What happens inside?
Spatial resolution techniques for catalytic reactors

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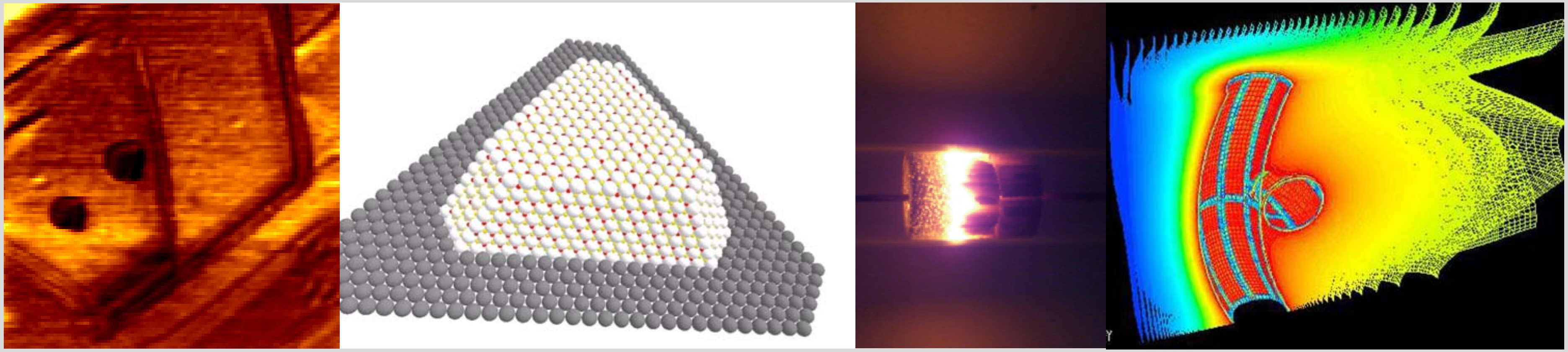
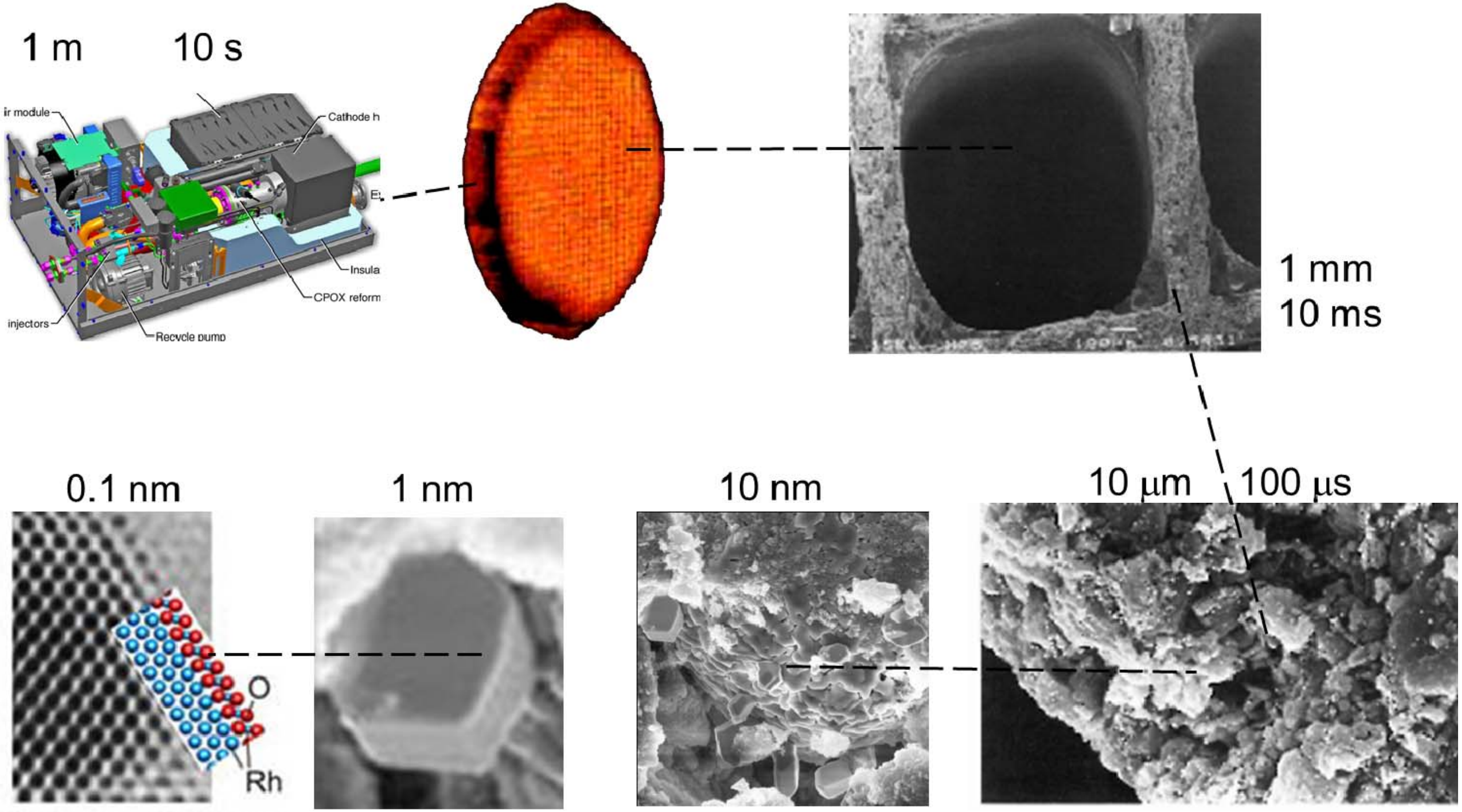
Institute for Chemical Technology and Polymer Chemistry (ITCP)

Institute for Catalysis Research and Technology (IKFT)



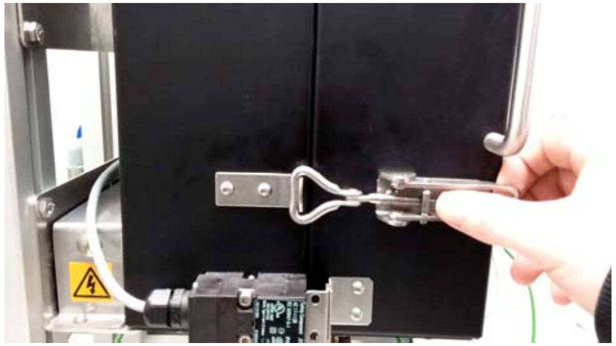
Challenge: Multi-scale interaction of physical and chemical processes: From 10^{-10} m and 10^{-13} s to 1 m and 10 s



Spatial resolution techniques for catalytic reactors
Motivation

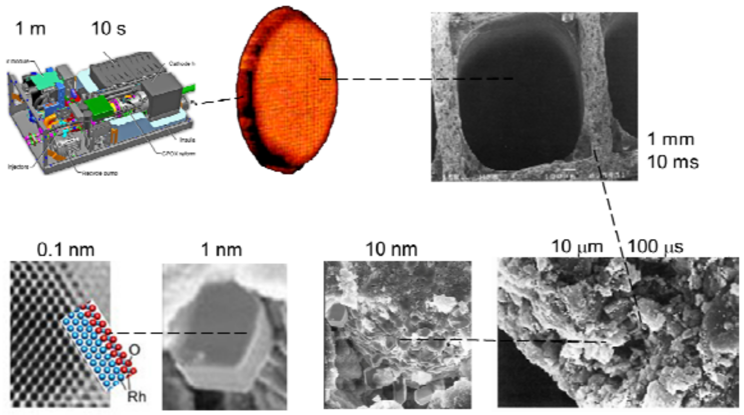
- Understanding and optimization of catalytic reactors demands the knowledge of

What happens inside?



- Approaches discussed here: Monitoring spatial and temporal profiles
  - Experimental observation
  - Numerical simulation

Spatial resolution techniques for catalytic reactors
Outline



- Motivation
- On the catalyst
  - Catalytic surface
  - Catalyst particle
  - Catalyst and support
- In the gas-phase
  - Reaction sequence
  - Kinetics, diffusion, and convection
  - Structured reactors
  - Fluidized beds
  - Packed beds
- Multi-phase systems

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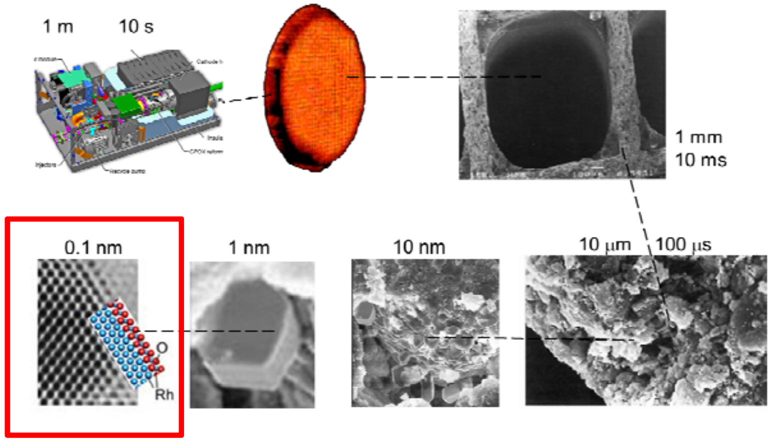
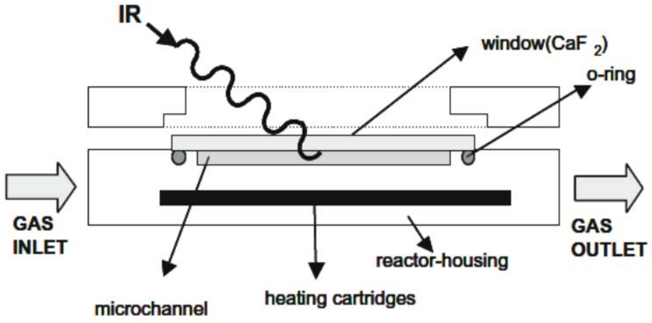
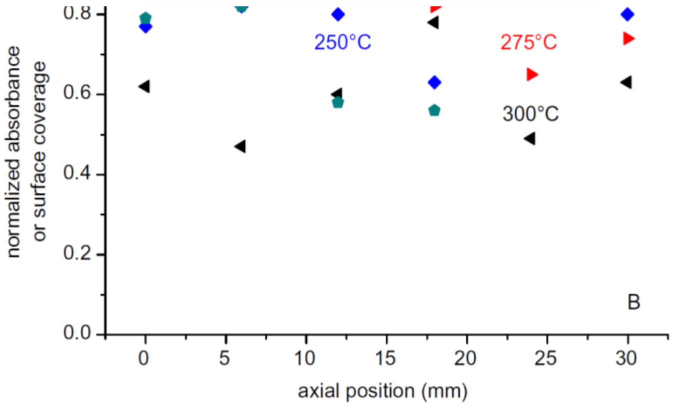


Spatially resolved surface coverage by DRIFTS and Raman analysis

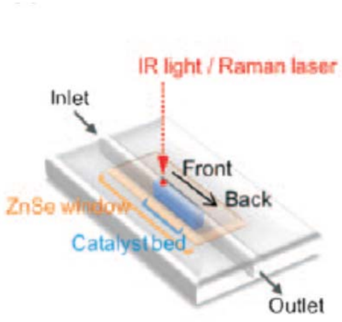
CO oxidation over Pt fixed bed reactor

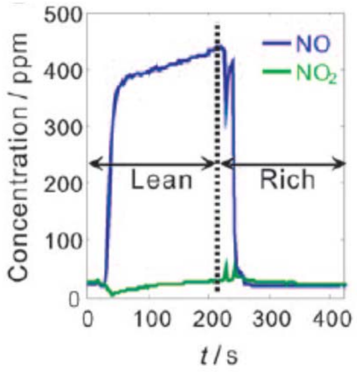


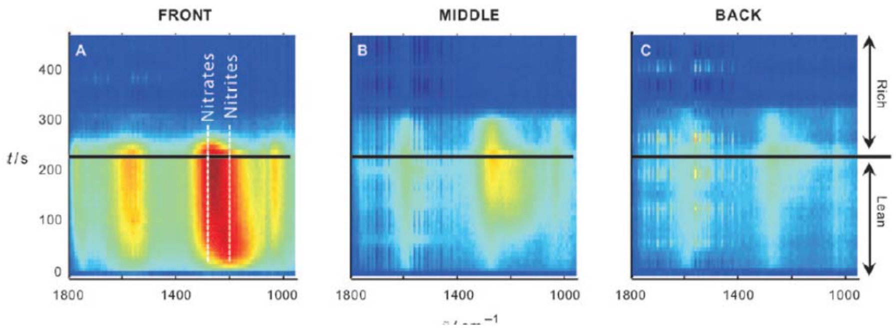


C. Daniel, M-O. Clarté, S.-P. Teh, O. Thinon, H. Provendier, A.C. Van Veen, B.J. Beccard, Y. Schuurman, C. Mirodatos. J. Catal. 272 (2010) 55

NOx storage reduction catalyst



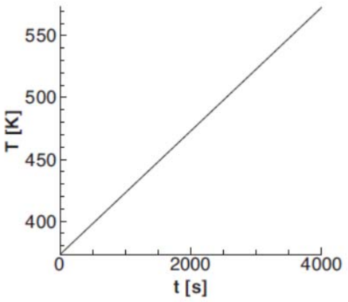


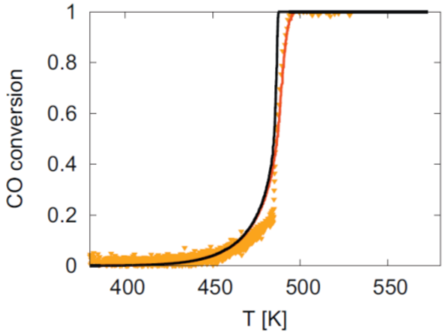


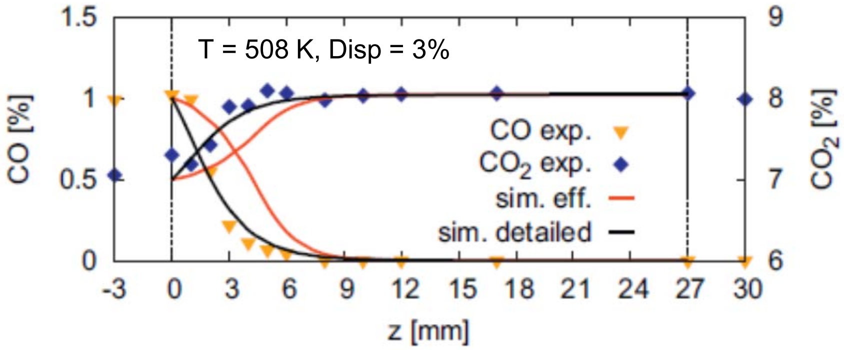
A. Urakawa, N. Maeda, A. Baiker. Angew. Chem. Int. Ed. 47 (2008) 9256.

Modeling of DOC light-off in laboratory test bench: Temporal variation of axial profiles

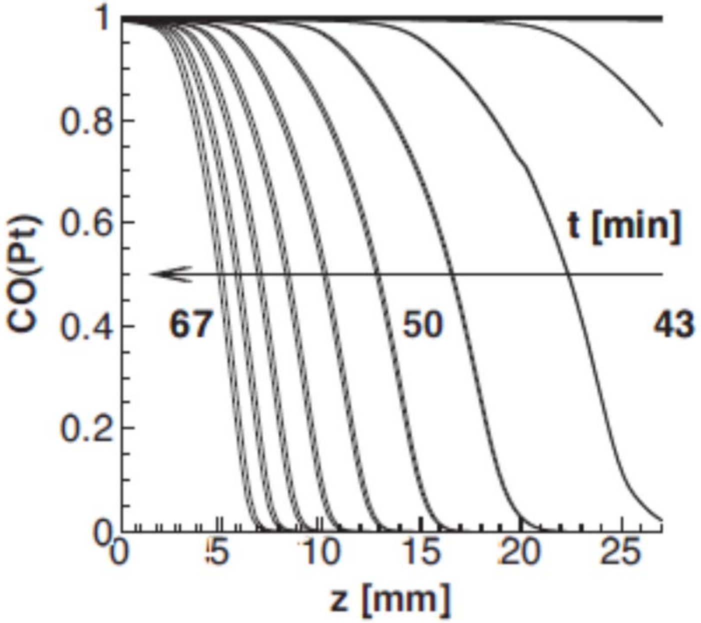
$$CO + 1/2\ O_2 \xrightarrow{Pt} CO_2$$





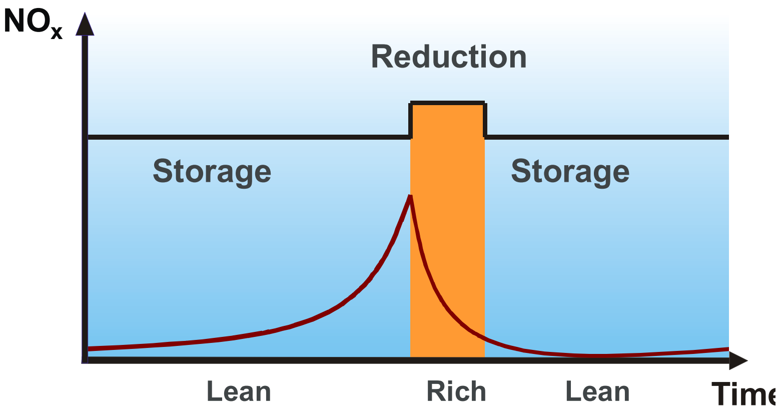


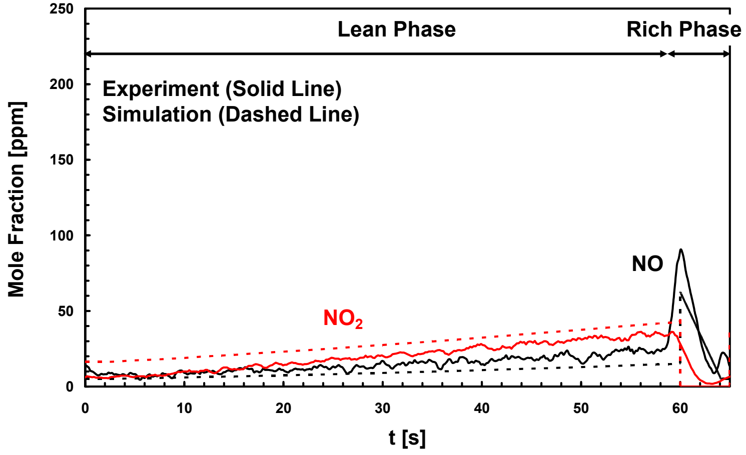
Reaction			A [mol, cm, s] / S^0	β	E_a [kJ/mol]
O_2 + (Pt)	⟶	O_2(Pt)	5.000×10^{-2}	0.000	0.00
O_2(Pt)	⟶	O_2 + (Pt)	5.243×10^{11}	−0.069	19.573
O_2(Pt) + (Pt)	⟶	O(Pt) + O(Pt)	8.325×10^{18}	0.000	39.933
O(Pt) + O(Pt)	⟶	O_2(Pt) + (Pt)	4.444×10^{21}	0.000	264.067 $-88.2 \times \Theta_O$
CO + (Pt)	⟶	CO(Pt)	8.400×10^{-1}	0.000	0.000
CO(Pt)	⟶	CO + (Pt)	7.635×10^{12}	−0.139	143.145 $-29.3 \times \Theta_{CO}$
CO_2 + (Pt)	⟶	CO_2(Pt)	3.193×10^{-3}	−0.035	2.686
CO_2(Pt)	⟶	CO_2 + (Pt)	1.894×10^{10}	0.139	21.855
CO(Pt) + O_2(Pt)	⟶	CO_2(Pt) + O(Pt)	4.124×10^{18}	0.069	9.494 $+44.1 \times \Theta_O$
CO_2(Pt) + O(Pt)	⟶	CO(Pt) + O_2(Pt)	2.910×10^{23}	−0.069	272.506 $+29.3 \times \Theta_{CO}$
CO(Pt) + O(Pt)	⟶	CO_2(Pt) + (Pt)	4.764×10^{18}	0.069	101.361 $-29.3 \times \Theta_{CO}$
CO_2(Pt) + (Pt)	⟶	CO(Pt) + O(Pt)	6.297×10^{20}	−0.069	140.239 $+44.1 \times \Theta_O$

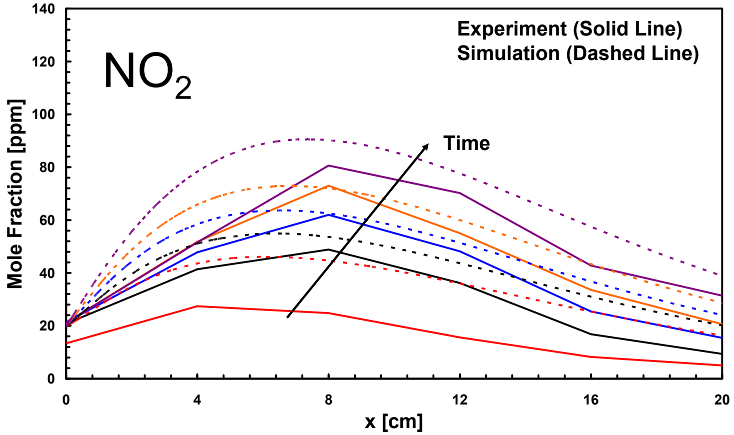


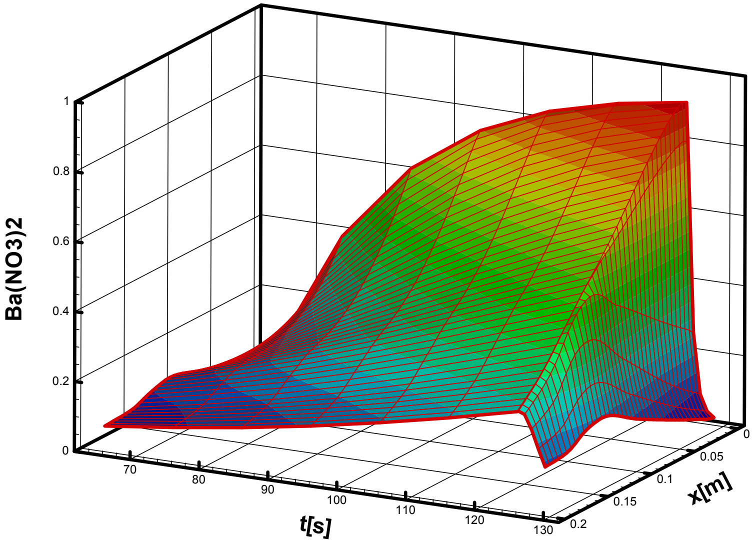
D. Chan, S. Tischer, J. Heck, C. Diehm, O. Deutschmann. Appl. Catal. B: Env. 156–157 (2014) 153.

Modeling NOx storage reduction catalyst
Spatial resolved axial profiles









Modeling: J. Koop, O. Deutschmann. SAE 2007-01-1142.
Experiment: V. Schmeißer, J. Perez, U. Tuttlies, G. Eigenberger, Top. Catal. 42 (2007) 15

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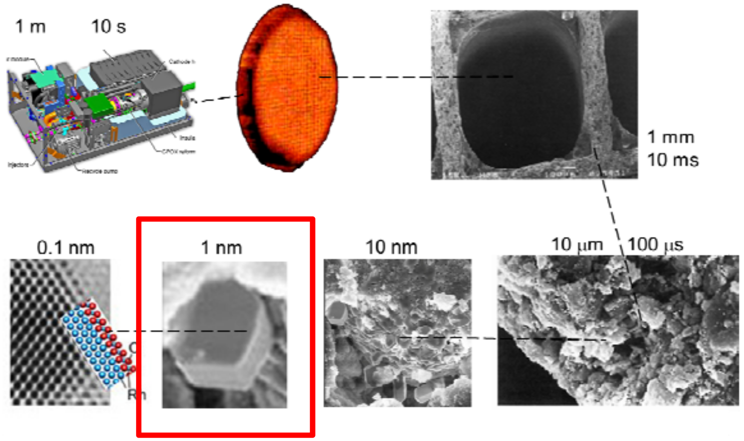
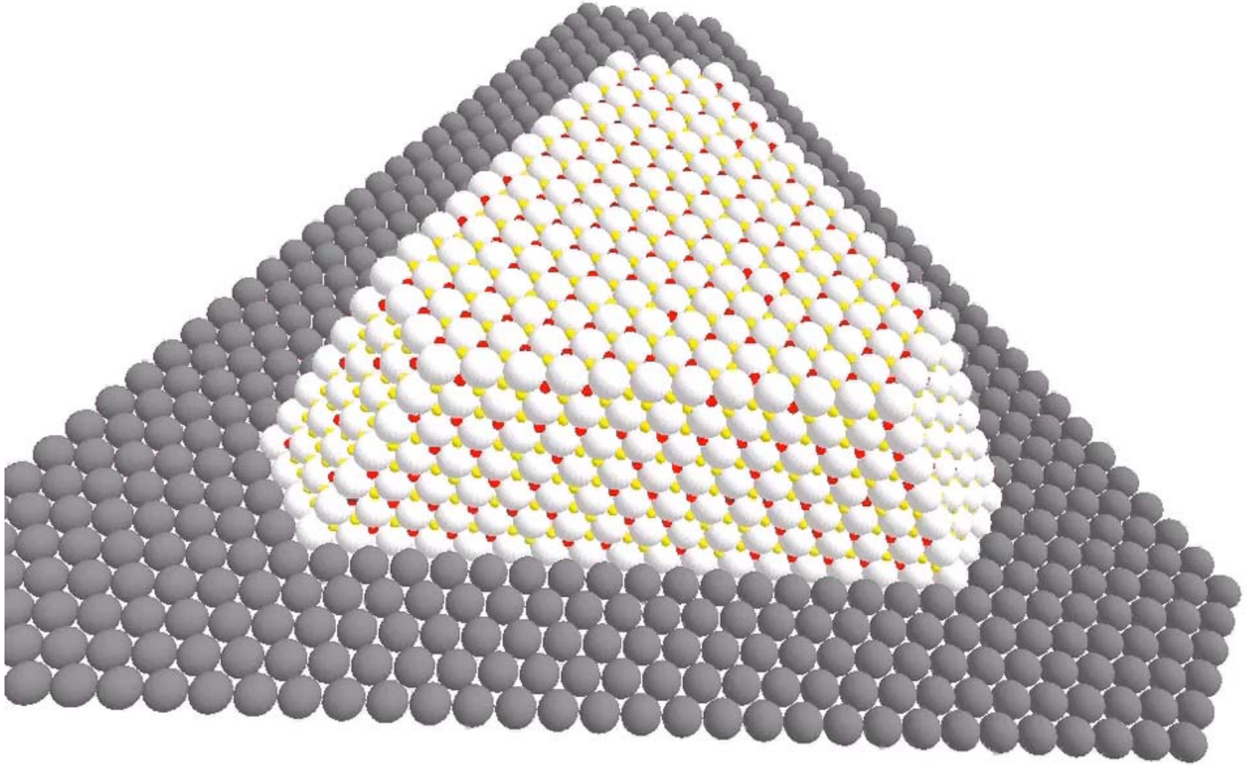


Kinetic Monte Carlo Simulation of surface reactions and diffusion: CO oxidation on Pt nanoperticle



$2\ CO + O_2 \rightarrow 2\ CO_2$

CO: blue   O: red

Catalyst atom (Pt): white

Washcoat molecule (Al_2O_3): grey

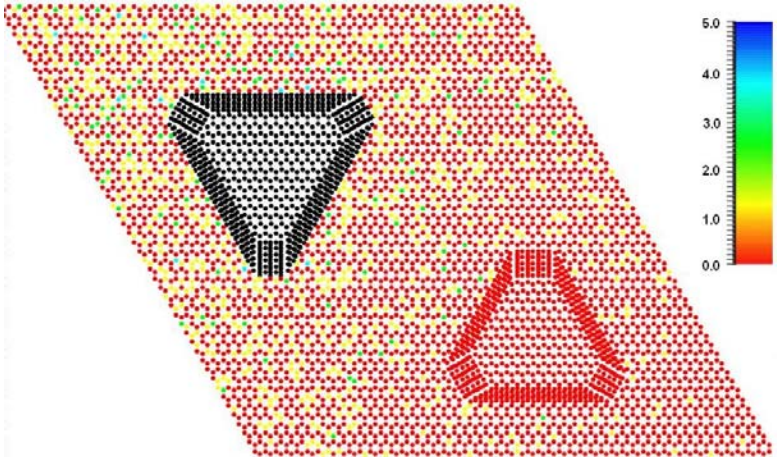
Adsorption sites: yellow

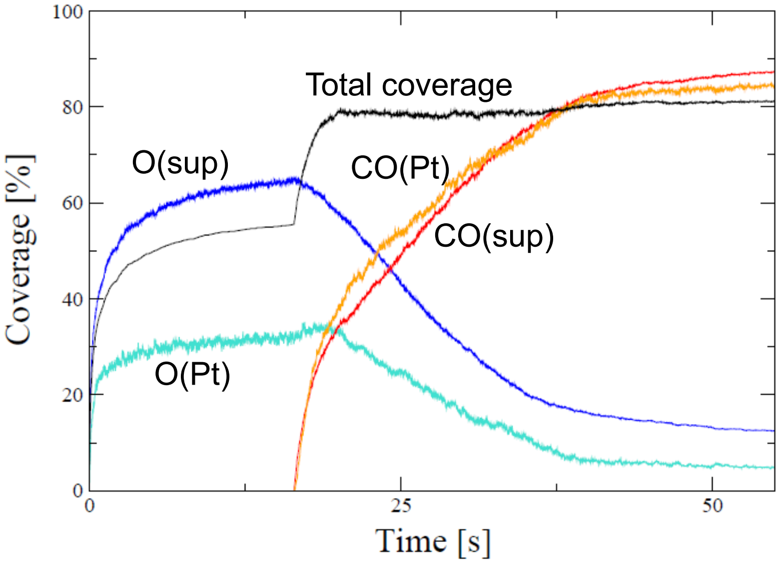
L. Kunz, F.M. Kuhn, O. Deutschmann. Journal of Chemical Physics 143 (2015) 044108.

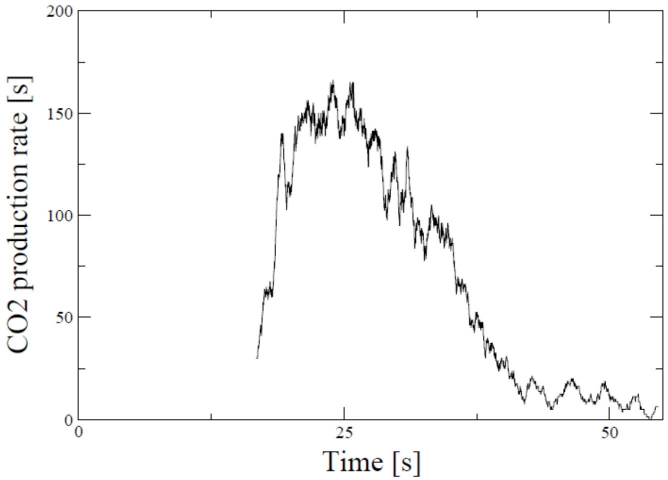
Kinetic Monte Carlo Simulation of surface reactions and diffusion with MoCKa: CO oxidation on Pt nanoparticle

Results of simulations:

- coverages over time on each facet
- reaction rates of each process
- number of times each process was used





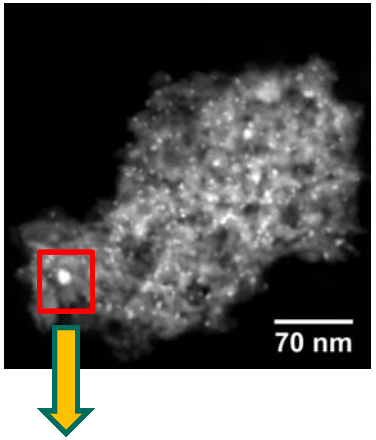


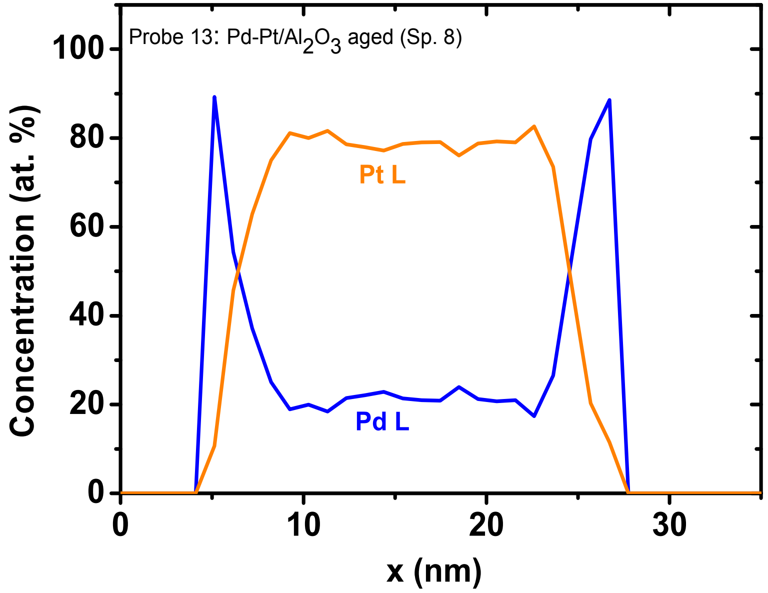
L. Kunz, F.M. Kuhn, O. Deutschmann. Journal of Chemical Physics 143 (2015) 044108.

Spatial resolution of the catalytic particle
Characterization by TEM and EDX after 100 h TOS

$$CH_4 + 2\ O_2 \xrightarrow{Pd/Pt_{0.1}} CO_2 + 2\ H_2O$$

- **Most particles d < 5 nm**
  - Homogenous alloy ($Pd_{100}Pt_0$ - $Pd_{89\pm5}Pt_{11\pm2}$)
- **Some particles d ≅ 10 nm**
  - Homogenous Alloy, higher Pt-content
- **Few large particles d > 30 nm**
  - Homogenous alloy
  - High Pt content
  - Formation of core-shell structure after 100 h, 1000 ppm CH_4, 10% O_2





A. T. Gremminger, H. W. Pereira de Carvalho, R. Popescu, J.-D. Grunwaldt, O. Deutschmann. Catalysis Today (2015) DOI 10.1016/j.cattod.2015.01.034

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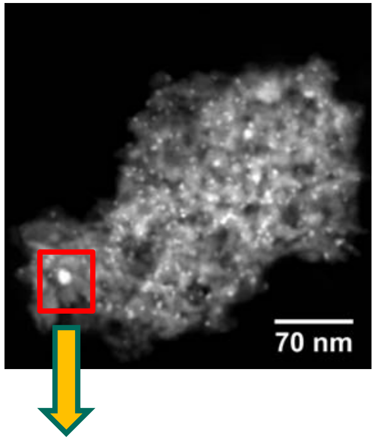
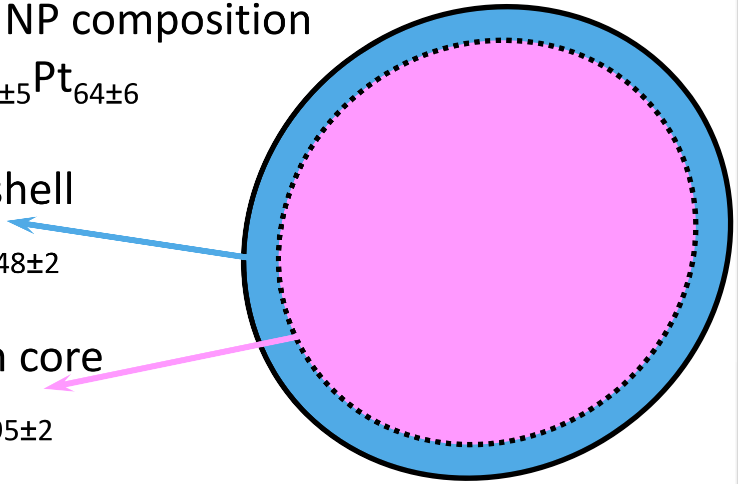


- Total NP composition $Pd_{36\pm5}Pt_{64\pm6}$



~ 3 nm shell $Pd_{52\pm4}Pt_{48\pm2}$

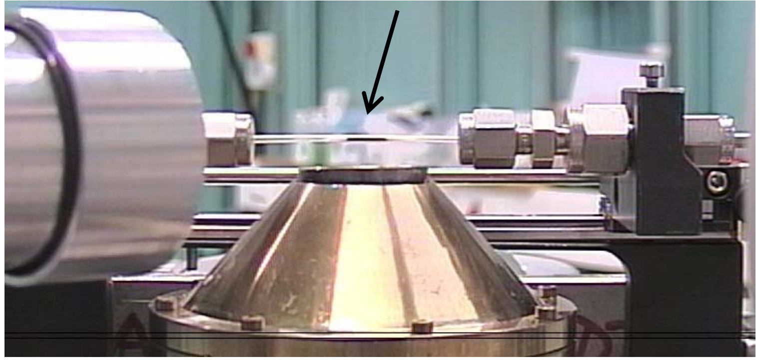
~ 22 nm core $Pd_{5\pm3}Pt_{95\pm2}$

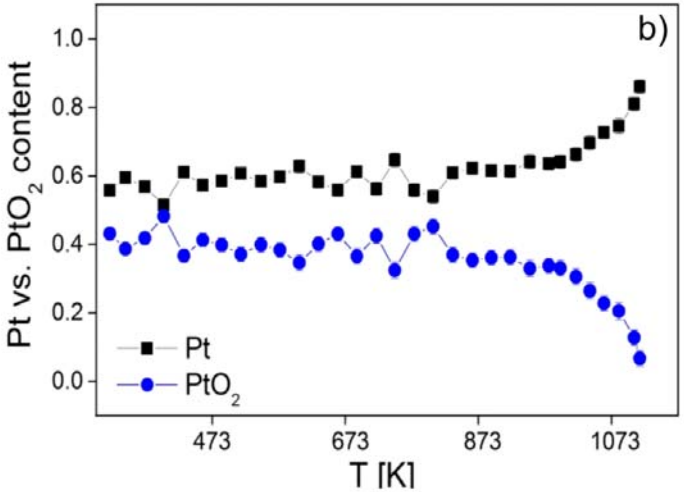
A. T. Gremminger, H. W. Pereira de Carvalho, R. Popescu, J.-D. Grunwaldt, O. Deutschmann. Catalysis Today (2015) DOI 10.1016/j.cattod.2015.01.034

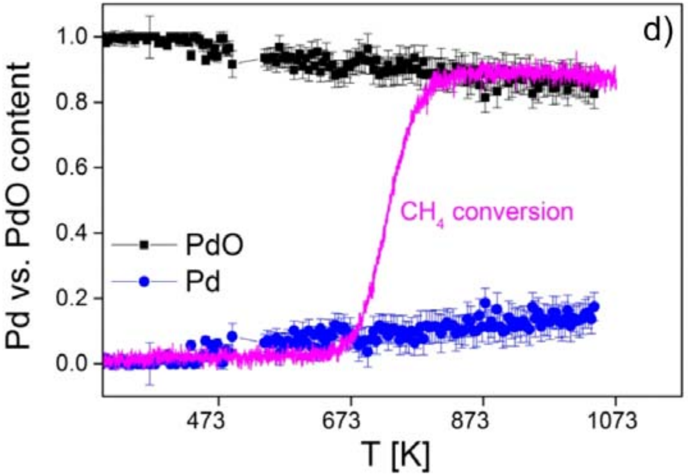
Oxidation state of the catalytic particle
Characterization by XANES

$$CH_4 + 2\,O_2 \xrightarrow{Pd/Pt_{0.1}} CO_2 + 2\,H_2O$$

Micro-reactor for X-ray spectroscopy







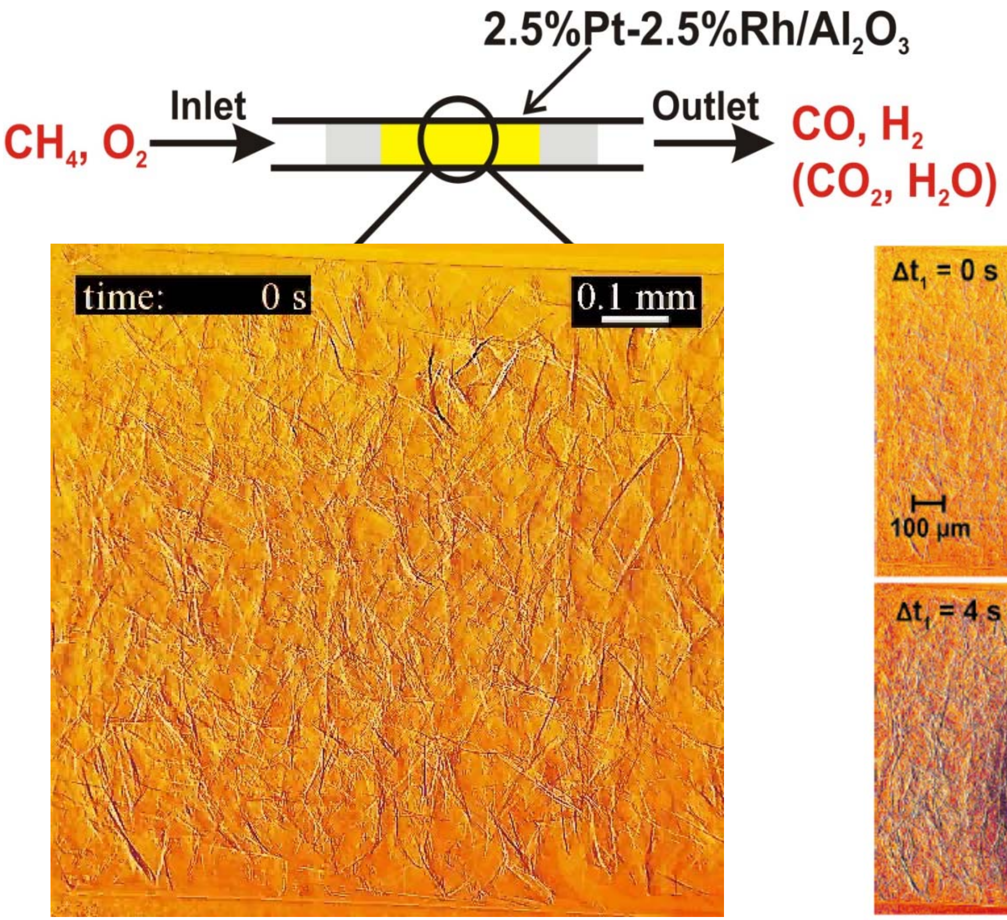
- PdO domintnt species in fresh and deactivated catalyst
- PdO stable under reaction conditions up to ~800 °C
- Pt present as metallic Pt and PtO_2 or PtO
- Reduction of PtO_x species at higher temperature

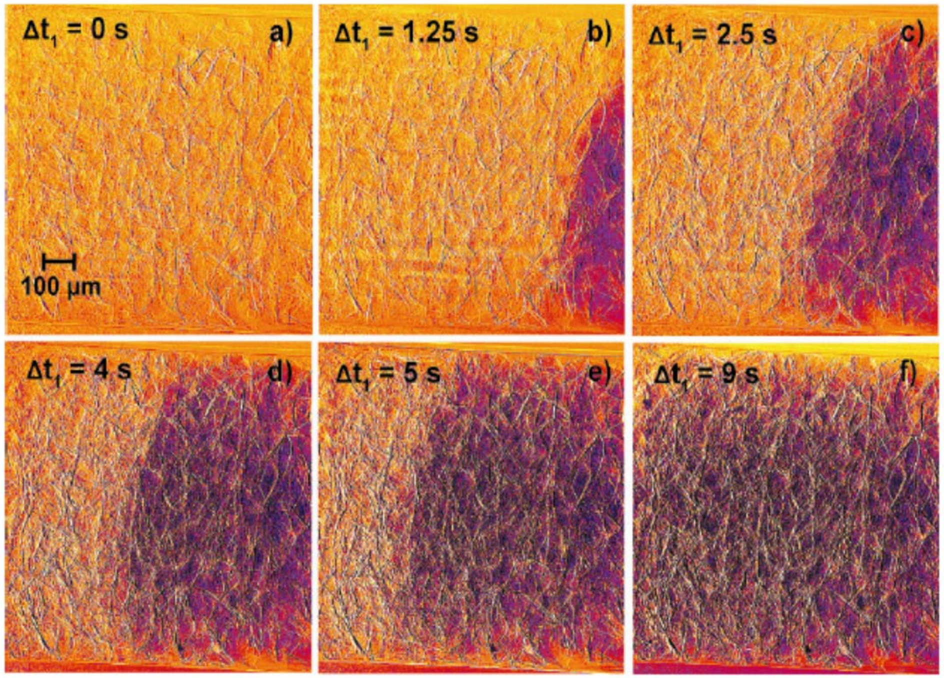
A. T. Gremminger, H. W. Pereira de Carvalho, R. Popescu, J.-D. Grunwaldt, O. Deutschmann. Catalysis Today (2015) DOI 10.1016/j.cattod.2015.01.034

Oxidation state of the catalytic particles spatially resolved: Transients in oxidation states during ignition

$$CH_4 + {}^1/_2\ O_2 \xrightarrow{\text{Pt/Rh}} CO + 2\ H_2$$

6%CH_4/3%O_2/He, ca. 320 °C





B. Kimmerle, J.-D. Grunwaldt, A. Baiker, P. Glatzel, P. Boye, S. Stephan, C.G. Schroer, Journal of Physical Chemistry C, 113 (2009) 3037.

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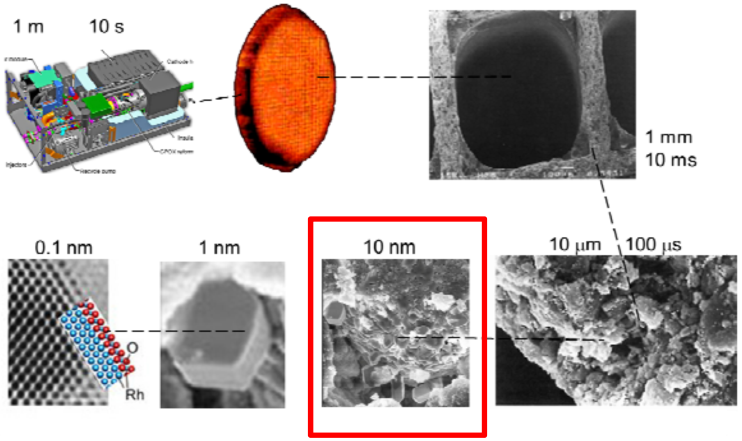
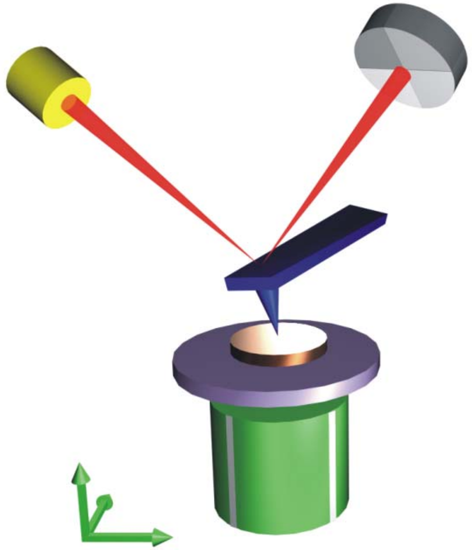
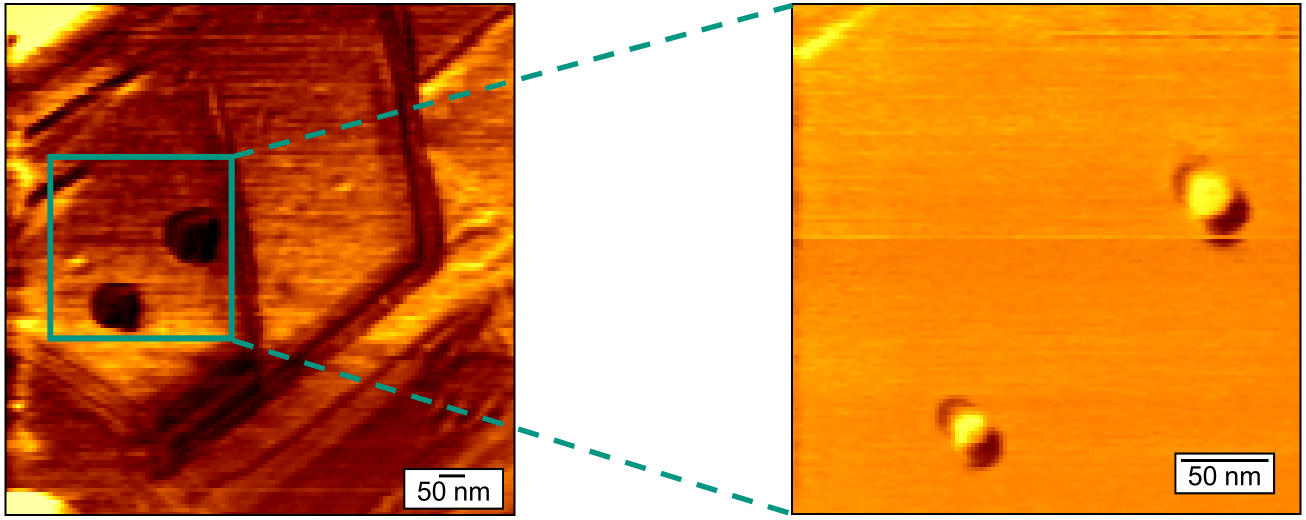


Coke formation in steam reforming of natural gas: Characterization by Atomic Force Microscopy (AFM)

$$CH_4 + H_2O \xrightarrow{Rh/Al2O3} CO + 3\ H_2$$





Scan 2 OFM

Scan 24 OFM

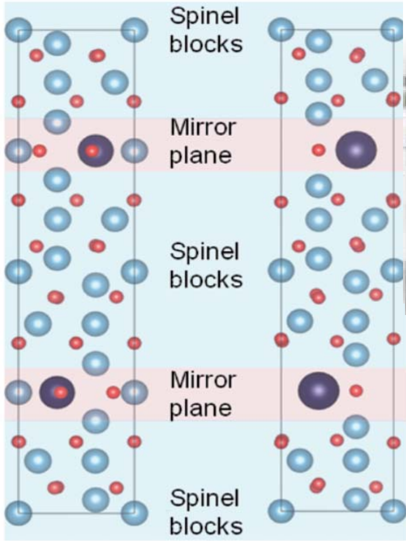
- After multiple scans: Change in the friction of the particles relatively to the substrate

→ Carbon is removed by the AFM-tip

C. Essmann, M. Seipenbusch, T. Schimmel, O. Deutschmann. Z. Phys. Chem. 225 (2011) 1207

From the chemist’s lab to the industrial plant: Dry-reforming of methane

$CH_4 + CO_2 \rightarrow 2\ H_2 + 2\ CO$




Cortesey of hte AG

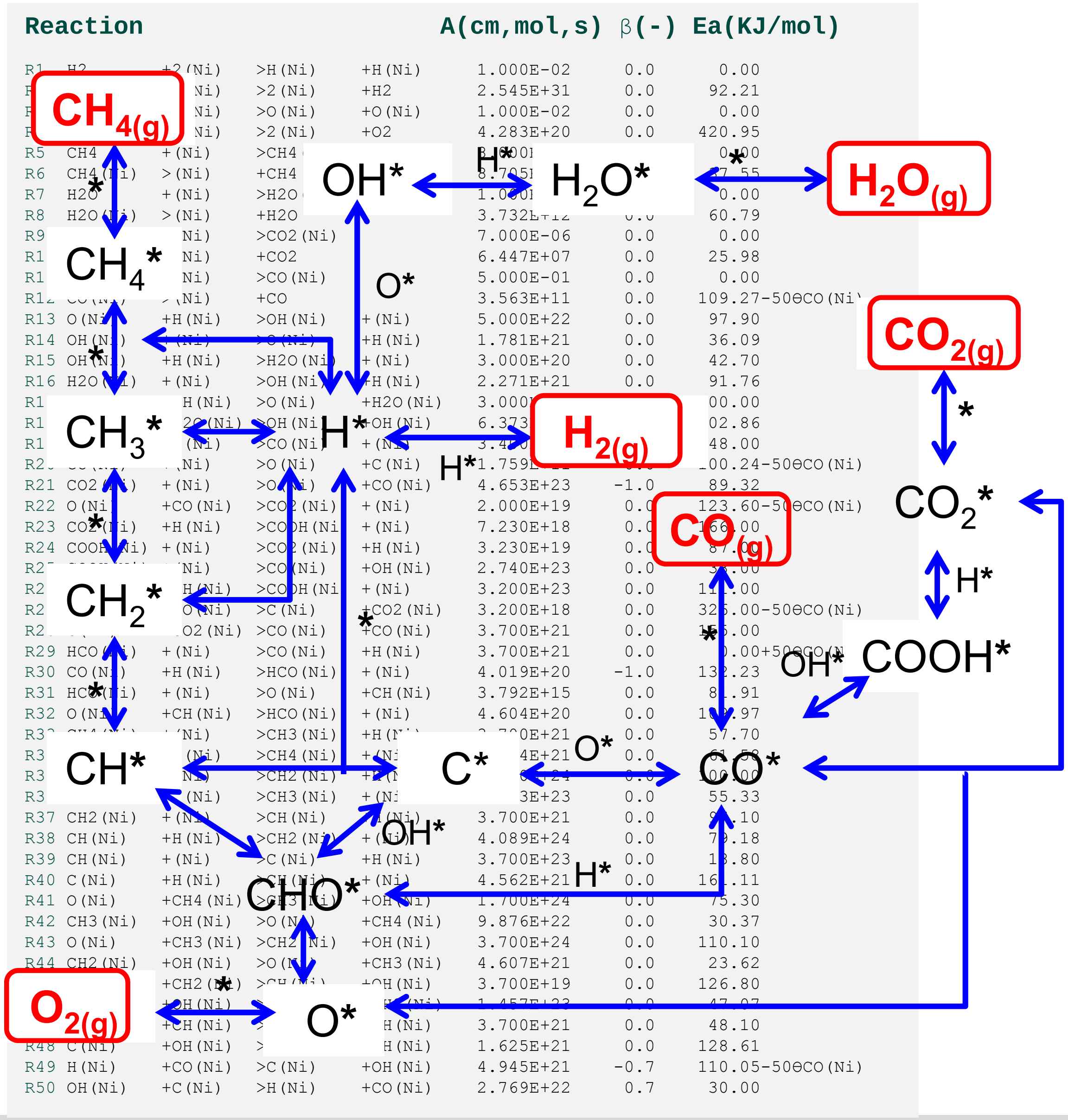

Cortesey of Linde AG

T. Roussière, L. Schulz, K. M. Schelkle, G. Wasserschaff, A. Milanov, E. Schwab, O. Deutschmann, A. Jentys, J. Lercher, S. A. Schunk. ChemCatChem 6 (2014) 1447.

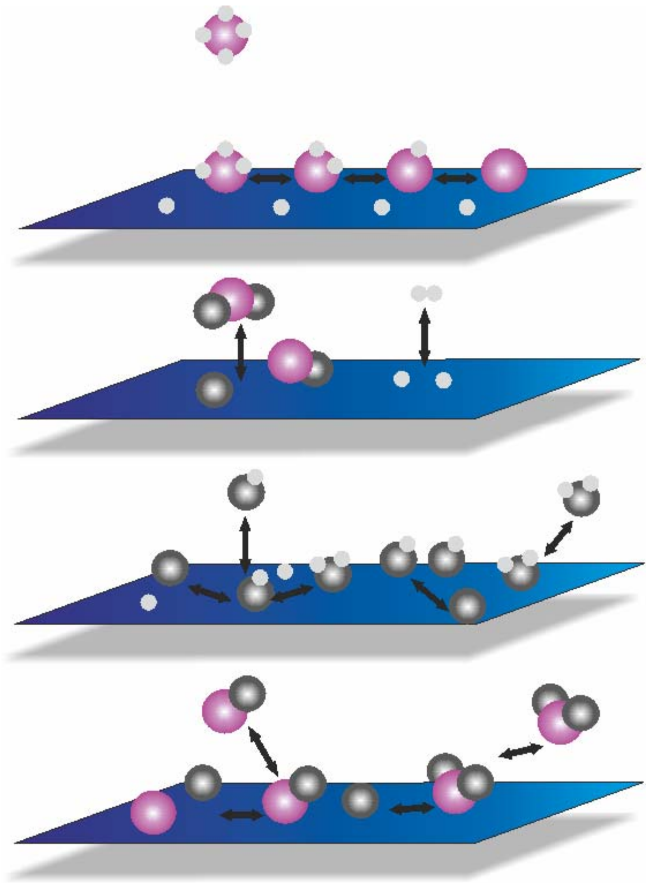
Bundesministerium
für Wirtschaft
und Technologie

DryRef: FKZ 0327856

Micro kinetic model for conversion of methane over Ni

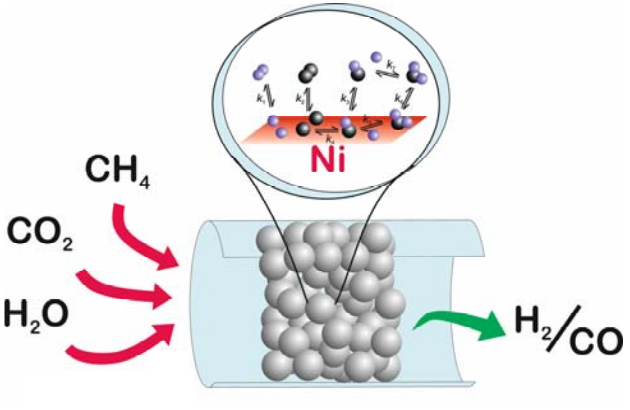


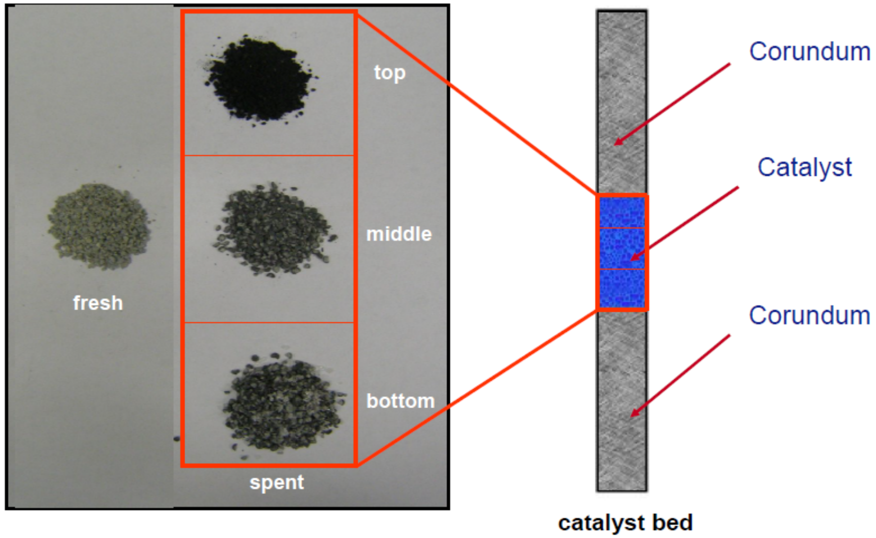
Reaction					A(cm,mol,s)	β(-)	Ea(KJ/mol)
R1	H2	+2(Ni)	>H(Ni)	+H(Ni)	1.000E-02	0.0	0.00
[illegible]	[illegible]	Ni)	>2(Ni)	+H2	2.545E+31	0.0	92.21
[illegible]	[illegible]	Ni)	>O(Ni)	+O(Ni)	1.000E-02	0.0	0.00
[illegible]	[illegible]	Ni)	>2(Ni)	+O2	4.283E+20	0.0	420.95
R5	CH4	+(Ni)	>CH4	[illegible]	[illegible]	[illegible]	0.00
R6	CH4(Ni)	>(Ni)	+CH4	[illegible]	8.705[illegible]	[illegible]	[illegible]7.55
R7	H2O	+(Ni)	>H2O	[illegible]	1.000[illegible]	[illegible]	0.00
R8	H2O(Ni)	>(Ni)	+H2O	[illegible]	3.732E+12	[illegible]	60.79
R9	[illegible]	Ni)	>CO2(Ni)		7.000E-06	0.0	0.00
R1	[illegible]	Ni)	+CO2		6.447E+07	0.0	25.98
R1	[illegible]	Ni)	>CO(Ni)		5.000E-01	0.0	0.00
R1	[illegible]	(Ni)	+CO		3.563E+11	0.0	109.27-50θCO(Ni)
R13	O(Ni)	+H(Ni)	>OH(Ni)	+(Ni)	5.000E+22	0.0	97.90
R14	OH(Ni)	[illegible]	[illegible]	+H(Ni)	1.781E+21	0.0	36.09
R15	OH(Ni)	+H(Ni)	>H2O(Ni)	+(Ni)	3.000E+20	0.0	42.70
R16	H2O(Ni)	+(Ni)	>OH(Ni)	+H(Ni)	2.271E+21	0.0	91.76
R1	[illegible]	H(Ni)	>O(Ni)	+H2O(Ni)	3.000[illegible]	[illegible]	[illegible]00.00
R1	[illegible]	2O(Ni)	>OH(Ni)	+OH(Ni)	6.373[illegible]	[illegible]	[illegible]02.86
R1	[illegible]	(Ni)	>CO(Ni)	+(Ni)	3.4[illegible]	[illegible]	48.00
R2	[illegible]	(Ni)	>O(Ni)	+C(Ni)	1.759[illegible]	[illegible]	[illegible]00.24-50θCO(Ni)
R21	CO2(Ni)	+(Ni)	>O(Ni)	+CO(Ni)	4.653E+23	-1.0	89.32
R22	O(Ni)	+CO(Ni)	>CO2(Ni)	+(Ni)	2.000E+19	0.0	123.60-50θCO(Ni)
R23	CO2(Ni)	+H(Ni)	>COOH(Ni	+(Ni)	7.230E+18	0.0	166.00
R24	COOH(Ni)	+(Ni)	>CO2(Ni)	+H(Ni)	3.230E+19	0.0	87.[illegible]
R2	[illegible]	(Ni)	>CO(Ni)	+OH(Ni)	2.740E+23	0.0	[illegible]
R2	[illegible]	H(Ni)	>COOH(Ni	+(Ni)	3.200E+23	0.0	1[illegible].00
R2	[illegible]	O(Ni)	>C(Ni)	+CO2(Ni)	3.200E+18	0.0	32[illegible].00-50θCO(Ni)
R2	[illegible]	O2(Ni)	>CO(Ni)	+CO(Ni)	3.700E+21	0.0	1[illegible]5.00
R29	HCO(Ni)	+(Ni)	>CO(Ni)	+H(Ni)	3.700E+21	0.0	[illegible].00+50θCO(Ni)
R30	CO(Ni)	+H(Ni)	>HCO(Ni)	+(Ni)	4.019E+20	-1.0	13[illegible].23
R31	HCO(Ni)	+(Ni)	>O(Ni)	+CH(Ni)	3.792E+15	0.0	8[illegible].91
R32	O(Ni)	+CH(Ni)	>HCO(Ni)	+(Ni)	4.604E+20	0.0	1[illegible].97
R3	[illegible]	(Ni)	>CH3(Ni)	+H(Ni)	[illegible]0E+21	0.0	57.70
R3	[illegible]	(Ni)	>CH4(Ni)	+(Ni	[illegible]4E+21	0.0	[illegible]
R3	[illegible]	Ni)	>CH2(Ni)	[illegible]	[illegible]	[illegible]	[illegible]
R3	[illegible]	(Ni)	>CH3(Ni)	+(Ni	[illegible]3E+23	0.0	55.33
R37	CH2(Ni)	+(Ni)	>CH(Ni)	[illegible]	3.700E+21	0.0	[illegible].10
R38	CH(Ni)	+H(Ni)	>CH2(Ni)	+(Ni)	4.089E+24	0.0	7[illegible].18
R39	CH(Ni)	+(Ni)	>C(Ni)	+H(Ni)	3.700E+23	0.0	1[illegible].80
R40	C(Ni)	+H(Ni)	[illegible]	+(Ni)	4.562E+21	0.0	16[illegible].11
R41	O(Ni)	+CH4(Ni)	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
R42	CH3(Ni)	+OH(Ni)	[illegible]	+CH4(Ni)	9.876E+22	0.0	30.37
R43	O(Ni)	+CH3(Ni)	[illegible]	+OH(Ni)	3.700E+24	0.0	110.10
R44	CH2(Ni)	+OH(Ni)	[illegible]	+CH3(Ni)	4.607E+21	0.0	23.62
[illegible]	[illegible]	+CH2(Ni)	[illegible]	[illegible]	3.700E+19	0.0	126.80
[illegible]	[illegible]	+OH(Ni)	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	+CH(Ni)	[illegible]	[illegible]	3.700E+21	0.0	48.10
[illegible]	[illegible]	+OH(Ni)	[illegible]	[illegible]	1.625E+21	0.0	128.61
R49	H(Ni)	+CO(Ni)	>C(Ni)	+OH(Ni)	4.945E+21	-0.7	110.05-50θCO(Ni)
R50	OH(Ni)	+C(Ni)	>H(Ni)	+CO(Ni)	2.769E+22	0.7	30.00

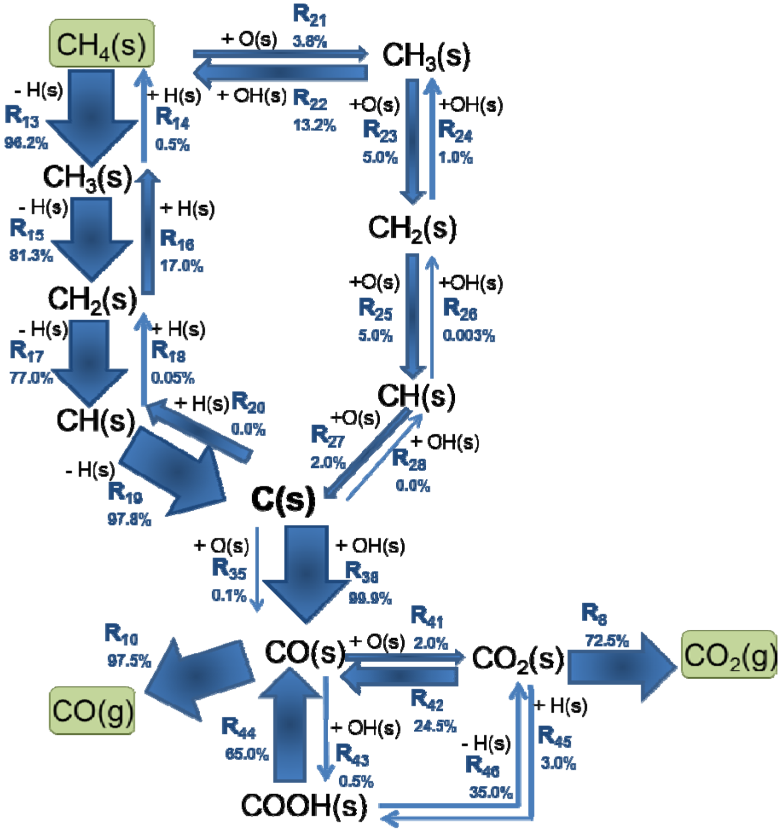


L. Maier, B. Schädel, K. Herrera Delgado, S. Tischer, O. Deutschmann, Top Catal. 54 (2011) 845.
K. Herrera Delgado, H. Stotz, L. Maier, S. Tischer, A. Zellner, O. Deutschmann. Catalysts 5 (2015) 871.

Micro kinetic model helps to understand the coking propensity in the different regions of the catalytic bed

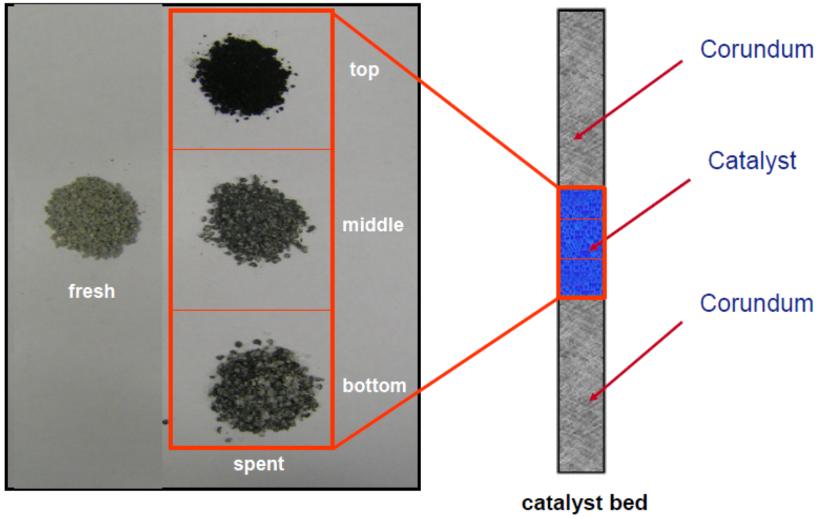


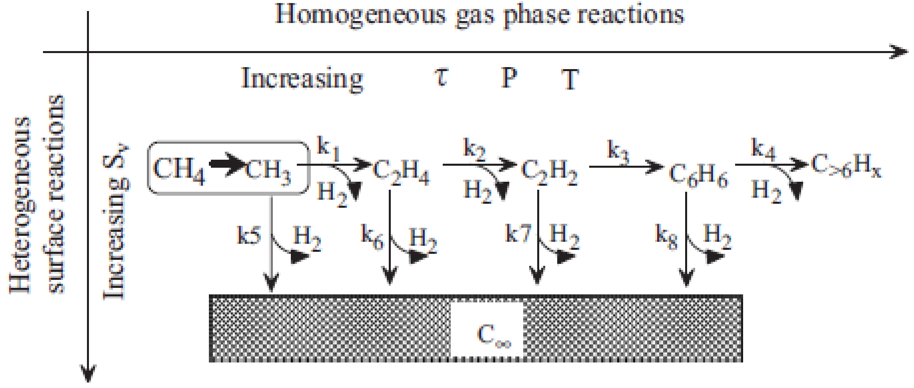


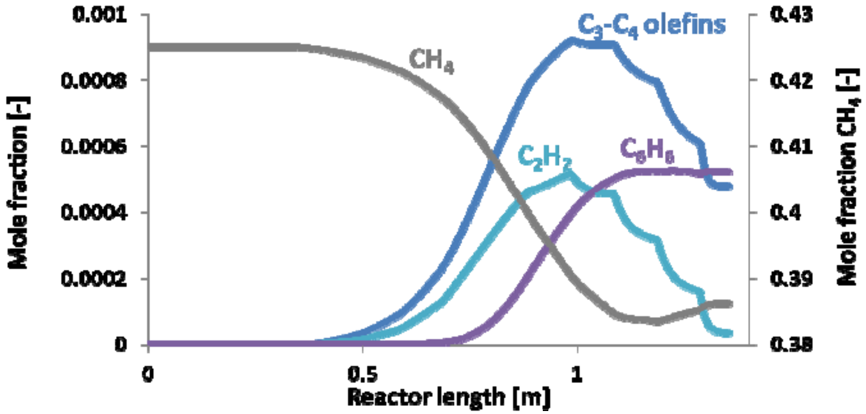


K. Herrera Delgado, H. Stotz, L. Maier, S. Tischer, A. Zellner, O. Deutschmann. Catalysts 5 (2015) 871.
L.C.S. Kahle, T. Roussière, L. Maier, K. Herrera Delgado, G. Wasserschaff, S.A. Schunk, O. Deutschmann. Industrial & Engineering Chemistry Research 52 (2013) 11920.

Dry-reforming of CH_4: Small olefins can lead to gas-phase molecular-weight growth and carbon deposits







$CH_4/CO_2 = 1$; 10 % H_2; 5 % Ar
$u^0 = 0{,}366$ m/s, ~1200 K, 20 bar

A. Li, O. Deutschmann. Chemical Engineering Science, 62(18-20):4976, 2007
L.C.S. Kahle, T. Roussière, L. Maier, K. Herrera Delgado, G. Wasserschaff, S.A. Schunk, O. Deutschmann. Industrial & Engineering Chemistry Res. 52 (2013) 11920.

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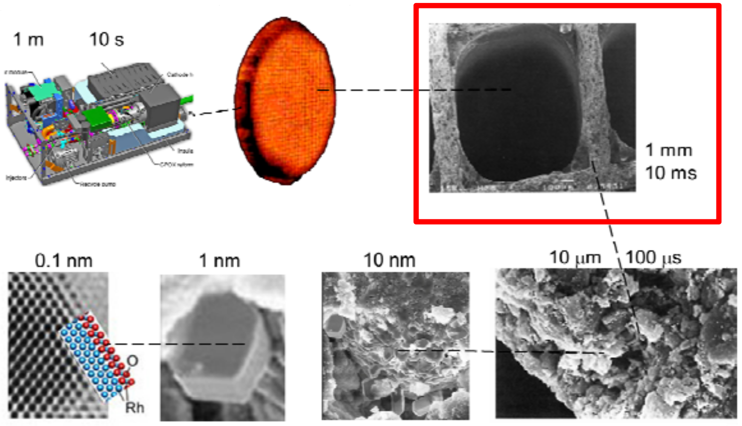
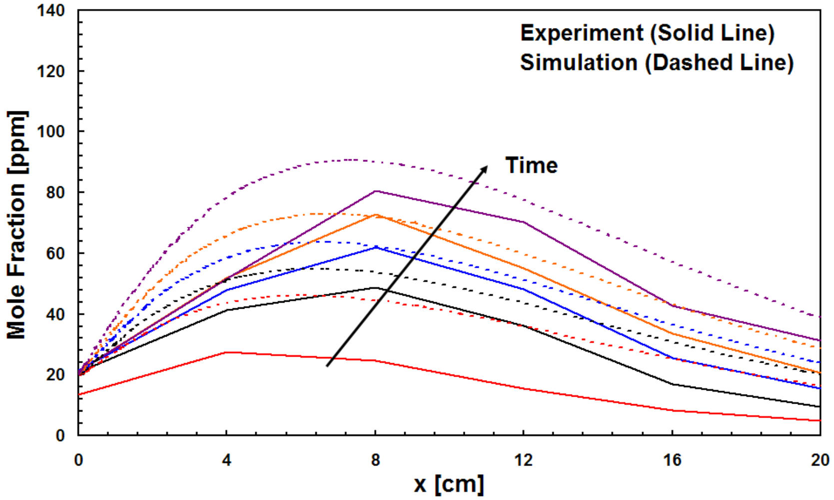


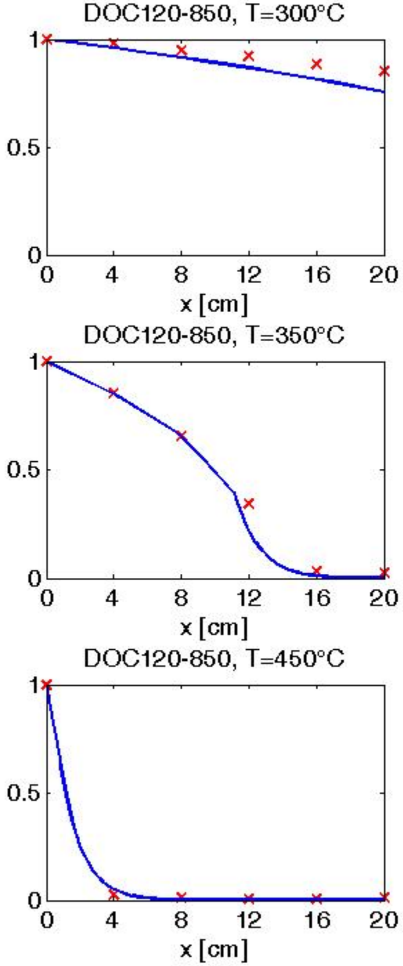
Isothermal flat bed reactor: Spatially and time-resolved exhaust-gas composition in catalyst channel

NO_2 profile in NSC during storage



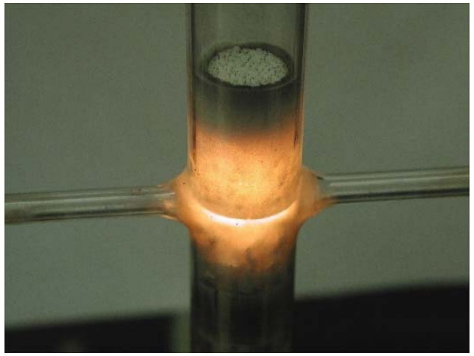
J. Koop, O. Deutschmann. SAE 2007-01-1142.

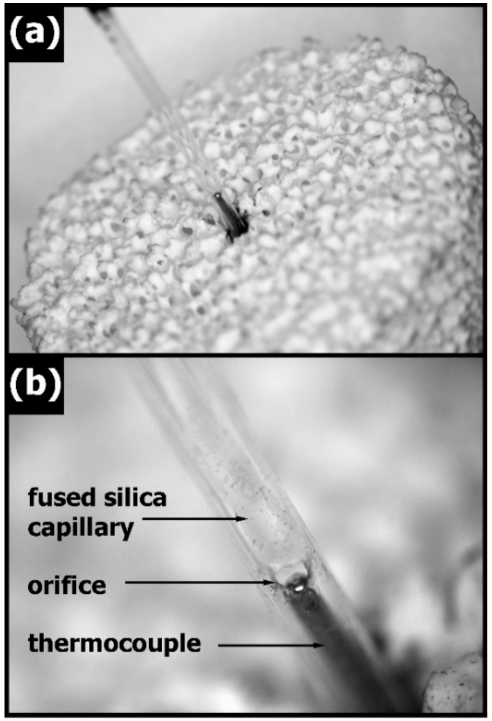
CO profile in DOC



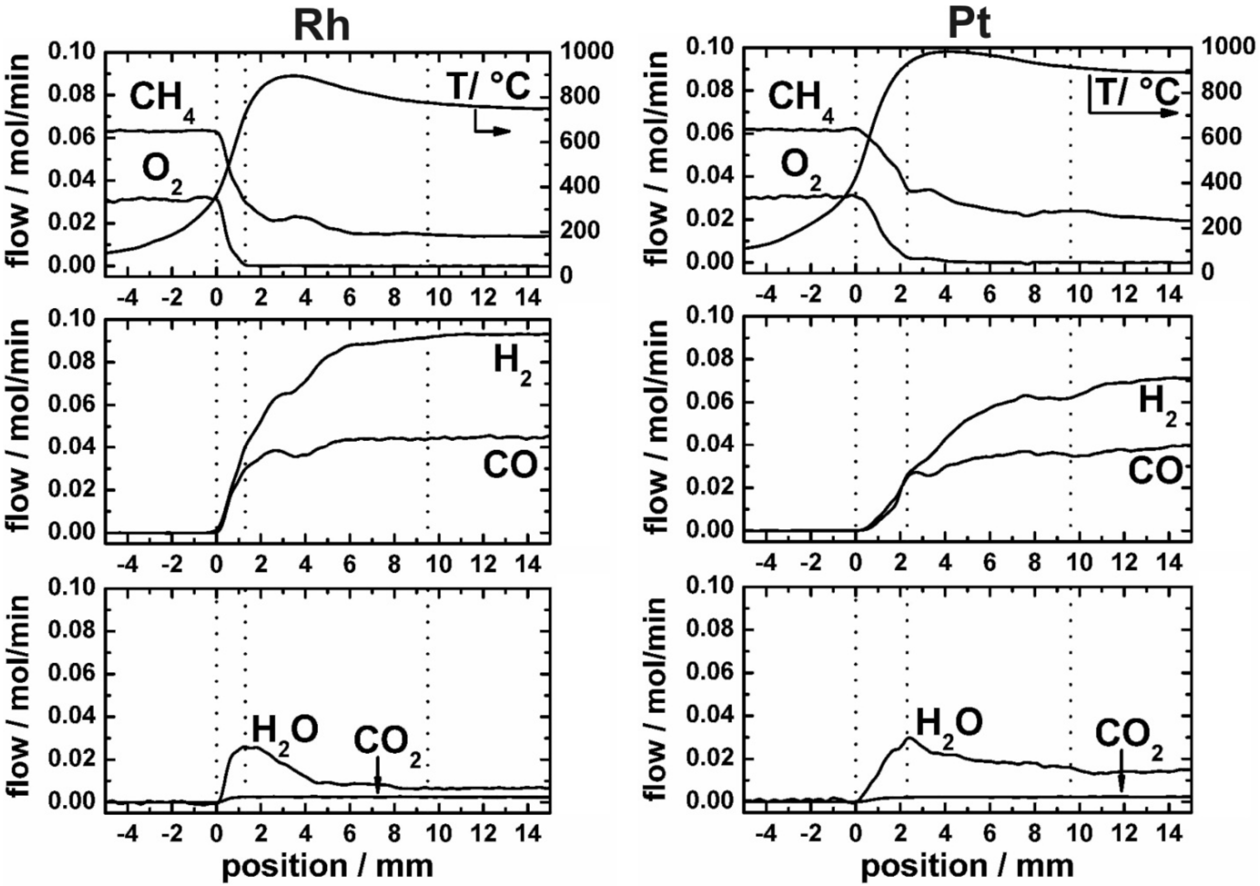
V. Schmeißer, J. Perez, U. Tuttlies, G. Eigenberger, Top. Catal. 42 (2007) 15

Spatially resolved profiles by moving a capillary: Autothermal conversion of methane in catalytic foams



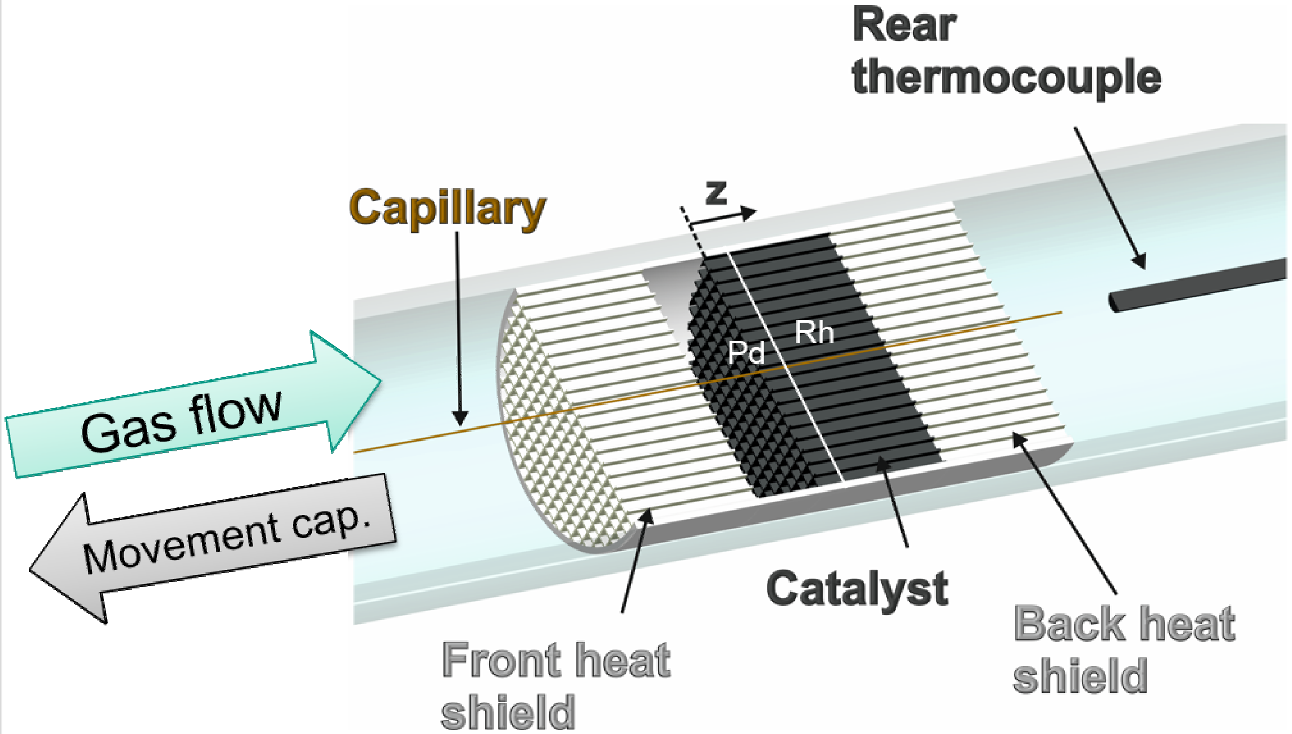


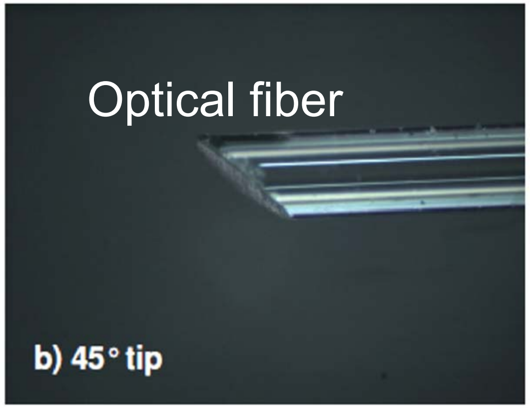
$$CH_4 + {}^1/_2\, O_2 \xrightarrow{Pt/Rh} CO + 2\, H_2$$



R. Horn, N. J. Degenstein, K. A. Williams, L. D. Schmidt. Catal. Lett. 110 (2006) 169.

In-situ probe technique: Resolution in flow direction with movable capillaries





$$\frac{}{A_{\text{channel}}} = 2{,}96\%$$

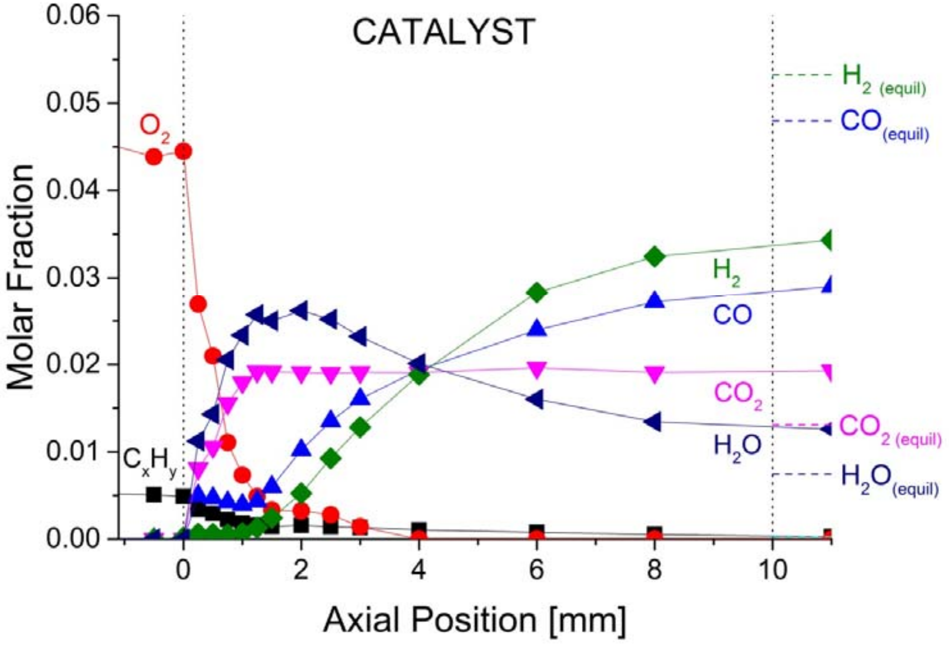
A. Donazzi, D. Livio, A. Beretta, G. Groppi, P. Forzatti, Applied Catalysis A: General, 402 (2011) 41-49.

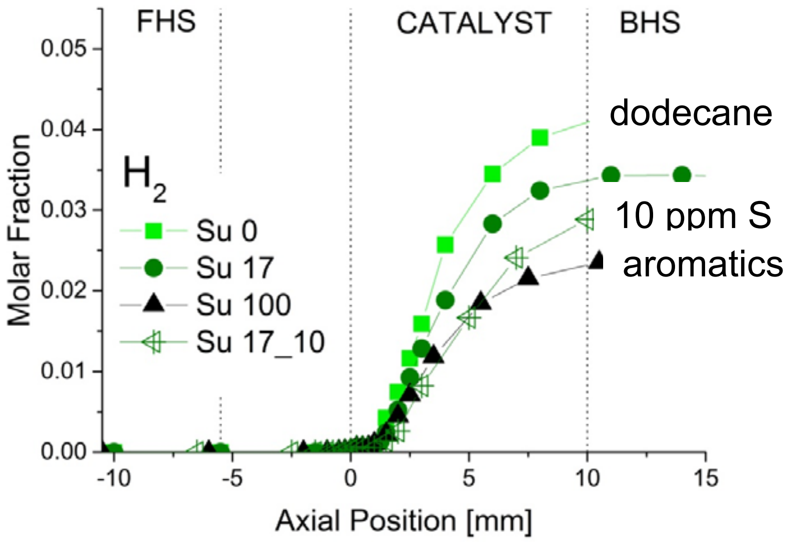
- Concentration profiles:
  - Gas sampled from catalyst channel with capillary (outer diameter = 170 µm)
  - Analysis of gas samples: FT- IR, MS
- Temperature profiles:
  - [illegible] inside of a capillary (outer diameter = 660 µm)
  - Gas phase temperature: Thermocouple
  - Surface temperature: Optical fiber connected to pyrometer
- Movement of capillary with motorized linear stage
  - Resolution: 0.25 mm

D. Livio, C. Diehm, A. Donazzi, A. Beretta, G. Groppi, O. Deutschmann, Appl. Catal. A 467 (2013) 530

Oxidative reforming of jet fuel surrogates in a Rh/Al_2O_3 coated monolith: Spatial concentration profiles

Effect of aromatics and sulfur





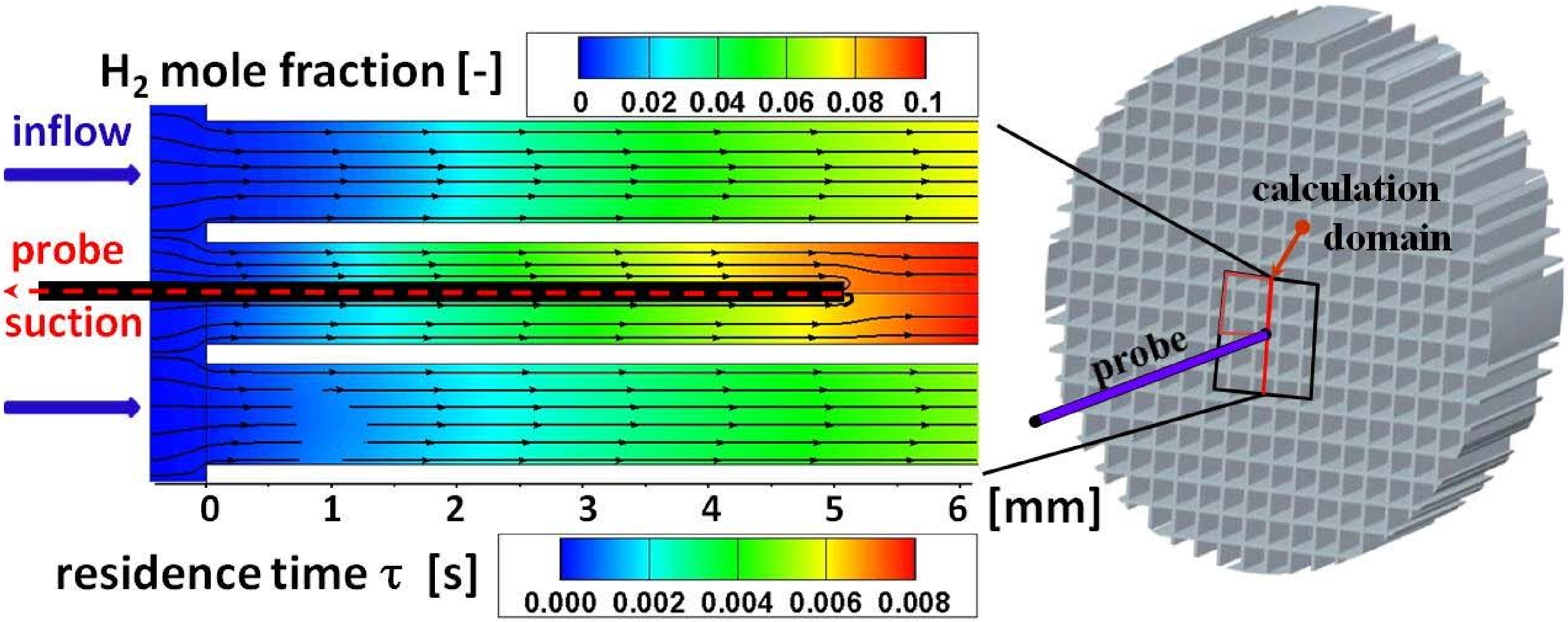
dodecane

10 ppm S

aromatics

J. Bär, C. Diehm, O. Deutschmann, Int. J. Hydrogen Energy, submitted

CFD simulations of impact of capillary on profiles
Hydrogen profile and residence time

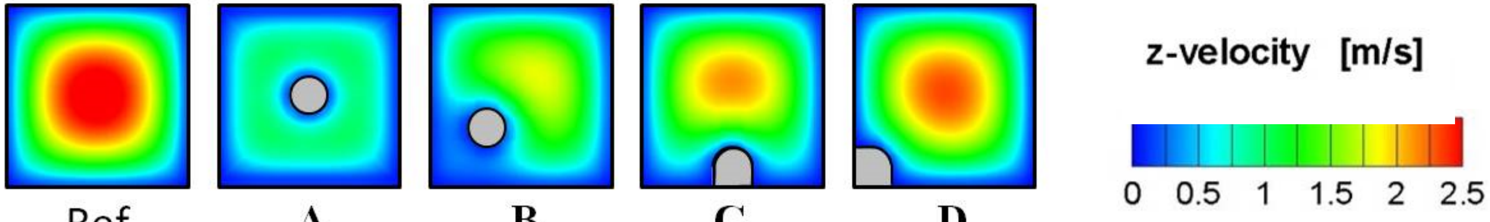


CPOX of CH4 over Rh/Al2O3
C/O = 1
Probe tip at z = 5 mm

M. Hettel, C. Diehm, B. Torkashvand, O. Deutschmann, Catalysis Today 216 (2013) 2

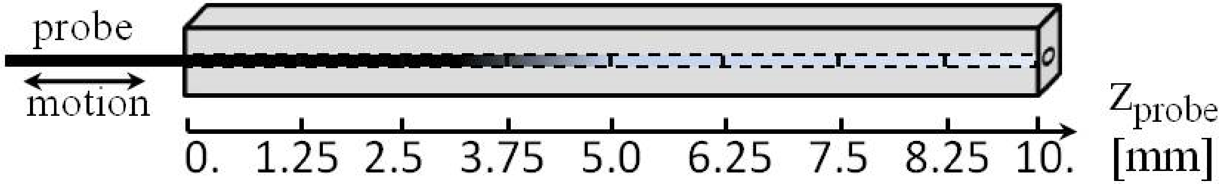
Impact of capillary position on volumetric flux though probe channel

Impact of radial position of capillary on axial velocity and volumetric flux



	Ref.	A	B	C	D
$\frac{\dot{V}_{channel,probe}}{\dot{V}_{channel,ref}}$	**1.00**	**0.46**	**0.62**	**0.79**	**0.91**

Impact of axial position of the tip for central location on volumetric flux



$\frac{\dot{V}_{channel,probe}}{\dot{V}_{channel,ref}}$	**0.96**	**0.75**	**0.62**	**0.52**	**0.46**

M. Hettel, C. Diehm, B. Torkashvand, O. Deutschmann, Catalysis Today 216 (2013) 2

Spatial resolution techniques for catalytic reactors
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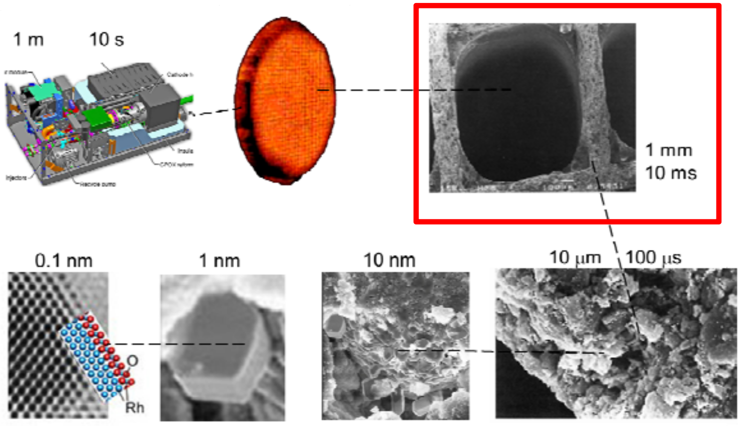
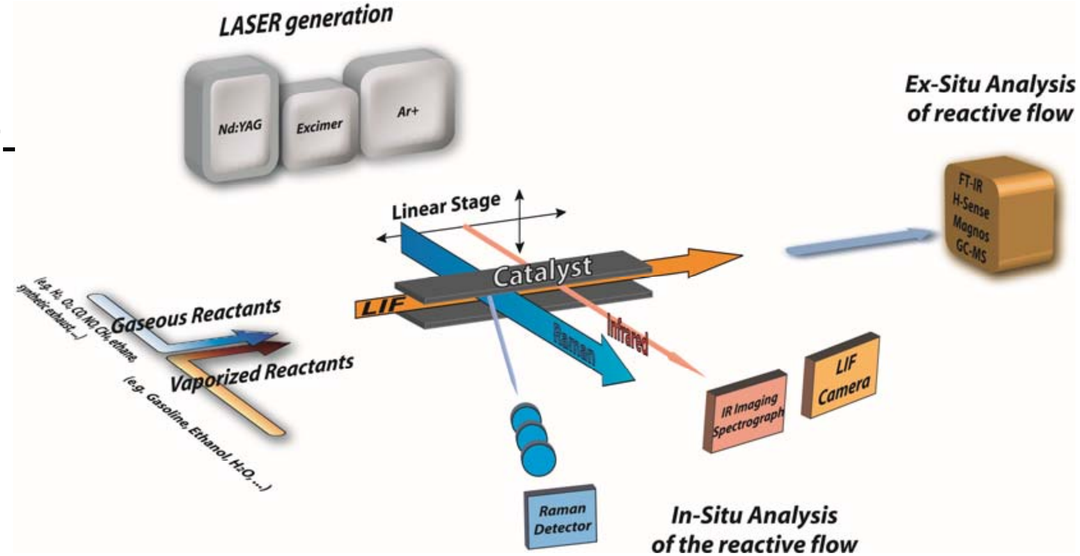
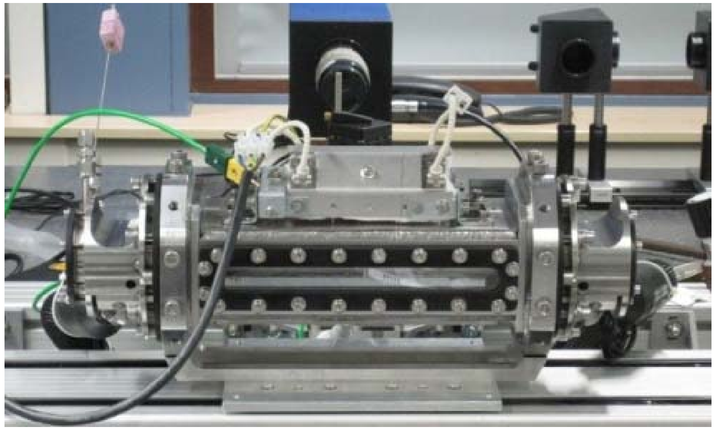


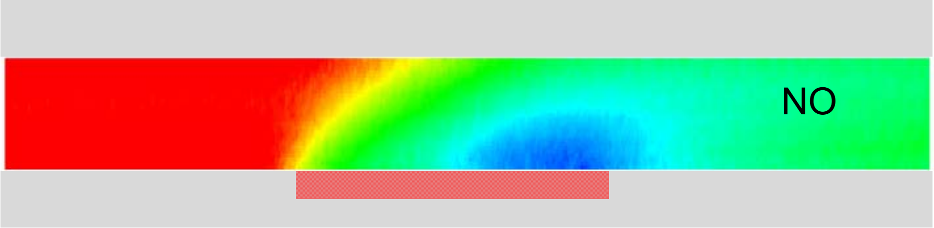
Two-dimensional spatial resolution of the gas-phase of catalytic reactors by laser spectroscopy

In-situ analysis of spatial and temporal profiles of species concentration and temperature in the gas phase above a catalytic surface using Raman and LIF-spectroscopy



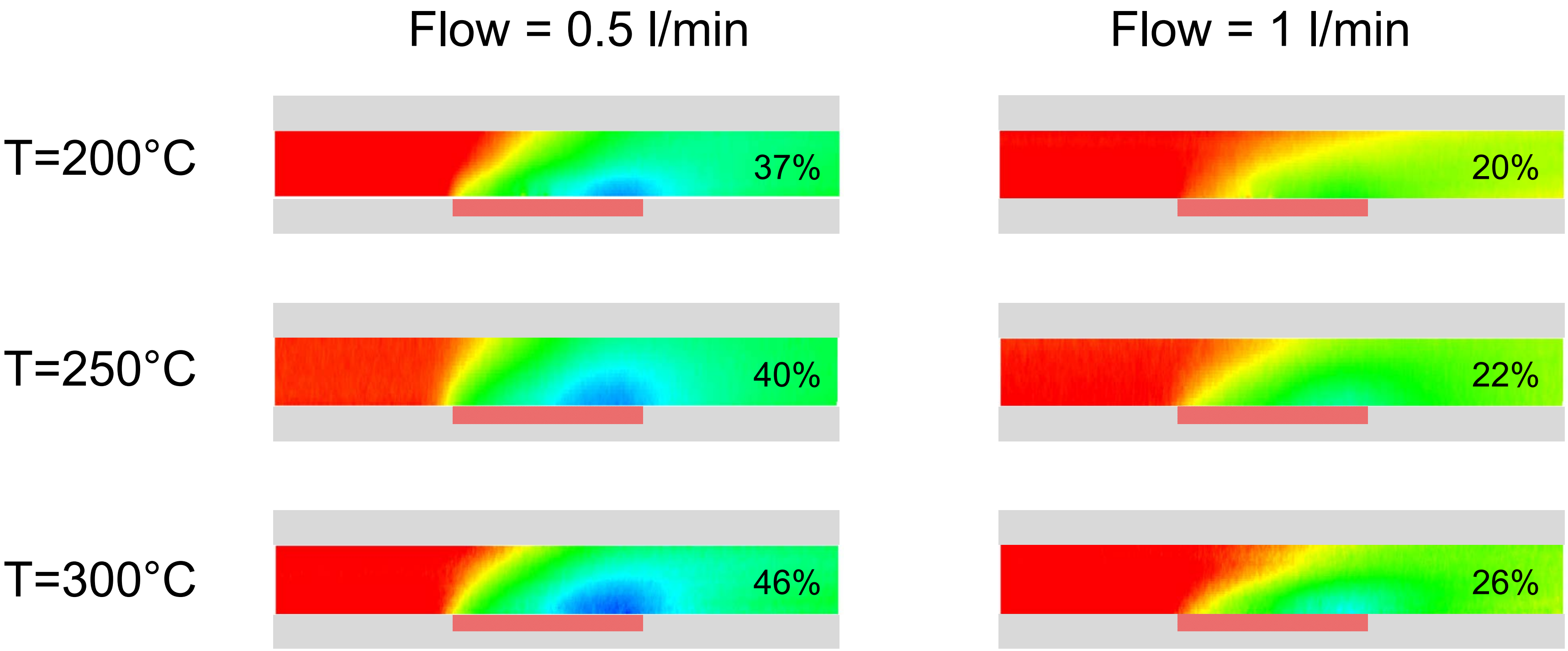


NO LIF profile during reduction by H_2 to NH_3 in Pt/Al_2O_3 one-side-coated single channel of a DOC

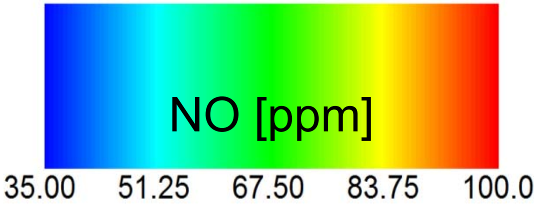


A. Zellner, R. Suntz, O. Deutschmann, Angew. Chem. 54 (2015) 2653.

NO reduction by H_2 to NH_3 over Pt - DOC catalyst: LIF monitored NO conversion



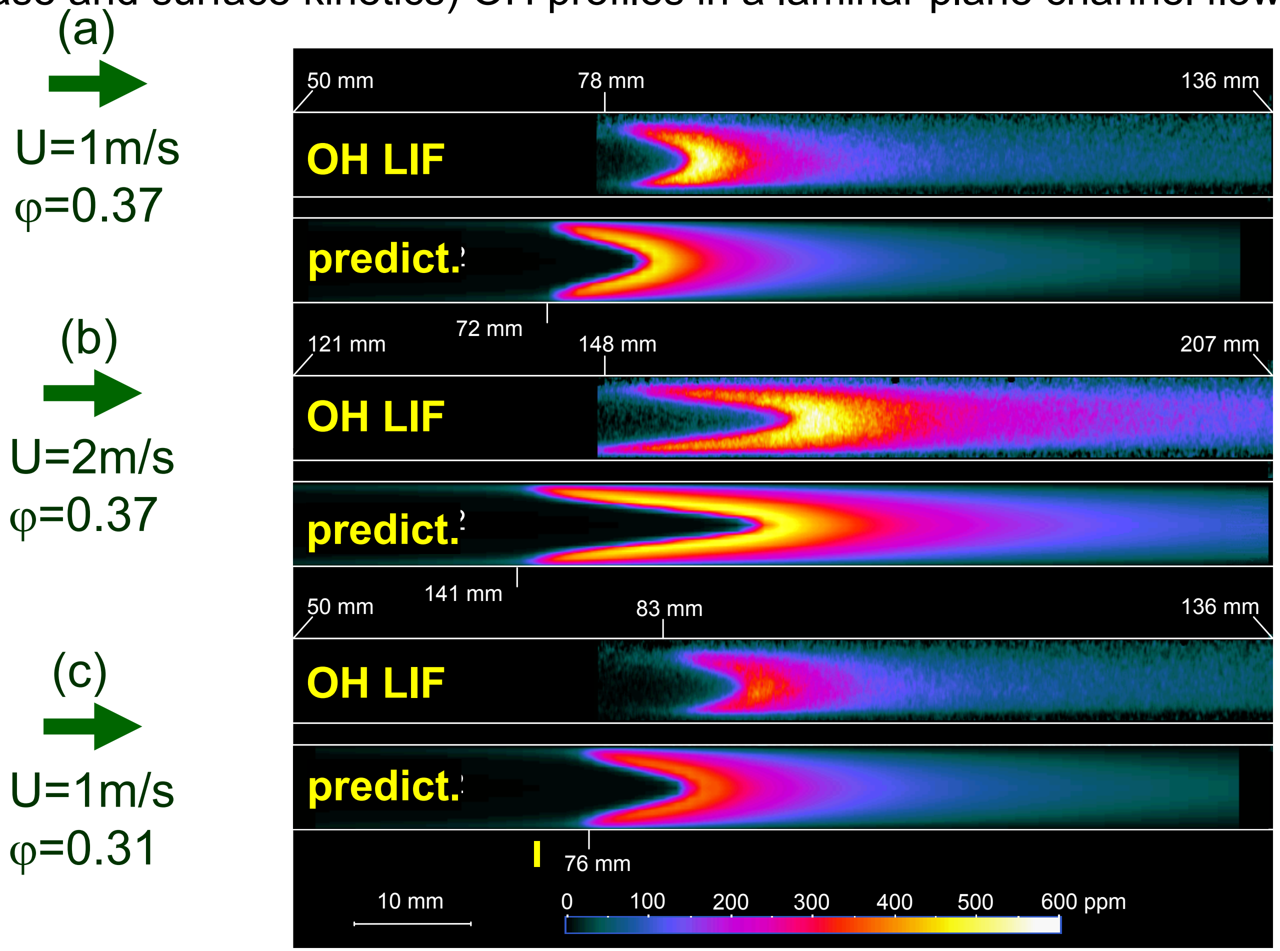
T = 200 – 300°C
p = 1 atm
Flow = 0.5 - 1 l/min
NO = 100 pmm
H_2 = 1.000 ppm



A. Zellner, R. Suntz, O. Deutschmann, Angew. Chem. 54 (2015) 2653

Homogeneous ignition in catalytic combustion of methane in a platinum coated channel

Comparison of experimentally observed (PLIF) and numerically predicted (2D NS model with detailed gas phase and surface kinetics) OH profiles in a laminar plane channel flow



U. Dogwiler, J. Mantzaras, C. Appel, P. Benz, B. Kaeppeli, R. Bombach, A. Arnold. Proc. Combust. Inst. 27 (1998) 2275

Spatial resolution techniques for catalytic reactors
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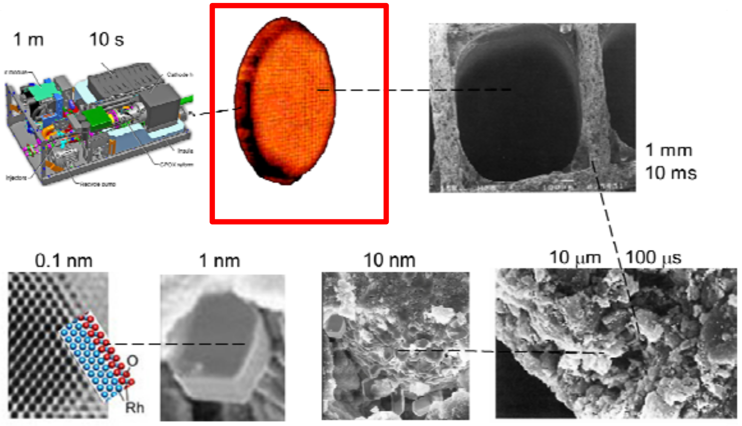

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DETCHEM$^{\text{MONOLITH}}$: Computer program for the numerical simulation of transients in catalytic monoliths

MONOLITH

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

transient

quasi-steady-state

temperature profile at the wall ↓

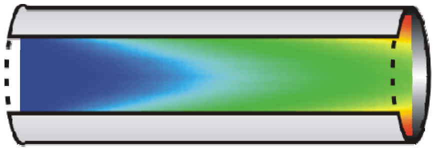
↑ heat source term

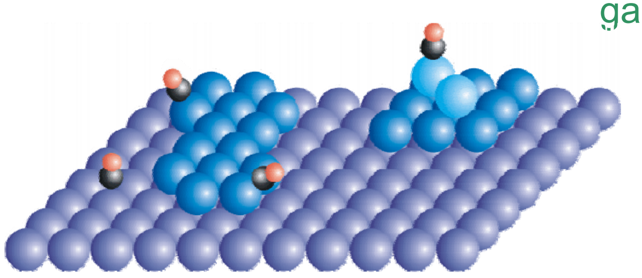
time scale ~ 1 s

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

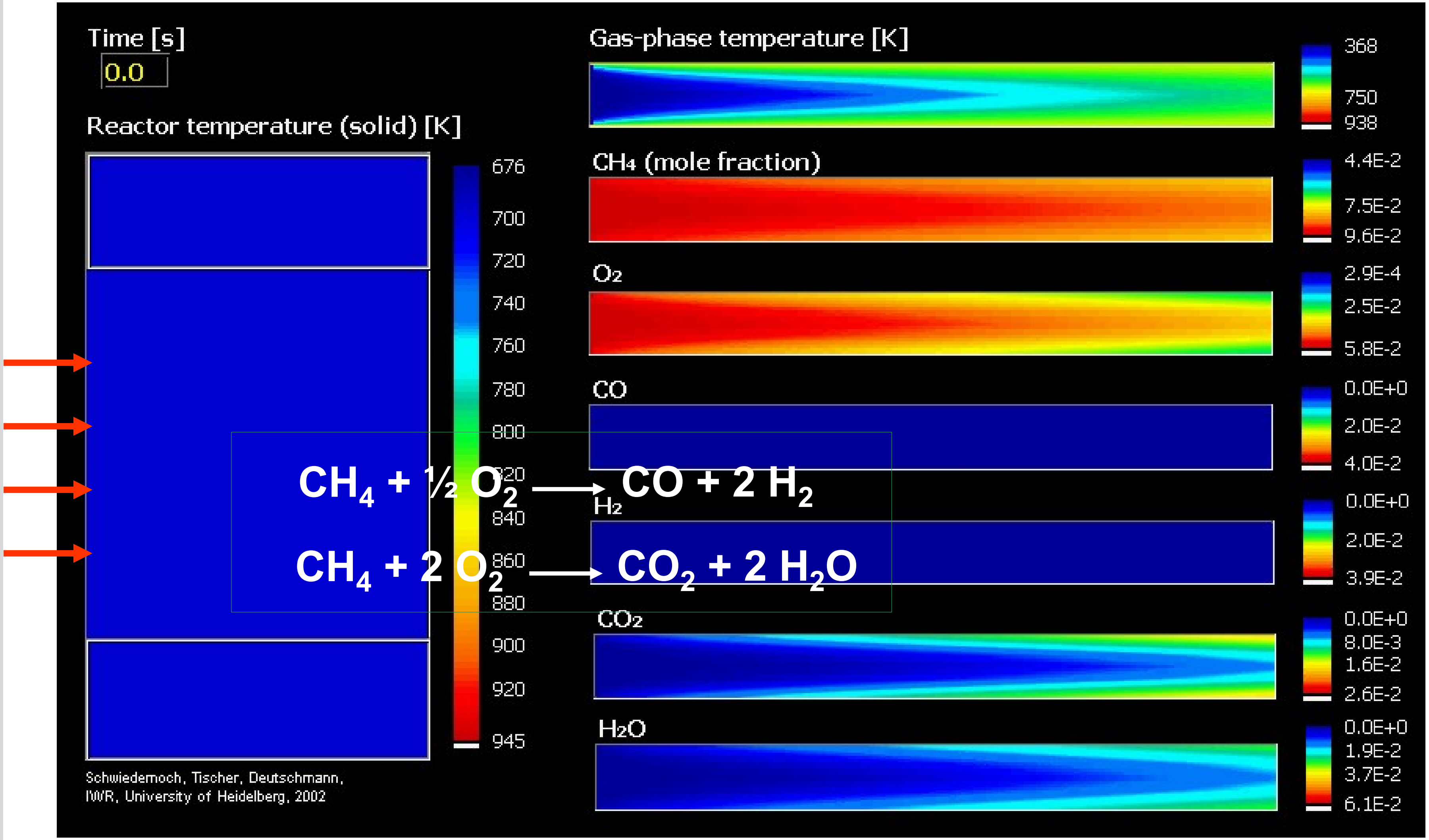
DETCHEM - Library

Thermodynamic and transport properties

Detailed reaction mechanisms for gas-phase & surface

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

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



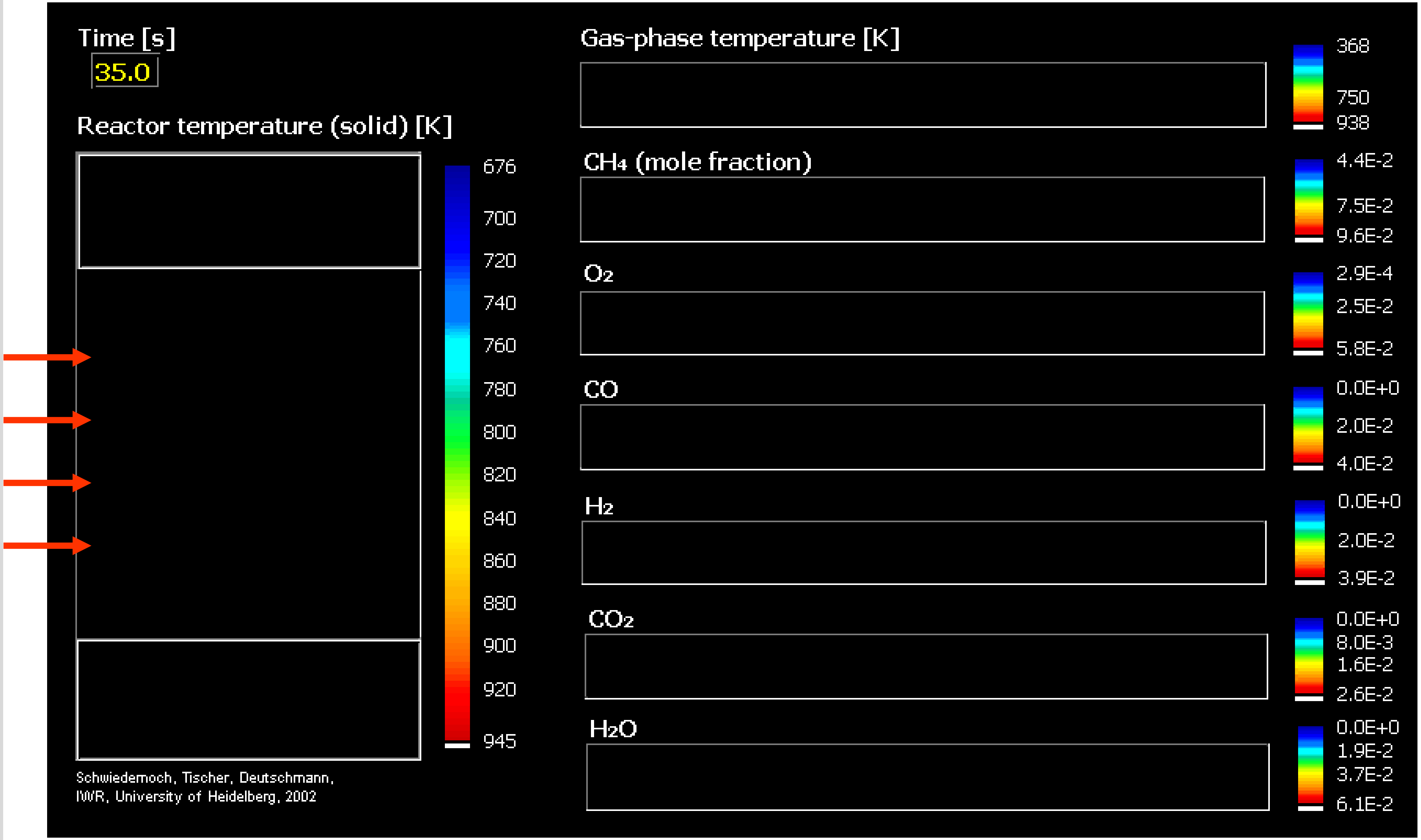
$CH_4 + ½\, O_2 \longrightarrow CO + 2\, H_2$

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

Schwiedernoch, Tischer, Deutschmann, IWR, University of Heidelberg, 2002

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

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



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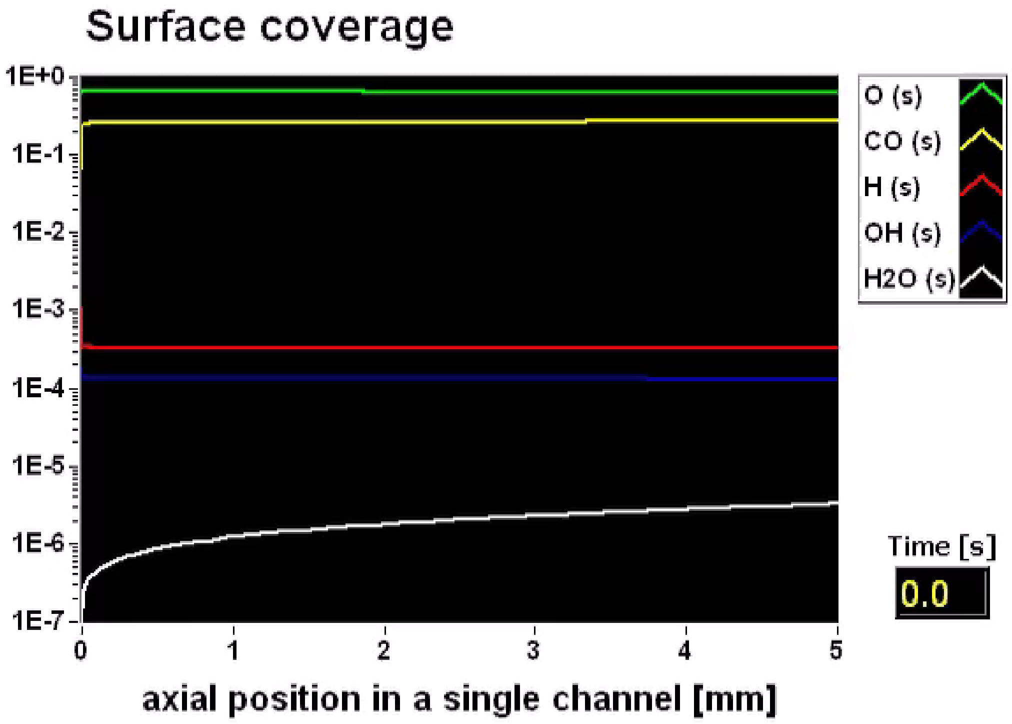
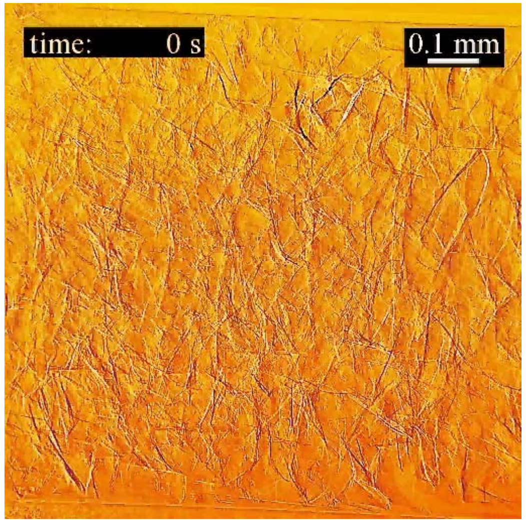
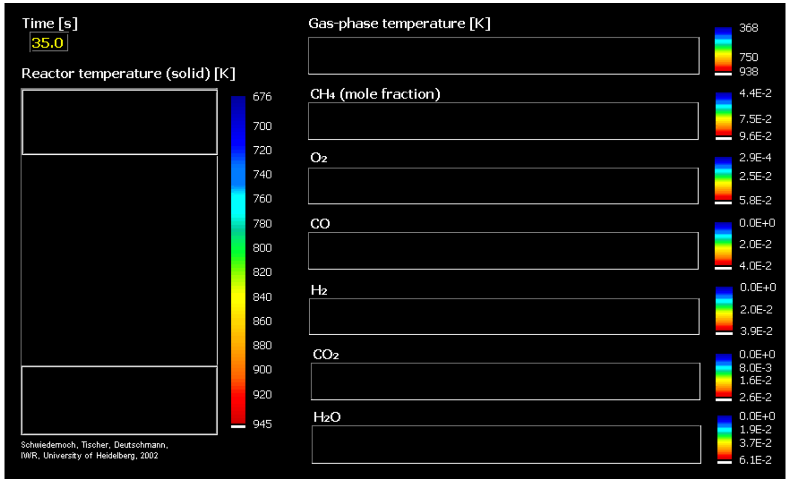


Schwiedernoch, Tischer, Deutschmann, IWR, University of Heidelberg, 2002



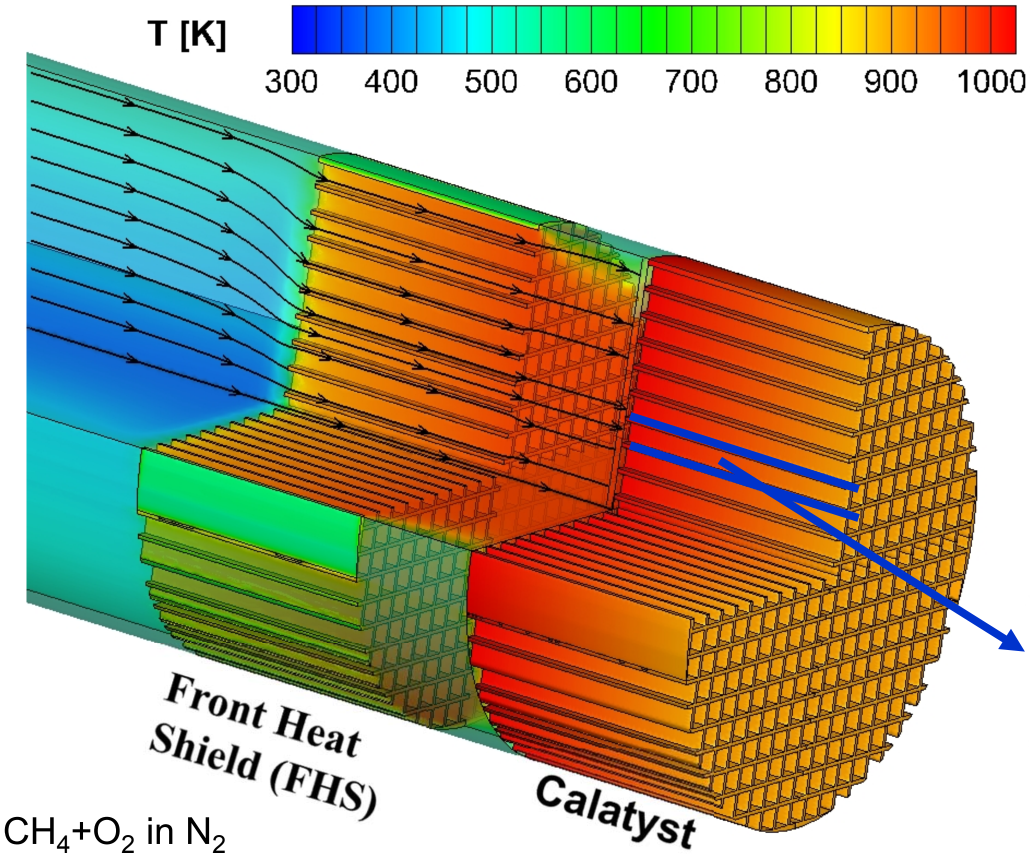


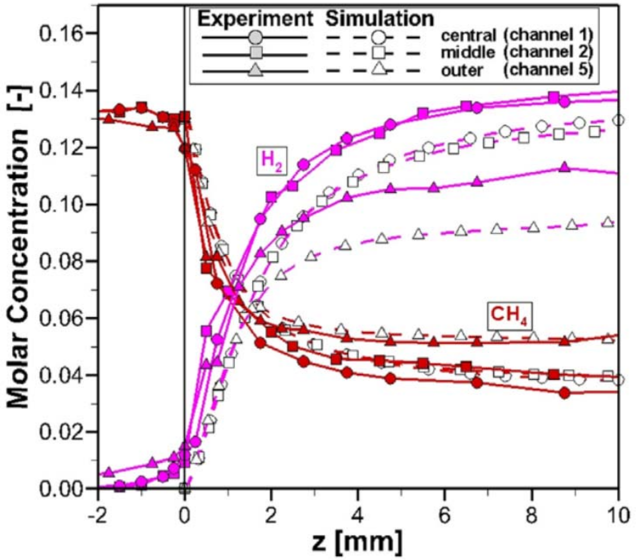
Schwiedernoch, Tischer, Deutschmann, IWR, University of Heidelberg, 2002

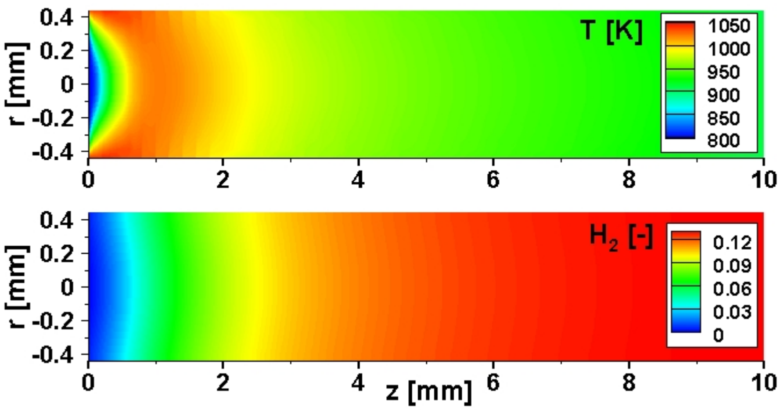
R. Schwiedernoch, S. Tischer, C. Correa, O. Deutschmann, Chem. Eng. Sci., 58 (2003) 633-642

B. Kimmerle, J.-D. Grunwaldt, A. Baiker, P. Glatzel, P. Boye, S. Stephan, C.G. Schroer, Journal of Physical Chemistry C, 113 (2009) 3037.

Syngas Formation in CPOX of CH_4 on Rh: CFD simulation using OpenFoam and DETCHEM







CH_4+O_2 in N_2
C/O = 1.0
Rh (10 mm)

M. Hettel, C. Diehm, O. Deutschmann, Catalysis Today, DOI: 10.1016/j.cattod.2015.02.011

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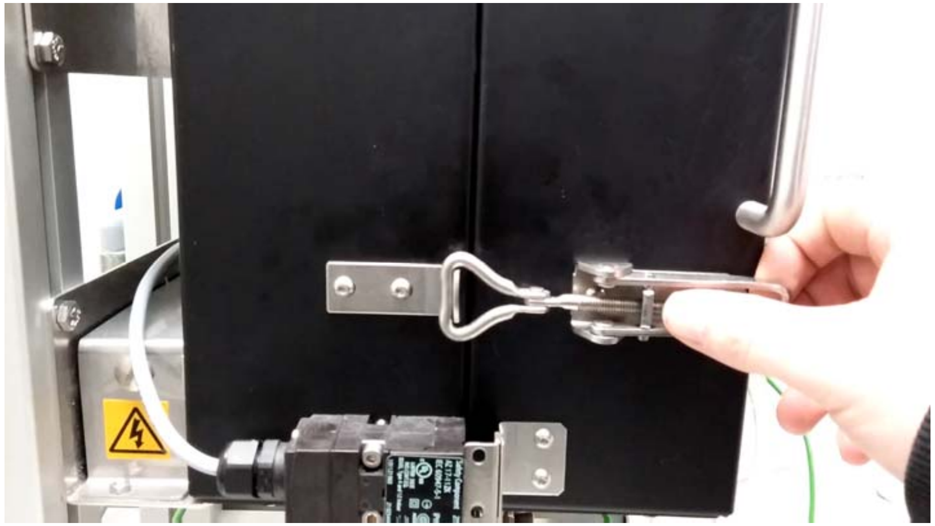
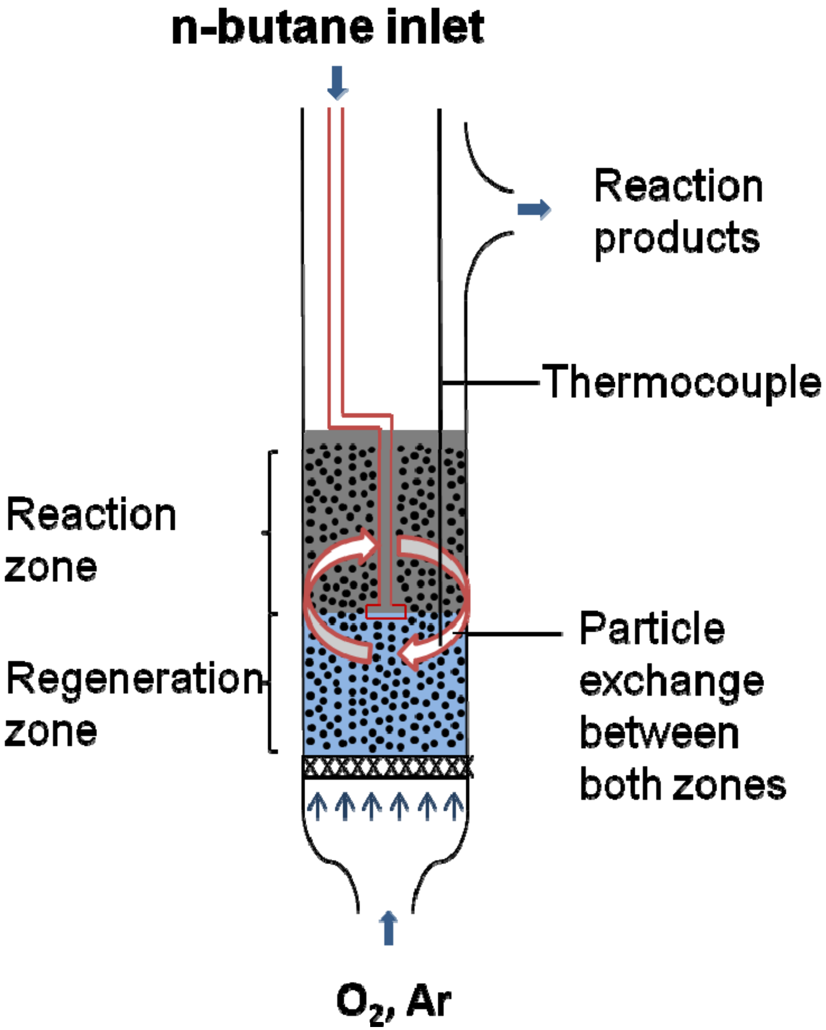
Potential route for butadiene production from n-butane: Two zone fluidized bed reactor with Mo-V catalysts

$$C_4H_{10} + O_2 \xrightarrow{\text{catalyst}} C_4H_6 + 2\ H_2O$$

570 °C, 6.5 Vol.% n-butane, O_2/n-butane ratio: 2.3





J. Rischard, C. Diehm, L. Maier, O. Deutschmann, APCATA, submitted

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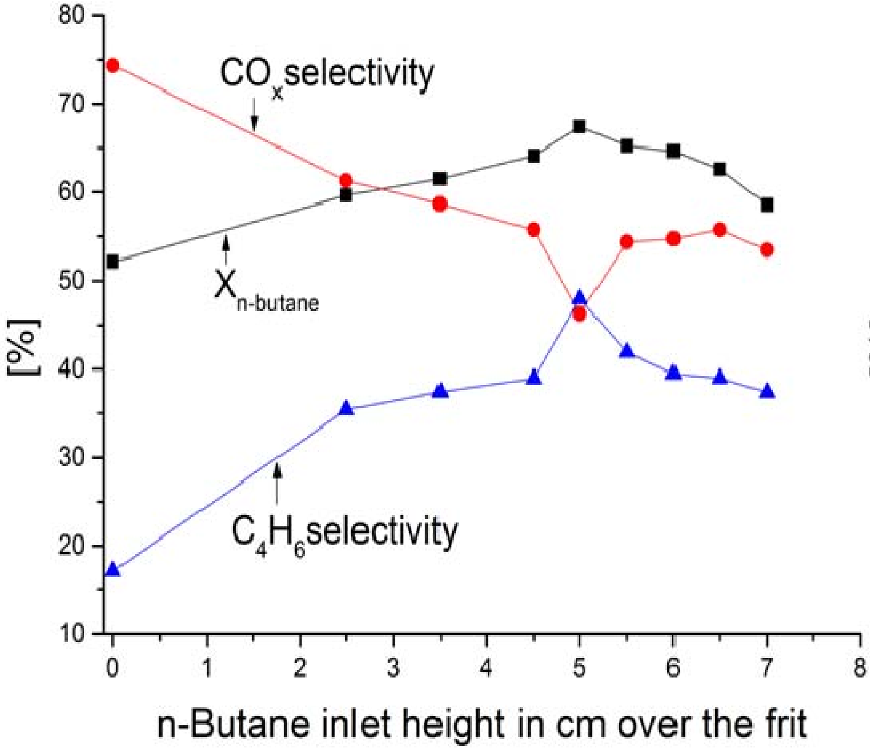
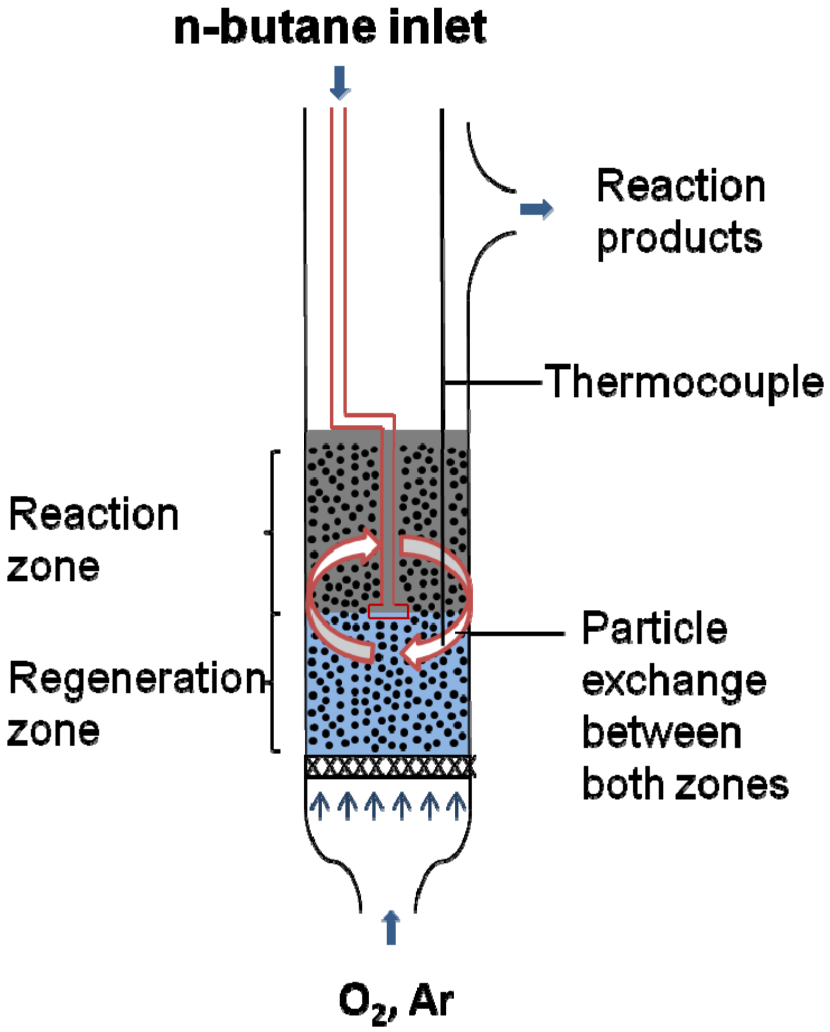
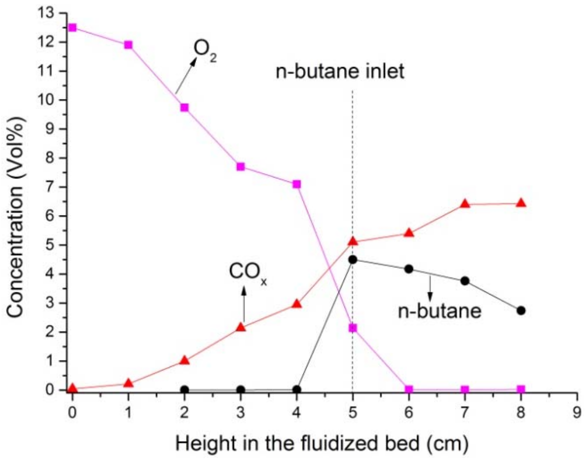


J. Rischard, C. Diehm, L. Maier, O. Deutschmann, APCATA, submitted

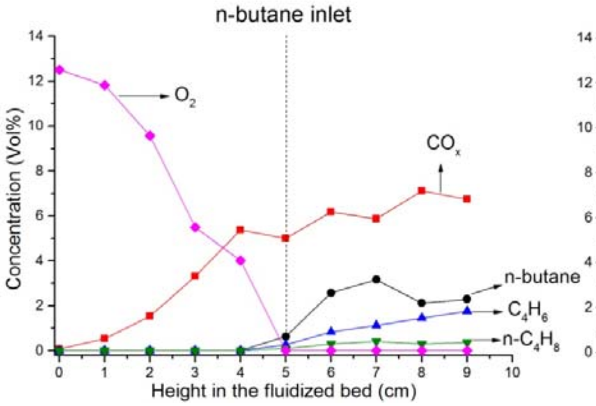


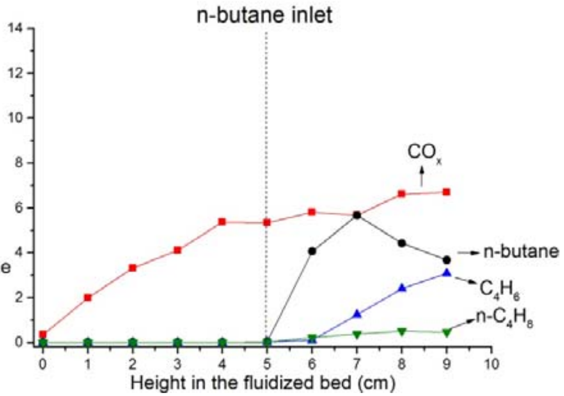
Two zone fluidized bed reactor setup:
Axial and radial species profiles by capillary sampling

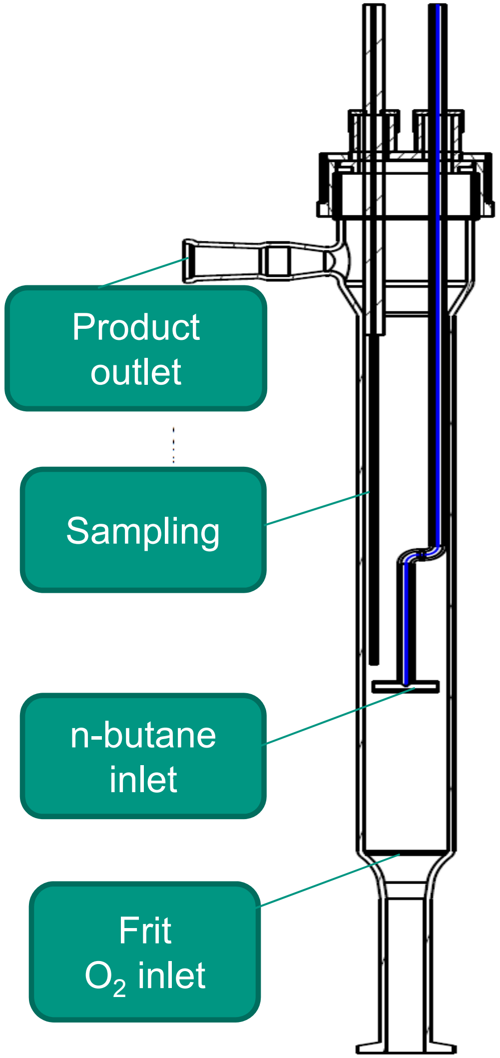
$$C_4H_{10} + O_2 \xrightarrow{\text{catalyst}} C_4H_6 + 2\ H_2O$$



Vertical concentration profiles inside the fluidized bed at different horizontal positions







Product outlet

Sampling

n-butane inlet

Frit
O_2 inlet

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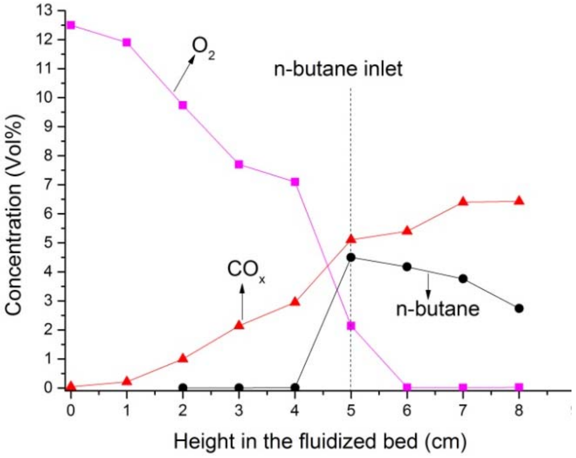
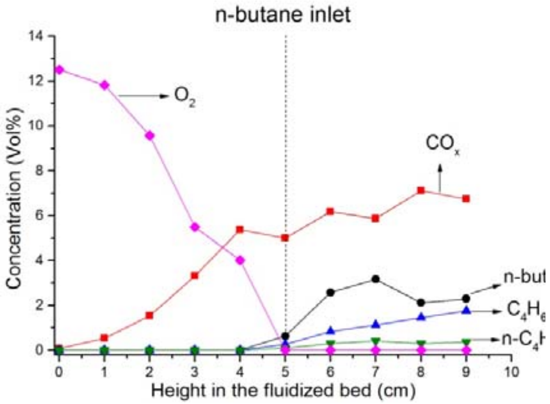
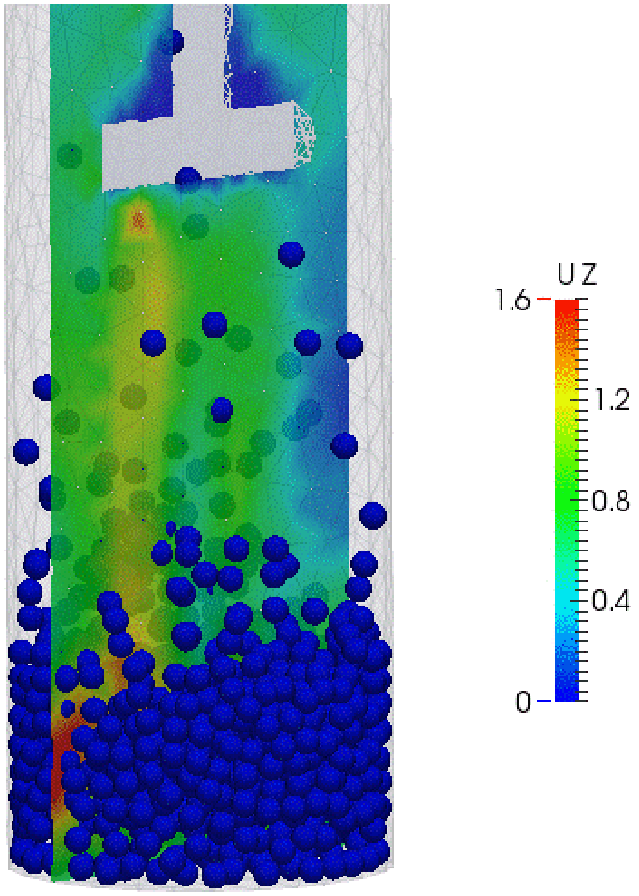
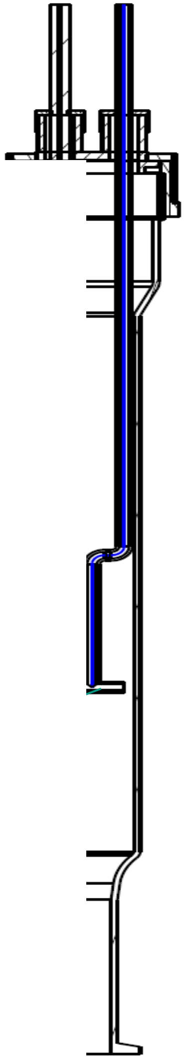






Height in the fluidized bed (cm)



M. Hettel, O. Deutschmann, 2015

Spatial resolution techniques for catalytic reactors
Outline

- Motivation

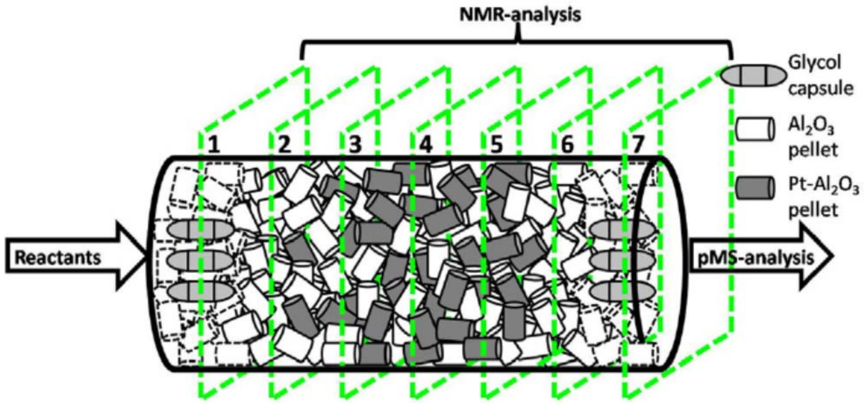
- On the catalyst
  - Catalytic surface
  - Catalyst particle
  - Catalyst and support

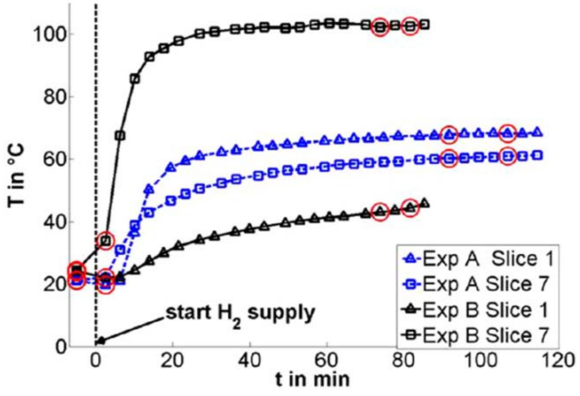
- In the gas-phase
  - Reaction sequence
  - Kinetics, diffusion, and convection
  - Structured reactors
  - Fluidized beds
  - Packed beds

- Multi-phase systems

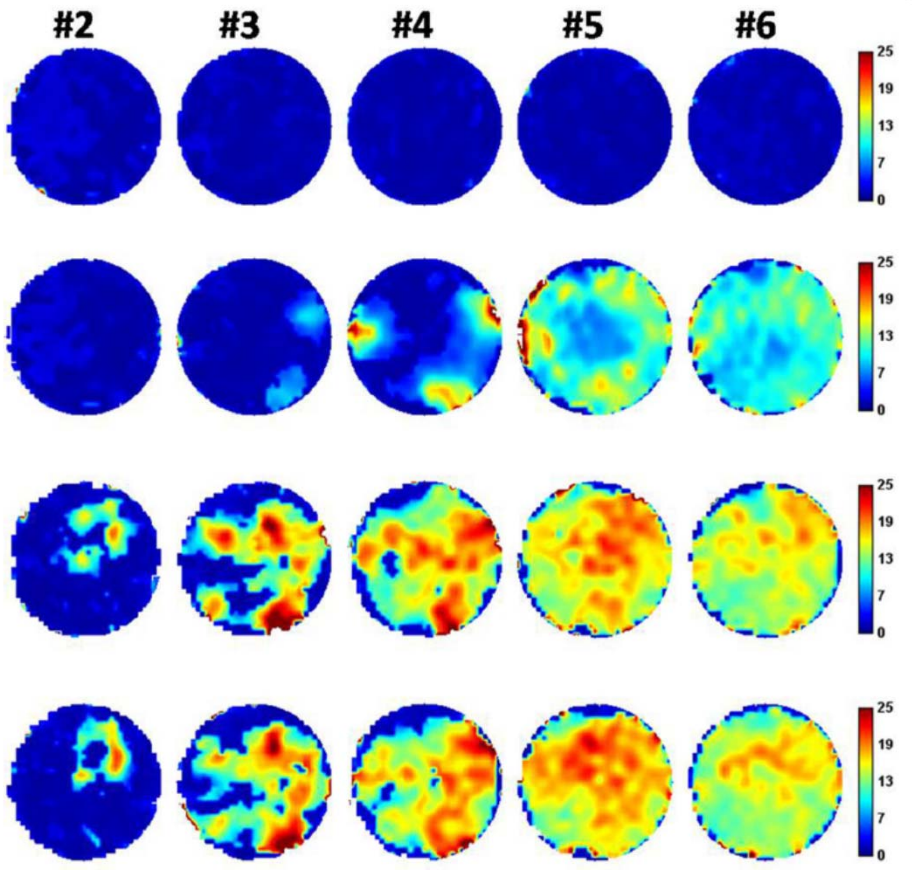
NMR imaging of gas-phase concentrations: Hydrogenation in a packed bed flow reactor

$$C_2H_4 + H_2 \xrightarrow{\text{catalyst}} C_2H_6$$





Temperature-dependent spatial evolution of ethane concentration



J. Ulpts, W. Dreher, M. Klink, J. Thöming. Applied Catalysis A: General 502 (2015) 340

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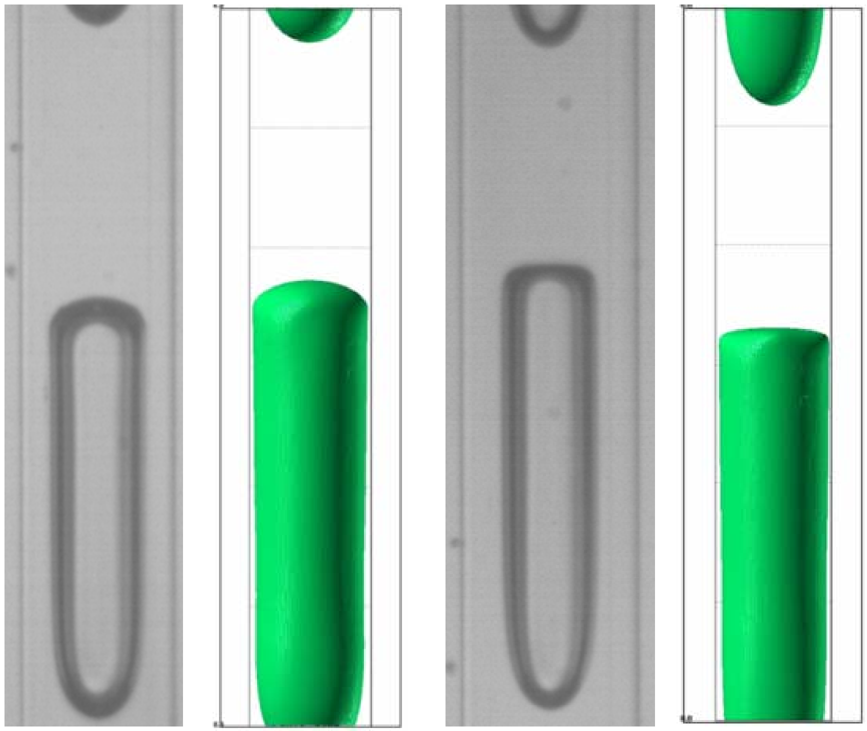
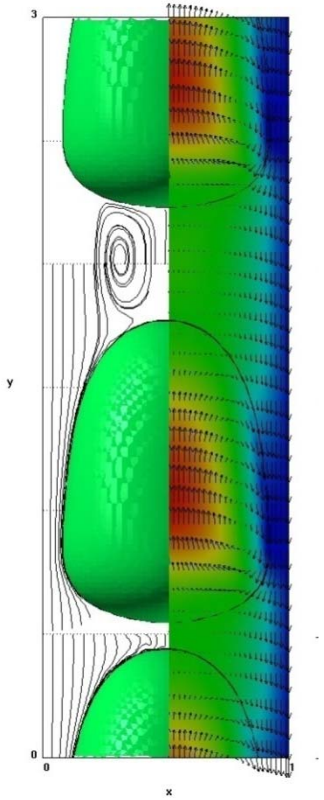
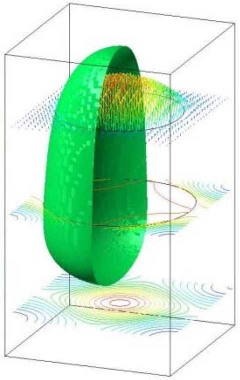
Monitoring and modeling gas bubbles in liquids

Hydrodynamics and mass transfer in Taylor flow



Ö. Keskin, M. Wörner, H.S. Soyhan,T. Bauer, O. Deutschmann, R. Lange. AIChE J 56 (2010) 1693

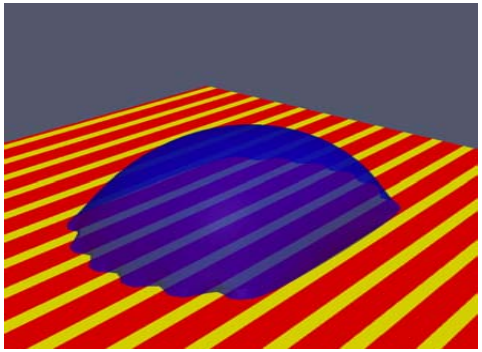




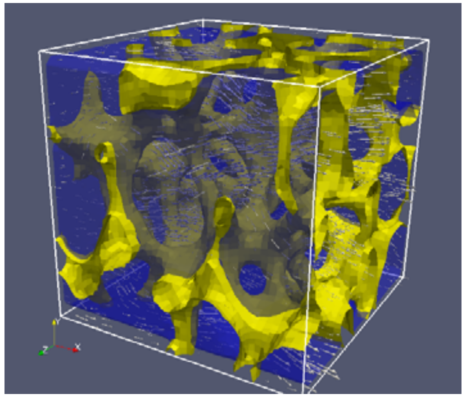
M. Wörner. Microfluidics and Nanofluidics 12 (2012) 841.
M.C. Öztaskin, M. Wörner, H.S. Soyhan. Physics of Fluids 21 (2009) 042108.

Spatial resolution of gas-liquid-solid interactions: Numerical simulation of wetting phenomena

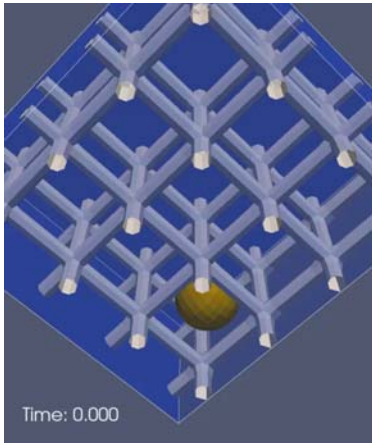
- Phase-field method in OpenFOAM® with adaptive mesh refinement near interface
- Method can handle real gas-liquid density and viscosity ratios



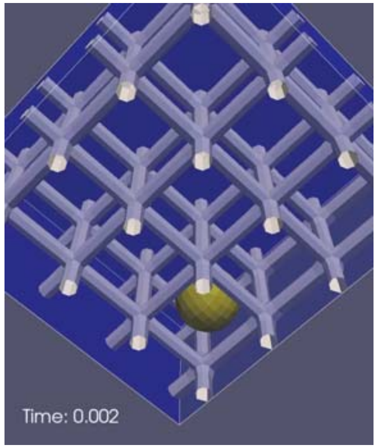
Spreading on a chemically patterned surface (hydrophilic / hydrophobic)



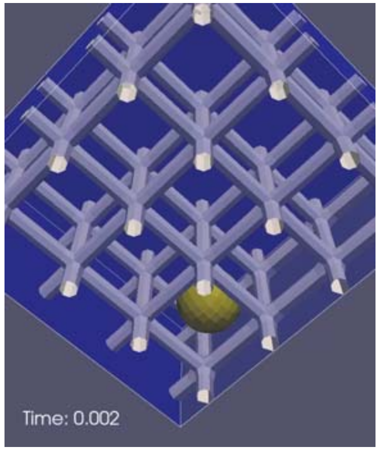
Gas-liquid flow through solid sponge



Air bubble rising through periodic open cell structure ($\theta_e = 90°$)



hydrophilic ($\theta_e = 0°$)



hydrophobic ($\theta_e = 135°$)

X. Cai, H. Marschall, M. Wörner, O. Deutschmann. Chem. Eng. & Technol. 38 (2015) DOI: 10.1002/ceat.201500089

KIT
Karlsruhe Institute of Technology

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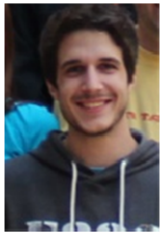
Alex Zellner


Lubow Maier


Claudia Diehm


Matthias Hettel


Rainer Suntz


Martin Wörner


Xuan Cai


Denise Chan


Mino Woo


Claudia Essmann


A.Gremminger


Steffen Tischer

Julius Rischard

Collaboration


J.-D. Grunwaldt

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KIC InnoEnergy

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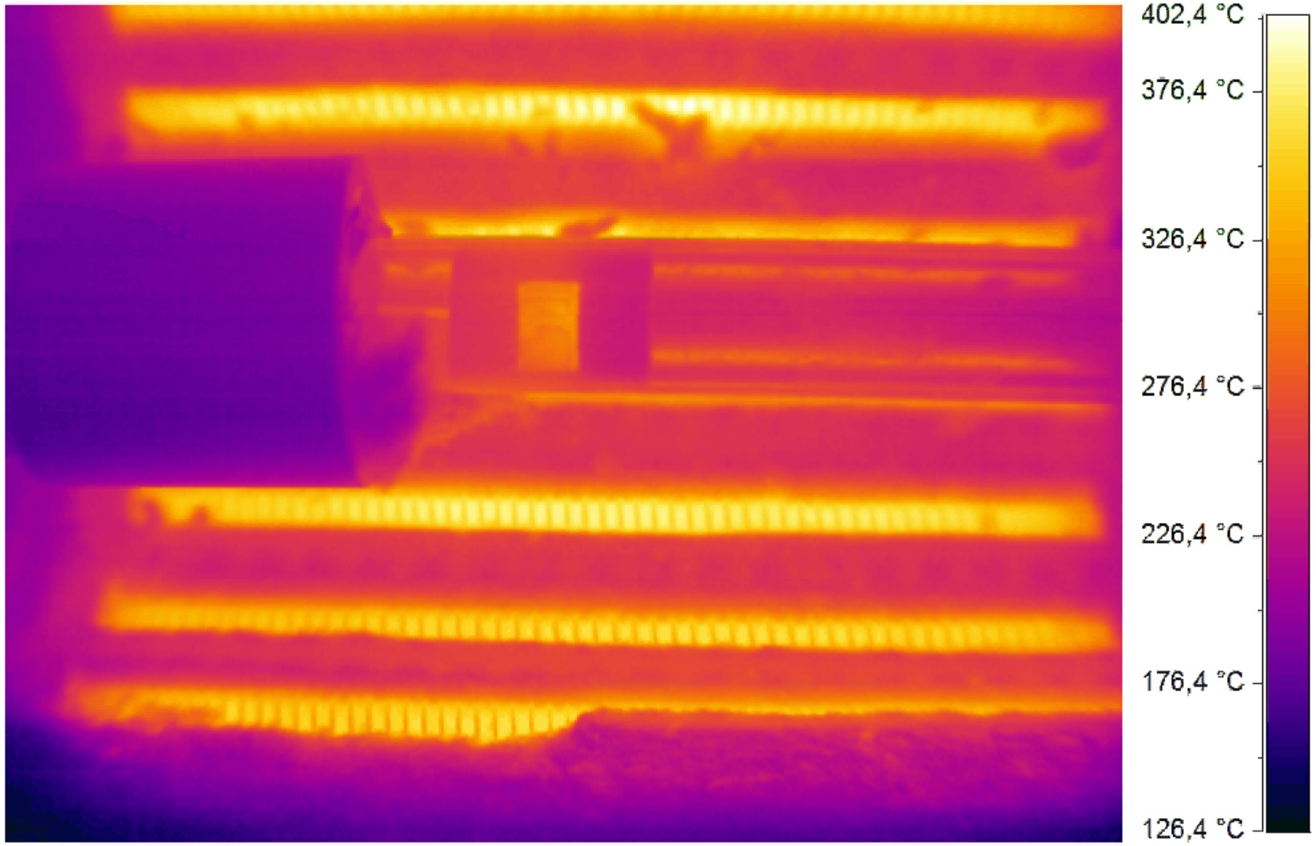
Thank you!



Light-off of CPOX of gasoline

T. Kaltschmitt, O. Deutschmann, 2011