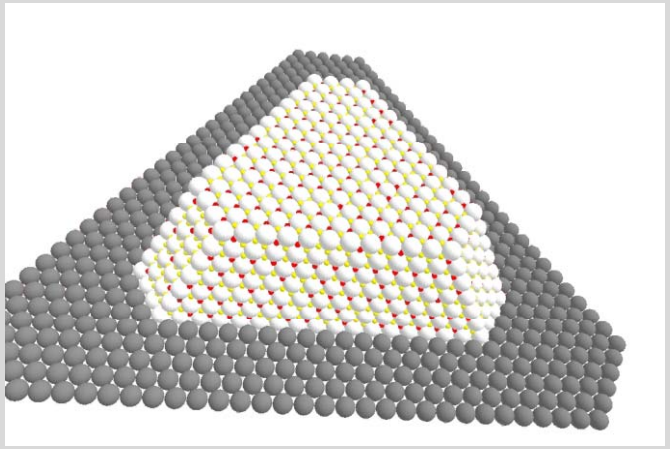
Olaf Deutschmann

Karlsruhe Institute of Technology (KIT), Germany

Institute for Chemical Technology and Polymer Chemistry (ITCP)

Institute for Catalysis Research and Technology (IKFT)





The University City of Karlsruhe

Karlsruhe:

founded 1715
300 000 people
located in Baden-Württemberg,SW state of Germany

Several federal institution such as German Supreme Court and Attorney General

Industry: chemical, automobile, energy, IT

2009: Fusion of the University of Karlsruhe and the National Research Center to the Karlsruhe Institute of Technology (KIT) with now 8000 employees and 20000 students

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Institute for Chemical Technology and Polymer Chemistry

Karlsruhe Institute of Technology (KIT): University and National Research Center

The members of Deutschmann groups at KIT are active at the University at Campus South as well as at the National Laboratory at Campus North.

- Institute for Catalysis Research and Technology (IKFT)
- Institute for Nuclear and Energy Technology (IKET)
- Helmholtz Research School Energy-Related Catalysis
- Institute for Chemical Technology and Polymer Chemistry (ITCP)
- Exhaust Gas Center

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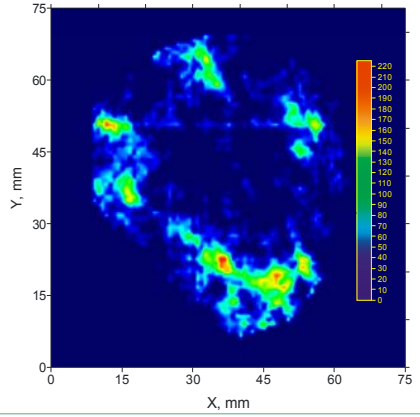
Heterogeneous reactions: Tools for chemicals and materials synthesis, emission control, and energy conversion

High-temperature catalysis

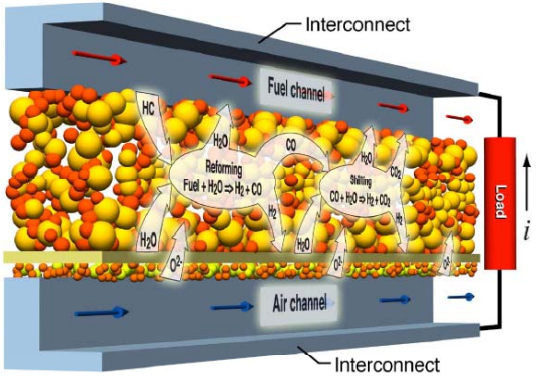
Emission control

Courtesy of J. Eberspächer GmbH& Co

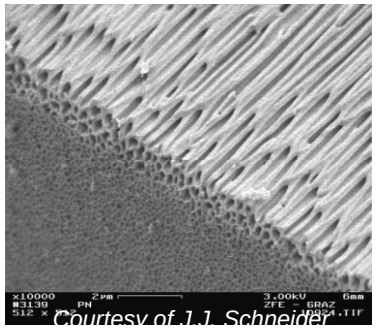
Combustion



Fuel cells (SOFC)

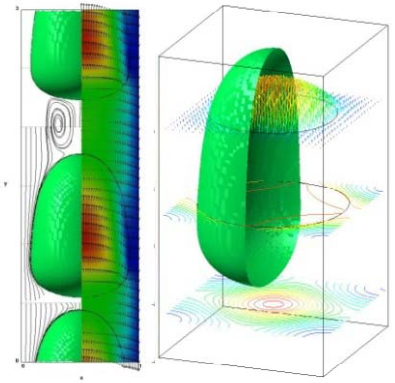


Carbon composite materials



Courtesy of J.J. Schneider

Multi-phase flow



Research methods: experiment, analytics and diagnostics, model development, numerical simulation, reactor and process design, optimization

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Catalytic combustion: Modeling and Simulation
Outline

1. **Motivation**
2. Principle of catalysis
3. Modeling the reactions on the catalytic surface
4. Modeling transport in reactions in porous media
5. Reactive flow and catalysis
6. Transient processes
7. Non-uniform inlet conditions
8. Gas-phase chemistry
9. Catalyst deactivation

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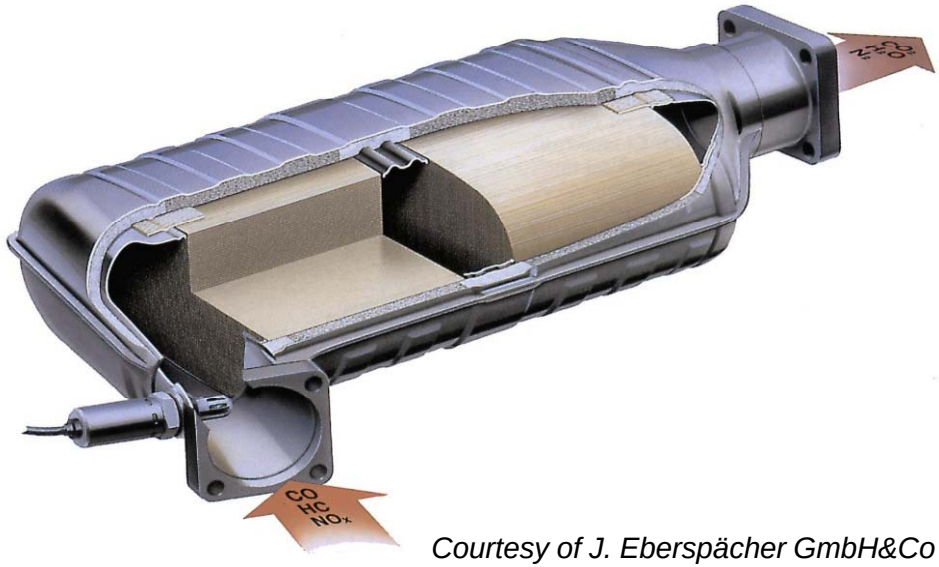
Catalytic combustion today: Wide variety of applications, mainly driven by environmental concerns

Objectives:

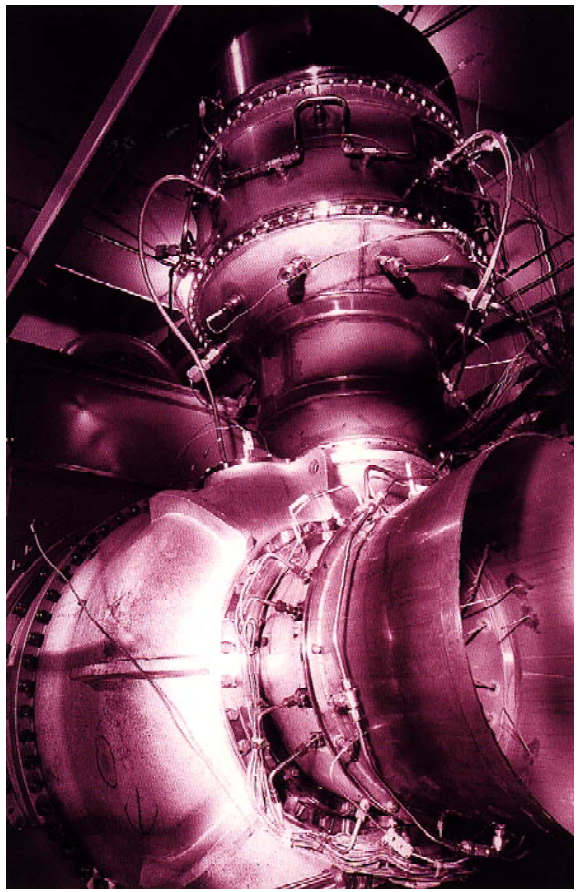
- remove pollutants
- reduce the formation of pollutants
- produce low temperature heat
- stabilize flames
- avoid and quench open flames

Automotive catalytic converter



Courtesy of J. Eberspächer GmbH&Co

Stationary gas turbine



Courtesy of Catalytica Combustion Sys.

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Catalytic combustion today: Wide variety of applications, mainly driven by environmental concerns

Objectives:

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- avoid and quench open flames

VOC removal

Courtesy of Catabrun, Taikisha Ltd.

Portable radiant heater

Courtesy of Catalyst SystemTechnologies

Domestic gas stove

Courtesy of L&S Fireplace Shoppe

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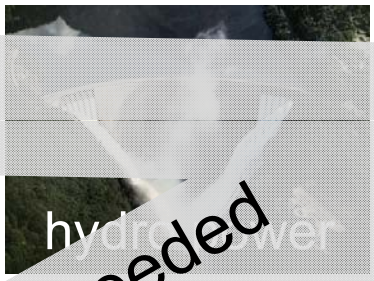
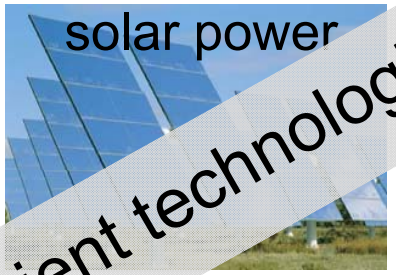
21th century: Diversification of raw materials for energy, fuels, and chemicals

mobility



Catalysis





efficient technologies needed

chemical products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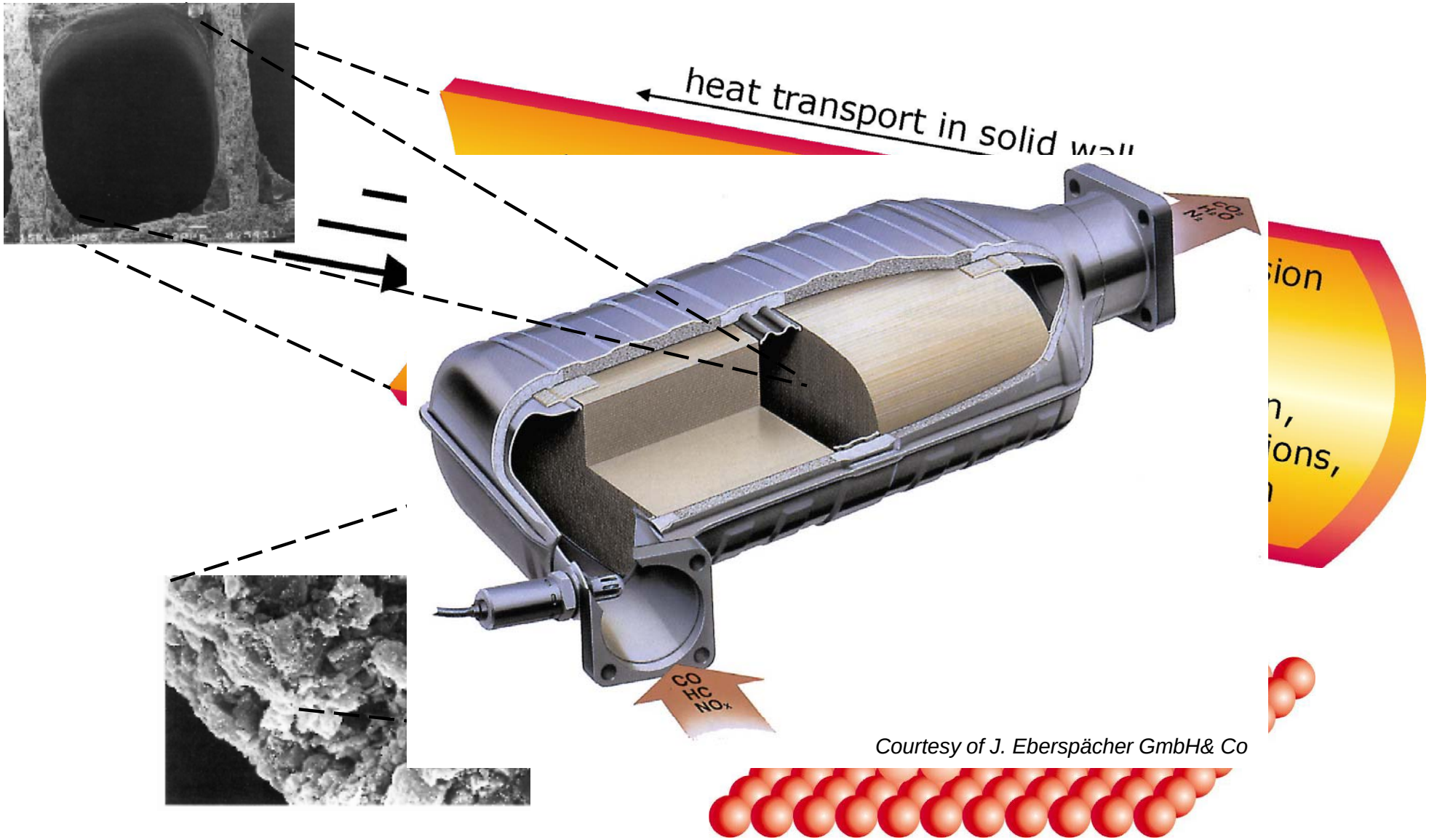
Complex interaction of physics and chemistry: Multi-scale modeling



Courtesy of J. Eberspächer GmbH& Co

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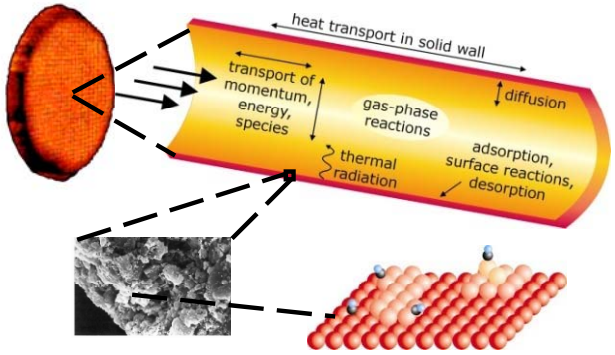
Objective of this lecture: Introduction into modeling of catalytic combustion and energy-related catalysis



Understanding of the underlying physical and chemical processes

Development of elementary reaction mechanisms (molecular level)

Coupling of chemistry with mass and heat transport of technical reactor
→stiff coupled non-linear PDE/DAE systems

Numerical solution of the resulting DAEs with appropriate inlet and boundary conditions

Optimization of reactor/burner design and operating conditions

Examples: Catalytic converters, radiant burners, and reformers

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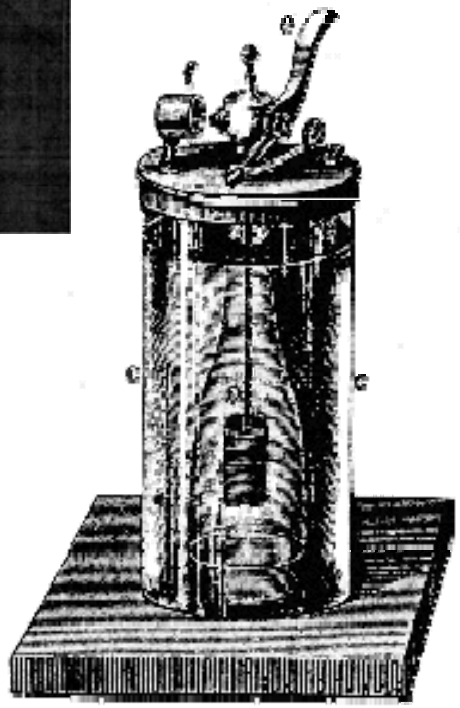
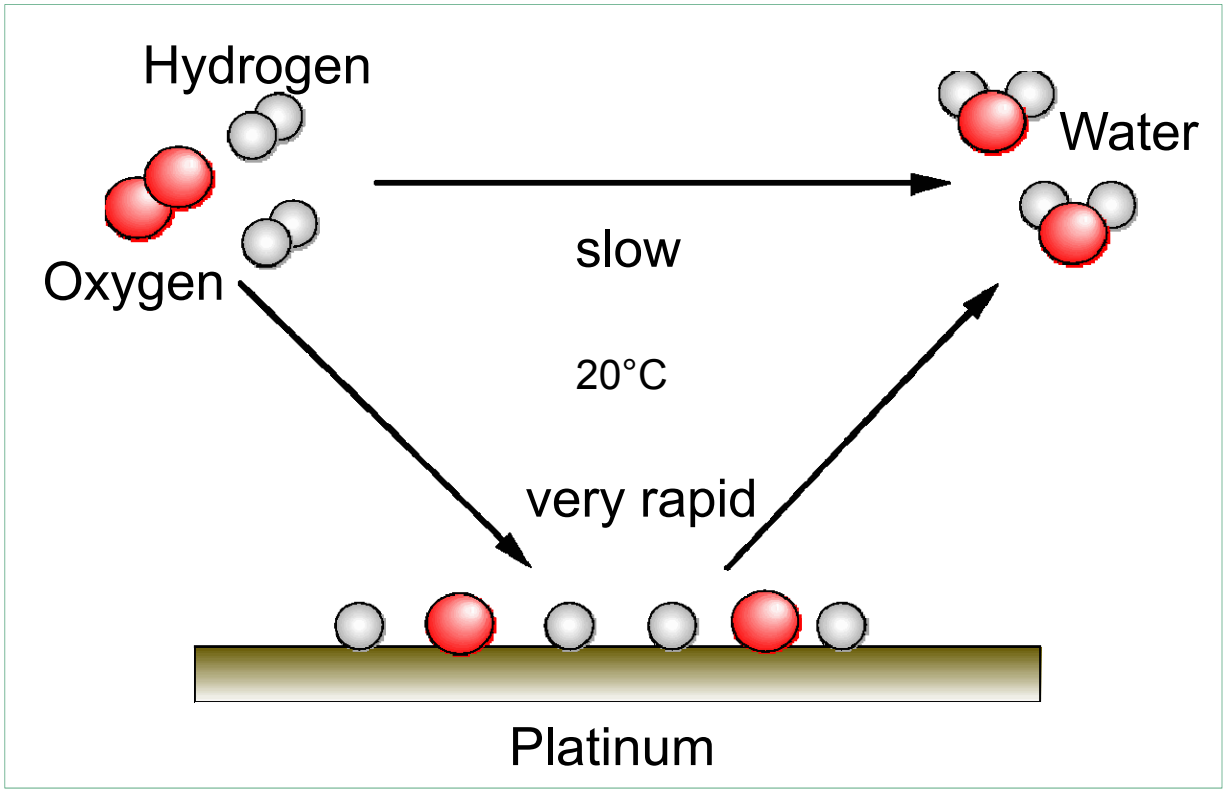
Heterogeneously catalyzed gas-phase reactions: Old concept but still new applications and challenges

Döbereiner´s lighter (1823)





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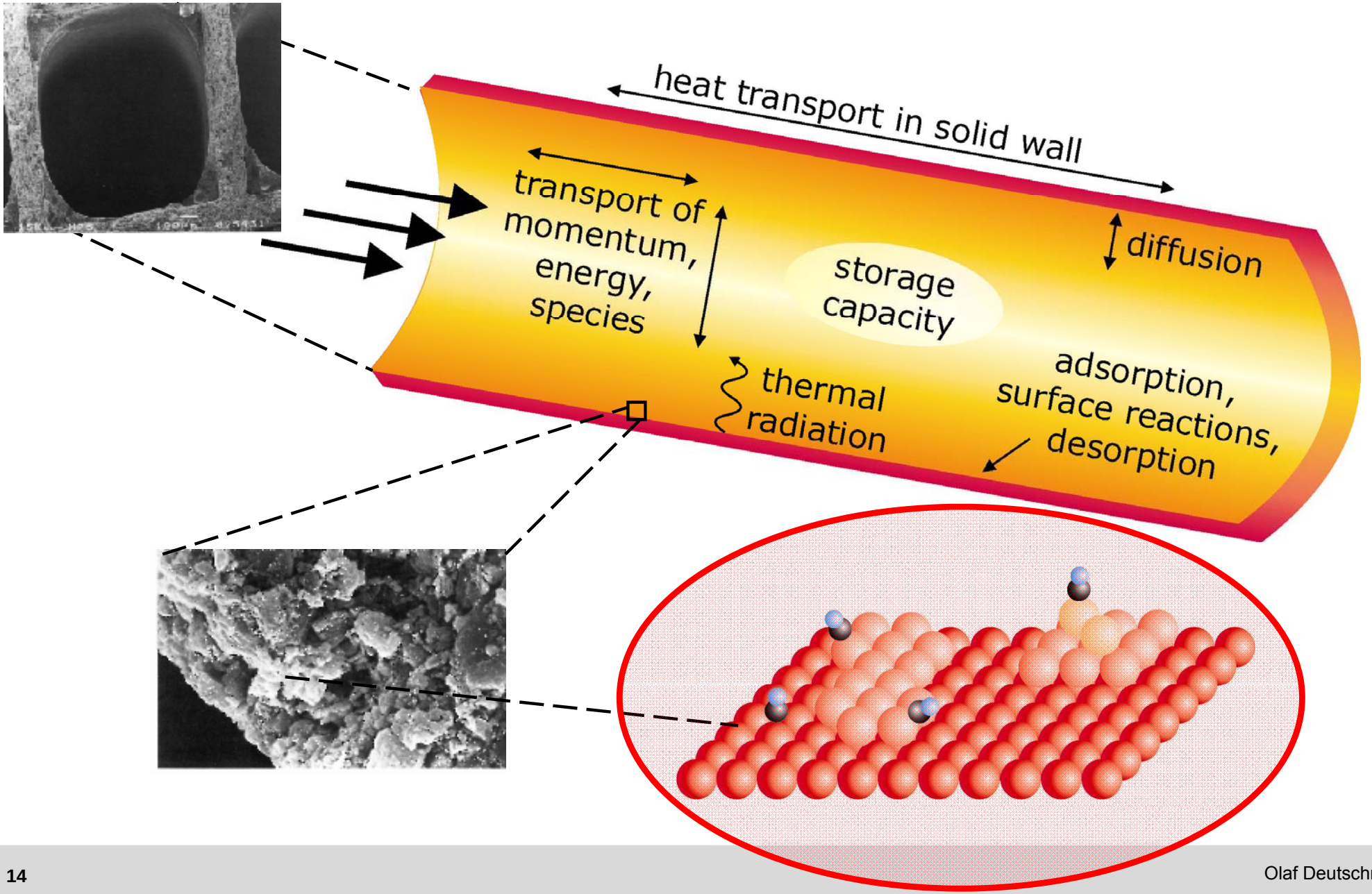
Heterogeneous catalytic reactions



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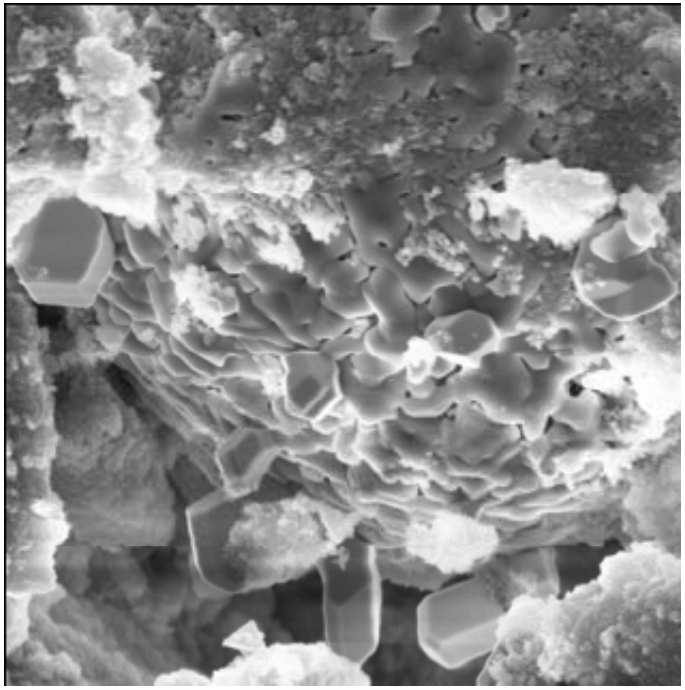
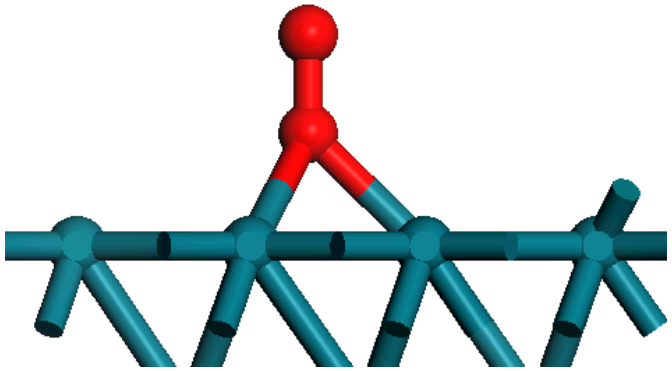
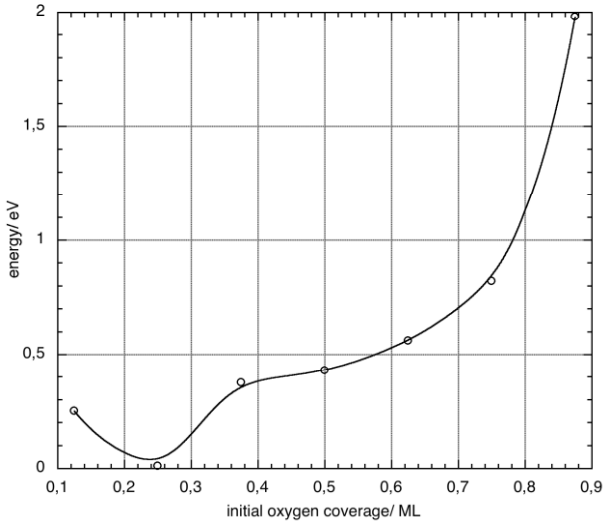
Elementary processes on catalytic reactions: DFT simulations provide thermo-chemical and kinetic data

Pt particles in highly-loaded DOC



O_2 - dissociation on Rh (111)





O.R. Inderwildi, D. Lebiedz, O. Deutschmann, J. Warnatz, J.Chem.Phys. 122 (2005) 034710

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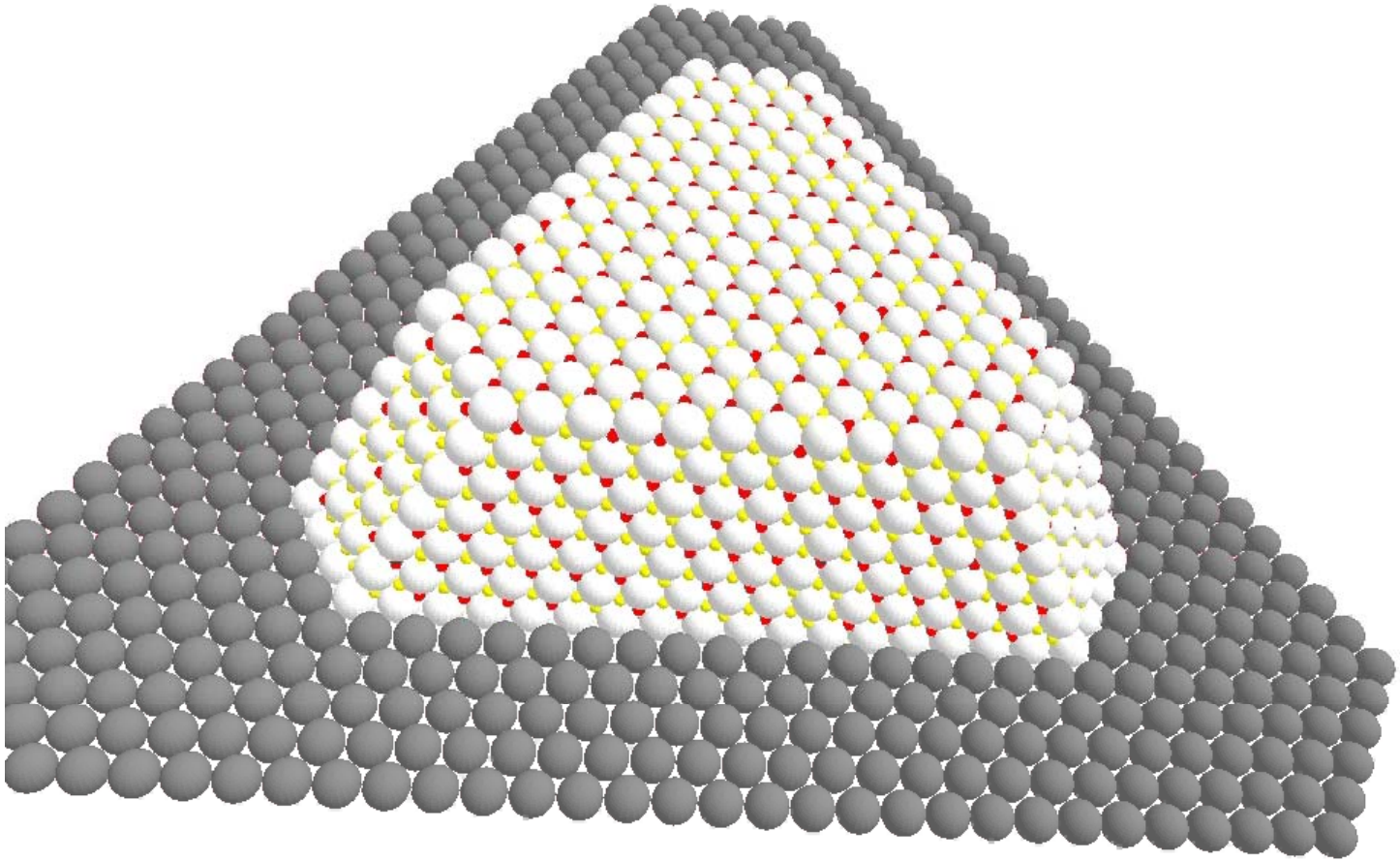
Kinetic Monte Carlo Simulation of surface reactions and diffusion: CO oxidation on Pt nanoperticle



$2\ CO + O_2 \rightarrow 2\ CO_2$
CO: blue O: red
Catalyst atom (Pt): white
Washcoat molecule (Al_2O_3): grey
Adsorption sites: yellow

Kunz, Deutschmann, 2006

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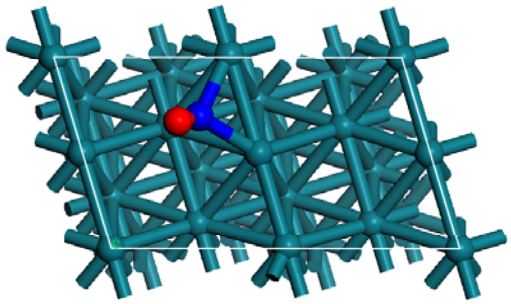
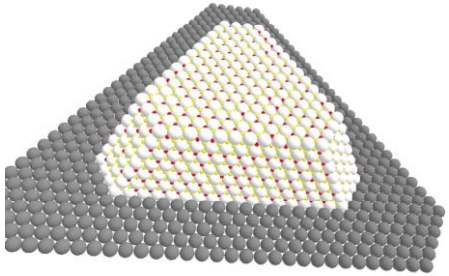
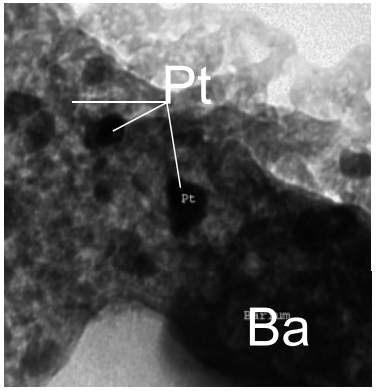
Modeling heterogeneous reactions: Molecular picture leads to mechanistic model







Surface coverage

$$\Theta_i = \frac{c_i \sigma_i}{\Gamma} \qquad \frac{\partial \Theta_i}{\partial t} = \frac{\dot{s}_i M_i}{\Gamma}$$

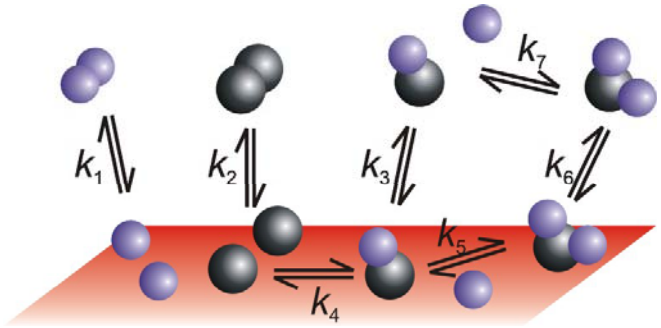
Surface reaction rate

$$\dot{s}_i = \sum_{k \in \mathbf{R}} \nu_{ik} k_{f_k} \prod_{j \in \mathbf{S}} c_j^{\nu'_{jk}}$$

Rate expression

$$k_{f_k} = A_k T^{\beta_k} \exp\left[\frac{-E_{a_k}}{RT}\right] \prod_{i=1}^{N_s} \Theta_i^{\mu_{ik}} \exp\left[\frac{\varepsilon_{i_k} \Theta_i}{RT}\right]$$

Locally resolved reaction rates depending on gas-phase concentration and surface coverages



O. Deutschmann. Chapter 6.6 in Handbook of Heterogeneous Catalysis, 2007

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Proposed surface reaction mechanism on Pt: Mean field approximation

	A (mole, cm, s)	E_a (kJ/mol)
Adsorption/desorption reactions		
$C_3H_6 + Pt(s) + Pt(s) \rightarrow C_3H_6(s)$	$S^0 = 0.98$	
$C_3H_6(s) \rightarrow Pt(s) + Pt(s) + C_3H_6$	3.7×10^{12}	74.4
$C_3H_6 + Pt(s) + O(s) \rightarrow C_3H_5(s) + OH(s)$	$S^0 = 0.05$ $\mu(\Theta_{Pt(s)}) = -0.9$	
$C_3H_5(s) + OH(s) \rightarrow O(s) + Pt(s) + C_3H_6$	3.7×10^{21}	31.0
$CH_4 + Pt(s) + Pt(s) \rightarrow CH_3(s) + H(s)$	$S^0 = 0.01$	
$O_2 + Pt(s) + Pt(s) \rightarrow O(s) + O(s)$	$S^0 = 0.07$	
$O(s) + O(s) \rightarrow Pt(s) + Pt(s) + O_2$	3.2×10^{21}	224.7 $-120\Theta_{O(s)}$
$H_2 + Pt(s) + Pt(s) \rightarrow H(s) + H(s)$	$S^0 = 0.046$ $\mu(\Theta_{Pt(s)}) = -1$	
$H(s) + H(s) \rightarrow Pt(s) + Pt(s) + H_2$	2.1×10^{21}	69.1 $-6\Theta_{H(s)}$
$H_2O + Pt(s) \rightarrow H_2O(s)$	$S^0 = 0.75$	
$H_2O(s) \rightarrow Pt(s) + H_2O$	5.0×10^{13}	49.2
$CO_2 + Pt(s) \rightarrow CO_2(s)$	$S^0 = 0.005$	
$CO_2(s) \rightarrow Pt(s) + CO_2$	3.6×10^{10}	23.7
$CO + Pt(s) \rightarrow CO(s)$	$S^0 = 0.84$	
$CO(s) \rightarrow Pt(s) + CO$	2.1×10^{13}	136.2 $-33\Theta_{CO(s)}$
$NO + Pt(s) \rightarrow NO(s)$	$S^0 = 0.85$	
$NO(s) \rightarrow Pt(s) + NO$	2.1×10^{12}	80.7
$NO_2 + Pt(s) \rightarrow NO_2(s)$	$S^0 = 0.9$	
$NO_2(s) \rightarrow Pt(s) + NO_2$	1.4×10^{13}	61.0
$N_2O + Pt(s) \rightarrow N_2O(s)$	$S^0 = 0.025$	
$N_2O(s) \rightarrow Pt(s) + N_2O$	1.2×10^{10}	0.7
$N(s) + N(s) \rightarrow Pt(s) + Pt(s) + N_2$	3.7×10^{21}	113.9 $-75\Theta_{CO(s)}$
Surface reactions		
Propylene oxidation		
$C_3H_6(s) \rightarrow C_3H_5(s) + H(s)$	1.0×10^{13}	75.4
$C_3H_5(s) + H(s) \rightarrow C_3H_6(s)$	3.7×10^{21}	48.8
$C_3H_5(s) + Pt(s) \rightarrow C_2H_3(s) + CH_2(s)$	3.7×10^{21}	108.2
$C_2H_3(s) + CH_2(s) \rightarrow C_3H_5(s) + Pt(s)$	3.7×10^{21}	3.3
$C_2H_3(s) + Pt(s) \rightarrow CH_3(s) + C(s)$	3.7×10^{21}	46.0
$CH_3(s) + C(s) \rightarrow C_2H_3(s) + Pt(s)$	3.7×10^{21}	46.5
$CH_3(s) + Pt(s) \rightarrow CH_2(s) + H(s)$	1.3×10^{22}	70.4
$CH_2(s) + H(s) \rightarrow CH_3(s) + Pt(s)$	2.9×10^{22}	0.4
$CH_2(s) + Pt(s) \rightarrow CH(s) + H(s)$	7.0×10^{22}	59.2
$CH(s) + H(s) \rightarrow CH_2(s) + Pt(s)$	8.1×10^{21}	0.7
$CH(s) + Pt(s) \rightarrow C(s) + H(s)$	3.1×10^{22}	0.0
$C(s) + H(s) \rightarrow CH(s) + Pt(s)$	5.8×10^{21}	128.9
$C_3H_5(s) + O(s) \rightarrow C_3H_4(s) + OH(s)$	5.0×10^{21}	70.0
$C_3H_4(s) + 4\,O(s) + 2\,Pt(s) \rightarrow 3\,C(s) + 4\,OH(s)$	2.6×10^{64}	0.0 [a]
$C_2H_3(s) + O(s) \rightarrow CH_3CO(s) + Pt(s)$	3.7×10^{19}	62.3
$CH_3CO(s) + Pt(s) \rightarrow C_2H_3(s) + O(s)$	7.9×10^{20}	191.4 $+60\Theta_{O(s)}$
$CH_3(s) + CO(s) \rightarrow CH_3CO(s) + Pt(s)$	3.7×10^{21}	82.9
$CH_3CO(s) + Pt(s) \rightarrow CH_3(s) + CO(s)$	1.8×10^{23}	6.1 $+33\Theta_{CO(s)}$
$CH_3(s) + O(s) \rightarrow OH(s) + CH_2(s)$	3.7×10^{21}	36.6
$OH(s) + CH_2(s) \rightarrow CH_3(s) + O(s)$	2.3×10^{22}	26.0
$CH_2(s) + O(s) \rightarrow OH(s) + CH(s)$	3.7×10^{21}	25.1
$OH(s) + CH(s) \rightarrow CH_2(s) + O(s)$	1.2×10^{21}	26.8
$CH(s) + O(s) \rightarrow OH(s) + C(s)$	3.7×10^{21}	25.1
$OH(s) + C(s) \rightarrow CH(s) + O(s)$	1.9×10^{21}	214.2
Carbon monoxide oxidation		
$CO(s) + O(s) \rightarrow CO_2(s) + Pt(s)$		
$CO_2(s) + Pt(s) \rightarrow CO(s) + O(s)$		
$C(s) + O(s) \rightarrow CO(s) + Pt(s)$		
$CO(s) + Pt(s) \rightarrow C(s) + O(s)$		
Reactions of hydroxyl species		
$H(s) + O(s) \rightarrow OH(s) + Pt(s)$		
$OH(s) + Pt(s) \rightarrow H(s) + O(s)$		
$OH(s) + H(s) \rightarrow H_2O(s) + Pt(s)$		
$H_2O(s) + Pt(s) \rightarrow OH(s) + H(s)$		
$OH(s) + OH(s) \rightarrow H_2O(s) + O(s)$	3.7×10^{21}	48.2
$H_2O(s) + O(s) \rightarrow OH(s) + OH(s)$	2.5×10^{20}	38.2
$CO(s) + OH(s) \rightarrow HCOO(s) + Pt(s)$	3.7×10^{21}	94.2
$HCOO(s) + Pt(s) \rightarrow CO(s) + OH(s)$	1.3×10^{21}	0.9
$HCOO(s) + O(s) \rightarrow OH(s) + CO_2(s)$	3.7×10^{21}	0.0
$OH(s) + CO_2(s) \rightarrow HCOO(s) + O(s)$	2.8×10^{21}	151.1
$HCOO(s) + Pt(s) \rightarrow H(s) + CO_2(s)$	3.7×10^{21}	0.0
$H(s) + CO_2(s) \rightarrow HCOO(s) + Pt(s)$	2.8×10^{21}	90.1
Reactions of NO and NO_2		
$NO(s) + Pt(s) \rightarrow N(s) + O(s)$	5.0×10^{20}	107.8 $+33\Theta_{CO(s)}$
$N(s) + O(s) \rightarrow NO(s) + Pt(s)$	1.0×10^{21}	122.6 $-60\Theta_{O(s)}$
$O(s) + NO \rightarrow NO_2(s)$	2.0×10^{13}	111.3 $+75\Theta_{CO(s)}$ $-60\Theta_{O(s)}$
$NO_2(s) \rightarrow O(s) + NO$	3.3×10^{14}	115.5
$N(s) + NO(s) \rightarrow N_2O(s) + Pt(s)$	1.0×10^{21}	90.9
$N_2O(s) + Pt(s) \rightarrow N(s) + NO(s)$	2.9×10^{24}	133.1
$O(s) + NO(s) \rightarrow NO_2(s) + Pt(s)$	1.3×10^{17}	133.0 $+75\Theta_{CO(s)}$
$NO_2(s) + Pt(s) \rightarrow O(s) + NO(s)$	8.1×10^{18}	58.0
$H(s) + NO(s) \rightarrow OH(s) + N(s)$	1.2×10^{21}	25.0 $+80\Theta_{CO(s)}$
$OH(s) + N(s) \rightarrow H(s) + NO(s)$	6.4×10^{21}	99.9
$NO_2(s) + H(s) \rightarrow OH(s) + NO(s)$	3.9×10^{21}	20.0
$OH(s) + NO(s) \rightarrow NO_2(s) + H(s)$	6.1×10^{22}	175.3

D. Chatterjee, O. Deutschmann, J. Warnatz. Faraday Discuss. 119 (2001) 371
J. Koop, O. Deutschmannn. Appl. Catal. B: Env. 91 (2009) 47

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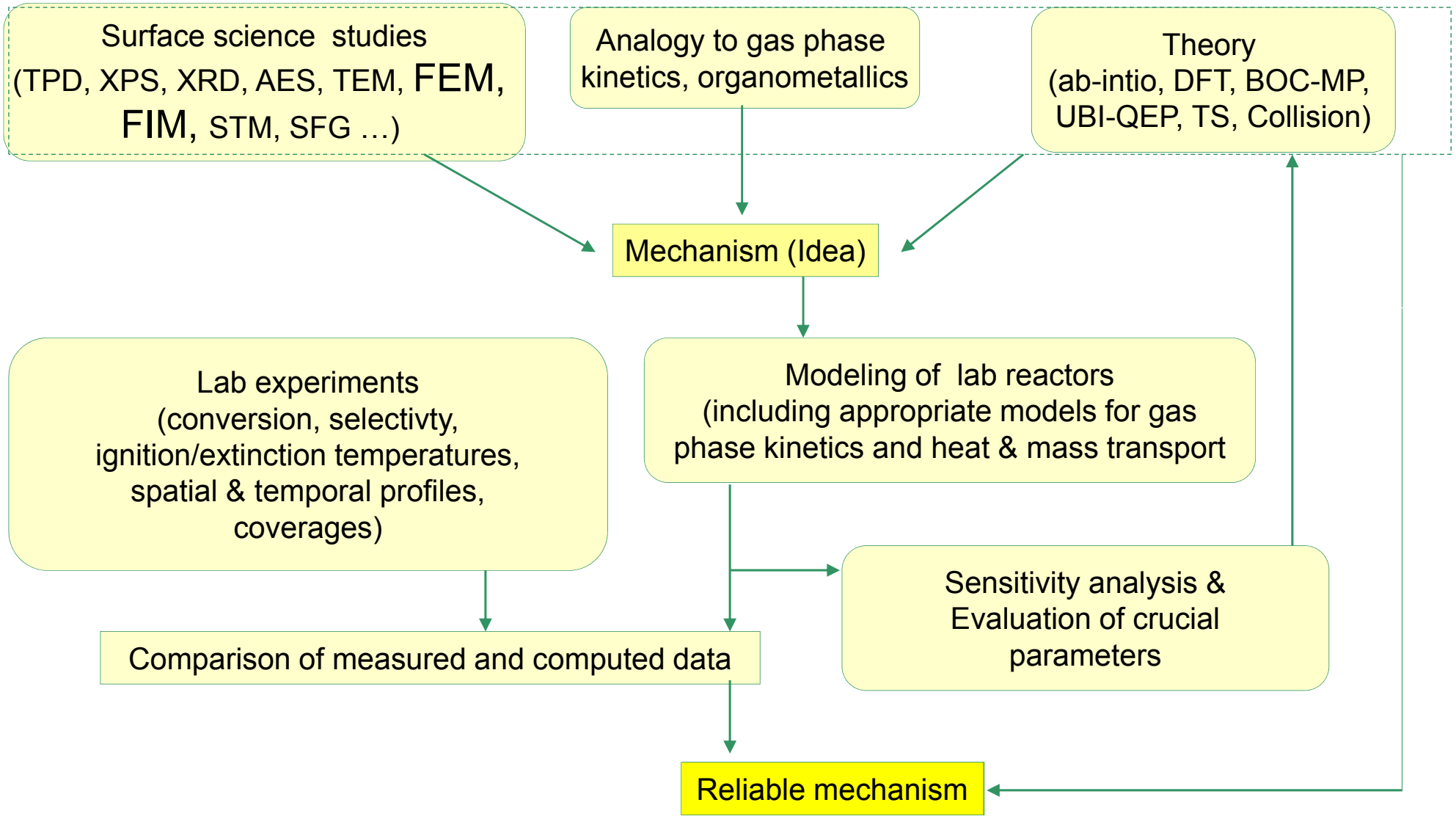
Development detailed reaction mechanisms for heterogeneously catalyzed gas-phase reactions



O. Deutschmann. Chapter 6.6 in Handbook of Heterogeneous Catalysis, 2007

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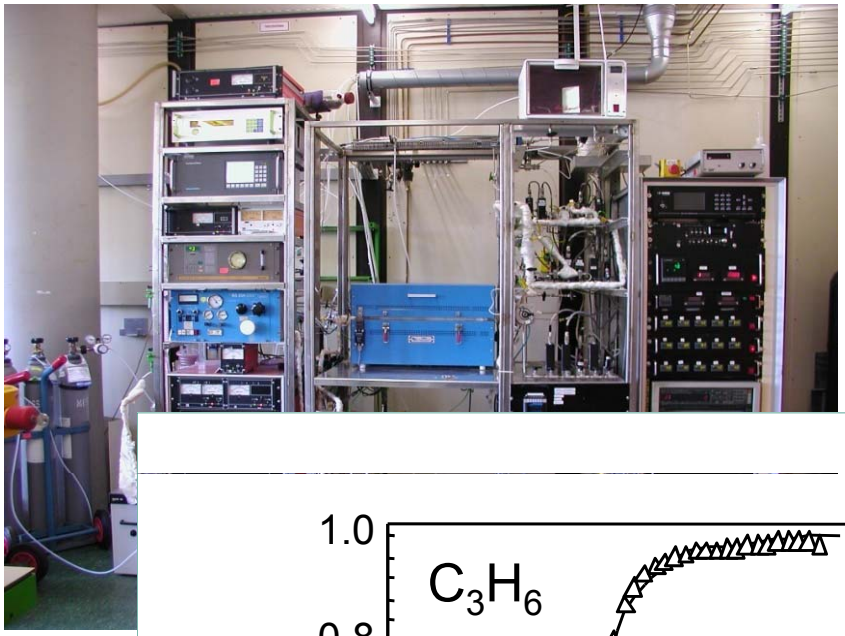
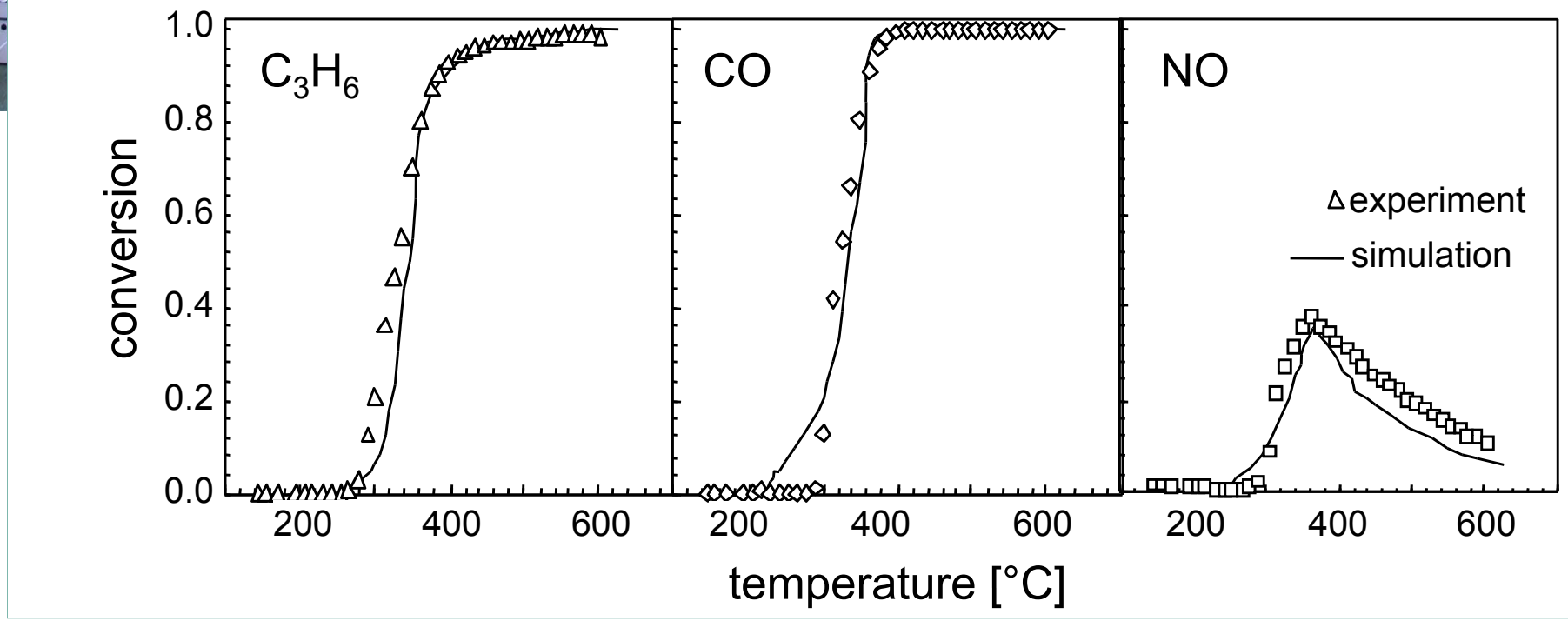
Conversion of a synthetic exhaust in a real three way catalyst: Steady-state conditions



Laboratory experiments at well-defined conditions, e.g. differentially operated reactors (no gradients),
are used for first model evaluation



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Institute for Chemical Technology and Polymer Chemistry

Different approaches to model reaction kinetics

Elementary Kinetics

	A (mole, cm, s
Adsorption/desorption reactions	
$C_3H_6 + Pt(s) + Pt(s) \rightarrow C_3H_6(s)$	$S^0 = 0.98$
$C_3H_6(s) \rightarrow Pt(s) + Pt(s) + C_3H_6$	3.7×10^{12}
$C_3H_6 + Pt(s) + O(s) \rightarrow C_3H_5(s) + OH(s)$	$S^0 = 0.05$
	$\mu(\Theta_{Pt(s)}) = -$
$C_3H_5(s) + OH(s) \rightarrow O(s) + Pt(s) + C_3H_6$	3.7×10^{21}
$CH_4 + Pt(s) + Pt(s) \rightarrow CH_3(s) + H(s)$	$S^0 = 0.01$
$O_2 + Pt(s) + Pt(s) \rightarrow O(s) + O(s)$	$S^0 = 0.07$
$O(s) + O(s) \rightarrow Pt(s) + Pt(s) + O_2$	3.2×10^{21}
$H_2 + Pt(s) + Pt(s) \rightarrow H(s) + H(s)$	$S^0 = 0.046$
	$\mu(\Theta_{Pt(s)}) = -$
$H(s) + H(s) \rightarrow Pt(s) + Pt(s) + H_2$	2.1×10^{21}
$H_2O + Pt(s) \rightarrow H_2O(s)$	$S^0 = 0.75$
$H_2O(s) \rightarrow Pt(s) + H_2O$	5.0×10^{13}
$CO_2 + Pt(s) \rightarrow CO_2(s)$	$S^0 = 0.005$

Global Kinetics

$$\frac{d[CO]}{dt} = \frac{k_1(T)\cdot[CO]\cdot[O_2]}{G_{Inhib.}\cdot G_{HC/CO}\cdot G_{NO}}$$

$$G_{NO} = \left(1 + K_{NO}\cdot[NO]^{0.7}\right)$$

Data based

Splines

Neural Networks

Look-up Tables

Adapted from M. Votsmeier

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Modeling surface reaction kinetics: Elementary Reactions versus Global Rate Expressions

Global: 13 Reactions

$$2\,CO + O_2 \leftrightarrow 2\,CO_2$$
$$2\,H_2 + O_2 \leftrightarrow 2\,H_2O$$
$$C_3H_6 + 4.5\,O_2 \leftrightarrow 3\,CO_2 + 3\,H_2O$$
$$CO + H_2O \leftrightarrow CO_2 + H_2$$
$$C_3H_6 + 6\,H_2O \leftrightarrow 3\,CO_2 + 9\,H_2$$
$$Ce_2O_3 + 0.5\,O_2 \leftrightarrow Ce_2O_4$$
$$Ce_2O_3 + NO \leftrightarrow Ce_2O_4 + 0.5\,N_2$$
$$Ce_2O_4 + CO \leftrightarrow Ce_2O_3 + CO_2$$
$$Ce_2O_4 + 2\,H_2 \leftrightarrow Ce_2O_3 + H_2O$$
$$9\,Ce_2O_4 + C_3H_6 \leftrightarrow 9\,Ce_2O_3 + 3\,CO_2 + 3\,H_2O$$
$$NO + 0.5\,O_2 \leftrightarrow NO_2$$
$$Pt + CO \leftrightarrow PtC + 0.5\,O_2$$
$$NO + Ce_2O_4 \leftrightarrow Ce_2O_4\text{-}NO$$

33 + ?? Parameter

Elementary: 16 Reactions

$$O_2 + 2\,Pt \leftrightarrow 2\,PtO$$
$$CO + Pt \leftrightarrow PtCO$$
$$H_2 + 2\,Pt \leftrightarrow 2\,PtH$$
$$NO + Pt \leftrightarrow PtNO$$
$$PtCO + PtO \leftrightarrow CO_2 + 2\,Pt$$
$$2\,PtH + PtO \leftrightarrow H_2O + 3\,Pt$$
$$PtC + PtO \leftrightarrow PtCO + Pt$$
$$CO + Ce_2O_3 + Pt \leftrightarrow Ce_2O_4 + PtC$$
$$C_3H_6 + 3\,PtO + 6\,Pt \leftrightarrow 3\,PtCO + 6\,PtH$$
$$PtNO + Pt \leftrightarrow PtO + PtN$$
$$PtNO + PtO \leftrightarrow PtNO_2 + Pt$$
$$2\,PtN \leftrightarrow N_2 + 2\,Pt$$
$$PtO + Ce_2O_3 \leftrightarrow Ce_2O_4 + Pt$$
$$O_2 + 2\,Ce_2O_3 \leftrightarrow 2\,Ce_2O_4$$
$$CO + Ce_2O_4 \leftrightarrow CO_2 + Ce_2O_3$$
$$2\,H_2 + Ce_2O_4 \leftrightarrow H_2O + Ce_2O_3$$

44 Parameter

Adapted from M. Votsmeier

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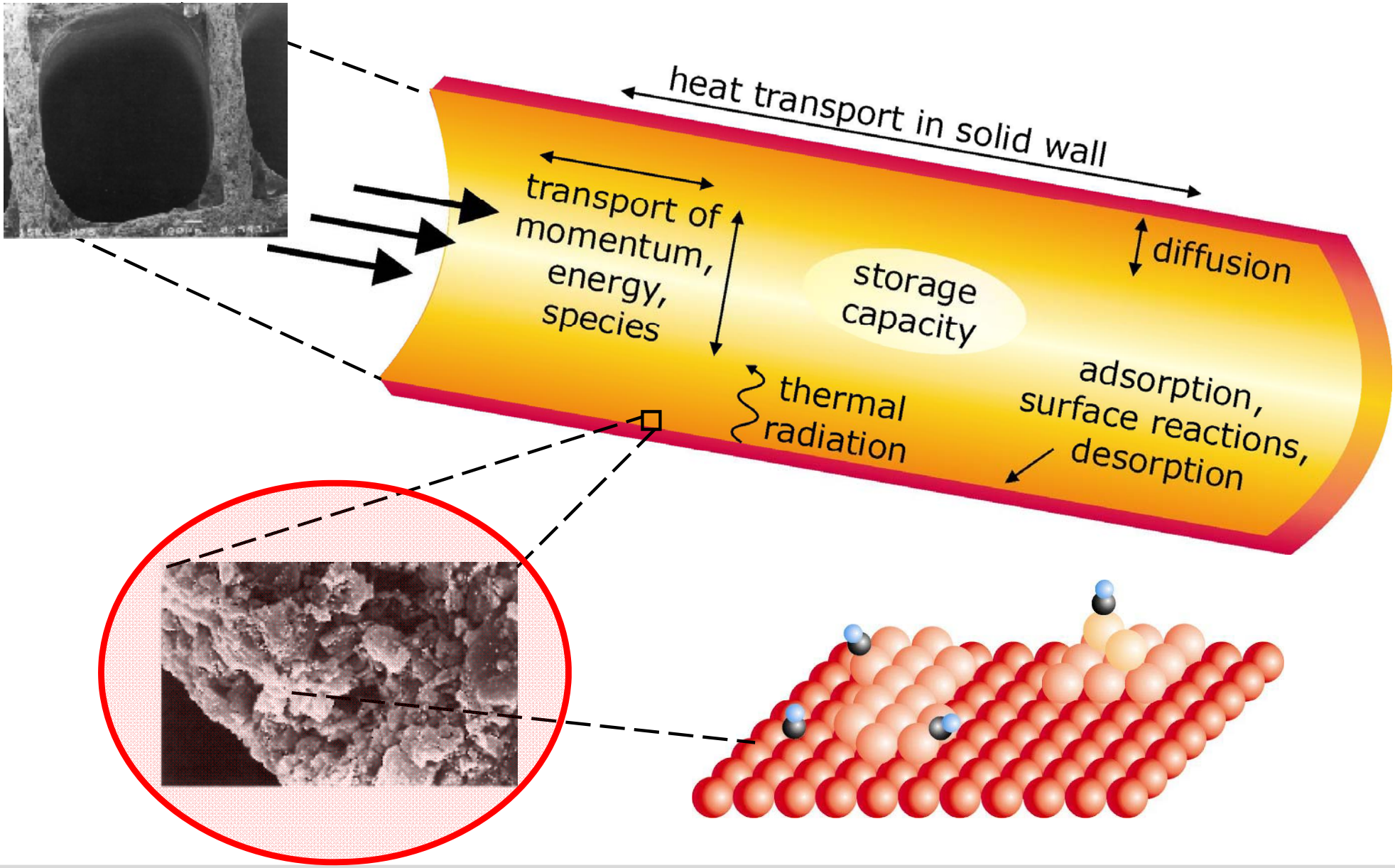
Coupling of diffusion and reaction



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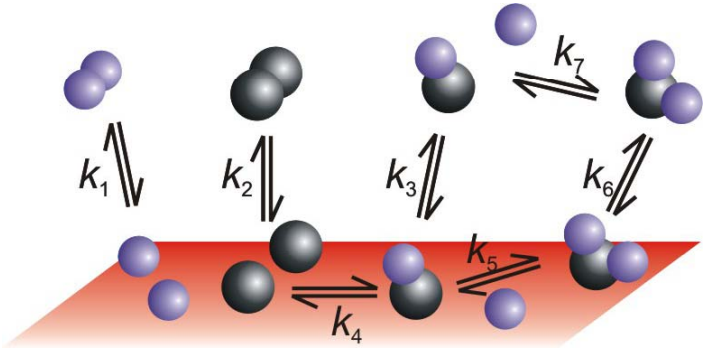
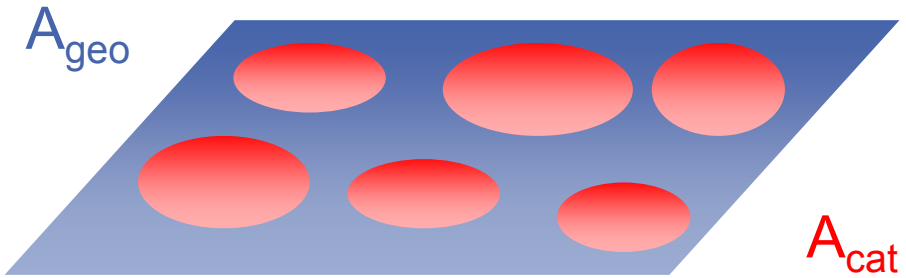
Coupling of surface reaction rate and flow field - Modeling transport limitation of reaction rate

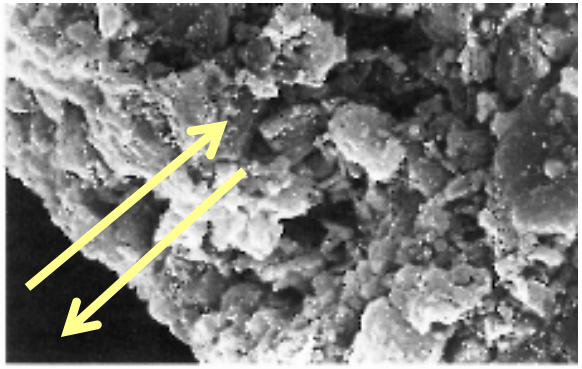


microscopic site density Γ



macroscopic catalyst area → $F_{cat/geo} = A_{cat} / A_{geo}$

$$j_{i,s} = F_{\text{cat/geo}}\, \eta_i\, M_i\, \dot{s}_i$$



Effectiveness factor $\eta_i = \dfrac{\tanh(\Phi_i)}{\Phi_i}$

$$\Phi_i = L \sqrt{\frac{\dot{s}_i\, \gamma}{D_{\text{eff},i}\, c_{i,0}}}$$

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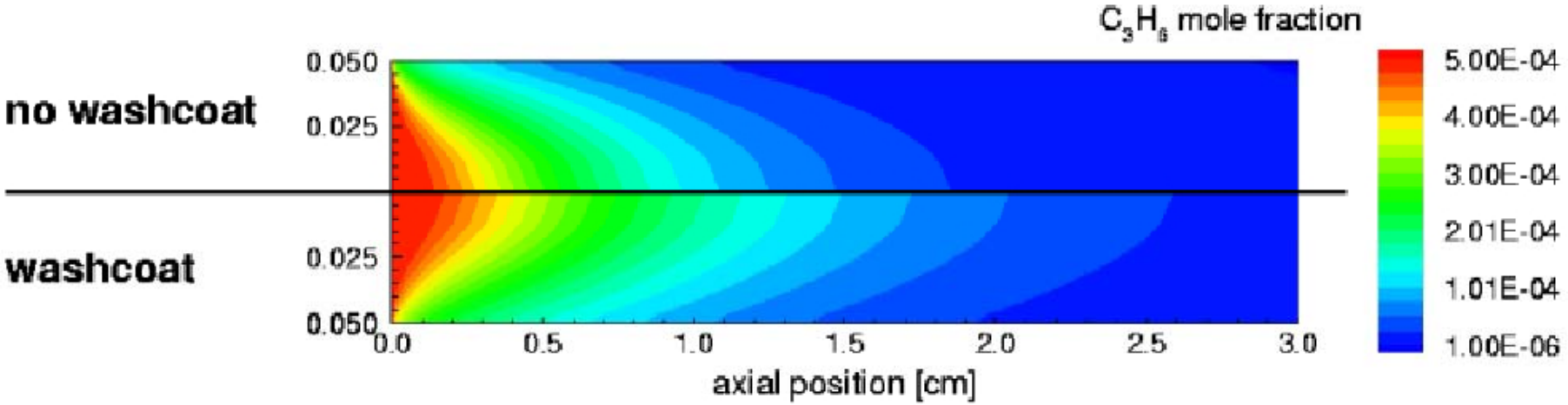
HC-SCR on Pt/Al_2O_3: Impact of washcoat transport limitation on conversion



Conditions:

500 ppm C_3H_6, 500 ppm NO, 5 Vol.-% O_2, in N_2, 6 slpm, u = 0.63 m/s; T = 570 K

D. Chatterjee, O. Deutschmann, 2000

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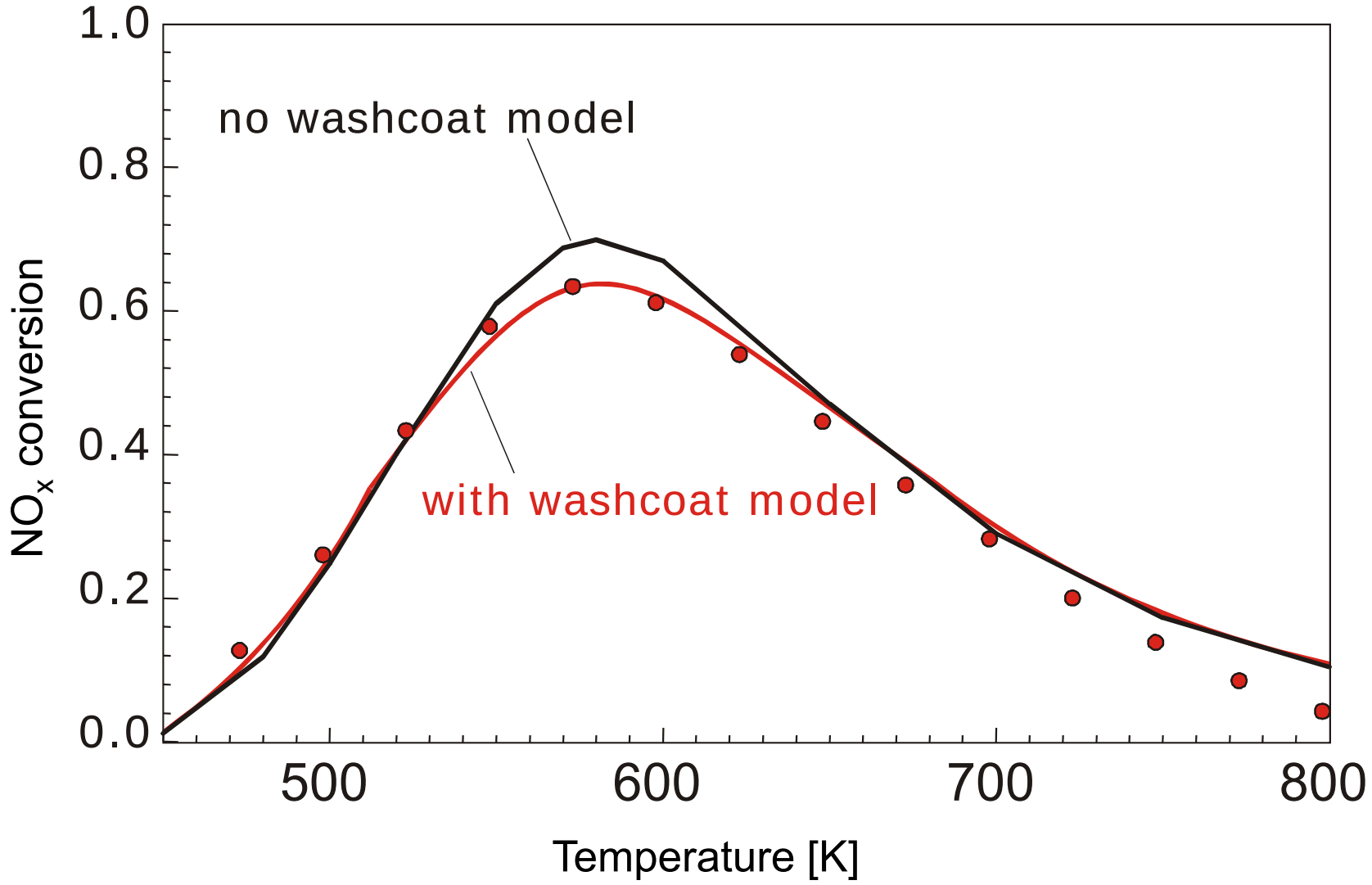
NO oxidation on Pt/Al_2O_3: Impact of washcoat transport limitation on conversion



Conditions: 500 ppm NO, 1 Vol.-% O_2 in N_2

D. Chatterjee, O. Deutschmann, 2000

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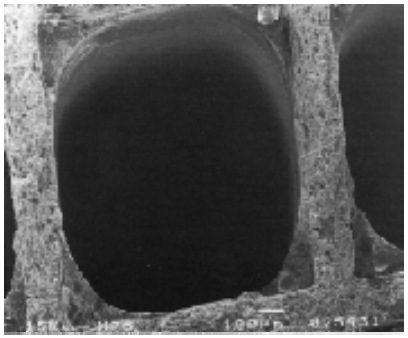
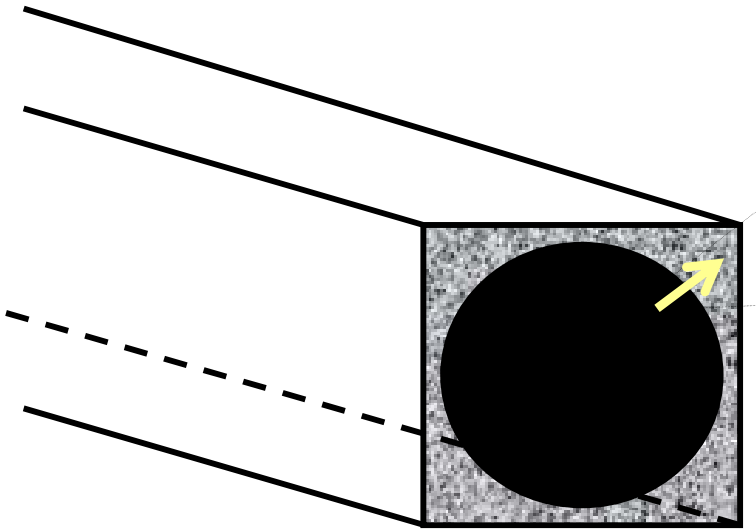
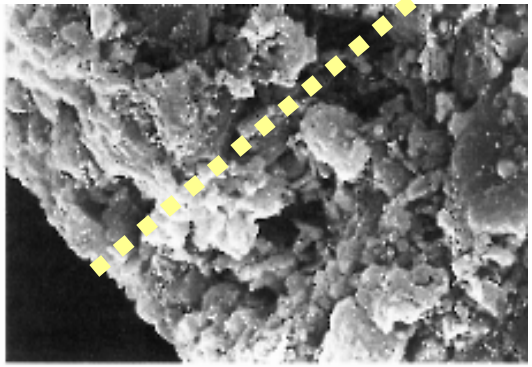
Modeling reaction and transport in porous media: 1d reaction-diffusion equations



Washcoat is treated as continuum





Discretization of the washcoat normal to the gas-phase-washcoat boundary at each radial and axial position

$$D_{\mathrm{eff},i}\frac{\partial c_i^{\mathrm{W}}}{\partial r}+\gamma\, M_i \dot{s}_i = 0 \qquad (i=1,\ldots,N_{\mathrm{g}})$$

$$\dot{s}_i = \sum_{k=1}^{K_s} \nu_{ik} k_{f_k} \prod_{j=1}^{N_g+N_s} c_j^{\nu'_{jk}}$$

$$\dot{s}_i = 0 \qquad (i=N_{\mathrm{g}}+1,\ldots,N_{\mathrm{g}}+N_{\mathrm{s}})$$

$$j_i^{\mathrm{surf}} = j_{r,i}^{\mathrm{W}}(r=0) = -D_{\mathrm{eff},i}\left.\frac{\partial c_i^{\mathrm{W}}}{\partial r}\right|_{r=0}$$

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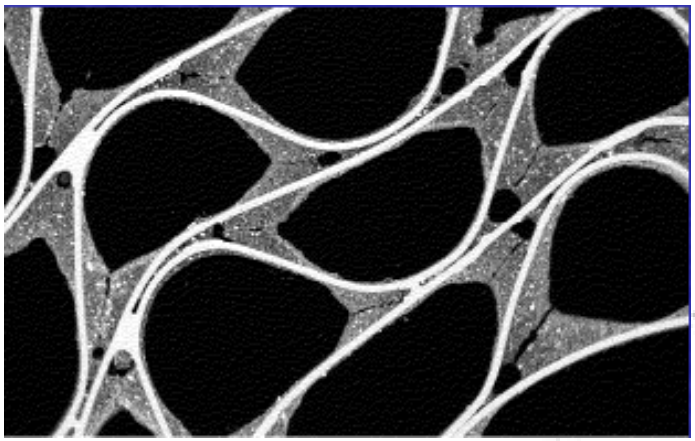
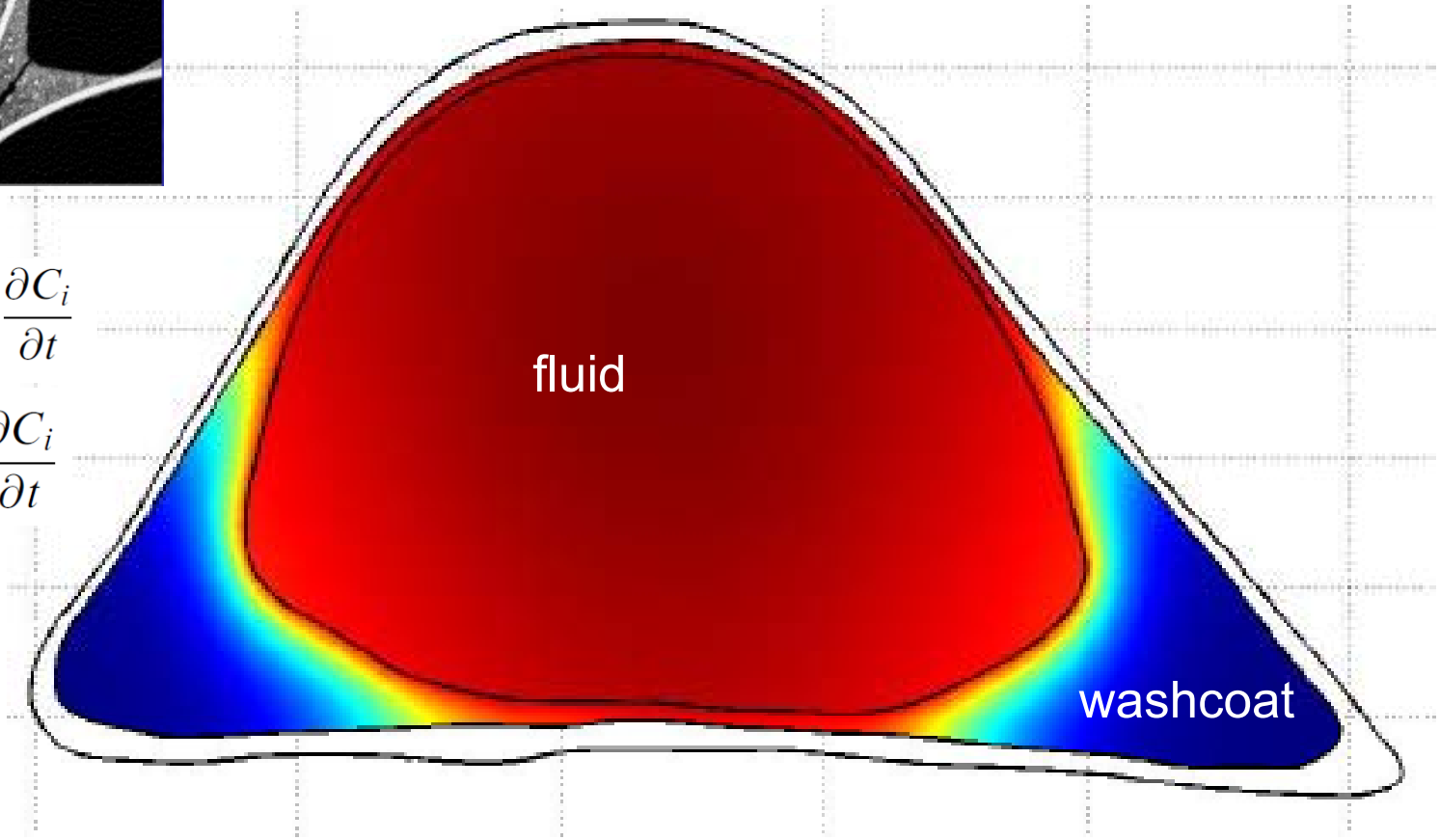
Understanding the interaction of diffusion and reaction: Potential for reduced catalyst costs by zone coating



Reactant concentration in a complex shaped channel

$$\nabla \cdot (D_i \nabla C_i) - \nabla \cdot (v C_i) = \frac{\partial C_i}{\partial t}$$

$$(D_{\text{eff}})_i \nabla^2 C_i - (-R_i) = \varepsilon \frac{\partial C_i}{\partial t}$$



R.E. Hayes, B. Liu, M. Votsmeier. Chem. Eng. Sci. 60 (2005) 2037.

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Catalytic combustion: Modeling and Simulation
Outline

1. Motivation
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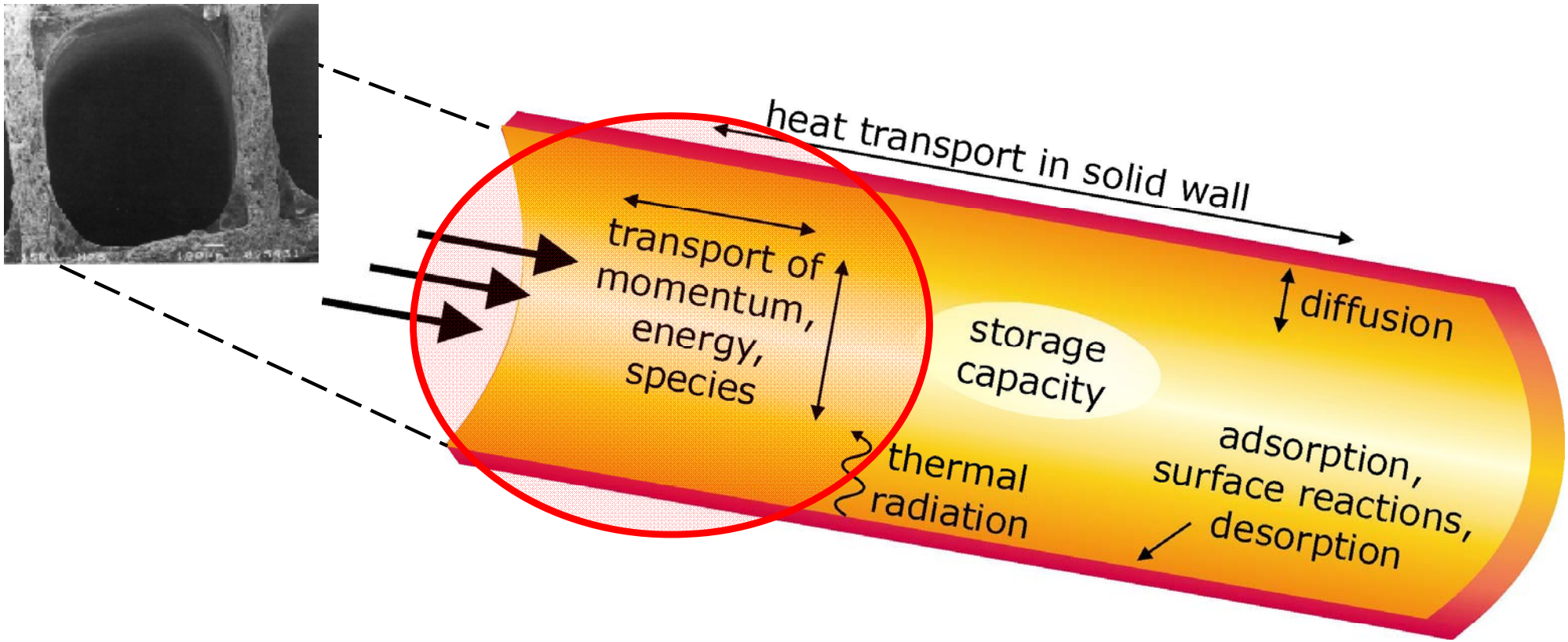
Modeling the flow in the channel



General:
Transient 3D Navier-Stokes equations + species mass balances + heat balances

Simplifying assumptions often made:
No direct transients, cylindrical channel, no axial (and radial) diffusion

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Most general approach for modeling laminar flow fields: Transient 3D Navier-Stokes equations

Karlsruhe Institute of Technology

Total mass

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v_i)}{\partial x_i} = S_{\mathrm{m}}$$

Momentum

$$\frac{\partial (\rho v_i)}{\partial t} + \frac{\partial (\rho v_i v_j)}{\partial x_j} + \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} = \rho g_i$$

$$\tau_{ij} = -\mu \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) + \left(\frac{2}{3}\mu - \kappa \right) \delta_{ij} \frac{\partial v_k}{\partial x_k}$$

Species' mass

$$\frac{\partial (\rho Y_i)}{\partial t} + \frac{\partial (\rho v_j Y_i)}{\partial x_j} + \frac{\partial (j_{i,j})}{\partial x_j} = R_i^{\mathrm{hom}}$$

$$j_{i,j} = -\rho \frac{Y_i}{X_i} D_i^{\mathrm{M}} \frac{\partial X_i}{\partial x_j} - \frac{D_i^{\mathrm{T}}}{T} \frac{\partial T}{\partial x_j}$$

Heat transport

$$\frac{\partial (\rho h)}{\partial t} + \frac{\partial (\rho v_j h)}{\partial x_j} + \frac{\partial j_{q,j}}{\partial x_j} = \frac{\partial p}{\partial t} + v_j \frac{\partial p}{\partial x_j} - \tau_{jk} \frac{\partial v_j}{\partial x_k} + S_{\mathrm{h}}$$

$$j_{q,j} = -\lambda \frac{\partial T}{\partial x_j} + \sum_{i=1}^{Ng} h_i j_{i,j}$$

solid phase

$$\frac{\partial (\rho h)}{\partial t} - \frac{\partial}{\partial x_j} \left(\lambda \frac{\partial T}{\partial x_j} \right) = S_{\mathrm{h}}$$

$$S_{h,\text{ext rad}} = -\varepsilon \sigma \left(T_{\text{solid}}^4 - T_{\text{ref}}^4 \right) A$$

temperature

$$h = \sum_{i=1}^{Ng} Y_i h_i(T)$$

Equation of state (perfect gas)

$$p = \frac{\rho R T}{\sum_{i=1}^{N_g} X_i M_i}$$

$$X_i = \frac{1}{\sum_{j=1}^{Ng} Y_j / M_j} \frac{Y_i}{M_i}$$

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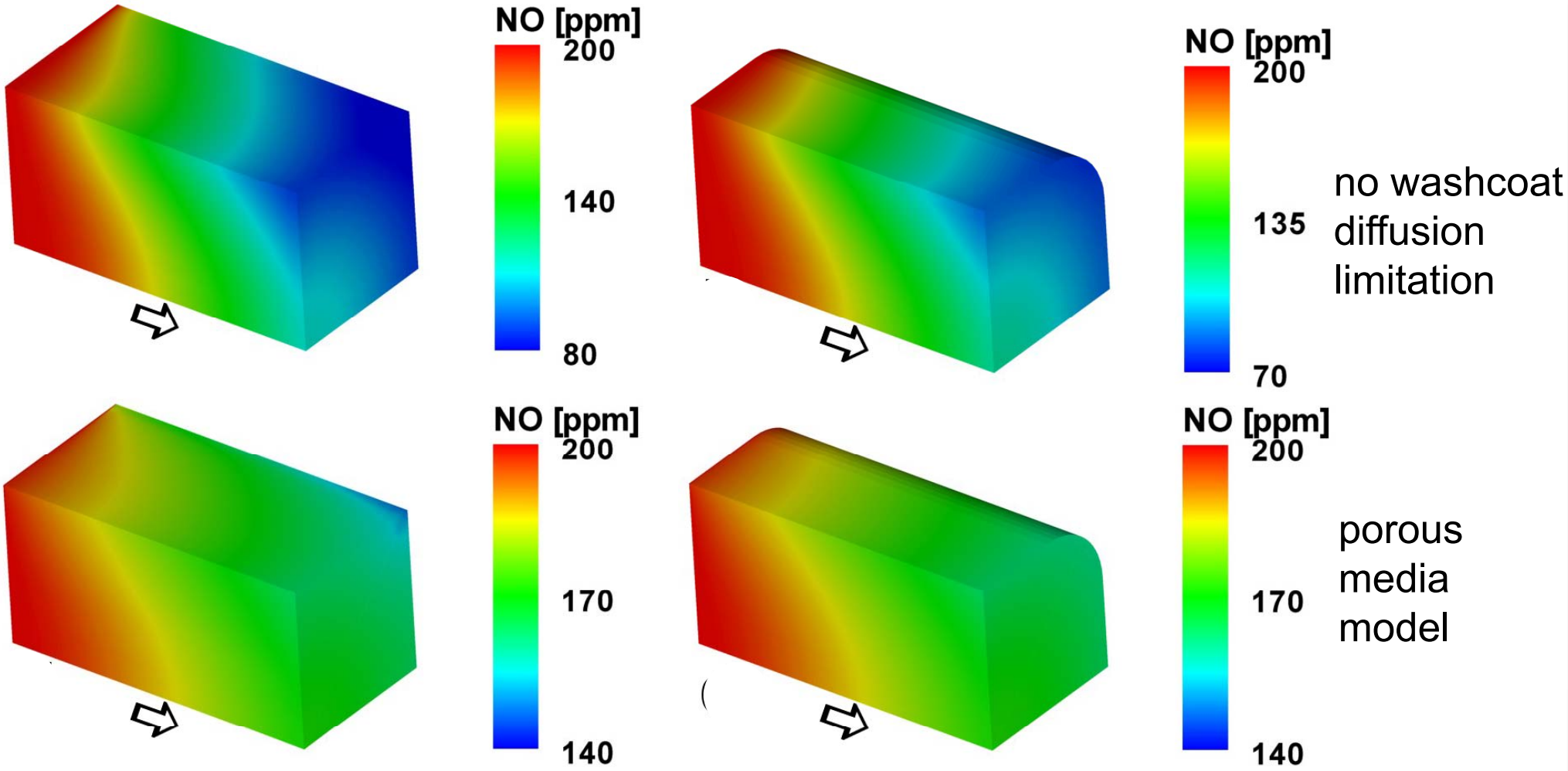
Institute for Chemical Technology and Polymer Chemistry

Impact of models for channel shape and washcoat diffusion on NO profiles in a DOC



NO profiles at lean conditions at 250°C (steady-state operation)
CFD code: Fluent + DETCHEM

N. Mladenov, J. Koop, S. Tischer, O. Deutschmann. Chem. Eng. Sci. 65 (2010) 812

Olaf Deutschmann
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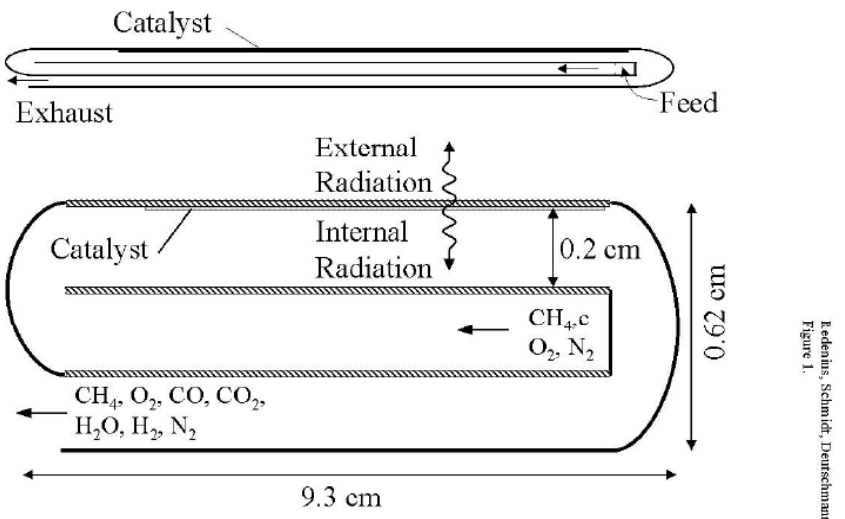
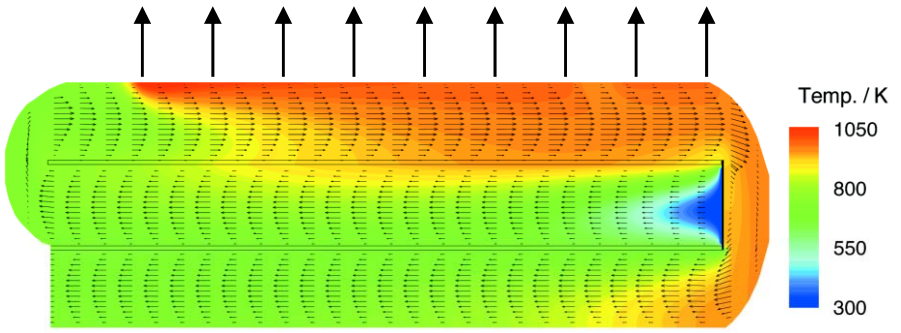
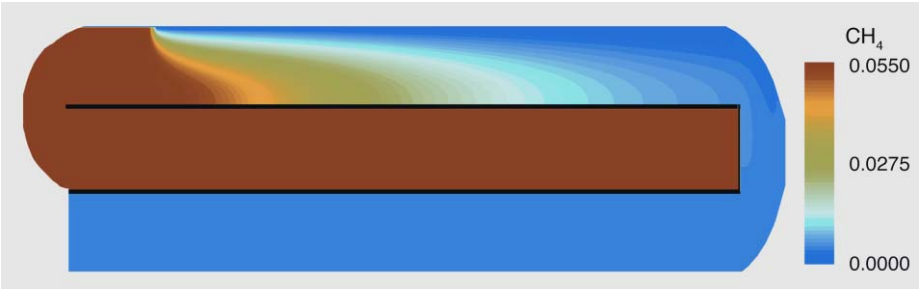
Simulation of a catalytic radiant burner with heat recuperation



- Steady-satet 2D laminar flow
- Detailed heterogeneous and homogeneoous gas-phase reaction
- External radiation heat loss
- Internal thermal radiation, and heat conduction in solid and gas-phase
- **FLUENT + DETCHEM (elliptisch)**





J.M. Redenius, L.D. Schmidt, O. Deutschmann. AIChE J. 47 (2001) 1177

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Model simplification by assuming a cylindrical channel and neglecting axial diffusion: Boundary-layer equations

Total mass flux

$$\frac{\partial(\rho u)}{\partial z} = -\frac{1}{r}\frac{\partial(r\rho v)}{\partial r}$$

Axial momentum flux

$$\frac{\partial(\rho u u)}{\partial z} = -\frac{1}{r}\frac{\partial(r\rho v u)}{\partial r} - \frac{\partial p}{\partial z} + \frac{1}{r}\frac{\partial}{\partial r}\left(\eta r \frac{\partial u}{\partial r}\right) + \rho g_z$$

Enthalpy flux

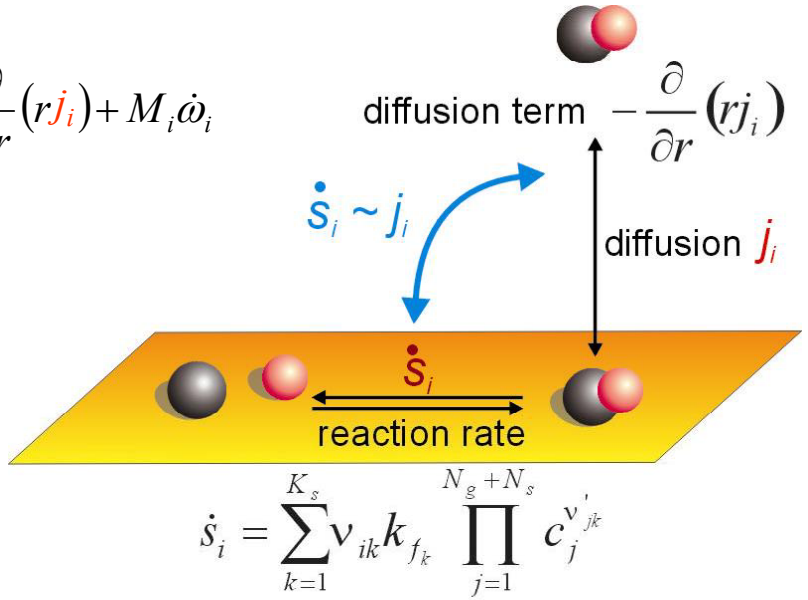
$$\frac{\partial(\rho u h)}{\partial z} = -\frac{1}{r}\frac{\partial(r\rho v h)}{\partial r} + u\frac{\partial p}{\partial z} - \frac{1}{r}\frac{\partial}{\partial r}(r q_r)$$

Species mass flux

$$\frac{\partial(\rho u Y_i)}{\partial z} = -\frac{1}{r}\frac{\partial(r\rho v Y_i)}{\partial r} - \frac{1}{r}\frac{\partial}{\partial r}(r j_i) + M_i \dot{\omega}_i$$

Coupling between surface reactions and flow field:

$$j_{i,wall} = F_{\text{cat/geo}}\ \eta_i M_i\ \dot{s}_i$$



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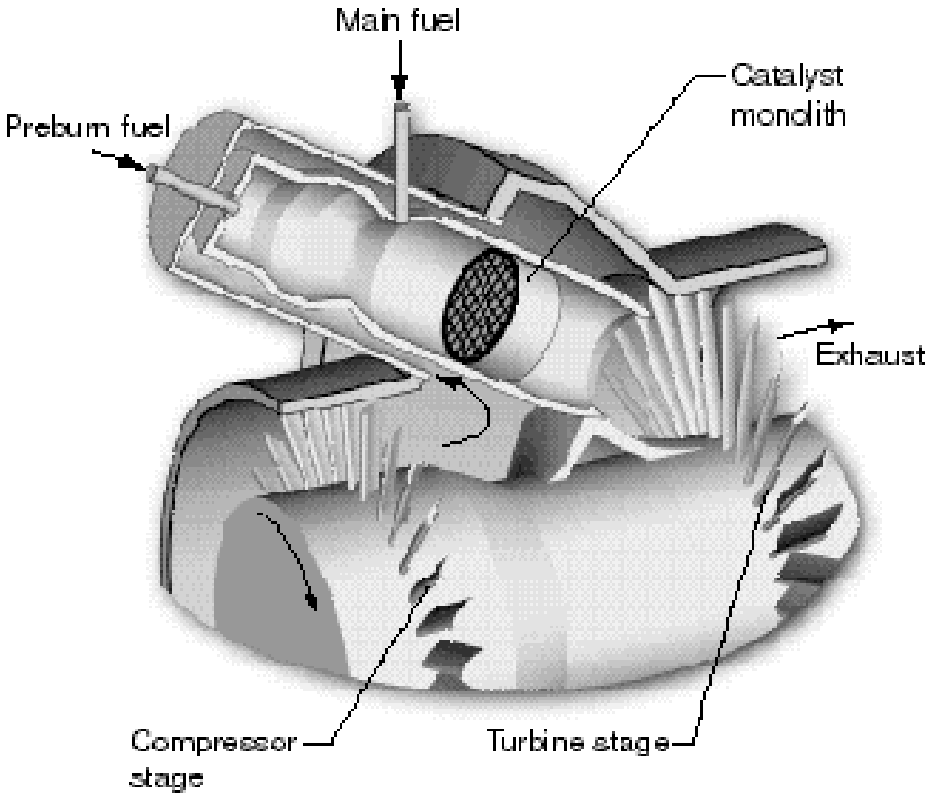
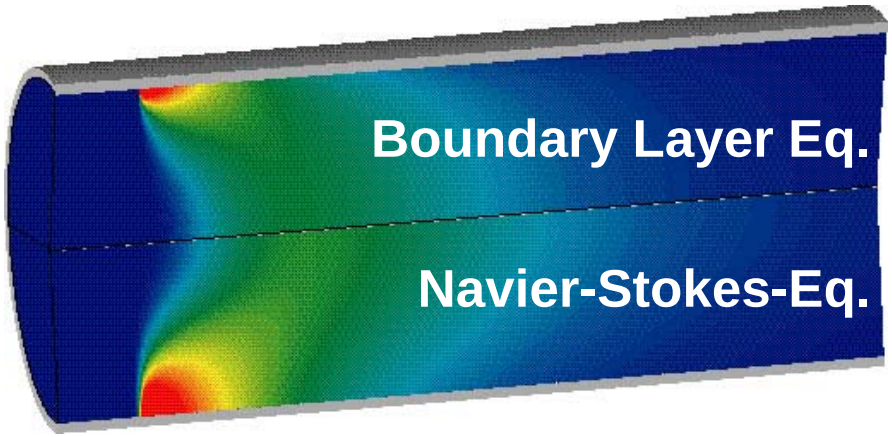
Institute for Chemical Technology and Polymer Chemistry

Catalytic combustion of natural gas in catalytic channel: 2D Navier-Stokes and 2D Boundary layer approach

$$CH_4 + 2\,O_2 \xrightarrow{Pt/Pd} CO_2 + 2\,H_2O$$



Picture: Courtesy of Robert J. Kee, Colorado School of Mines



L. L. Raja, R. J. Kee, O. Deutschmann, J. Warnatz, L. D. Schmidt. Catalysis Today 59 (2000) 47-60.

Computed CO concentrations in single monolith channel

⇒ No significant differences

⇒ Axial diffusion can be neglected

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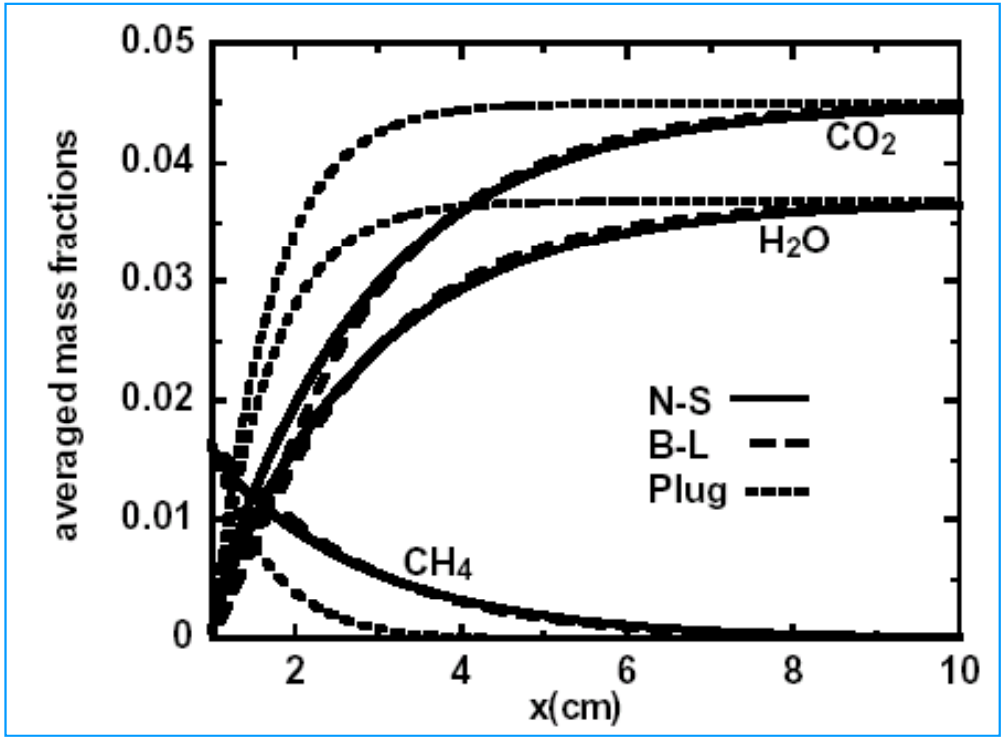
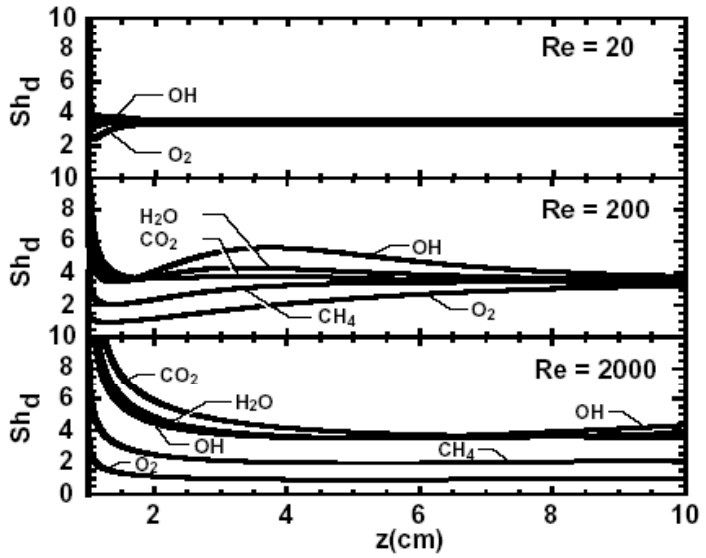
Institute for Chemical Technology and Polymer Chemistry

Catalytic combustion of natural gas in catalytic channel: 2D Navier-Stokes, 2D Boundary layer, and 1d Plug flow approach

1D – Plug-Flow-Model over estimates conversion





Use of mass transfer coefficient is difficult due to large reaction rate causing strong variation oif the Sherwood number

L. L. Raja, R. J. Kee, O. Deutschmann, J. Warnatz, L. D. Schmidt. Catalysis Today 59 (2000) 47-60.

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Institute for Chemical Technology and Polymer Chemistry

DETCHEM^{MONOLITH}: Computer program for the numerical simulation of transients in catalytic monoliths

Karlsruhe Institute of Technology

MONOLITH

Temperature of the solid structure incl. canning
by a 2D / 3D heat balance

transient
quasi-steady-state

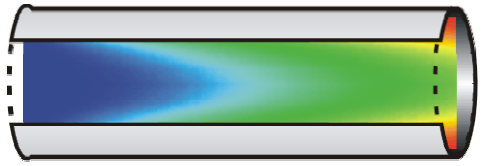
temperature profile
at the wall

heat source term

time scale ~ 1 s
residence time < 100 ms

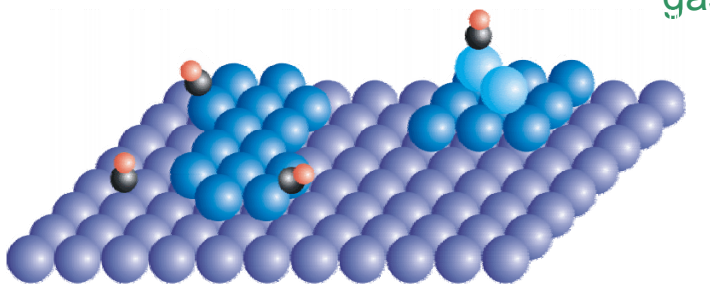
CHANNEL or PLUG

1D or 2D-flow field simulations for a representative number of channels using boundary layer or plug flow equations



gas phase concentrations
temperature

chemical source term
transport coefficients



DETCHEM - Library

Thermodynamic and transport properties
Detailed reaction mechanisms for gas-phase & surface

S. Tischer, O. Deutschmann, Catal. Today 105 (2005) 407, www.detchem.de

Olaf Deutschmann
Institute for Chemical Technology and Polymer Chemistry

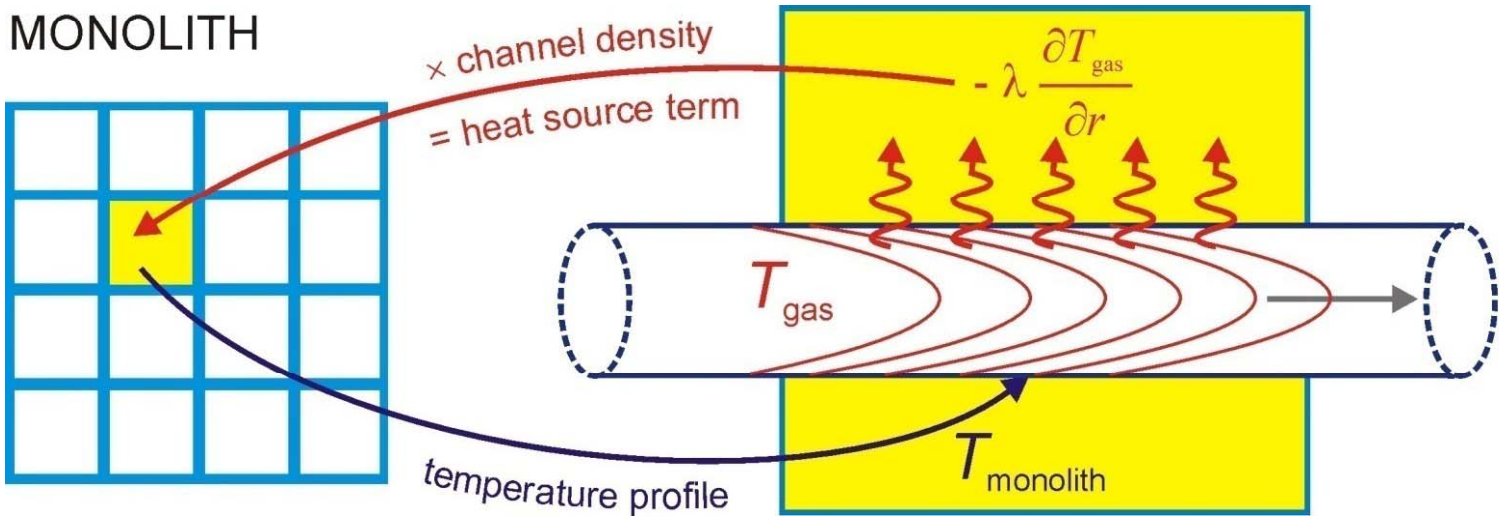
Modeling the temperature of the solid phase of the monolith: Transient three-dimensional heat balance

Temperature

$$\frac{\partial T_{\text{monolith}}}{\partial t} = \nabla^2 \left(\frac{\lambda T_{\text{monolith}}}{\rho c_p} \right) + \frac{q}{\rho c_p}$$

Heat source term

$$q = -\sigma \cdot 2\pi r \, \lambda \frac{\partial T_{\text{gas}}}{\partial r}\bigg|_{\text{surface}}$$



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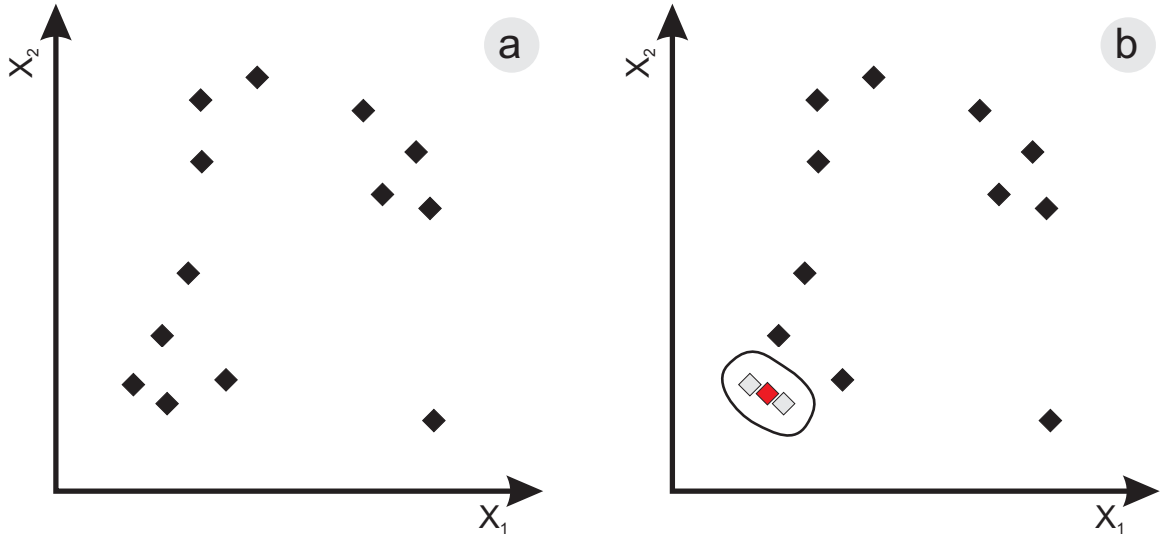
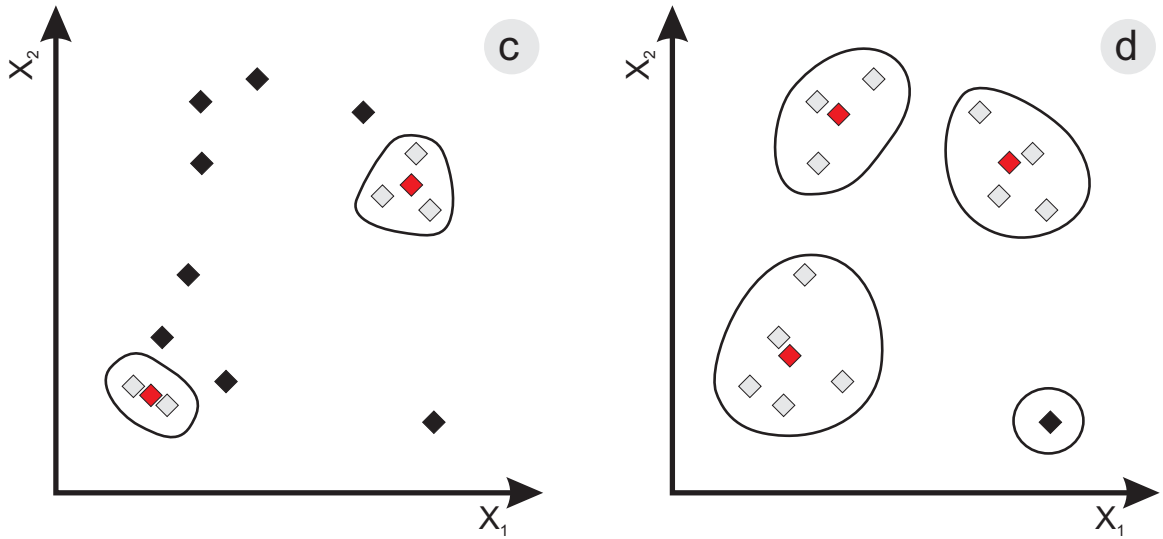
DETCHEM^{MONOLITH}
Selecting representative channels

- Cluster-Agglomeration:
- channels may differ in:
  wall temperature profile
  inlet conditions
- ➔ discrete vectors
- $x=(x_1,x_2,..)$



Clustering of „similair“ vectors

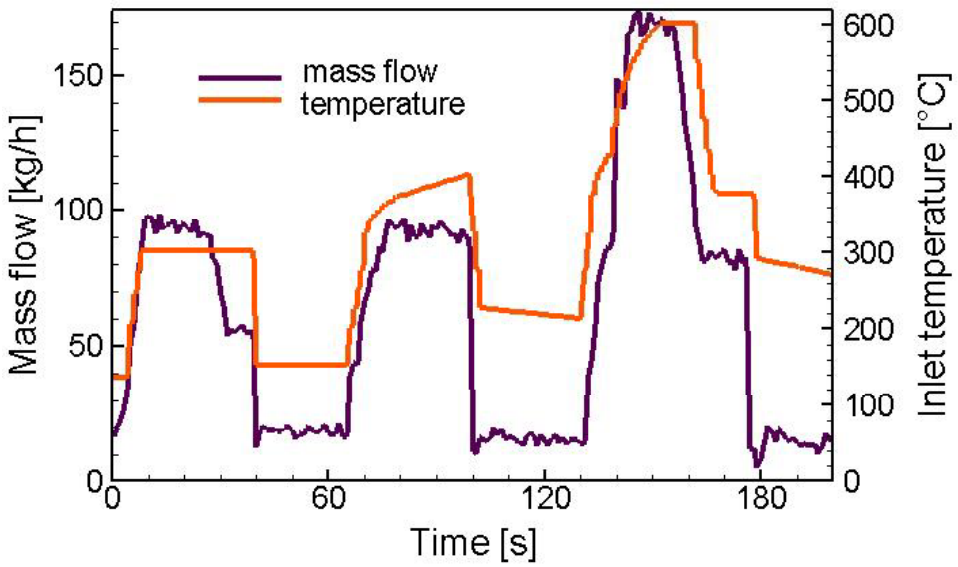
Vectors in one cluster are represented by an averaged vector

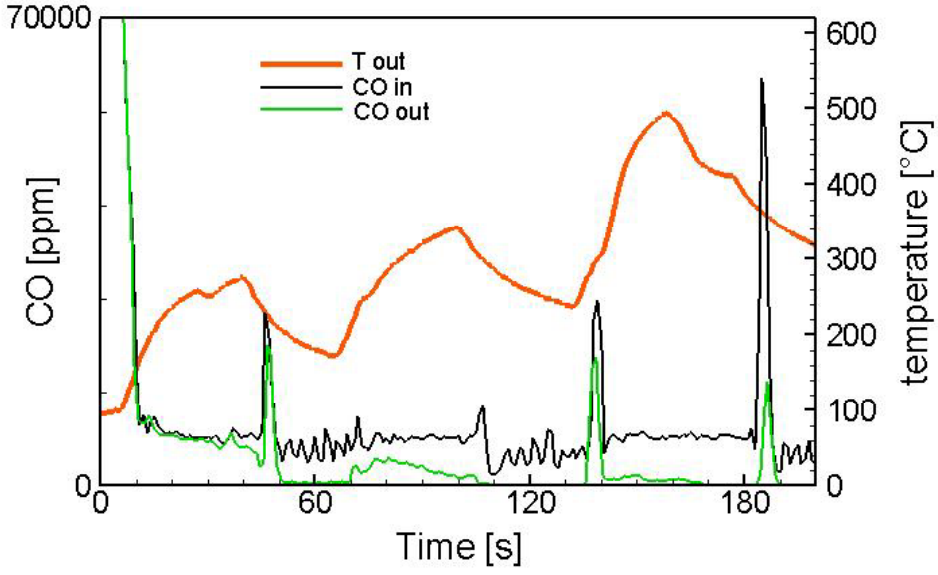


S. Tischer, O. Deutschmann. Catalysis Today 105 (2005) 407-413

Olaf Deutschmann
Institute for Chemical Technology and Polymer Chemistry

Simulation at real driving conditions is very challenging: Continuous variation of all inlet variables





J. Braun, T. Hauber, H. Többen, J. Windmann, P. Zacke, D. Chatterjee, C. Correa, O. Deutschmann, L. Maier, S.Tischer, J. Warnatz, SAE paper 2002-01-0065

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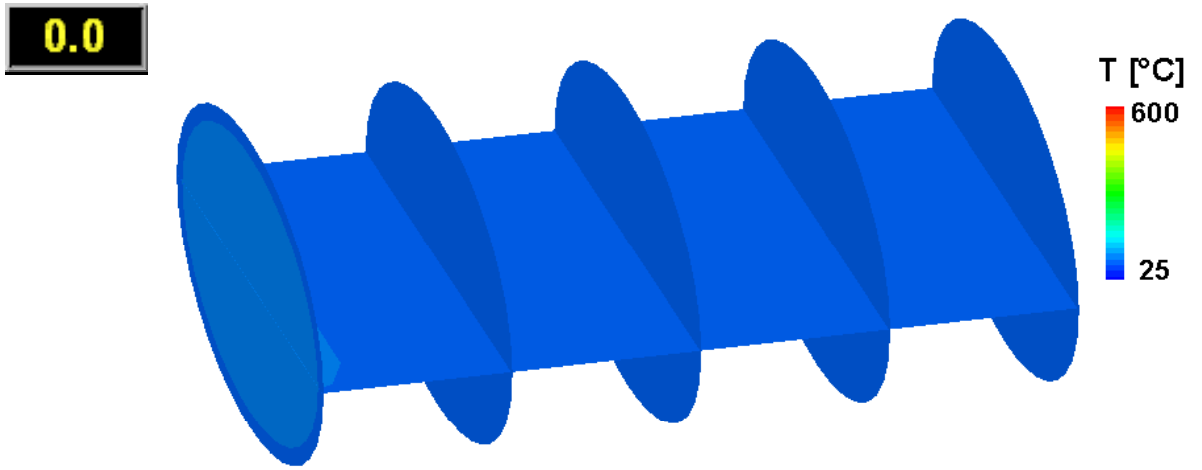
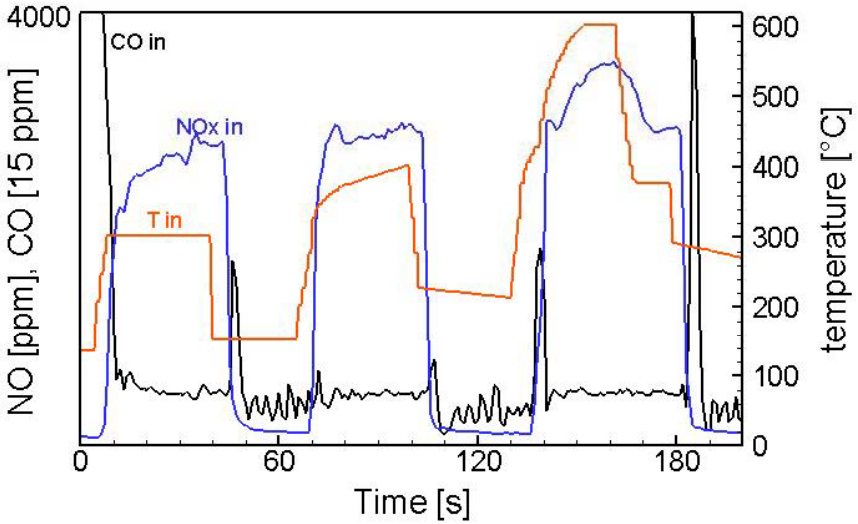
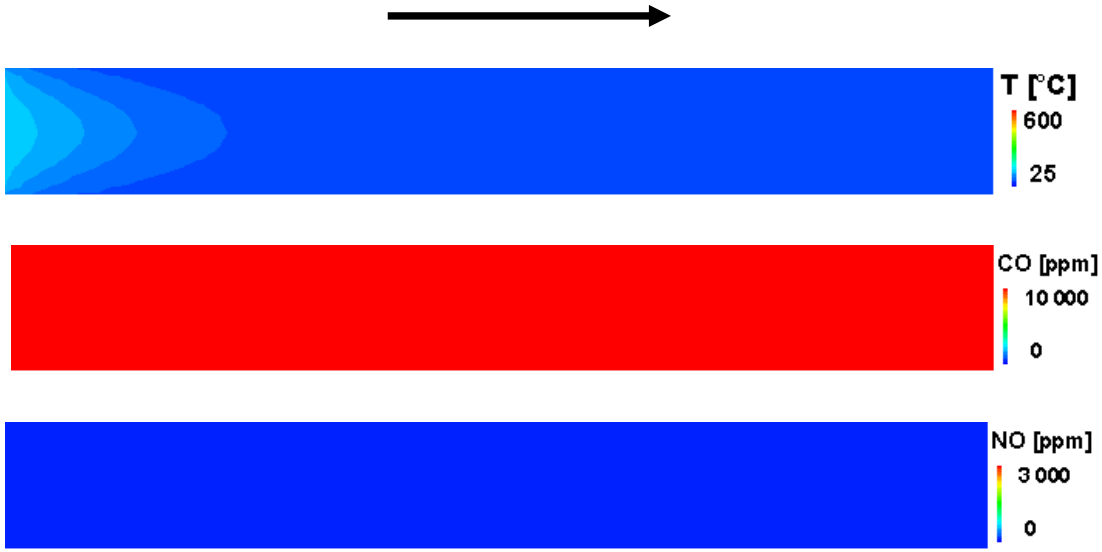
Pollutant reduction in a three-way catalyst during cold start-up: Simulation of a driving cycle







J. Braun, T. Hauber, H. Többen, J. Windmann, P. Zacke, D. Chatterjee, C. Correa, O. Deutschmann, L. Maier, S.Tischer, J. Warnatz, SAE paper 2002-01-0065

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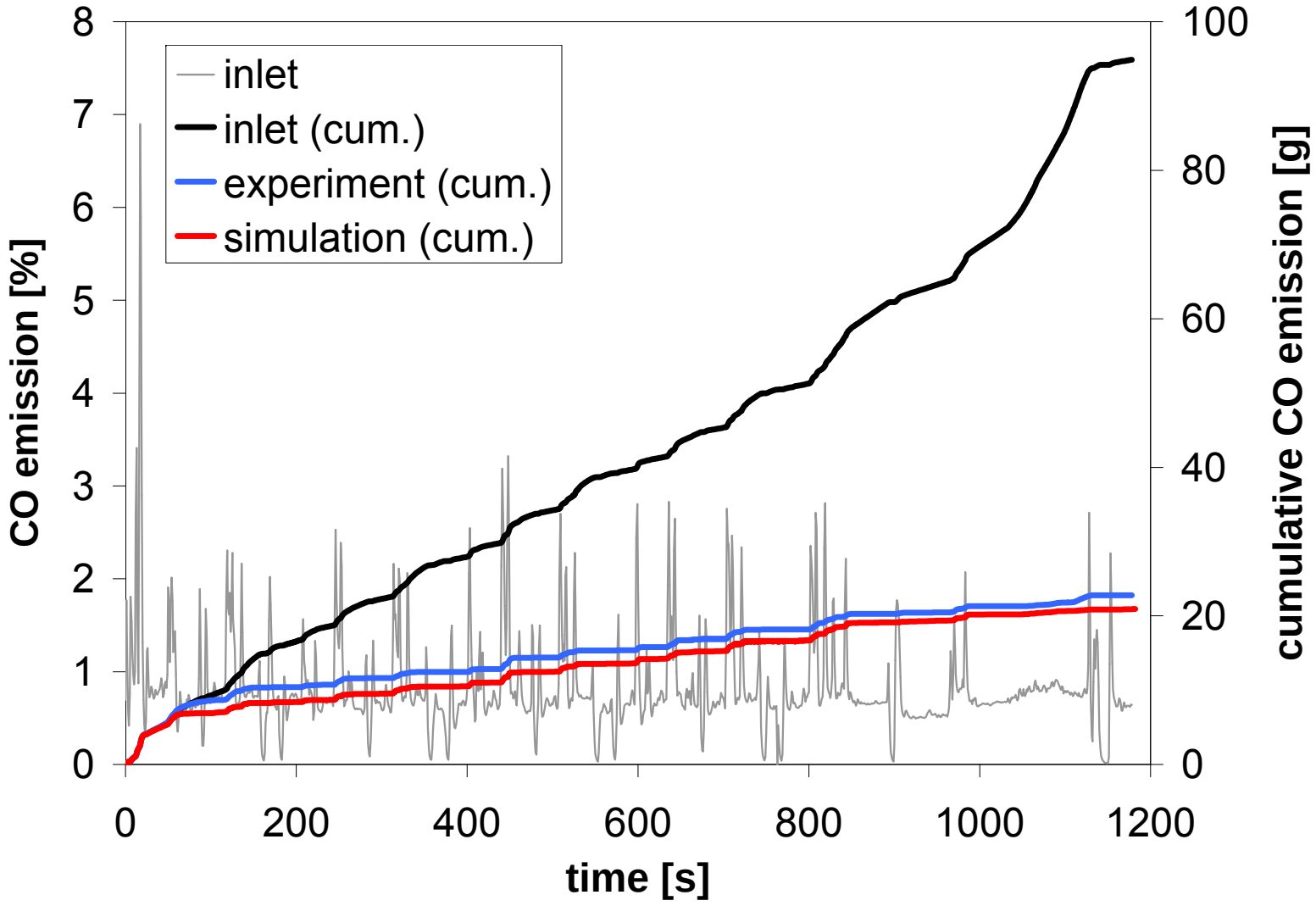
Cumulative CO emission in MEVG cycle: Experiment vs. simulation



Funded by Corning, 2006-2009

Tischer et al. SAE Technical paper 2007-01-1072 2007

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Catalytic combustion: Modeling and Simulation
Outline

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8. Gas-phase chemistry
9. Catalyst deactivation

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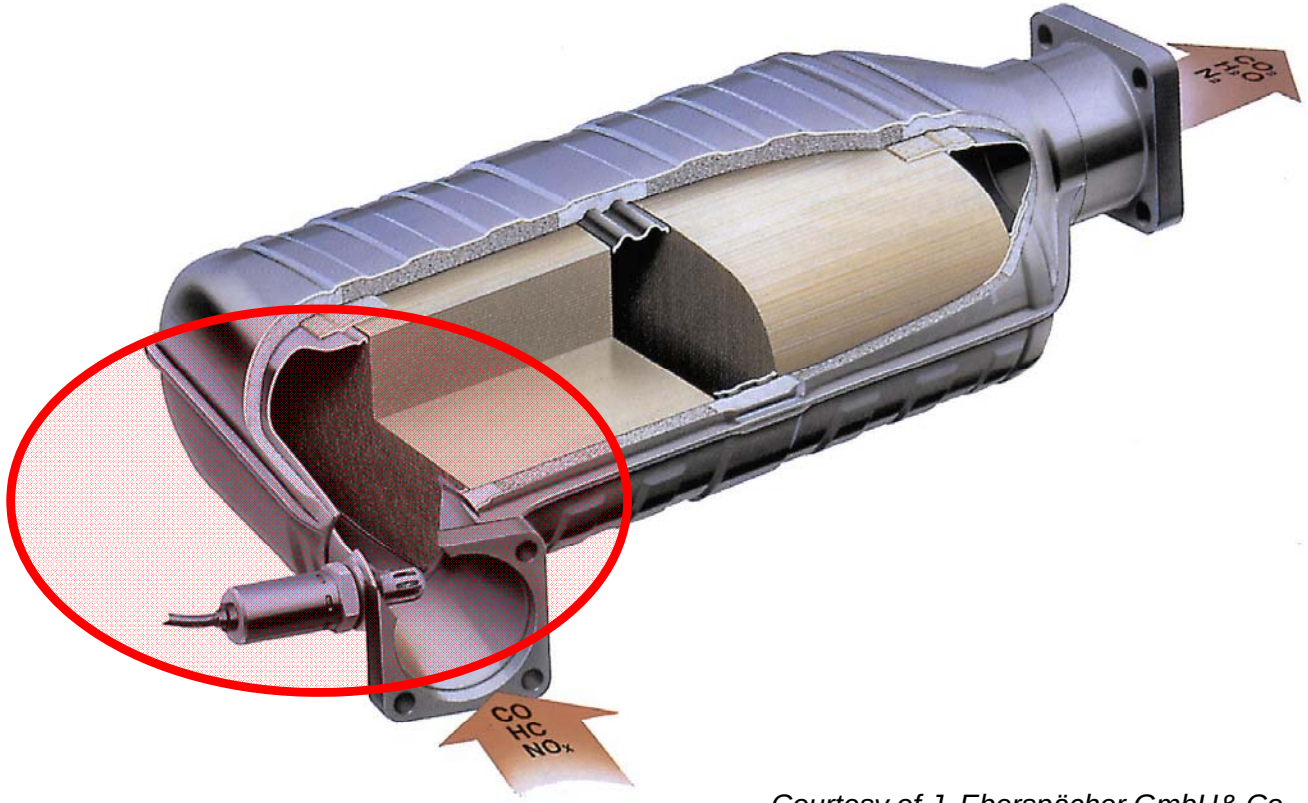
Spatially non-uniform inlet conditions: Non-efficient use of catalyst materials



Courtesy of J. Eberspächer GmbH& Co

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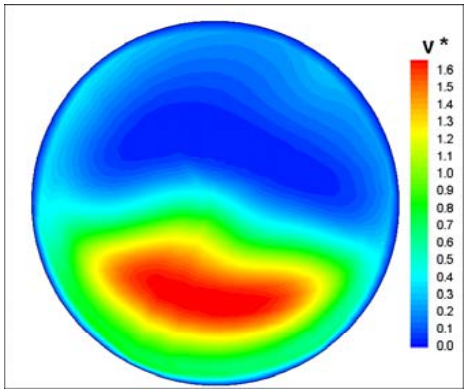
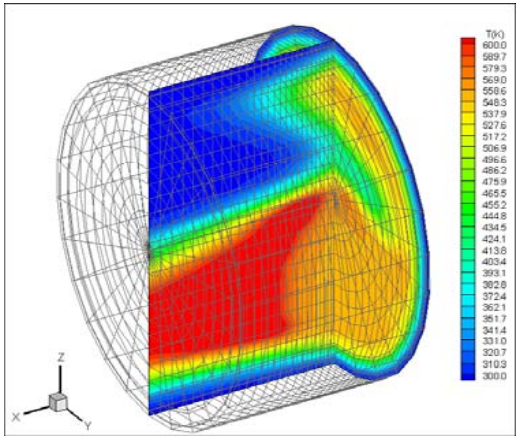
Simulation reveals consequences of design restrictions: Spatial non-uniformity increases pollution emissions

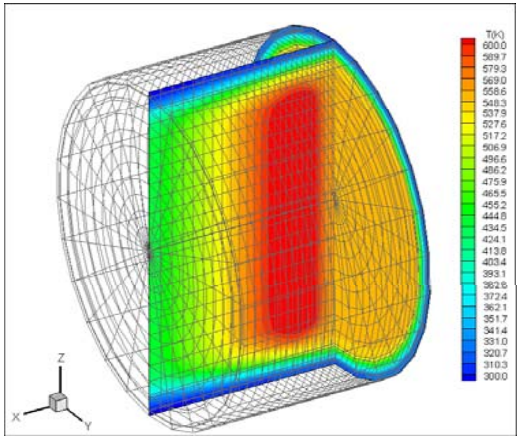
Non-uniform flow distribution at converter front face

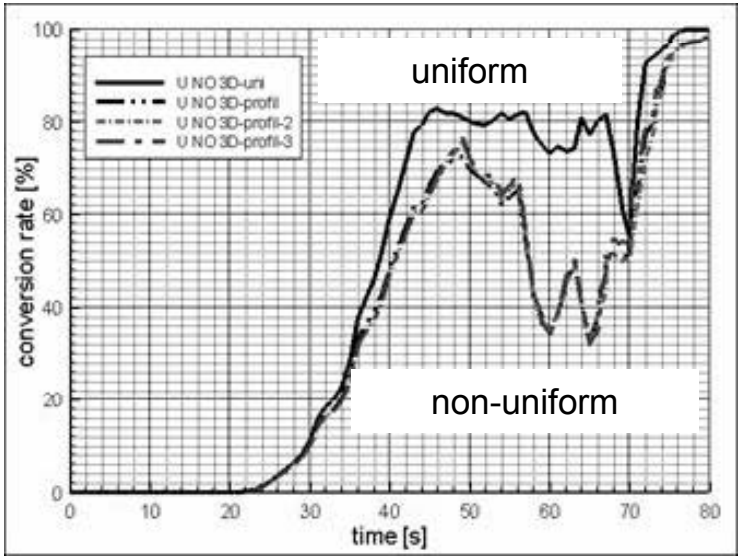


Temperature after 40 s Non-uniform flow distribution



Temperature after 40 s Uniform flow distribution

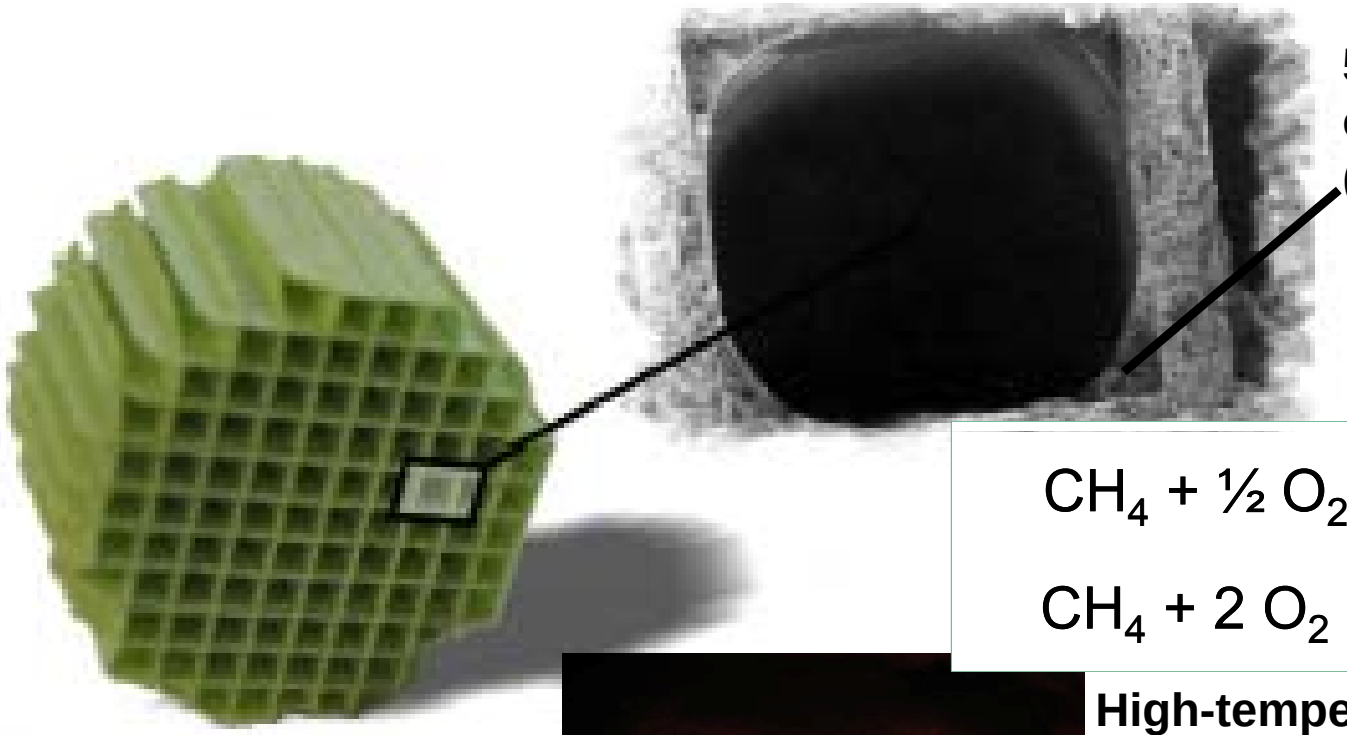




J. Windmann, P. Zacke, S.Tischer, O. Deutschmann, J. Warnatz, SAE paper 2003-01-0937 (2003)

Olaf Deutschmann
Institute for Chemical Technology and Polymer Chemistry

High-temperature catalysis: Compact and autothermal production of hydrogen in few milliseconds



5-50 μm thick oxide layer containing catalyst particles (Pt, Rh) of nm-size

$$CH_4 + ½\ O_2 \longrightarrow CO + 2\ H_2$$

$$CH_4 + 2\ O_2 \longrightarrow CO_2 + 2\ H_2O$$

High-temperature (1000°C) Rh catalyst converting natural gas into CO and H_2 in less than 5 ms without any additional energy supply

D.A. Hickman, L.D. Schmidt, Science 259 (1993) 343

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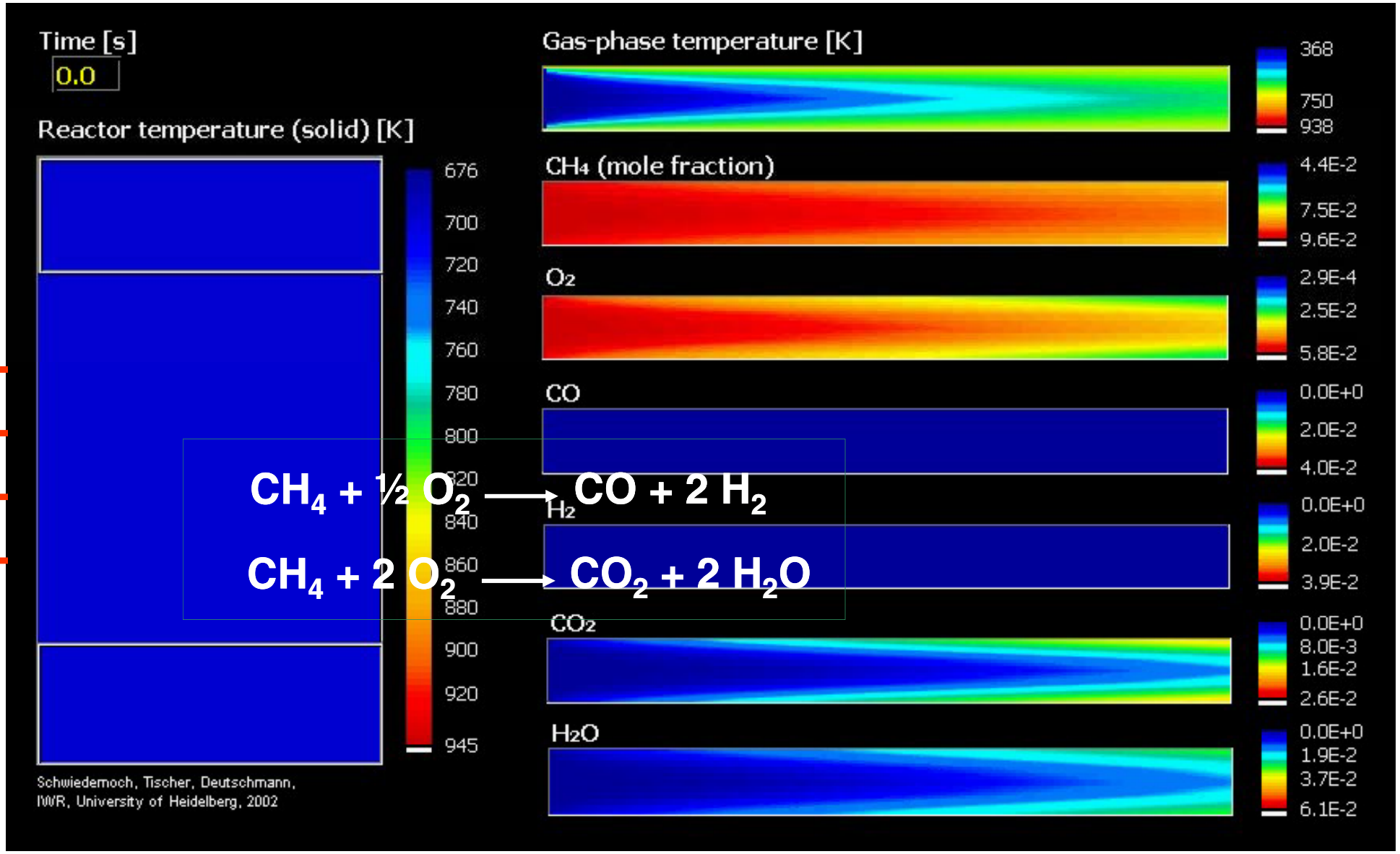
Partial oxidation of CH_4 on Rh at 1 bar: Computed temperature and concentration profiles during light-off



R. Schwiedernoch, S. Tischer, C. Correa, O. Deutschmann, Chem. Eng. Sci., 58 (2003) 633-642

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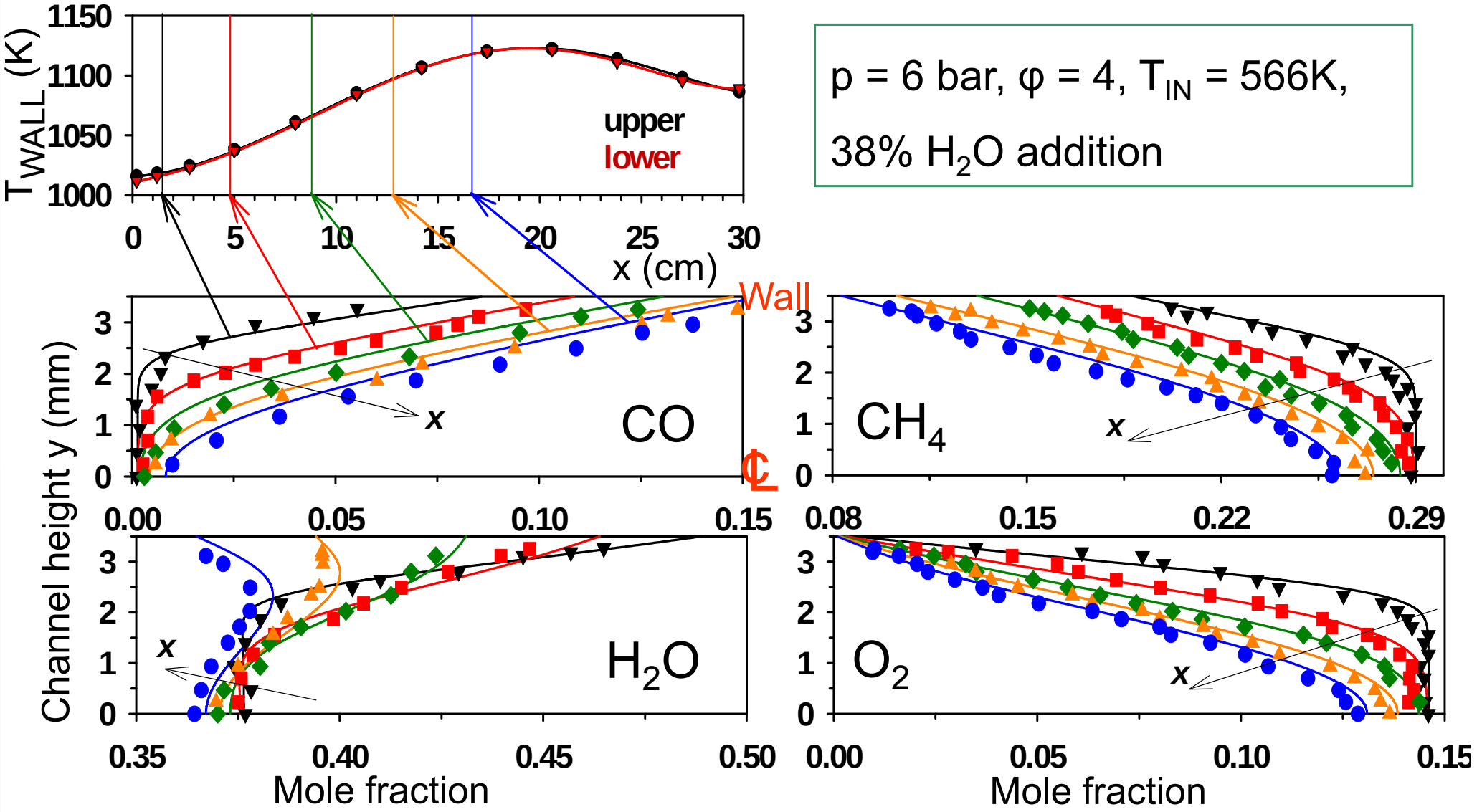
CPOX of CH_4 on Rh in single channel at steady state: 2d Raman profiles vs. computation (Mantzaras et al.)



p = 6 bar, φ = 4, T_{IN} = 566K,

38% H_2O addition

A. Schneider, J. Mantzaras, P. Jansohn et al. Proc. Comb. Inst. 31 (2007)

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High temperature catalysis: Technology for production of hydrogen, syngas, olefins, and liquid hydrocarbons

Natural gas → Synthesis gas

$$CH_4 + ½\ O_2 \longrightarrow CO + 2\ H_2$$

→ MeOH, DME, Diesel

O. Deutschmann, L.D. Schmidt., AIChE J. 44 (1998) 2465-2476

Paraffins → Olefins

$$C_2H_6 + ½\ O_2 \longrightarrow C_2H_4 + 2\ H_2O$$

D.K. Zerkle, M.D. Allendorf, M. Wolf, O. Deutschmann. J. Catal. 196 (2000) 18-39

Ethanol → Hydrogen

$$CH_3CH_2OH + ½\ O_2 + 2\ H_2O \longrightarrow 5\ H_2 + 2\ CO_2$$

N. Hebben, C. Diehm, O. Deutschmann, Appl. Catal. A 388 (2010) 225

Gasoline, Diesel → Hydrogen

$$C_nH_m + {}^{n}/_{2}\ O_2 + n\ H_2O \longrightarrow (n+m/2)\ H_2 + n\ CO_2$$

M. Hartmann, L. Maier, O. Deutschmann, Combustion and Flame 157 (2010) 1771

Steam reforming

$$C_nH_m + 2n\ H_2O \longrightarrow n\ CO_2 + (2n+{}^{m}/_{2})\ H_2$$

B. Schädel, O. Deutschmann, Stud. Surf. Sci. & Catal. 167 (2007) 207

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Catalytic combustion: Modeling and Simulation
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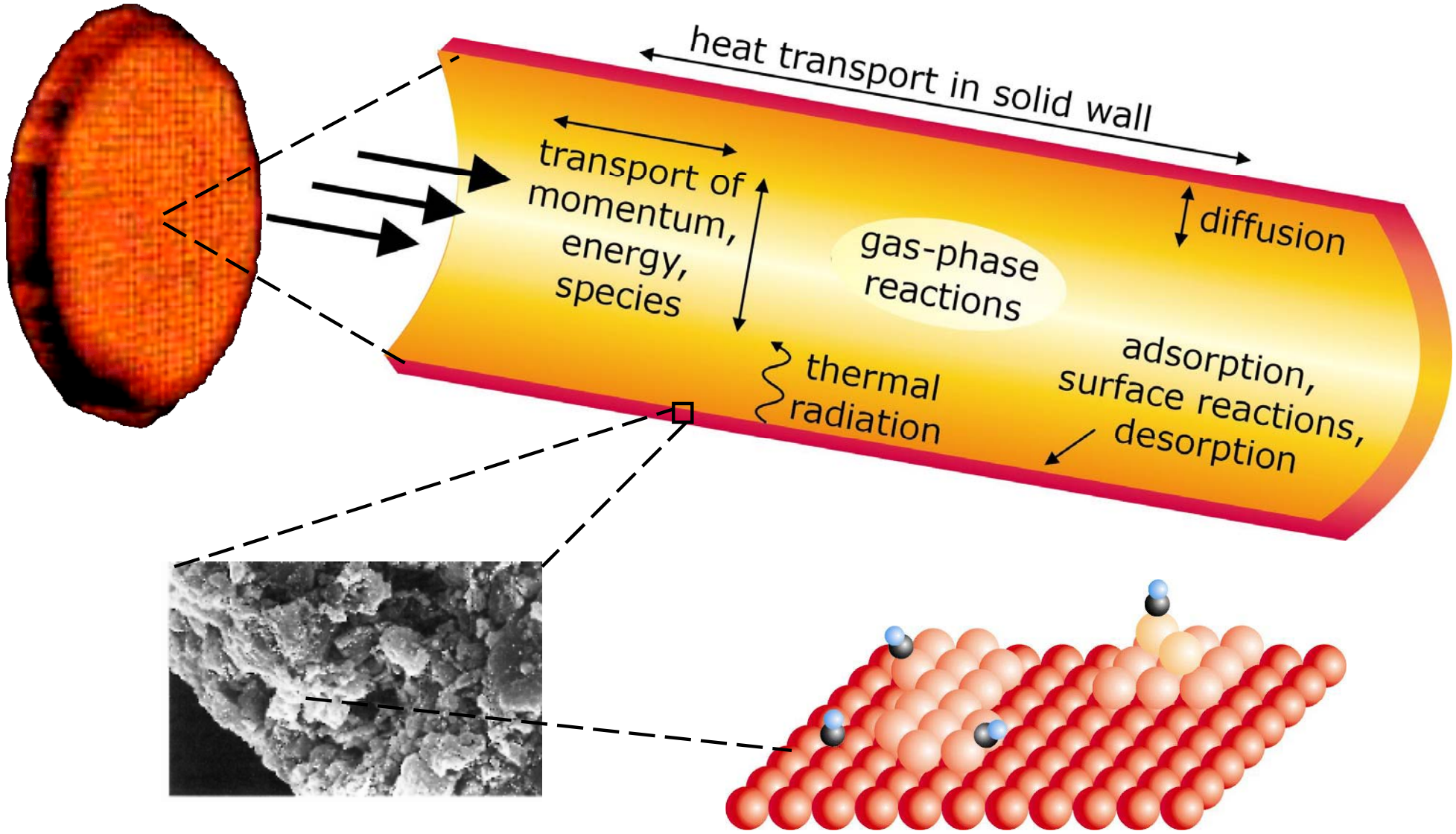
Interaction of physical and chemical processes in catalytic monoliths



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Example: More efficient technology for auxiliary power supply in automobile vehicles needed

Idling long-haul trucks consumes 1 billion gallons of diesel fuel annually in the USA
→11 million tons CO_2, 180,000 tons NO_x, 5000 tons particulates!

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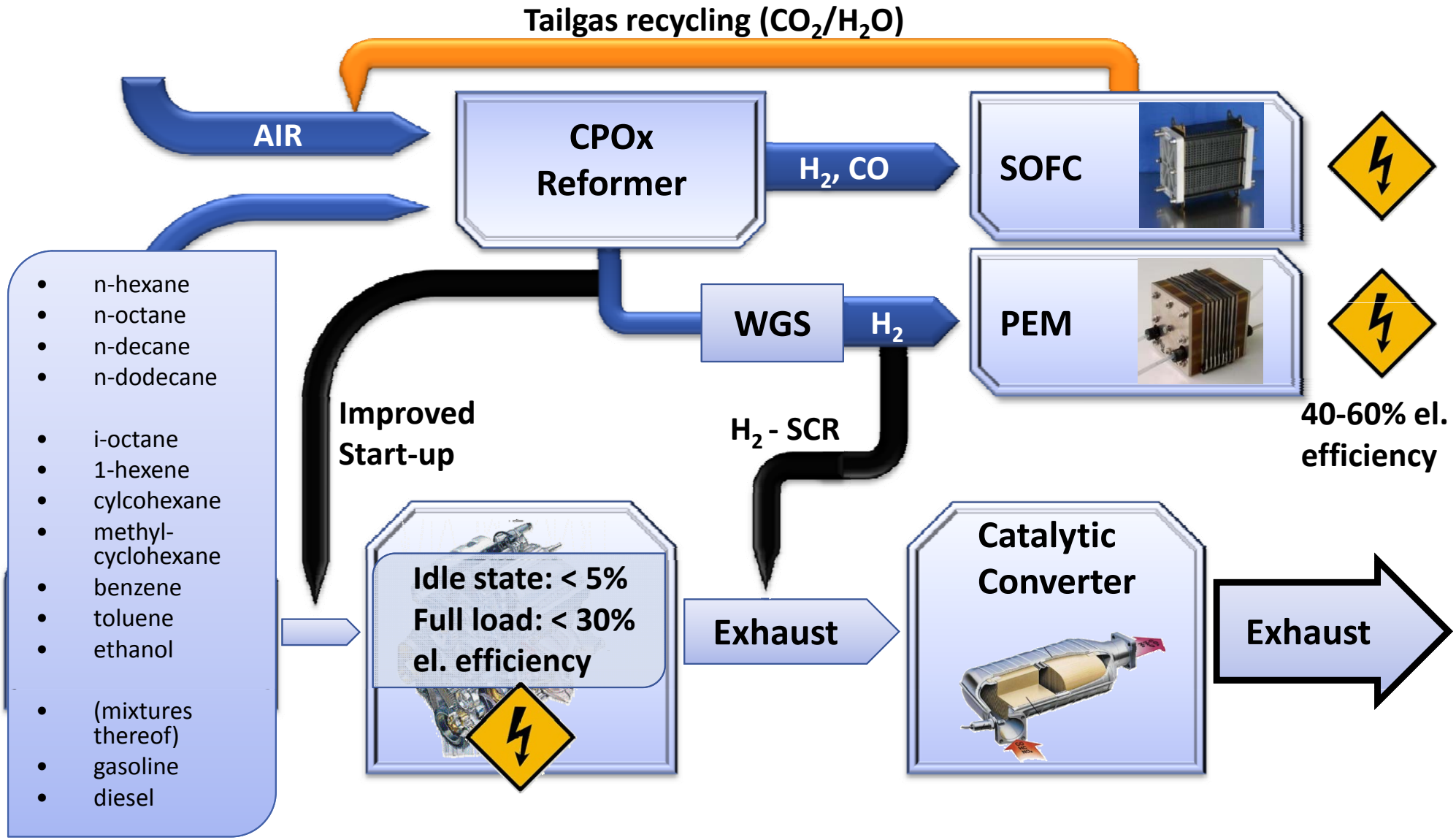
Institute for Chemical Technology and Polymer Chemistry

On-board catalytic partial oxidation (CPOX) of logistic fuels provides electricity and reduces pollutant emissions



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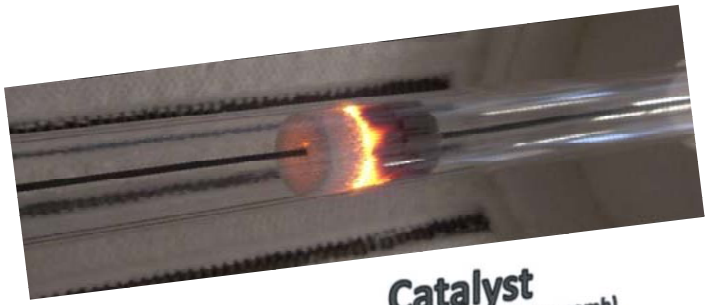
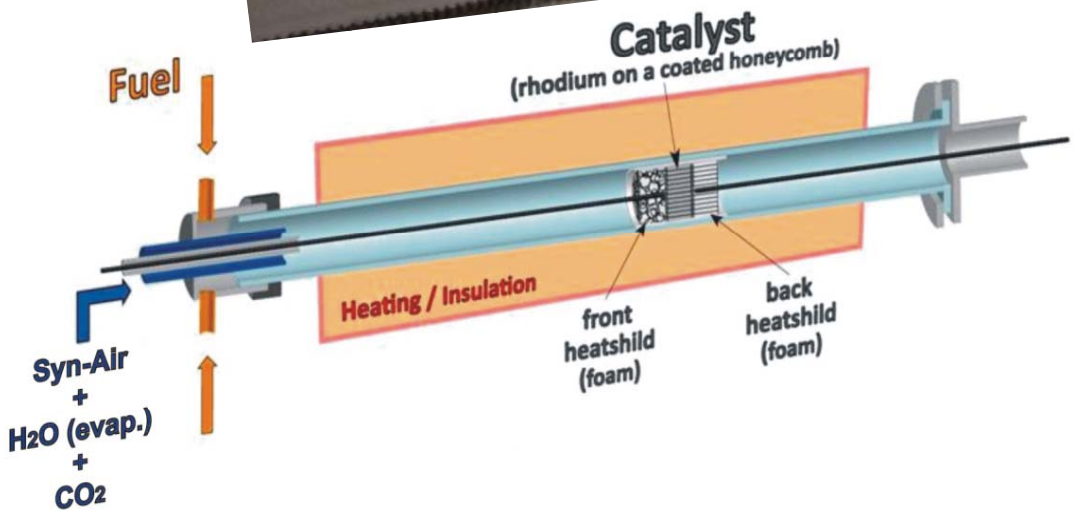
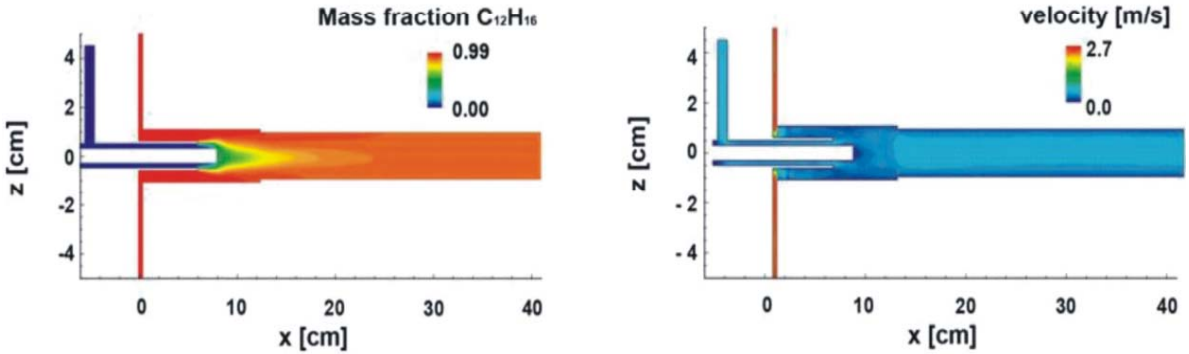
CPOX lab reactor set-up:
Well-defined inlet and boundary conditions







M. Hartmann, T. Kaltschmitt, O. Deutschmann. Catalysis Today 147 (2009) S204

Pulse-free rapid mixing of up to eight gaseous reactants below auto-ignition temperature

900 cpsi Rh coated honeycomb

Autothermal operation

C/O: 0.8 – 2.0

Flow rate: 2 – 6 splm

w/ & w/o CO_2 and H_2O addition

Product analysis:

FT-IR, MS, GC/MS, O_2 sensor

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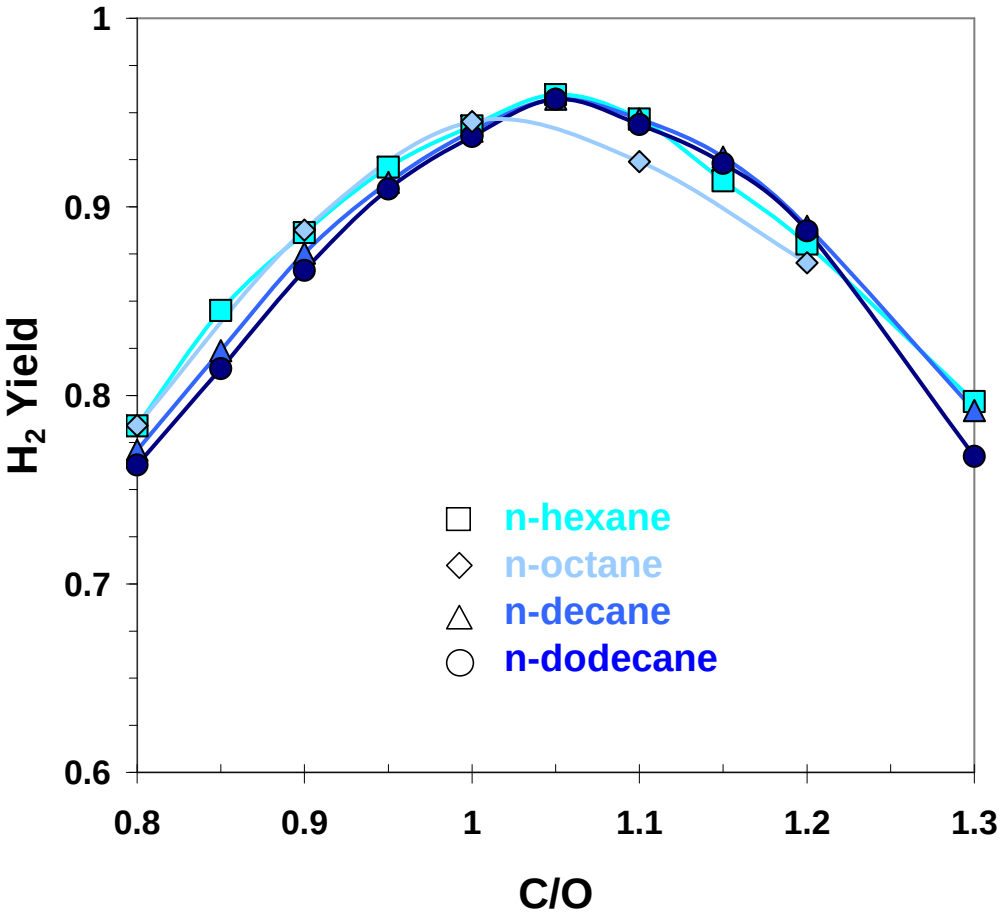
Institute for Chemical Technology and Polymer Chemistry

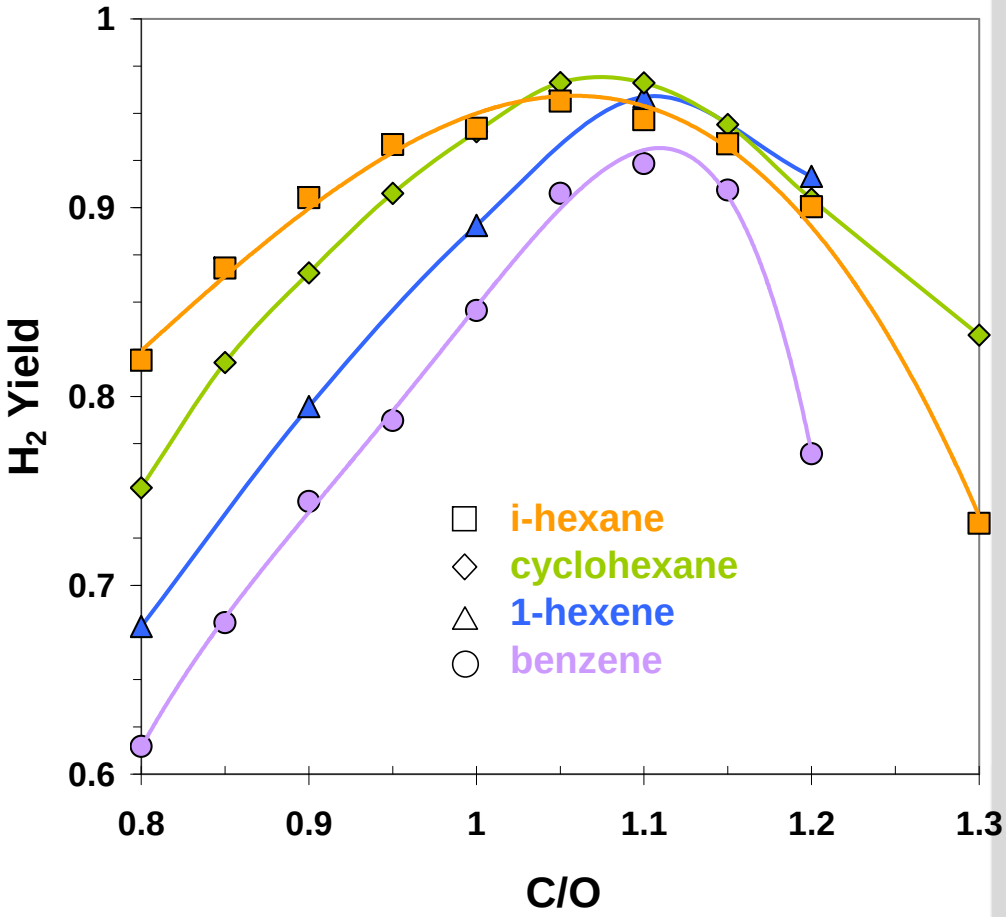
Fuel composition (aliphats, aromatics, olefins) and C/O ratio determines both yields in hydrogen and coke precursors

Karlsruhe Institute of Technology

Variation of chain length



Variation of structure



M. Hartmann, T. Kaltschmitt, O. Deutschmann. Catalysis Today 147 (2009) S204

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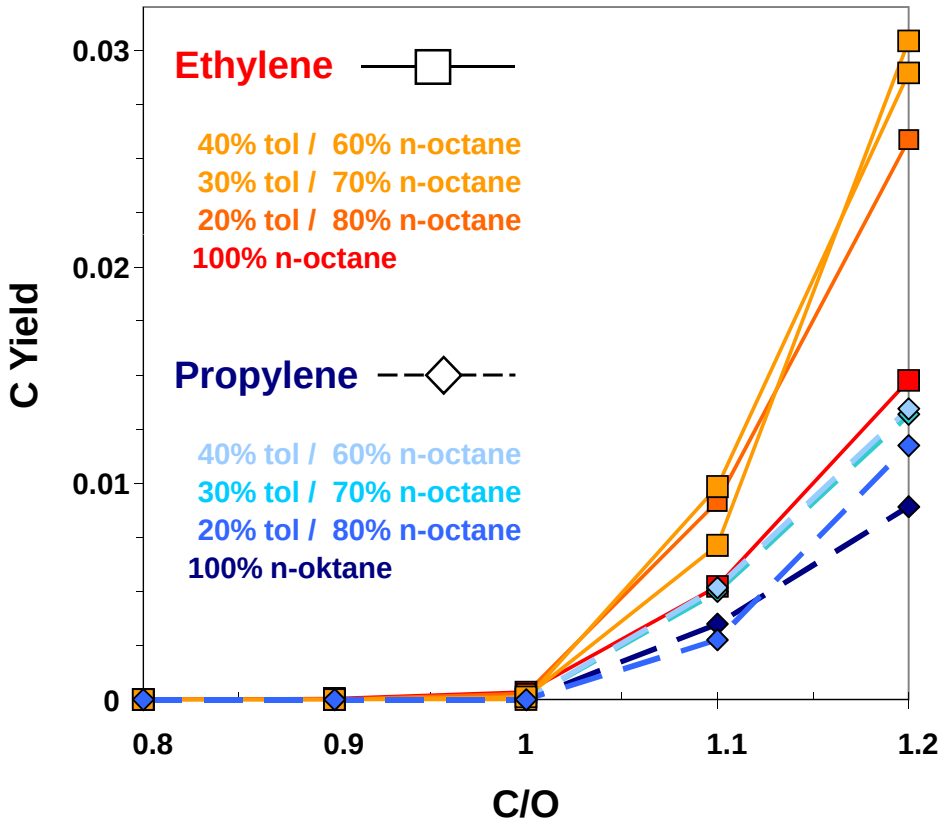
Institute for Chemical Technology and Polymer Chemistry

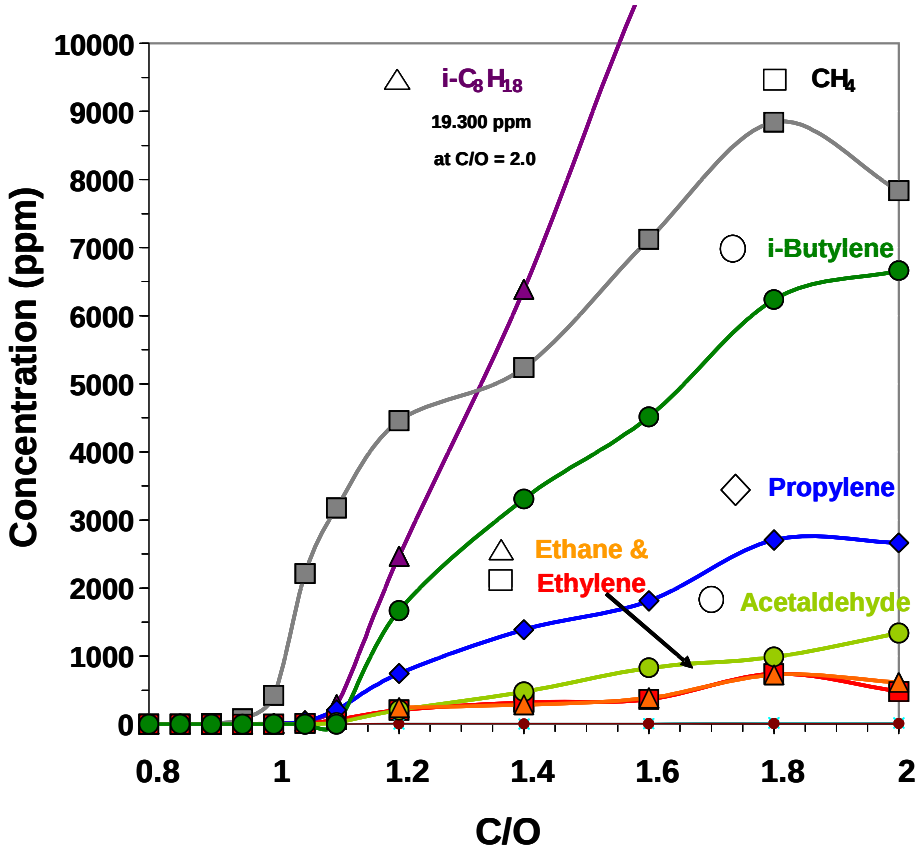
Fuel composition (aliphats, aromatics, olefins) and C/O ratio determines both yields in hydrogen and coke precursors

Karlsruhe Institute of Technology

Coke precursors



By-products in CPOX of iso-octane



M. Hartmann, T. Kaltschmitt, O. Deutschmann. Catalysis Today 147 (2009) S204

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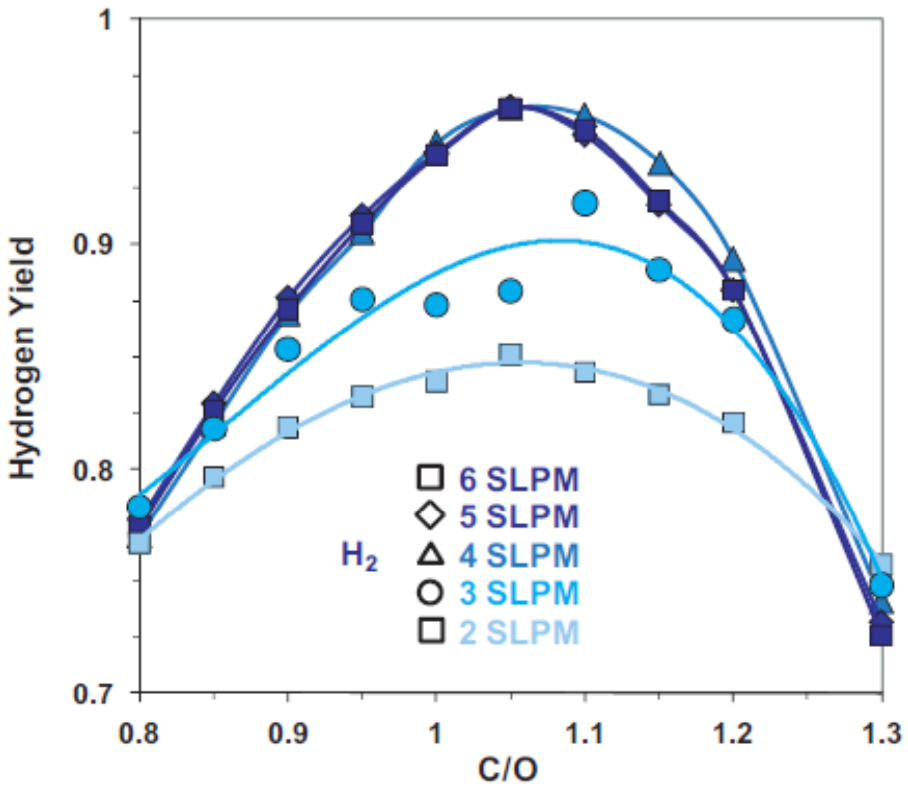
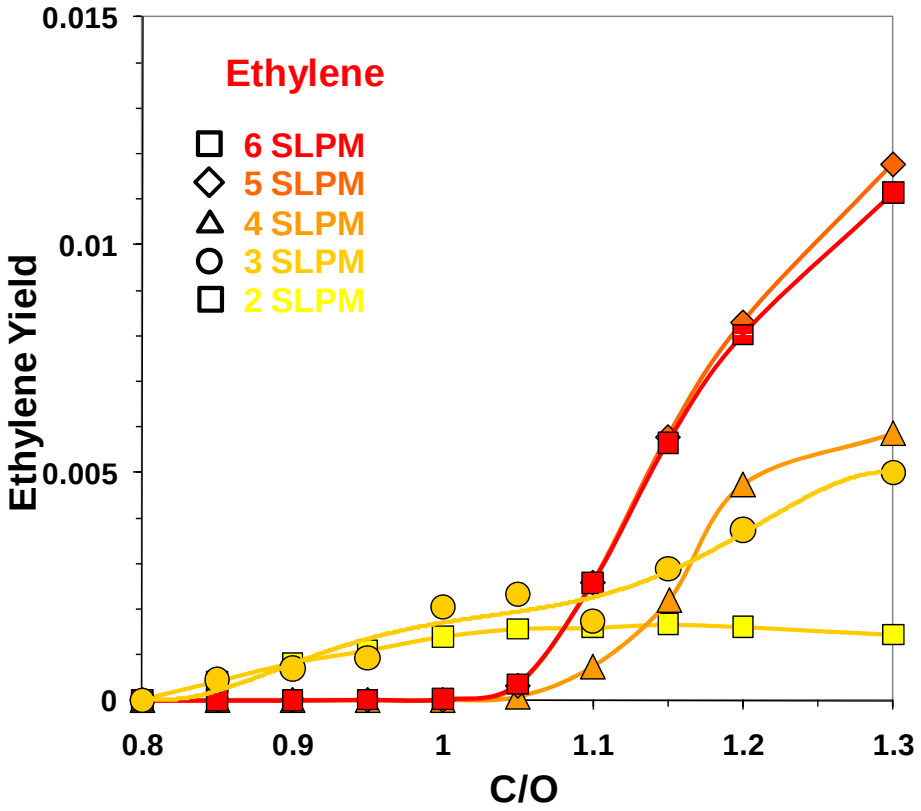
CPOX of iso-octane over rhodium: Influence of residence time and C/O ratio on hydrogen formation and by-product formation





M. Hartmann, L. Maier, O. Deutschmann, Applied Catalysis A: General 391 (2011) 144–152.
L. Maier, M. Hartmann, O. Deutschmann, Combust. Flame 158 (2011) 796-808.

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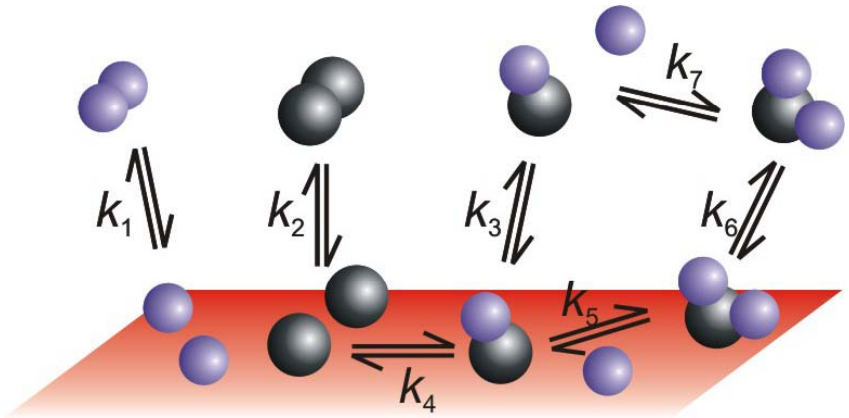
CPOX of i-octane: Modeling based on detailed reaction mechanisms on the catalyst and in the gas-phase

Surface reactions

Detailed reaction mechanism for C_1-C_3 species:
111 reactions, 31 surface species



C_{4+} hydrocarbons: lumped steps assuming a fast dissociation leading to adsorbed C_1-C_3 species

M. Hartmann, L. Maier, O. Deutschmann, Combustion and Flame 2010, 157, 1771.

Elementary-step gas-phase reaction mechanisms

LLNL: 7193 reactions among 857 species and 17 third bodies
H. J. Curran, P. Gaffuri, W.J. Pitz, C.K. Westbrook. Combustion and Flame 129 (2002) 253

Golovichev, Chalmers University: 690 reactions, 130 species
V. I. Golovitchev, F. Tao, L. Chomial, in SAE paper 1999-01-3552

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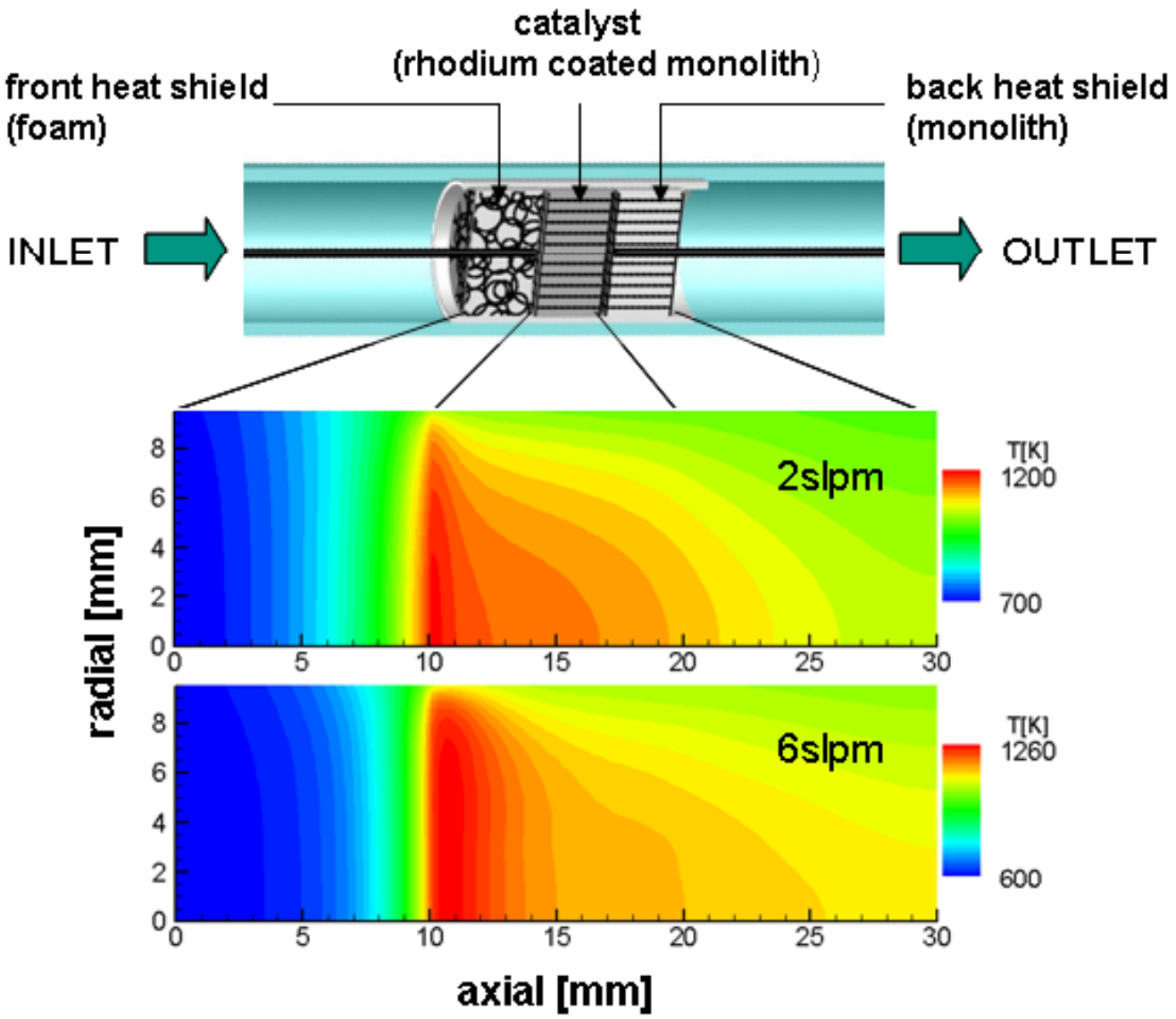
CPOX of i-octane:
Computed temperature distribution in the reactor



L. Maier, M. Hartmann, O. Deutschmann, Combust. Flame 158 (2011) 796–808.

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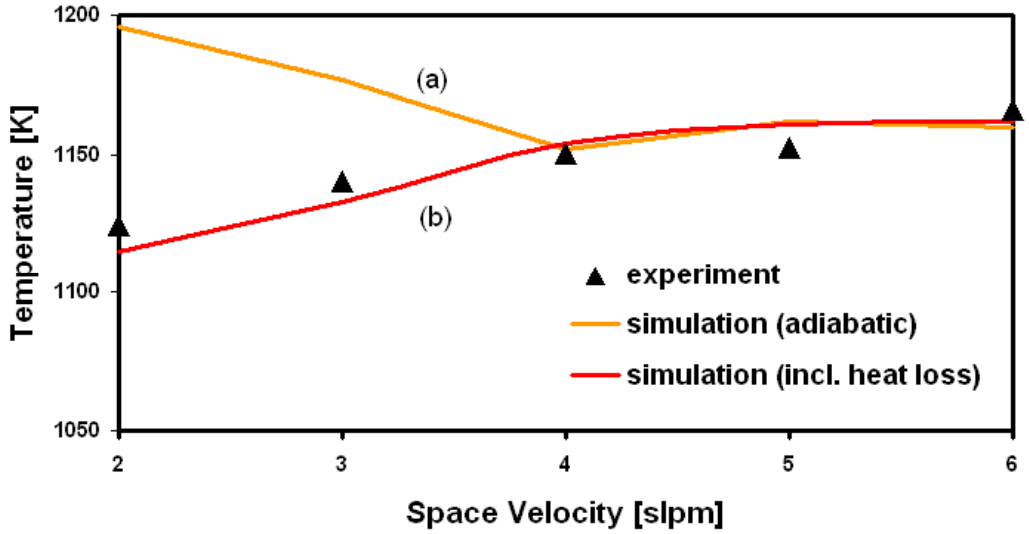
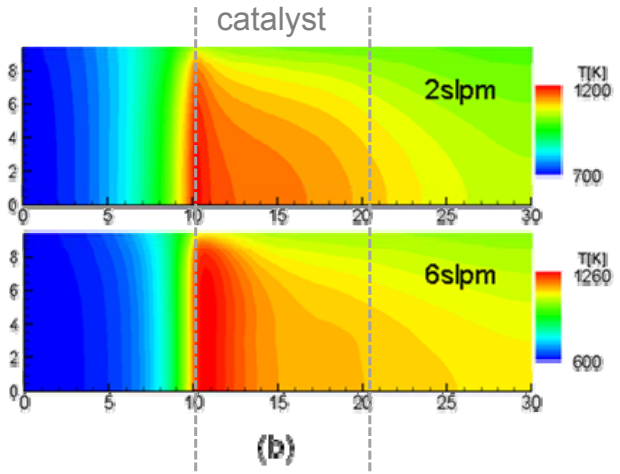
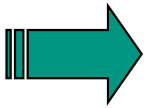
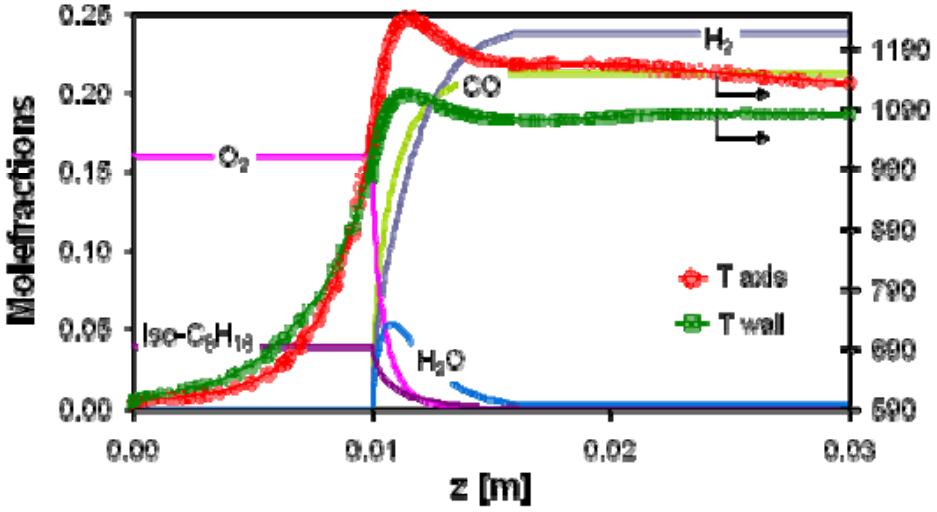
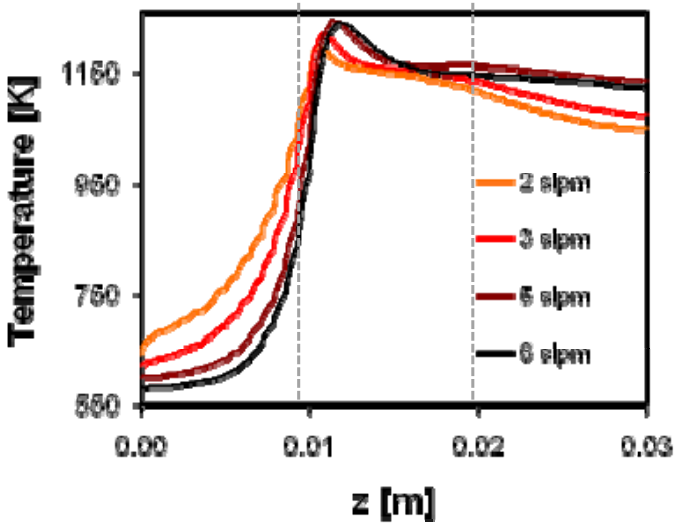
CPOX of HC: Counter-intuitive increase of yields with decreasing residence time understood

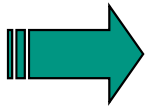












L. Maier, M. Hartmann, O. Deutschmann, Combust. Flame 158 (2011) 796–808.

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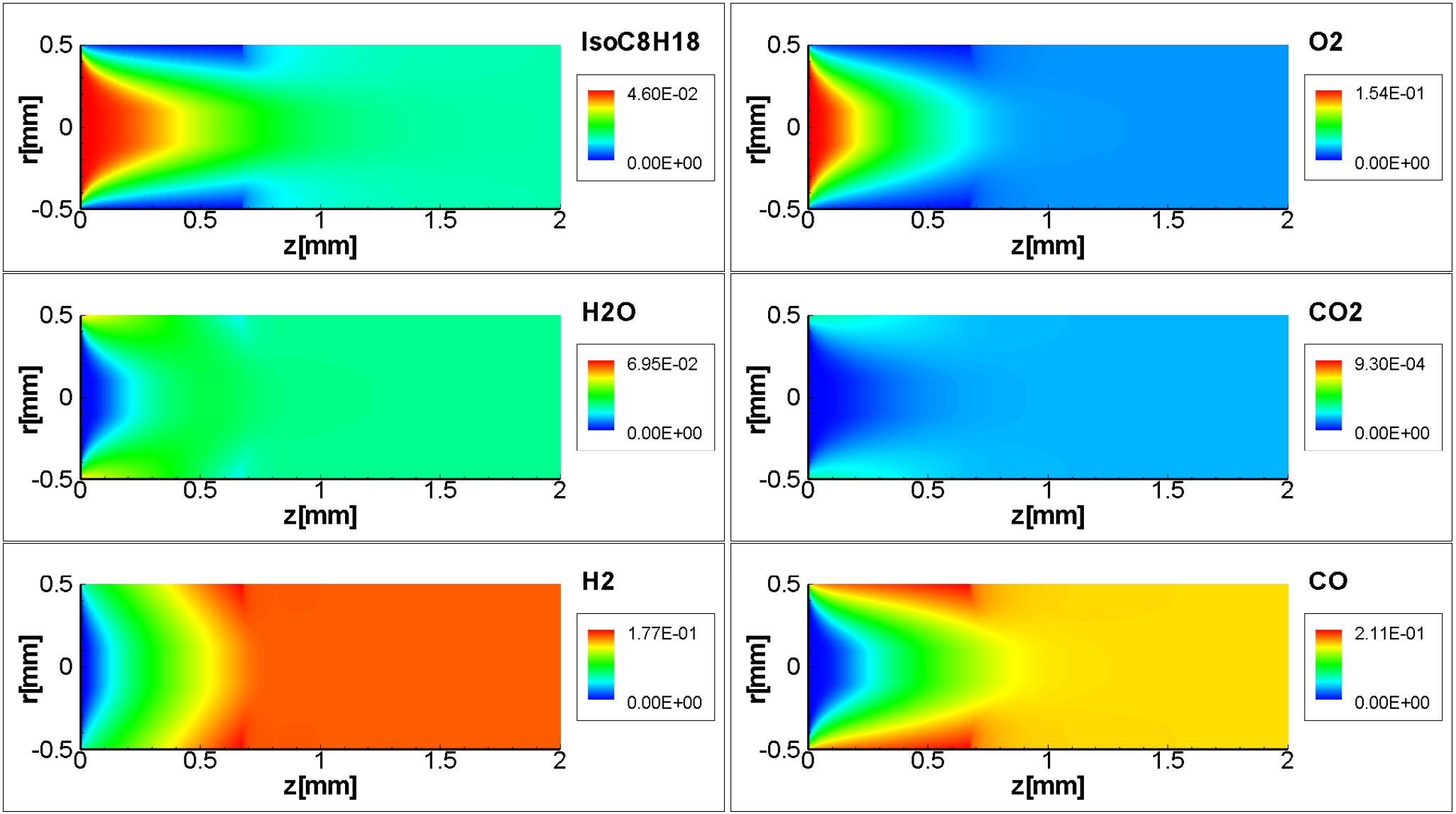
CPOX of iso-octane in catalytic channel: Numerically predicted 2D species profiles in gas-phase



C/O = 1.2, 800°C

M. Hartmann, L. Maier, O. Deutschmann, Combust. Flame 157 (2010) 1771

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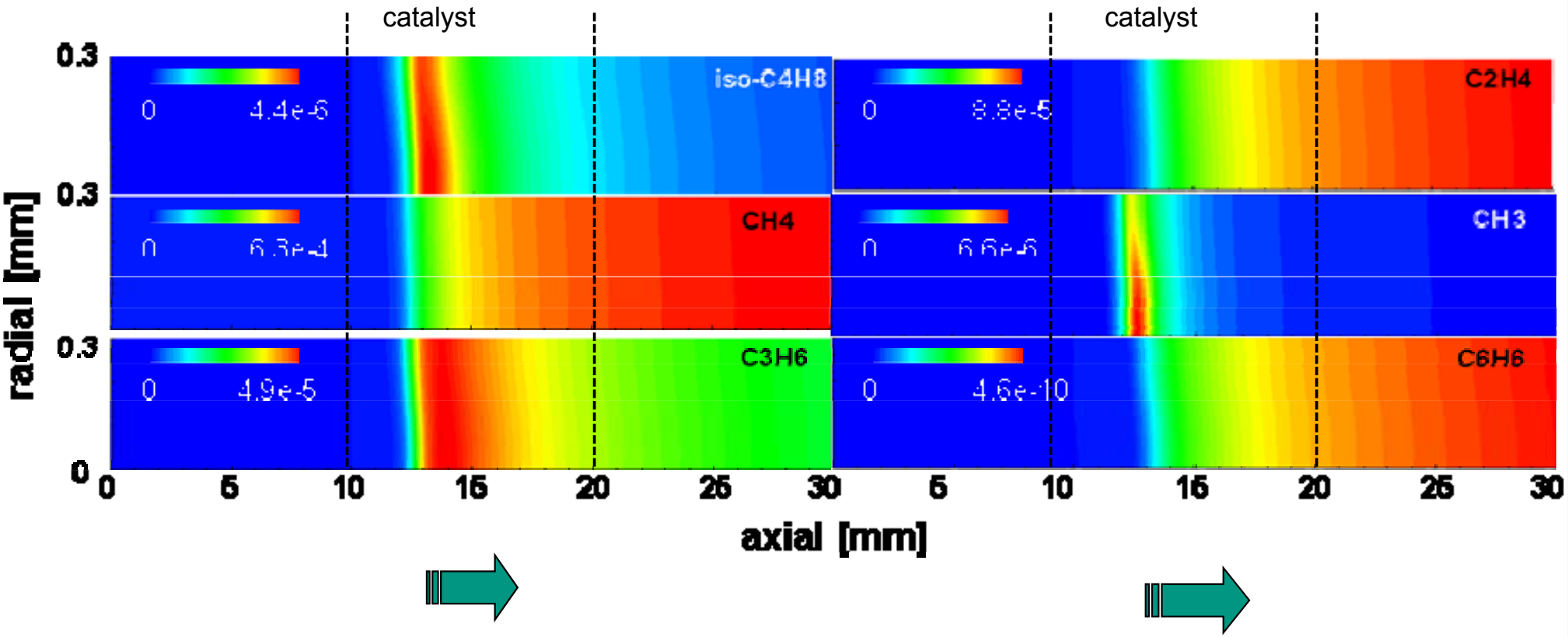
CPOX of i-octane: Coke precursors are formed in the gas phase in the catalytic zone and downstream



C/O = 1.0 5 slpm

L. Maier, M. Hartmann, O. Deutschmann, Combust. Flame 158 (2011) 796–808.

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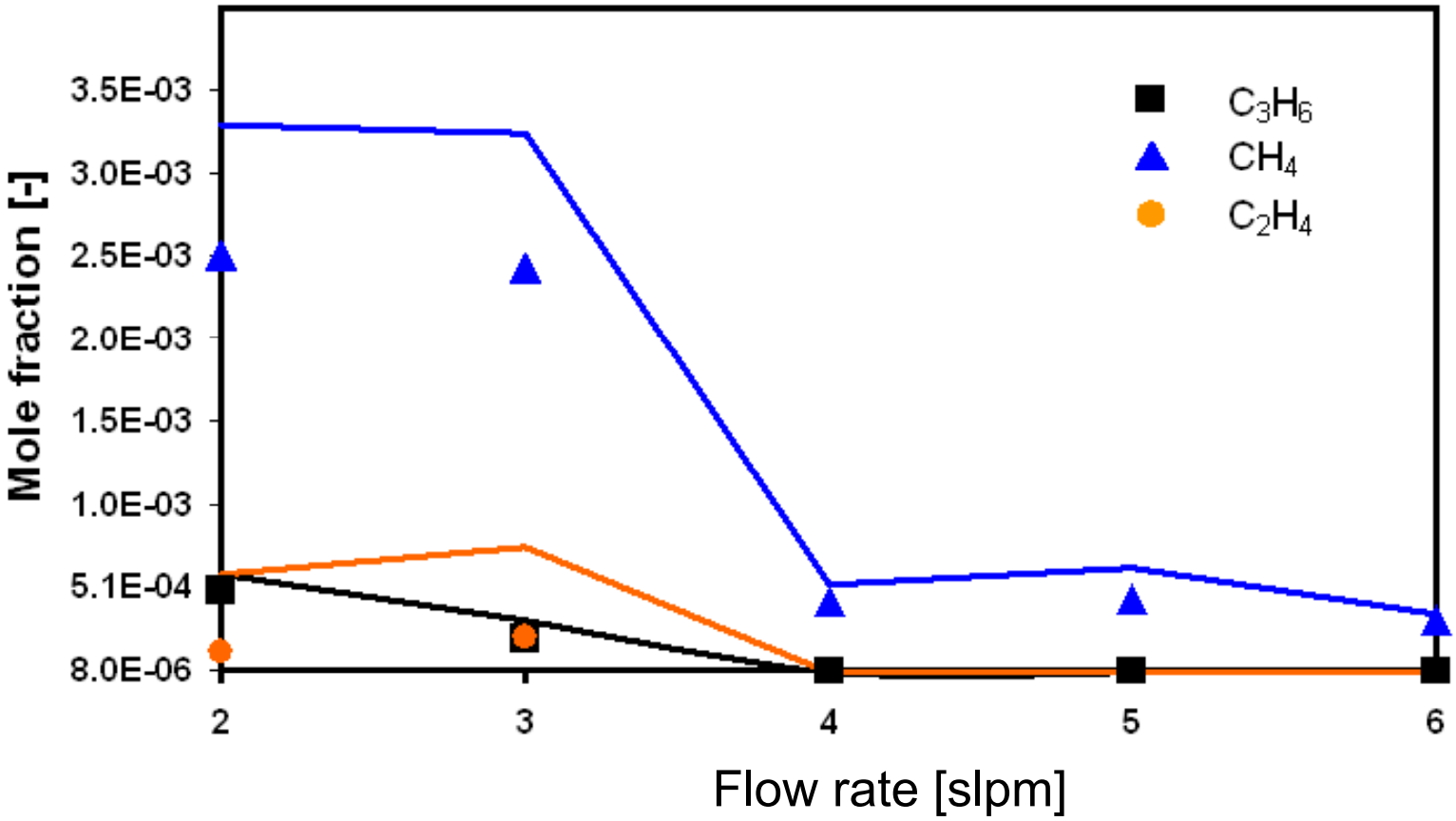
Institute for Chemical Technology and Polymer Chemistry

CPOX of iso-octane:
Coke precursor formation also depends on flow rate

Modeling (lines) versus experiment (symbols)



C/O = 1.0

L. Maier, M. Hartmann, O. Deutschmann, Combust. Flame 158 (2011) 796–808.

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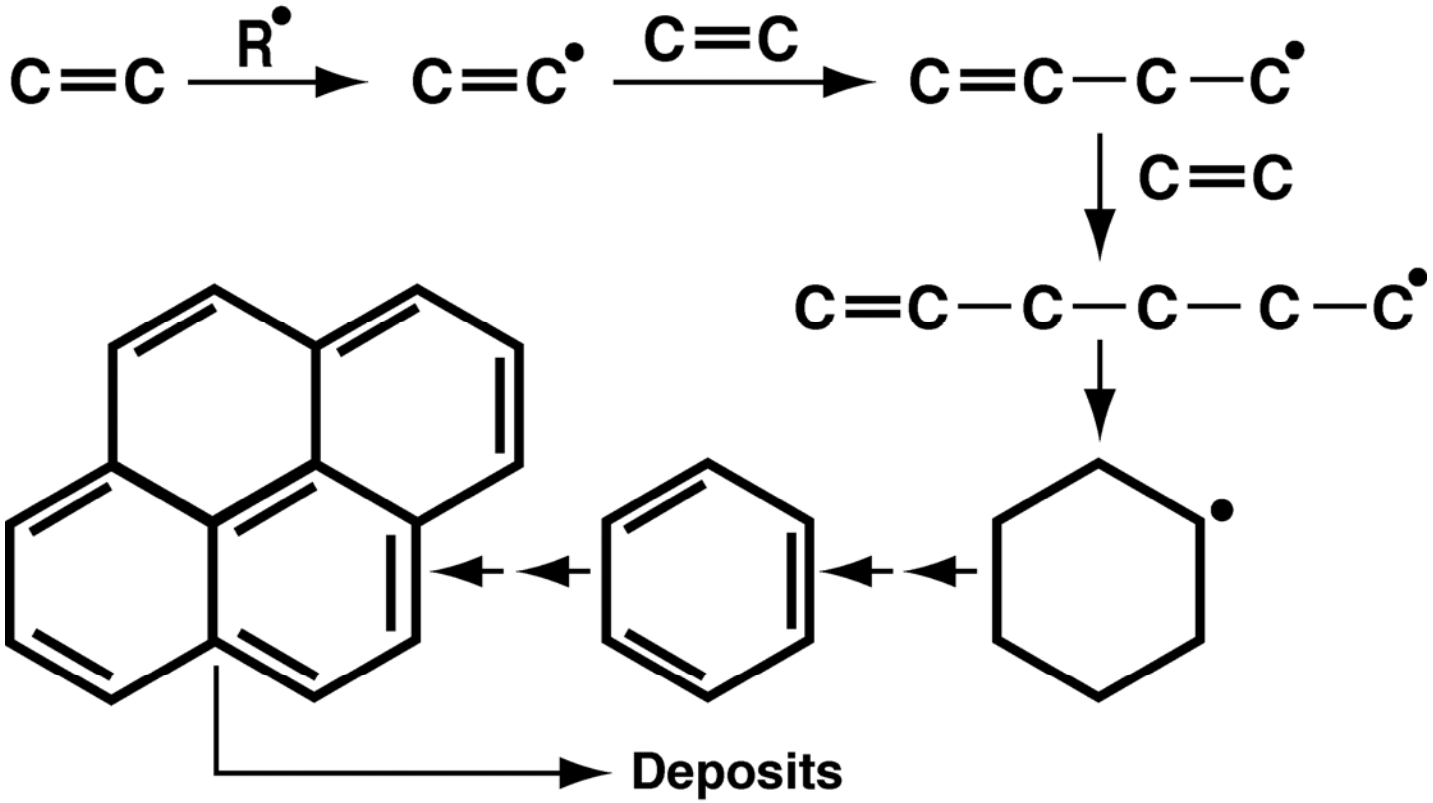
Small olefins in reformate gas can lead to gas-phase molecular-weight growth and carbon deposits



A. Dean, Colorado School of Mines

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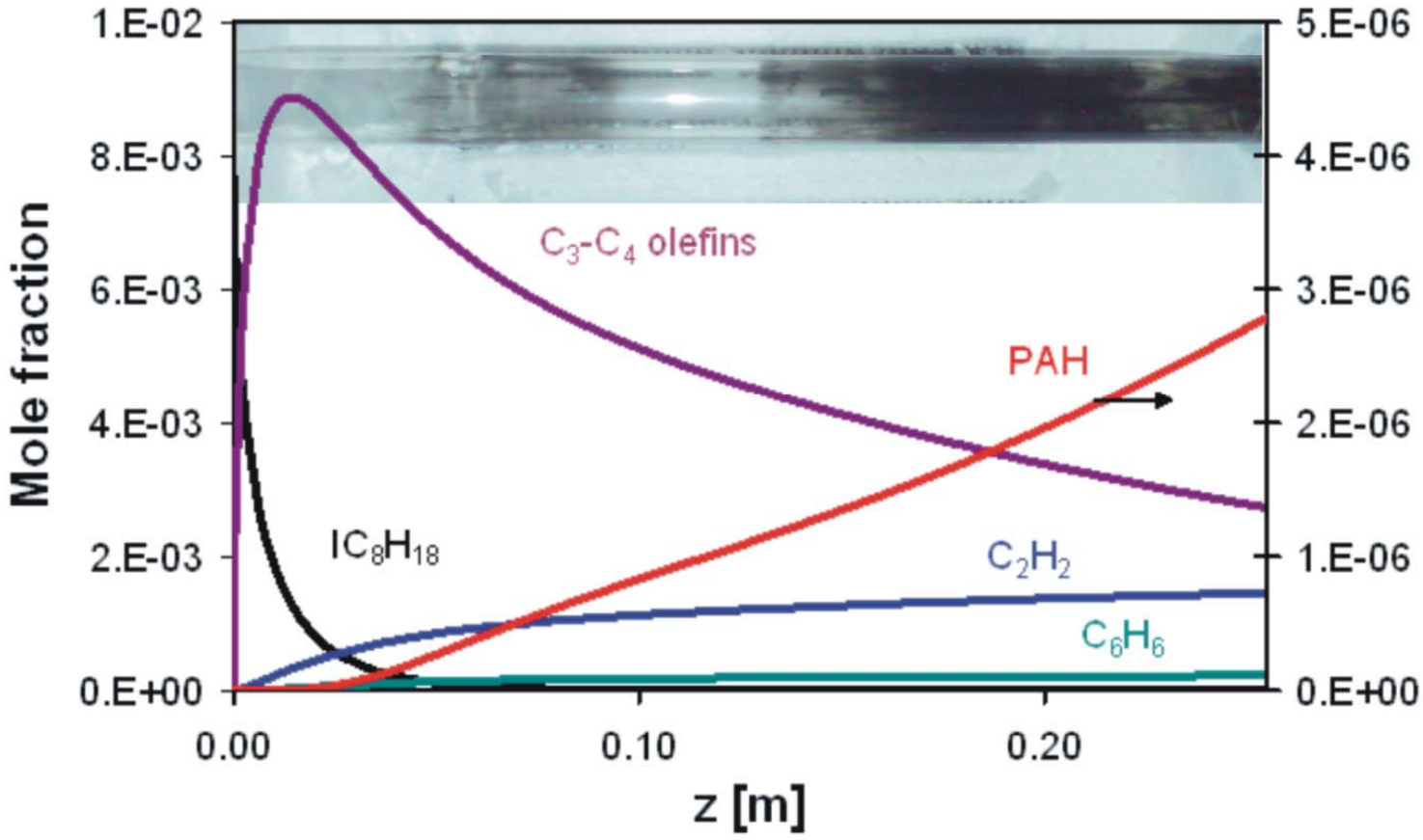
Coke formation in partial oxidation of iso-octane: Carbon distribution along the reactor (w/o catalyst)



C/O = 1.6, 1108 K, 6 SLPM. C_3-C_4 olefins contain 1,2-propadiene, propene, propyne, n-butene (1-buten, 2-butene), iso-butene, 1,3-butadiene; PAH contains naphthalene, anthracene, pyrene. Embedded photo shows the tubular quartz reactor after operation.

T. Kaltschmitt, L. Maier, O. Deutschmann. Proceedings of the Combustion Institute 33 (2011) 3177

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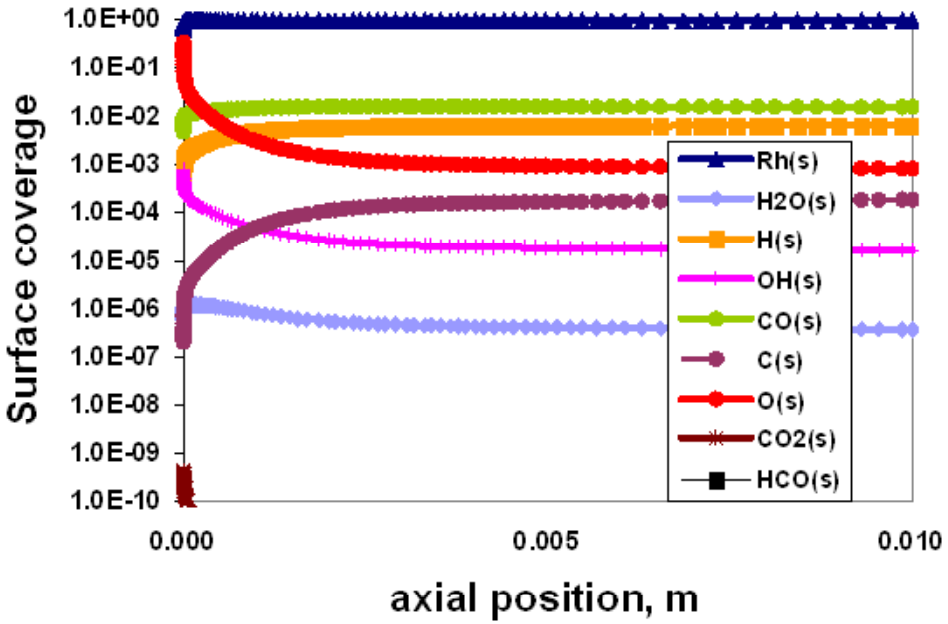
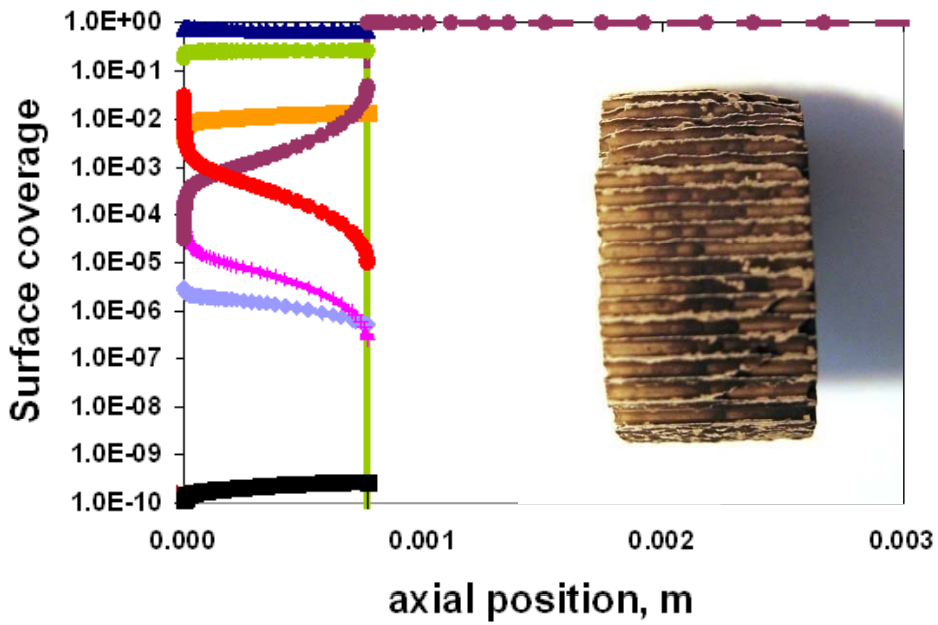
CPOX of i-octane: Coke formation on the downstream section of the catalyst at rich conditions

Numerically predicted surface coverage along the monolithic catalyst

C/O = 0.8



C/O = 1.2



M. Hartmann, L. Maier, O. Deutschmann, Combust. Flame 157 (2010) 1771

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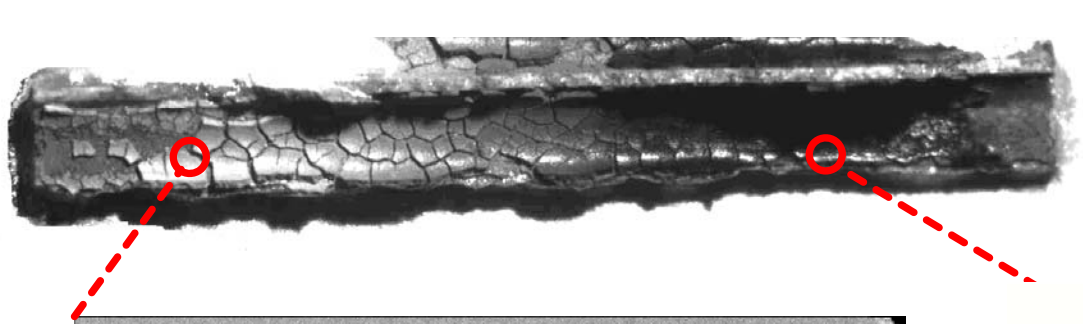
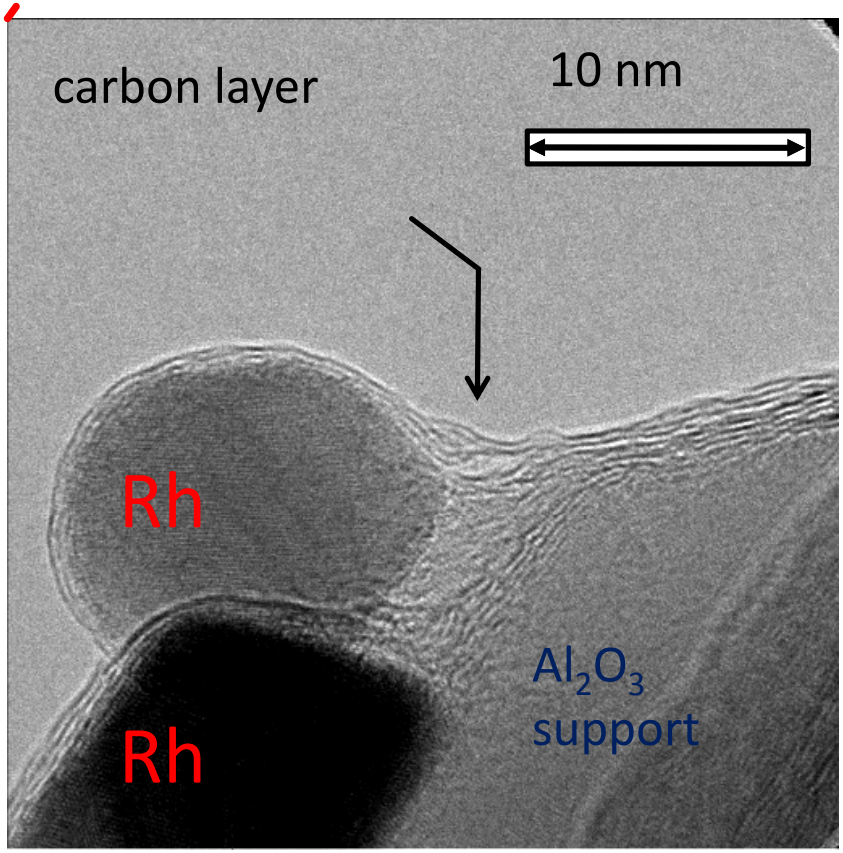
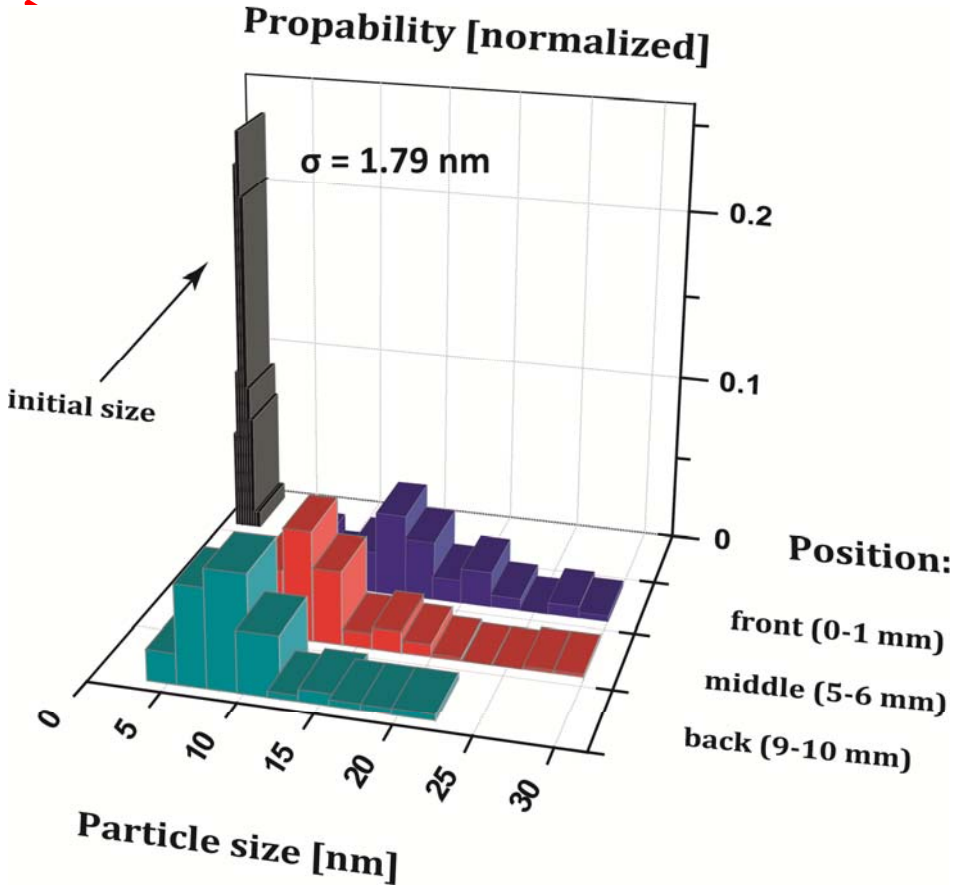
Catalyst deactivation by coking: TEM-Images of the Rh particles



d = 0.6 mm





M. Hartmann, B. Reznik, O. Deutschmann, 2010, to be published

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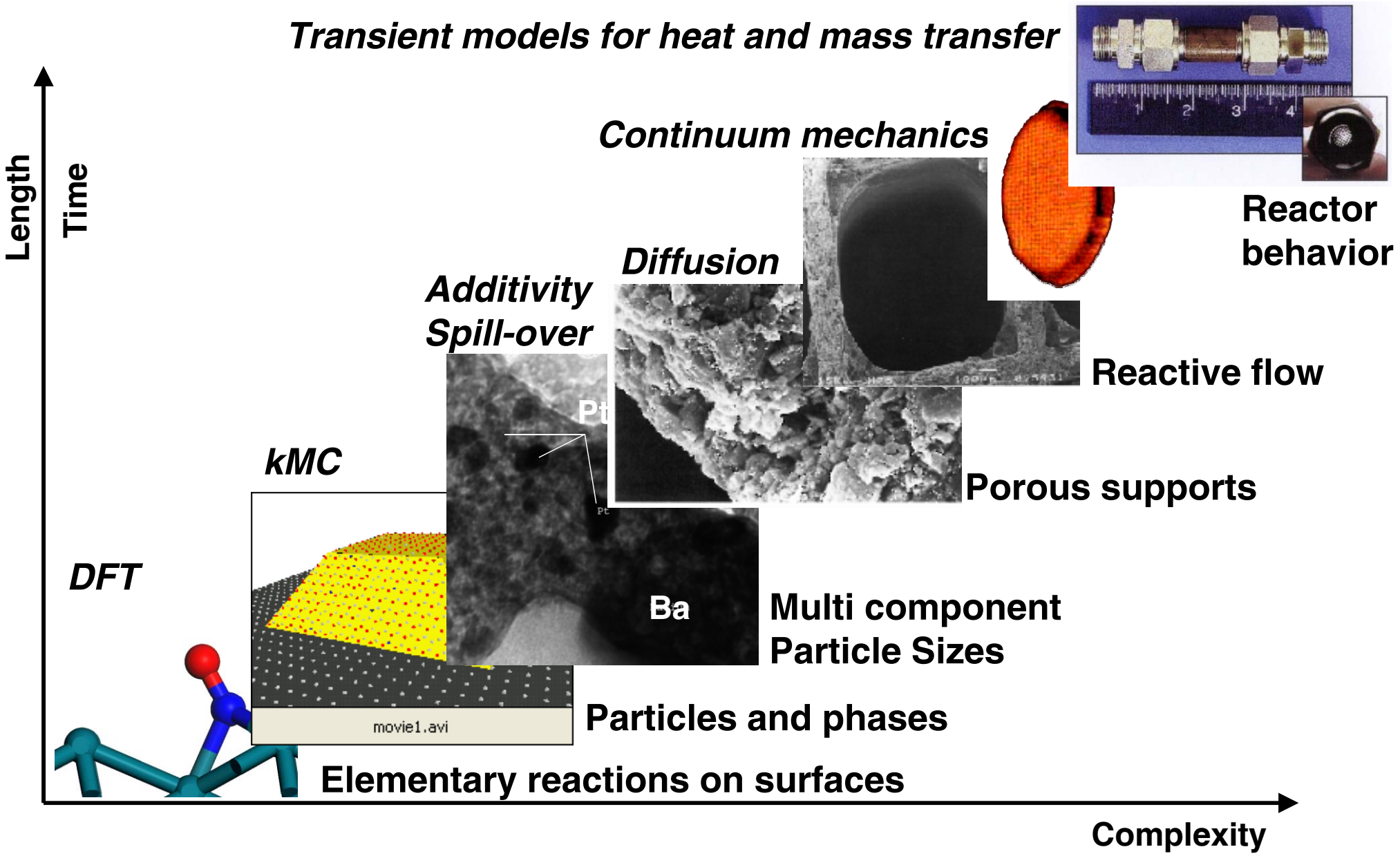
Hierarchical modeling in catalytic combustion: Reactor simulation from first principles



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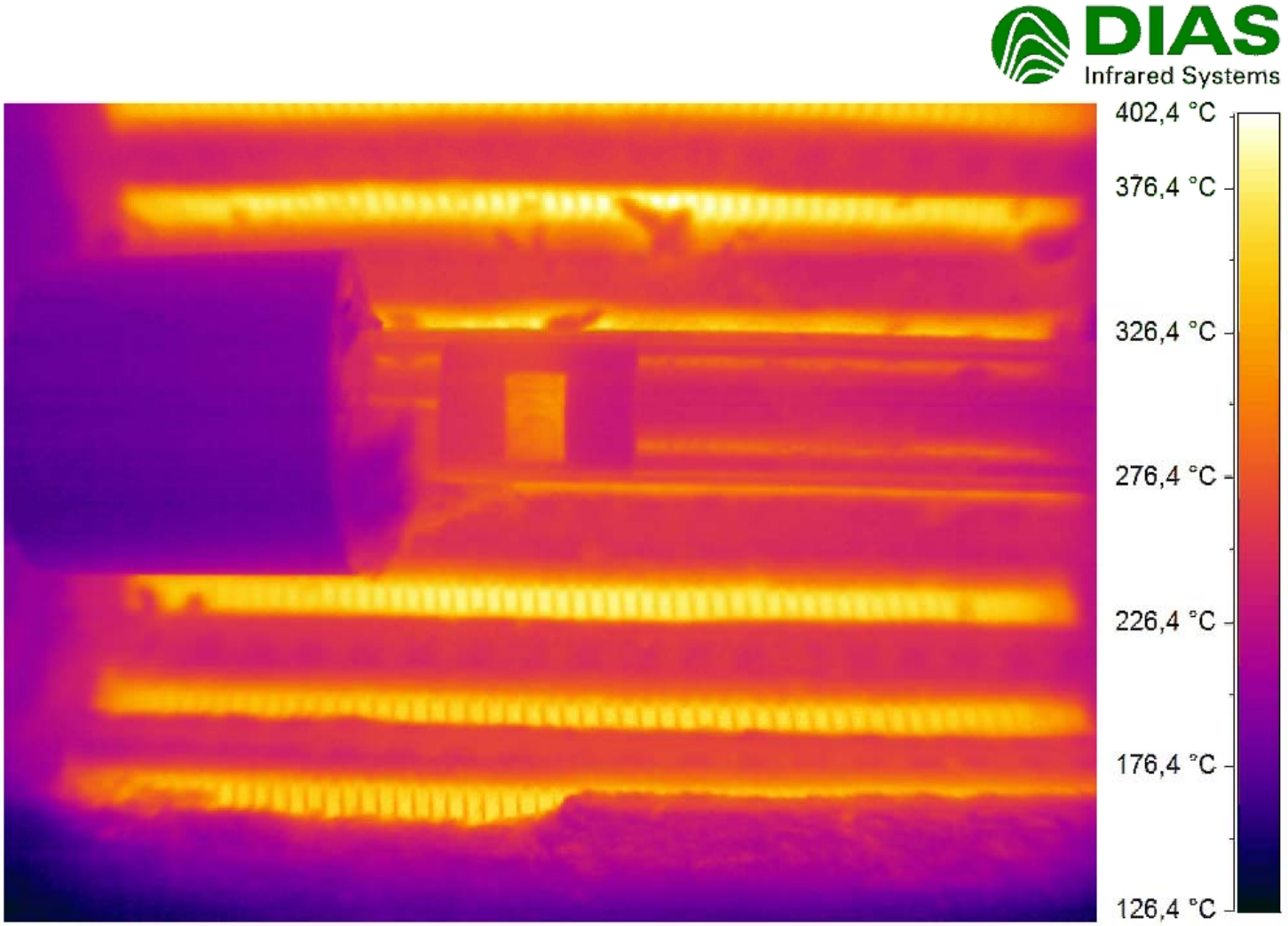
Schleicher-Stiftung
Baden-Baden

Muito obrigado!



Light-off of CPOX of gasoline

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