

## Reviewed Publications Olaf Deutschmann et. al. overview

2024

(329) P. Lott, K. Schäfer, O. Deutschmann, M. Werner, P. Weinmann, L. Zimmermann, H. Toebben. Reducing emissions from lean-burn hydrogen combustion engines using a state-of-the-art oxidation catalyst and a VWTi-based SCR catalyst: Potentials and challenges . SAE Technical Paper (2024) 2024-01-2634. <https://www.sae.org/publications/technical-papers/content/2024-01-2634>

(328) J. Chawla, S. Schardt, P. Lott, S. Angeli, S. Tischer, L. Maier, O. Deutschmann. Detailed Kinetic Modeling of Catalytic Oxidative Coupling of Methane, Chem. Eng. J. (2024) 148719. <https://doi.org/10.1016/j.cej.2024.148719>

(327) Y. Wang, J. Shib, X. Gu, O. Deutschmann, Y. Shi, N. Cai. Toward Mobility of Solid Oxide Fuel Cells. Progress in Energy and Combustion Science, accepted 31.12.2023

## 2023

- (326) D. Hodonj, M. Borchers, L. Zeh, G. T. Hoang, S. Tischer, P. Lott, O. Deutschmann. Impact of operation parameters and lambda input signal during lambda-dithering of three-way catalysts for low-temperature performance enhancement. *Applied Catalysis B: Environmental* 345 (2024) 123657.  
<https://doi.org/10.1016/j.apcatb.2023.123657>
- (325) R. Chacko, H. Gossler, S. Angeli, O. Deutschmann. Interconnected Digital Solutions to Accelerate Modeling of the Reaction Kinetics in Catalysis. *ChemCatChem* (2024) e202301355.  
<http://dx.doi.org/10.1002/cctc.202301355>
- (324) M. Mokashi, A. Shirsath, P. Lott, H. Müller, S. Tischer, L. Maier, O. Deutschmann. Understanding of gas-phase methane pyrolysis towards hydrogen and solid carbon with detailed kinetic simulations and experiments, *Chemical Engineering Journal* 479 (2024) 147556.  
<https://doi.org/10.1016/j.cej.2023.147556>
- (323) S. Wan, T. Häber, P. Lott, R. Suntz, O. Deutschmann. Experimental investigation of NO reduction by H<sub>2</sub> on Pd using planar laser-induced fluorescence. *Applications in Energy and Combustion Science* 16 (2023) 100229.  
<https://doi.org/10.1016/j.jaecs.2023.100229>
- (322) P. Blanck, G. Kass, K.P. Kinzel, O. Deutschmann. Dry reforming of steelworks off-gases in a pilot plant integrated into a steel mill: influence of operating parameters. *Energy Advances* 3 (2024) 123-130.  
<https://doi.org/10.1039/d3ya00227f>
- (321) A. Çelik, I.B. Othman, H. Müller, P. Lott, O. Deutschmann. Pyrolysis of biogas for carbon capture and carbon dioxide-free production of hydrogen. *Reaction Chemistry & Engineering* 9 (2024) 108-118.  
<https://doi.org/10.1039/D3RE00360D>
- (320) P. Lott, M. Casapu, J.-D. Grunwaldt, O. Deutschmann. A review on exhaust gas after-treatment of lean-burn natural gas engines – From fundamentals to application. *Appl. Catal. B: Env.* 340 (2024) 123241.  
<https://doi.org/10.1016/j.apcatb.2023.123241>
- (319) B. Kreitz, P. Lott, A.J. Medford, F. Studt, O. Deutschmann; C.F. Goldsmith. Automated Generation of Microkinetics for Heterogeneously Catalyzed Reactions Considering Correlated Uncertainties. *Angew. Chemie Intl. Ed.* 62 (2023) e20230651.  
<https://doi.org/10.1002/anie.202306514>
- (318) H. Többen, A. Paule, P. Weinmann, T. Wolf, L. Zimmermann, P. Lott, S. Bastian, O. Deutschmann. Formation of N<sub>2</sub>O in the Exhaust Line of Combustion Engines. *SAE Technical Paper* 2023-01-5045 (2023).  
<https://doi.org/10.4271/2023-01-5045>
- (317) A.B. Shirsath, M.L. Schulte, B. Kreitz, S. Tischer, J.-D. Grunwaldt, O. Deutschmann. Spatially-resolved investigation of CO<sub>2</sub> methanation over Ni/γ-Al<sub>2</sub>O<sub>3</sub> and Ni<sub>3.2</sub>Fe/γ-Al<sub>2</sub>O<sub>3</sub> catalysts in a packed-bed reactor. *Chem. Eng. J.* 469 (2023) 143847.  
<https://doi.org/10.1016/j.cej.2023.143847>
- (316) K. Keller, P. Lott, S. Tischer, M. Casapu, J.-D. Grunwaldt, O. Deutschmann. Methane oxidation over PdO: Towards a better understanding of the influence of the support material. *ChemCatChem* 15 (2023) e202300366.  
<https://doi.org/10.1002/cctc.202300366>

(315) L. Wehrle, A. Ashar, O. Deutschmann, R.J. Braun. Modeling High-Power Density Ceria-Based Direct Ammonia Fueled SOFC Stacks for Mobile Applications. *ECS Transactions* 111 (2023) 753-762.  
<https://doi.org/10.1149/11106.0753ecst>

(314) O. Furst, L. Wehrle, D. Schmidler, J. Dailly, O. Deutschmann. Systematic Determination of Optimal Design-Points of Fully Integrated Power-to-SNG Process Chains Via Detailed Simulation of SOEC Stacks. *ECS Transactions* 111 (2023) 1965-1973.  
<https://doi.org/10.1149/11106.1965ecst>

(313) R. Chacko, K. Keller, S. Tischer, A.B. Shirsath, P. Lott, S. Angeli, O. Deutschmann. Automating the optimization of catalytic reaction mechanism parameters using Basin-Hopping: a proof of concept. *Journal of Phys. Chem. C* 127 (2023), 7628–7639.  
<https://doi.org/10.1021/acs.jpcc.2c08179>

(312) A.B. Shirsath, M. Mokashi, P. Lott, H. Müller, R. Pashminehazar, T. Sheppard, S. Tischer, L. Maier, J.-D. Grunwaldt, O. Deutschmann. Soot formation in methane pyrolysis reactor: modeling soot growth and particle characterization. *J. Phys. Chem. A* 127 (2023) 2136–2147.  
<https://doi.org/10.1021/acs.jpca.2c06878>

(311) C. Kuntz, P.J. Jägerfeld, J. Mmbaga, R.E. Hayes, O. Deutschmann. Coupling of Liquid and Surface Chemistry in Urea SCR Systems. *Emission Control Science and Technology* 9 (2023) 77–92.  
<https://doi.org/10.1007/s40825-023-00224-1>

(310) L. Warmuth, P. Lott, O. Deutschmann, C. Feldmann. MOx@VOx-Pd-type Nanorods and Nanotubes as Catalyst Support for Selective Catalytic Reduction of NO. *ChemCatChem* 15 (2023) e202201354.  
<https://doi.org/10.1002/cctc.202201354>

(309) P. Lott, S. Bastian, H. Többen, L. Zimmermann, O. Deutschmann. Formation of nitrous oxide over Pt-Pd oxidation catalysts: Secondary emissions by interaction of hydrocarbons and nitric oxide. *Applied Catalysis A, General* 651 (2023) 119028.  
<https://doi.org/10.1016/j.apcata.2023.119028>

**2022**

(308) S. Hanf, S. Angeli, D. Dussol, C. Fritsch, L. Maier, M. Müller, O. Deutschmann, S. A. Schunk. Methane Dry Reforming, Chapter 9 in Chemical Valorisation of Carbon Dioxide, ed. by G. Stefanidis, A. Stankiewicz. Green Chemistry Series, Vol. 74, The Royal Society of Chemistry, 2022.

<https://doi.org/10.1039/9781839167645>

(307) P. Mishra, H. Gossler, O. Deutschmann. Optimization of operating conditions of an internal combustion engine used as chemical reactor for methane reforming using ozone as an additive. Applications in Energy and Combustion Science 13 (2023) 100109.

<https://doi.org/10.1016/j.jaecs.2022.100109>

(306) P. Lott, M.B. Mokashi, H. Müller, D.J. Heitlinger, S. Lichtenberg, A.B. Shirsath, C. Janzer, S. Tischer, L. Maier, O. Deutschmann. Hydrogen Production and Carbon Capture by Gas Phase Methane Pyrolysis: A Feasibility Study. ChemSusChem 16 (2022) e202201720.

<http://dx.doi.org/10.1002/cssc.202201720>

(305) C. Kuhn, A. Düll, P. Rohlf, S. Tischer, M. Börnhorst, O. Deutschmann. Iron as recyclable energy carrier: Feasibility study and kinetic analysis of iron oxide reduction. Application in Energy and Combustion Science 12 (2022) 100096.

<https://doi.org/10.1016/j.jaecs.2022.100096>

(304) M. Borchers, P. Lott, O. Deutschmann. Selective Catalytic Reduction with Hydrogen for Exhaust gas aftertreatment of Hydrogen Combustion Engines. Topics in Catalysis (2022).

<https://doi.org/10.1007/s11244-022-01723-1>

(303) A. Boubnov, A. Gremminger, M. Casapu, O. Deutschmann, J.-D. Grunwaldt. Dynamics of the Reversible Inhibition during Methane Oxidation on Bimetallic Pd-Pt Catalysts Studied by Modulation-Excitation XAS and DRIFTS. ChemCatChem 14 (2022) e202200573.

<https://doi.org/10.1002/cctc.202200573>

(302) C. Karakaya, M. Kidder, C. Wolden, R.J. Kee, O. Deutschmann. Mechanistic interpretations and insights for the oxidative dehydrogenation of propane via CO<sub>2</sub> over Cr<sub>2</sub>O<sub>3</sub>/Al<sub>2</sub>O<sub>3</sub> catalysts. Ind. Eng. Chem. Res. 61 (2022) 14482–14493.

<https://doi.org/10.1021/acs.iecr.2c02298>

(301) B. Kreitz, P. Lott, J. Bae, K. Blöndal, S. Angeli, Z.W. Ulissi, F. Studt, C.F. Goldsmith, O. Deutschmann. Detailed Microkinetics for the Oxidation of Exhaust Gas Emissions through Automated Mechanism Generation. ACS Catal. 12 (2022) 11137–11151.

<https://doi.org/10.1021/acscatal.2c03378>

(300) H. Gossler, J. Riedel, E. Daymo, R. Chacko, S. Angeli, O. Deutschmann. A New Approach to Research Data Management with a Focus on Traceability: Adacta. Chemie Ingenieur Technik 94 (2022) 1798-1807.

<https://doi.org/10.1002/cite.202200064>

(299) C. Karakaya, E. White, D. Jennings, M. Kidder, O. Deutschmann, R.J. Kee. CO<sub>2</sub> hydrogenation to hydrocarbons over Fe/BZY catalysts. ChemCatChem (2022).

<https://doi.org/10.1002/cctc.202200802>

- (298) J. Pazdera, D. Issayeva, R. Gläser, O. Deutschmann, A. Jentys. Impact of the local environment of amines on the activity for CO<sub>2</sub> hydrogenation over bifunctional basic – metallic catalysts. *ChemCatChem* 14 (2022) e202200620.  
<https://doi.org/10.1002/cctc.202200620>
- (297) K. Keller, S. Wan, M. Borchers, P. Lott, R. Suntz, O. Deutschmann. Treating NO<sub>x</sub> emission of hydrogen fueled combustion engines by NO<sub>x</sub> storage and reduction catalysts: A transient kinetic study including PLIF measurements. *Proc. Combust. Inst.* 39 (2022) 4247-4256.  
<https://doi.org/10.1016/j.proci.2022.07.027>
- (296) P. Lott, O. Deutschmann. Heterogeneous chemical reactions – a cornerstone in emission reduction of local pollutants and greenhouse gases. *Proc. Combust. Inst.* 39 (2022) 3183-3215.  
<https://doi.org/10.1016/j.proci.2022.06.001>
- (295) L. Wehrle, D. Schmider, J. Dailly, A. Banerjee, O. Deutschmann. Benchmarking solid oxide electrolysis cell-stacks for industrial Power-to-Methane systems via hierarchical multi-scale modelling. *Applied Energy* 317 (2022) 119143.  
<https://doi.org/10.1016/j.apenergy.2022.119143>
- (294) S. Wan, K. Keller, P. Lott, A.B. Shirsath, S. Tischer, T. Häber, R. Suntz, O. Deutschmann. Experimental and Numerical Investigation of NO Oxidation on Pt/Al<sub>2</sub>O<sub>3</sub>- and NO<sub>x</sub> Storage on Pt/BaO/Al<sub>2</sub>O<sub>3</sub>-Catalysts. *Catal. Sci. & Technol.* 12 (2022), 4456 – 4470.  
<https://doi.org/10.1039/D2CY00572G>
- (293) M. Eck, P. Lott, D. Schweigert, M. Börnhorst, O. Deutschmann. Spatially resolved measurements of HNCO hydrolysis over SCR catalysts. *Chemie Ingenieur Technik* 94 (2022) 738-746.  
<https://doi.org/10.1002/cite.202100192>
- (292) A. Düll, P. Rohlf, O. Deutschmann, M. Börnhorst. Performance evaluation of KBH<sub>4</sub> as energy carrier for shipping applications. *Chemie Ingenieur Technik* 94 (2022) 747–759.  
<https://doi.org/10.1002/cite.202100193>
- (291) C. Kuntz, H. Weickenmeier, M. Börnhorst, O. Deutschmann. Deposition and decomposition of urea and its by-products on TiO<sub>2</sub> and VWT-SCR catalysts. *International Journal of Heat and Fluid Flow* 95 (2022) 108969.  
<https://doi.org/10.1016/j.ijheatfluidflow.2022.108969>
- (290) J. Chawla, S. Schardt, S. Angeli, P. Lott, S. Tischer, L. Maier, O. Deutschmann. Oxidative Coupling of Methane over Pt/Al<sub>2</sub>O<sub>3</sub> at High Temperature: Multiscale Modeling of the Catalytic Monolith. *Catalysts* 12 (2022) 189.  
<https://doi.org/10.3390/catal12020189>
- (289) S. Wang, P. Rohlf, M. Börnhorst, A. Schillaci, H. Marschall, O. Deutschmann, M. Wörner. Bubble cutting by cylinder - elimination of wettability effects by a separating liquid film. *Chemie Ingenieur Technik* 94 (2022) 385-392.  
<https://doi.org/10.1002/cite.202100145>
- (288) M. Stein, V. Bykov, C. Kuntz, M. Börnhorst, O. Deutschmann, U. Maas. Modelling the decomposition of urea-water-solution in films and droplets under SCR conditions with chemistry in the liquid phase. *International Journal of Heat and Fluid Flow* 94 (2022) 108936.  
<https://doi.org/10.1016/j.ijheatfluidflow.2022.108936>
- (287) E. A. Daymo, M. Hettel, O. Deutschmann, G. D. Wehinger. Accelerating particle-resolved CFD simulations of catalytic fixed-bed reactors with DUO. *Chem. Eng. Sci.* 250 (2022) 117408.  
<https://doi.org/10.1016/j.ces.2021.117408>

(286) P. Lott, U. Wagner, T. Koch, O. Deutschmann. Der Wasserstoffmotor – Chancen und Herausforderungen auf dem Weg zu einer dekarbonisierten Mobilität. Chemie Ingenieur Technik 94 (2022) 217-229.

<https://doi.org/10.1002/cite.202100155>

## 2021

(285) S. Erdogan, T. Schulenberg, O. Deutschmann, M. Wörner. Evaluation of models for bubble-induced turbulence by DNS and utilization in two-fluid model computations of an industrial bubble column: *Chemical Engineering Research and Design* 175 (2021) 283-295.

<https://doi.org/10.1016/j.cherd.2021.09.012>

(284) L. Wehrle, Y. Wang, P. Boldrin, N.P. Brandon, O. Deutschmann, A. Banerjee. Optimizing solid oxide fuel cell performance to re-evaluate its role in the mobility sector. *ACS Environmental Au* 2 (2022) 42-64.

<https://doi.org/10.1021/acsenvironau.1c00014>

(283) M. Börnhorst, O. Deutschmann. Advances and challenges of ammonia delivery by urea-water sprays in SCR systems. *Progress in Energy and Combustion Science* 87 (2021) 100949.

<https://doi.org/10.1016/j.pecs.2021.100949>

(282) L. Wehrle, D. Schmider, J. Dailly, A. Banerjee, O. Deutschmann. Model-Based Optimization of Solid Oxide Electrolysis Cells and Stacks for Power- to-Gas Applications. *ECS Transactions* 103 (2021) 545-554.

<https://doi.org/10.1149/10301.0545ecst>

(281) C. Kuntz, C. Kuhn, H. Weickenmeier, S. Tischer, M. Börnhorst, O. Deutschmann. Kinetic modeling and simulation of high-temperature by-product formation from urea decomposition. *Chem. Eng. Sci.* 246 (2021) 116876.

<https://doi.org/10.1016/j.ces.2021.116876>

(280) S. Gossler, L. Ruwe, W. Yu, J. Yang, X. Chen, S. Schmitt, L. Maier, K. Kohse-Höinghaus, Fei Qi, O. Deutschmann. Exploring the interaction kinetics of butene isomers and NO<sub>x</sub> at low temperatures and diluted conditions. *Combust. Flame* 233 (2021) 111557.

<https://doi.org/10.1016/j.combustflame.2021.111557>

(279) D. Schmider, L. Maier, O. Deutschmann. Reaction Kinetics of CO and CO<sub>2</sub> methanation over nickel. *Ind. & Eng. Chem. Res.* 60 (2021) 5792-5805.

<https://doi.org/10.1021/acs.iecr.1c00389>

(278) C. Wulf, M. Beller, T. Boenisch, O. Deutschmann, S. Hanf, N. Kockmann, R. Kraehnert, M. Oezaslan, S. Palkovits, S. Schimmmler, S.A. Schunk, K. Wagemann, D. Linke. A Unified Research Data Infrastructure for Catalysis Research - Challenges and Concepts. *ChemCatChem* 13 (2021) 3223-3236.

<https://doi.org/10.1002/cctc.202001974>

(277) S. Angeli, S. Gossler, S. Lichtenberg, G. Kass, A. Agrawal, M. Valerius, K. P. Kinzel, O. Deutschmann. Reduction of CO<sub>2</sub> emission from off-gases of steel industry by dry reforming of methane. *Angew. Chemie Intl. Ed.* 60 (2021) 11852-11857.

<https://doi.org/10.1002/anie.202100577>

<https://doi.org/10.1002/ange.202100577>

(276) J. Schütz, H. Störmer, P. Lott, O. Deutschmann. Effects of hydrothermal aging on CO and NO oxidation activity over monometallic and bimetallic Pt-Pd catalysts. *Catalysts* 11 (2021) 300.

<https://doi.org/10.3390/catal11030300>

(275) D. Zengel, M. Stehle, O. Deutschmann, M. Casapu, J.-D. Grunwaldt. Impact of gas phase reactions and catalyst poisons on the NH<sub>3</sub>-SCR activity of a V<sub>2</sub>O<sub>5</sub>-WO<sub>3</sub>/TiO<sub>2</sub> catalyst at pre-turbine position. *Applied Catalysis B: Environmental* 288 (2021) 119991.

<https://doi.org/10.1016/j.apcatb.2021.119991>

(274) F. Maurer, A. Gänzler, P. Lott, B. Betz, M. Votsmeier, S. Loidant, P. Vernoux, V. Murzin, B. Bornmann, R. Frahm, O. Deutschmann, M. Casapu, J.-D. Grunwaldt. Spatiotemporal investigation of the temperature

and structure of a Pt/CeO<sub>2</sub> oxidation catalyst for CO and hydrocarbon oxidation during pulse activation. *Ind. & Eng. Chem. Res.* 60 (2021) 6621-6675.

<https://doi.org/10.1021/acs.iecr.0c05798>

(273) M. Wörner, N. Samkhaniani, X. Cai, Y. Wu, A. Majumdar, H. Marschall, B. Frohnappel, O. Deutschmann. Spreading and rebound dynamics of sub-millimeter urea-water-solution droplets impinging on substrates of varying wettability. *Applied Mathematical Modeling* 95 (2021) 53–73.

<https://doi.org/10.1016/j.apm.2021.01.038>

(272) M. Borchers, K. Keller, P. Lott, O. Deutschmann. Selective catalytic reduction of NO<sub>x</sub> with H<sub>2</sub> for cleaning exhausts of hydrogen engines: Impact of H<sub>2</sub>O, O<sub>2</sub>, and NO/H<sub>2</sub>-ratio. *Ind. & Eng. Chem. Res.* 60 (2021) 6613-6626.

<http://dx.doi.org/10.1021/acs.iecr.0c05630>

(271) A. Abai- Bertóiné, D. Zengel, C. Janzer, L. Maier, J.-D. Grunwaldt, M. Olzmann, O. Deutschmann. Effect of NO<sub>2</sub> on Gas-Phase Reactions in lean NO<sub>x</sub>/NH<sub>3</sub>/O<sub>2</sub>/H<sub>2</sub>O Mixtures at Conditions Relevant for Exhaust Gas Aftertreatment. *SAE Technical Paper* (2021) 2021-01-5005.

<https://doi.org/10.4271/2021-01-5005>



**2020**

(270) C. Ates, M. Börnhorst, R. Koch, M. Eck, O. Deutschmann, H.-J. Bauer. Morphological characterization of urea derived deposits in SCR systems. *Chem. Eng. J.* 409 (2021) 128230.

<https://doi.org/10.1016/j.cej.2020.128230>

(269) M. Woo, L. Maier, S. Tischer, O. Deutschmann, M. Wörner. A qualitative numerical study on catalytic hydrogenation of nitrobenzene in gas-liquid Taylor flow with detailed reaction mechanism. *Fluids* 5 (2021) 234.

<https://doi.org/10.3390/fluids5040234>

(268) P. Lott, O. Deutschmann. Lean-Burn Natural Gas Engines: Challenges and Concepts for an Efficient Exhaust Gas Aftertreatment System. *Emission Control Science and Technology* 7 (2021) 1-6.

<https://doi.org/10.1007/s40825-020-00176-w>

(267) S. Wan, Y. Guo, T. Häber, R. Suntz, O. Deutschmann. Spatially and Temporally Resolved Measurements of NO Adsorption/Desorption over NO<sub>x</sub>-Storage Catalyst. *ChemPhysChem* 21 (2020) 2497-2501.

<https://doi.org/10.1002/cphc.202000765>

(266) A. Giehr, L. Maier, S. Angeli, S.A. Schunk, O. Deutschmann. Dry and Steam Reforming of CH<sub>4</sub> on Co-Hexaaluminate: On the Formation of Metallic Co and Its Influence on Catalyst Activity. *Ind. Eng. Chem. Res.* 59, 42 (2020) 18790-18797.

<https://dx.doi.org/10.1021/acs.iecr.0c03522>

(265) D. Schweigert, B. Damson, H. Lüders, C. Becker, O. Deutschmann. New experimental insights in AdBlue-spray/wall interaction and its impacts on EGT system design. In: M. Bargende, H.C. Reuss, A. Wagner, J. Wiedemann (eds.) 19. Internationales Stuttgarter Symposium. Proceedings. Springer Vieweg, Wiesbaden, 2019.

[https://doi.org/10.1007/978-3-658-25939-6\\_13](https://doi.org/10.1007/978-3-658-25939-6_13)

(264) C. Karakaya, O. Deutschmann, R. J. Kee. Reactive utilization of CO<sub>2</sub> for oxidative dehydrogenation of alkanes to produce olefins. *Chemie Ingenieur Technik* 92 (2020) 1271-1271.

<https://doi.org/10.1002/cite.202055353>

(263) S. Schmitt, S. Schwarz, L. Ruwe, J. Horstmann, F. Sabath, L. Maier, O. Deutschmann, K. Kohse-Höinghaus. Homogeneous conversion of NO<sub>x</sub> and NH<sub>3</sub> with CH<sub>4</sub>, CO, and C<sub>2</sub>H<sub>4</sub> at the diluted conditions of exhaust-gases of lean operated natural gas engines. *International Journal of Chemical Kinetics* 53 (2020) 213-229.

<https://dx.doi.org/10.1002/kin.21435>

(262) M. Woo, S. Tischer, O. Deutschmann, M. Wörner. A step toward the numerical simulation of catalytic hydrogenation of nitrobenzene in Taylor flow at practical conditions. *Chemical Engineering Science* 230 (2021) 116132.

<https://doi.org/10.1016/j.ces.2020.116132>

(261) B. Atakan, S. A. Kaiser, J. Herzler, S. Porras, K. Banke, O. Deutschmann, T. Kasper, M. Fikri, R. Schießl, D. Schröder, C. Rudolph, D. Kaczmarek, H. Gossler, S. Drost, V. Bykovb, U. Maas, C. Schulz. Flexible energy conversion and storage via high-temperature gas-phase reactions: The piston engine as a polygeneration reactor. *Renewable and Sustainable Energy Reviews* 133 (2020) 110264.

<https://doi.org/10.1016/j.rser.2020.110264>

(260) Y. Wang, L. Wehrle, A. Banerjee, Y. Shi, O. Deutschmann. Analysis of a biogas-fed SOFC CHP system based on multi-scale hierarchical modeling. *Renewable Energy* 163 (2021) 78-87.

<https://doi.org/10.1016/j.renene.2020.08.091>

(259) H. Karadeniz, C. Karakaya, S. Tischer, O. Deutschmann. Numerical Simulation of Methane Reforming Over a Porous Rh/Al<sub>2</sub>O<sub>3</sub> Catalyst in Stagnation Flows: Impact of Internal Diffusion on Species Profiles. *Catalysts* 10 (2020) 915.

<https://doi.org/10.3390/catal10080915>

(258) K. Keller, P. Lott, H. Stotz, L. Maier, O. Deutschmann. Microkinetic modeling of the oxidation of methane over PdO catalysts – Towards a better understanding of the water inhibition effect. *Catalysts* 10 (2020) 922.

<https://doi.org/10.3390/catal10080922>

(257) W. Yuan, L. Ruwe, S. Schwarz, C. Cao, J. Yang, O. Deutschmann, K. Kohse-Höinghaus, F. Qi. Insights into the interaction kinetics between propene and NO<sub>x</sub> at moderate temperatures with experimental and modeling methods. *Proceedings of the Combustion Institute* 38 (2021) 795-803.

<https://doi.org/10.1016/j.proci.2020.07.041>

(256) P. Lott, M. Eck, D. Doronkin, A. Zimina, R. Popescu, S. Belin, V. Briois, M. Casapu, J.-D. Grunwaldt, O. Deutschmann. Understanding Sulfur Poisoning of Bimetallic Pd-Pt Methane Oxidation Catalysts and their Regeneration. *Applied Catalysis B: Environmental* 278 (2020) 119244.

<https://doi.org/10.1016/j.apcatb.2020.119244>

(255: en) D. Zengel, P. Koch, B. Torkashvand, J.-D. Grunwaldt, M. Casapu, O. Deutschmann. Emission of toxic HCN during NO<sub>x</sub> removal by ammonia SCR in the exhaust of lean-burn natural gas engines. *Angew. Chem. Int. Ed.* 59 (2020) 14423-14428.

<https://doi.org/10.1002/anie.202003670>

(255: de) Freisetzung von toxischem HCN bei der Stickoxidreduktion mittels NH<sub>3</sub>-SCR in mager betriebenen Erdgasmotoren. *Angew. Chemie* 132 (2020) 14530-14535.

<https://doi.org/10.1002/ange.202003670>

(254) K.A. Karinshak, P. Lott, M.P. Harold, O. Deutschmann. In situ activation of bimetallic Pd-Pt methane oxidation catalysts. *ChemCatChem* 12 (2020) 3712-3720.

<https://dx.doi.org/10.1002/cctc.202000603>

(253) K. Wiranarongkorn, A. Banerjee, O. Deutschmann, A. Arpornwichanop. Performance analysis and temperature gradient of solid oxide fuel cell stacks operated with bio-oil sorption-enhanced steam reforming. *Intl. J. Hydrogen Energy* 45 (2020) 12108-12120.

<https://doi.org/10.1016/j.ijhydene.2020.02.120>

(252) D. Schweigert, B. Damson, H. Lüders, P. Stephan, O. Deutschmann. The effect of wetting characteristics, thermophysical properties, and roughness on spray-wall heat transfer in selective catalytic reduction systems. *International Journal of Heat and Mass Transfer* 52 (2020) 119554.

<https://doi.org/10.1016/j.ijheatmasstransfer.2020.119554>

(251) U. Budziankou, M. Börnhorst, C. Kuntz, O. Deutschmann, T. Lauer. Deposit Formation from Urea Injection: a Comprehensive Modeling Approach. *Emiss. Control Sci. Technol.* 6 (2020) 211-227.

<https://doi.org/10.1007/s40825-020-00159-x>

(250) M. Woo, O. Deutschmann, M. Wörner. Influence of liquid composition on diffusive mass transfer in the lubricating film of Taylor flow - A study related to the hydrogenation of nitrobenzene. *Chemical Engineering & Processing: Process Intensification* 149 (2020) 107835.

<https://doi.org/10.1016/j.cep.2020.107835>

(249) A. Gremminger, J. Phil, M. Casapu, J.-D. Grunwaldt, T. J. Toops, O. Deutschmann. PGM based catalysts for exhaust-gas after-treatment under typical Diesel, gasoline and gas engine conditions with focus on methane and formaldehyde oxidation. *Applied Catalysis B: Environmental* 265 (2020) 118571.

<https://doi.org/10.1016/j.apcatb.2019.118571>

(248) J. Dörnhöfer, M. Börnhorst, C. Ates, N. Samkhaniani, J. Pfeil, M. Wörner, R. Koch, H.-J. Bauer, O. Deutschmann, B. Frohnäpfel, T. Koch. A Holistic View on Urea Injection for NO<sub>x</sub> Emission Control: Impingement, Re-atomization and Deposit Formation. *Emission Control Science and Technology* (2020) 228-243.

<https://doi.org/10.1007/s40825-019-00151-0>

**2019**

(247) S. Wan, T. Häber, R. Suntz, O. Deutschmann. Investigation of HCHO Catalytic Oxidation over Platinum using Planar Laser-induced Fluorescence. *Applied Catalysis B: Environmental* 264 (2020) 118473.

<https://doi.org/10.1016/j.apcatb.2019.118473>

(246) M. Hettel, E. Daymo, T. Schmidt, O. Deutschmann. CFD-Modeling of Fluid Domains with Embedded Monoliths with Emphasis on Automotive Converters. *Chemical Engineering & Processing: Process Intensification* 147 (2020) 107728.

<https://doi.org/10.1016/j.cep.2019.107728>

(245) A.M. Gänzler, M. Casapu, D.E. Doronkin, F. Maurer, P. Lott, P. Glatzel, M. Votsmeier, O. Deutschmann, J.-D. Grunwaldt. Unravelling the Different Reaction Pathways for Low Temperature CO Oxidation on Pt/CeO<sub>2</sub> and Pt/Al<sub>2</sub>O<sub>3</sub> by Spatially Resolved Structure-Activity Correlations. *The Journal of Physical Chemistry Letters* 10 (2019) 7698-7705.

<https://dx.doi.org/10.1021/acs.jpcllett.9b02768>

(244) M. Börnhorst, C. Kuntz, S. Tischer, O. Deutschmann. Urea derived deposits in diesel exhaust gas after-treatment: Integration of urea decomposition kinetics into a CFD simulation. *Chem. Eng. Sci.* 211 (2019) 115319.

<https://doi.org/10.1016/j.ces.2019.115319>

(243) M. Börnhorst, X. Cai, M. Wörner, O. Deutschmann. Maximum spreading of urea water solution during drop impingement. *Chemical Engineering & Technology* 42 (2019) 2419-2427.

<https://doi.org/10.1002/ceat.201800755>

(242) S. Tischer, M. Börnhorst, G. Schoch, O. Deutschmann. Thermodynamics and reaction mechanism of urea decomposition. *Physical Chemistry Chemical Physics* 21 (2019) 16785-16797.

<https://doi.org/10.1039/c9cp01529a>

(241) K. Nishad, M. Stein, F. Ries, V. Bykov, U. Maas, O. Deutschmann, J. Janicka, A. Sadiki. Thermal decomposition of a single AdBlue droplet including wall-film formation in turbulent cross-flow in a SCR system. *Energies* 12 (2019) 2600.

<https://doi.org/10.3390/en12132600>

(240) D. Schweigert, H. Lüders, B. Damson, M. Börnhorst, O. Deutschmann. Heat transfer during spray/wall interaction with urea water solution: an experimental parameter study. *International Journal of Heat and Fluid Flow* 78 (2019) 108432.

<https://doi.org/10.1016/j.ijheatfluidflow.2019.108432>

(239) P. Lott, P. Dolcet, M. Casapu, J.-D. Grunwaldt, O. Deutschmann. The effect of prereduction on the performance of Pd/Al<sub>2</sub>O<sub>3</sub> and Pd/CeO<sub>2</sub> catalysts during methane oxidation. *Industrial & Engineering Chemistry Research* 58 (2019) 12561-12570.

<https://doi.org/10.1021/acs.iecr.9b01267>

(238) Y. Wang, A. Banerjee, L. Wehrle, Y. Shi, N. Brandon, O. Deutschmann. Performance analysis of a reversible solid oxide cell (r-SOC) system based on multi-scale hierarchical SOC modelling. *Energy Conversion and Management* 96 (2019) 484-496.

<https://doi.org/10.1016/j.enconman.2019.05.099>

(237) D.E. Doronkin, F. Benzi, L. Zheng, L. Amidani, P.W. Roesky, M. Casapu, O. Deutschmann, J.-D. Grunwaldt. NH<sub>3</sub>-SCR over V-W/TiO<sub>2</sub> Investigated by Operando X-ray Absorption and Emission Spectroscopy. *J. Phys Chem C* 123 (2019) 23, 14338-14349.

<https://doi.org/10.1021/acs.jpcc.9b00804>

(236) H. Gossler, S. Drost, S. Porras, R. Schießl, U. Maas, O. Deutschmann. The Internal Combustion Engine as a CO<sub>2</sub> Reformer. *Combustion and Flame* 207 (2019) 186-195.

<https://doi.org/10.1016/j.combustflame.2019.05.031>

(235) L. Wehrle, Y. Wan, A. Banerjee, N. Brandon, O. Deutschmann. Dynamic modeling of reversible solid oxide cells (rSOCs). *Chemie Ingenieur Technik* 91 (2019) 833-842.

<https://doi.org/10.1002/cite.201800188>

(234) H. Gossler, L. Maier, S. Angeli, S. Tischer, O. Deutschmann. CaRMEN: An Improved Computer-Aided Method for Developing Catalytic Reaction Mechanisms. *Catalysts* 9 (2019) 227.

<https://doi.org/10.3390/catal9030227>

(233) W. Benzinger, E. Daymo, M. Hettel, L. Maier, C. Antinori, P. Pfeifer, O. Deutschmann. Reverse Water Gas Shift (RWGS) over Ni - Spatially-Resolved Measurements and Simulations. *Chemical Engineering Journal* 362 (2019) 430-441.

<https://doi.org/10.1016/j.cej.2019.01.038>

(232) O. Deutschmann, R. Dittmeyer, J.-D. Grunwaldt, G. Kolb, S. Löbbbecke, G.D. Wehinger. Trendbericht Technische Chemie. *Nachrichten aus der Chemie* 67 (6) (2019) 50-58.

<https://doi.org/10.1002/nadc.20194088095>

(231) D. Demtröder, O. Deutschmann, B. Eck, R. Gläser, L. Goosen, J.-D. Grunwaldt, R. Krähnert, U. Kragl, W. Leitner, G. Mestl, K. Reuter, F. Rosowski, A. Schäfer, M. Scheffler, R. Schlögl, F. Schüth, Stephan A. Schunk, F. Studt, K. Wagemann, C. Wöll. White Paper: The Digitalization of Catalysis-Related Sciences. Frankfurt am Main: German Catalysis Society (GeCatS) (2019).

[https://www.dechema.de/Digitale\\_Katalyse](https://www.dechema.de/Digitale_Katalyse)

**2018**

(230) M. Hettel, M. Wörner, O. Deutschmann. Computational Fluid Dynamics of Catalytic Reactors. Chapter 6-1 in Handbook of Materials Modeling, W. Andreoni, S. Yip (eds.), Springer Nature 2018.

[https://doi.org/10.1007/978-3-319-50257-1\\_6-1](https://doi.org/10.1007/978-3-319-50257-1_6-1)

(229) H. Stotz, L. Maier, A. Boubnov, A.T. Gremminger, J.-D. Grunwaldt, O. Deutschmann. Surface Reaction Kinetics of Methane Oxidation over PdO. Journal of Catalysis 370 (2019) 152-175.

<https://doi.org/10.1016/j.jcat.2018.12.007>

(228) T. Schedlbauer, P. Lott, M. Casapu, H. Störmer, O. Deutschmann, J.-D. Grunwaldt. Impact of the support on the catalytic performance, inhibition effects and SO<sub>2</sub> poisoning resistance of Pt-based formaldehyde oxidation catalysts. Topics in Catalysis 62 (2019) 198-205.

<https://doi.org/10.1007/s11244-018-1122-z>

(227) P. Lott, M. Eck, D.E. Doronkin, R. Popescu, M. Casapu, J.-D. Grunwaldt, O. Deutschmann. Regeneration of sulfur poisoned Pd-Pt/CeO<sub>2</sub>-ZrO<sub>2</sub>-Y<sub>2</sub>O<sub>3</sub>-La<sub>2</sub>O<sub>3</sub> and Pd-Pt/Al<sub>2</sub>O<sub>3</sub> methane oxidation catalysts. Topics in Catalysis 62 (2019) 164-171.

<https://doi.org/10.1007/s11244-018-1121-0>

(226) Y. Wang, A. Banerjee, O. Deutschmann. Dynamic behavior and control strategy study of CO<sub>2</sub>/H<sub>2</sub>O co-electrolysis in solid oxide electrolysis cells. J. Power Sources 412 (2019) 255-264.

<https://doi.org/10.1016/j.jpowsour.2018.11.047>

(225) L. Zheng, M. Casapu, M. Stehle, O. Deutschmann, J.-D. Grunwaldt. Selective catalytic reduction of NO<sub>x</sub> with ammonia and hydrocarbon oxidation over V<sub>2</sub>O<sub>5</sub>-MoO<sub>3</sub>/TiO<sub>2</sub> and V<sub>2</sub>O<sub>5</sub>-WO<sub>3</sub>/TiO<sub>2</sub> SCR catalysts. Topics in Catalysis 62 (2019) 164-171.

<https://doi.org/10.1007/s11244-018-1097-9>

(224) B. Torkashvand, L. Maier; P. Lott; T. Schedlbauer, J.-D. Grunwaldt, O. Deutschmann. Formaldehyde Oxidation Over Platinum: On the Kinetics Relevant to Exhaust Conditions of Lean-Burn Natural Gas Engines. Topics in Catalysis 62 (2019) 206-213.

<https://doi.org/10.1007/s11244-018-1087-y>

(223) B. Torkashvand, L. Maier, T. Schedlbauer, M. Casapu, J.-D. Grunwaldt, O. Deutschmann. On the challenges and constrains of ultra-low emission limits: Formaldehyde oxidation in catalytic sinusoidal-shaped channels. Chem. Eng. Sci. 195 (2019) 841-850.

<https://doi.org/10.1016/j.ces.2018.10.031>

(222) F. Jamshidi, H. Heimel, M. Hasert, X. Cai, O. Deutschmann, H. Marschall, M. Wörner. On suitability of phase-field and algebraic volume-of-fluid OpenFOAM<sup>®</sup> solvers for gas-liquid microfluidic applications. Computer Physics Communications 236 (2019) 72–85.

<https://doi.org/10.1016/j.cpc.2018.10.015>

(221) M. Börnhorst, S. Langheck, H. Weickenmeier, C. Dem, R. Suntz, O. Deutschmann. Characterization of solid deposits from urea water solution injected into a hot gas test rig. Chemical Engineering Journal 377 (2019) 119855.

<https://doi.org/10.1016/j.cej.2018.09.016>

- (220) A. Banerjee, Y. Wang, J. Diercks, O. Deutschmann. Hierarchical Modeling of Solid Oxide Cells and Stacks producing Syngas via H<sub>2</sub>O/CO<sub>2</sub> Co-electrolysis for Industrial Applications. *Appl. Energy* 230 (2018) 996-1013.  
<https://doi.org/10.1016/j.apenergy.2018.08.122>
- (219) B. Torkashvand, P. Lott, D. Zengel, L. Maier, J.-D. Grunwaldt, O. Deutschmann. Homogeneous oxidation of light alkanes in the exhaust of turbocharged lean-burn gas engines. *Chemical Engineering Journal* 377 (2019) 119800.  
<https://doi.org/10.1016/j.cej.2018.08.186>
- (218) T. Schedlbauer, A. Gremminger, M. Casapu, O. Deutschmann, J.-D. Grunwaldt. Impact of the gas mixture and aging conditions on formaldehyde conversion over a series of commercial Pt-based catalysts, SAE Technical Paper 2018-01-5021 (2018).  
<https://doi.org/10.4271/2018-01-5021>
- (217) H. Gossler, L. Maier, S. Angeli, S. Tischer, O. Deutschmann. CaRMeN – A tool for analyzing and deriving kinetics in the real world. *Physical Chemistry Chemical Physics* 20 (2018) 10857-10876.  
<https://doi.org/10.1039/C7CP07777G>
- (216) M. Stein, V. Bykov, A. Bertotiné Abai, C. Janzer, U. Maas, O. Deutschmann, M. Olzmann. A reduced model for the evaporation and decomposition of urea-water solution droplets. *International Journal of Heat and Fluid Flow* 70 (2018) 216-225.  
<https://doi.org/10.1016/j.ijheatfluidflow.2018.02.005>
- (215) V. Kappings, C. Grün, D. Ivannikov, I. Hebeiss, S. Kattge, I. Wendland, B.E. Rapp, M. Hettel, O. Deutschmann, U. Schepers. vasQchip: A novel microfluidic, artificial blood vessel scaffold for vascularized 3D tissues. *Advanced Materials Technologies* (2018) 1700246.  
<https://doi.org/10.1002/admt.201700246>
- (214) M. Hettel, E. Daymo, O. Deutschmann. 3D Modeling of a CPOX-Reformer including Detailed Chemistry and Radiation Effects with DUO. *Computers & Chemical Engineering* 109 (2018) 166-178.  
<https://doi.org/10.1016/j.compchemeng.2017.11.005>
- (213) B. Böck, O. Deutschmann, U. Nieken. Chemie Ingenieur Technik und ACHEMA–Zwei Partner mit langer Tradition. *Chemie Ingenieur Technik* 90 (2018) 747.  
<https://doi.org/10.1002/cite.201870062>
- (212) M. Börnhorst, O. Deutschmann. Single droplet impingement of urea water solution on a heated substrate. *International Journal of Heat and Fluid Flow* 69 (2018) 55-61.  
<https://doi.org/10.1016/j.ijheatfluidflow.2017.10.007>
- (211) A. Giehr, L. Maier, S. Schunk, O. Deutschmann. Thermodynamic considerations on the stability of Co/γ-Al<sub>2</sub>O<sub>3</sub> and Ni/γ-Al<sub>2</sub>O<sub>3</sub> catalysts under dry and steam reforming conditions. *ChemCatChem* 10 (2018) 751-757.  
<https://doi.org/10.1002/cctc.201701376>

**2017**

(210) O. Deutschmann, D. Chatterjee. Modeling of Exhaust-Gas After-Treatment. *Emission Control Science and Technology* 3 (2017) 247-248.

<https://doi.org/10.1007/s40825-017-0077-z>

(209) Spatially Resolved Operando Measurements in Heterogeneous Catalytic Reactors. Eds.: A. Dixon, O. Deutschmann. *Advances in Chemical Engineering*, vol. 50, Elsevier, 2017. ISBN 978-0-12-812589-2.

(208) T. Rammelt, B. Torkashvand, C. Hauck, J. Böhm, R. Gläser, O. Deutschmann, Nitric Oxide Reduction of Heavy-Duty Diesel Off-Gas by NH<sub>3</sub>-SCR in Front of the Turbocharger. *Emission Control Science and Technology* 3 (2017) 275-288.

<https://doi.org/10.1007/s40825-017-0078-y>

(207) S. Kannepalli, A. Gremminger, S. Tischer, O. Deutschmann. Optimization of axial catalyst loading in transient-operated zone-structured monoliths: Reduction of cumulative emissions in automotive oxidation catalysts. *Chem. Eng. Sci.* 174 (2017) 189-202.

<https://doi.org/10.1016/j.ces.2017.09.013>

(206) S. Kannepalli, A. Bürger, S. Tischer, O. Deutschmann. Model based optimization of ammonia dosing in NH<sub>3</sub>-SCR of NO<sub>x</sub> for transient driving cycle: Model development and simulation. *Emission Control Science and Technology* 3 (2017) 249-262.

<https://doi.org/10.1007/s40825-017-0072-4>

(205) M. Woo, M. Wörner, S. Tischer, O. Deutschmann. Validation of a numerical method for interface-resolving simulation of multicomponent gas-liquid mass transfer and evaluation of multicomponent diffusion models. *Heat and Mass Transfer* (2017).

<https://doi.org/10.1007/s00231-017-2145-x>

(204) X. Cai, M. Wörner, H. Marschall, O. Deutschmann. CFD Simulation of Liquid Back Suction and Gas Bubble Formation in a Circular Tube with Sudden or Gradual Expansion. *Emission Control Science and Technology* 3 (2017) 289-301.

<https://doi.org/10.1007/s40825-017-0073-3>

(203) A. Gremminger, P. Lott, M. Merts, M. Casapu, J.-D. Grunwaldt, O. Deutschmann. Sulfur poisoning and regeneration of bimetallic Pd-Pt methane oxidation catalysts. *Applied Catalysis B: Environmental* 218 (2017) 833-843.

<https://doi.org/10.1016/j.apcatb.2017.06.048>

(202) B. Torkashvand, A. Gremminger, S. Valchera, M. Casapu, J.-D. Grunwaldt, O. Deutschmann. The impact of pre-turbine catalyst placement on methane oxidation in lean-burn gas engines: An experimental and numerical study. *SAE Technical Paper* 2017-01-1019 (2017).

<https://dx.doi.org/10.4271/2017-01-1019>

(201) H. Dubbe, J. Schütz, O. Deutschmann, U Nieken. De- and Reactivation Behaviour of Pt/Pd Diesel Oxidation Catalysts. *MTZ worldwide* 78 (6), 72-75.

<https://doi.org/10.1007/s38313-017-0061-6>





**2016**

(200) J.N. Bär, C. Antinori, L. Maier, O. Deutschmann. Catalysts Spatial concentration profiles for the catalytic partial oxidation of jet fuel surrogates in a Rh/Al<sub>2</sub>O<sub>3</sub> coated monolith. *Catalysts* 6 (2016) 207.  
<https://dx.doi.org/10.3390/catal6120207>

(199) A. Banerjee, O. Deutschmann. Elementary Kinetics of the Oxygen Reduction Reaction on LSM-YSZ Composite Cathodes. *Journal of Catalysis* 346 (2017) 30-49.  
<https://dx.doi.org/10.1016/j.jcat.2016.11.035>

(198) C. Karakaya, L. Maier, H. Karadeniz, O. Deutschmann. Surface reaction kinetics of the oxidation and reforming of propane over Rh/Al<sub>2</sub>O<sub>3</sub> catalysts. *ChemCatChem* 9 (2016) 685-695.  
<https://dx.doi.org/10.1002/cctc.201601237>

(197) Y. Wang, H. Zeng, A. Banerjee, Y. Shi, O. Deutschmann, N. Cai. Elementary Reaction Modeling and Experimental Characterization on Methane Partial Oxidation within a Catalyst-Enhanced Porous Media Combustor. *Energy & Fuels* 30 (9) (2016) 7778-7785.  
<https://dx.doi.org/10.1021/acs.energyfuels.6b01624>

(196) M. Hettel, C. Antinori, O. Deutschmann. CFD evaluation of in-situ probe techniques for catalytic honeycomb monoliths. *J. Emission Control Science and Technology* Volume 2, Issue 4 (2016) 188-203.  
<https://dx.doi.org/10.1007/s40825-016-0043-1>

(195) J. Rischard, R. Franz, C. Antinori, O. Deutschmann. Oxidative Dehydrogenation of a C<sub>4</sub> Raffinate-2 towards 1,3-Butadiene in a Two-Zone Fluidized Bed. *Chem. Ing. Tech.* 88 (2016) 1723-1729.  
<https://dx.doi.org/10.1002/cite.201600055>

(194) J. Rischard, R. Franz, C. Antinori, O. Deutschmann. Oxidative dehydrogenation of butenes over Bi-Mo and Mo-V based catalysts in a two-zone fluidized bed reactor. *AIChE J.* 63 (2016) 43-50.  
<https://dx.doi.org/10.1002/aic.15368>

(193) T. Günter, K. Schäfer, J. Pesek, A. Bertótiné Abai, M. Casapu, O. Deutschmann, J.-D. Grunwaldt. Cu-SSZ-13 as pre-turbine NO<sub>x</sub>-removal-catalyst: Impact of pressure and catalyst poisons. *Appl. Catal. B* 198 (2016) 548-557.  
<https://dx.doi.org/10.1016/j.apcatb.2016.06.005>

(192) J. Rink, B. Mozaffari, S. Tischer, O. Deutschmann, M. Votsmeier. Real-time simulation of dual-layer catalytic converters. *Topics in Catalysis* (2016) 1-5.  
<https://dx.doi.org/10.1007/s11244-016-0602-2>

(191) H. Gossler, B. L. Kee, H. Zhu, M. Hettel, O. Deutschmann, R. J. Kee. Flow and pressure characteristics in rectangular channels with internal cylindrical bodies. *Chem Eng. Sci.* 149 (2016) 296-305.  
<https://dx.doi.org/10.1016/j.ces.2016.04.033>

(190) H. Stotz, L. Maier, O. Deutschmann. Methane Oxidation over Palladium: On the Mechanism in Fuel-Rich Methane-Oxygen Mixtures at High Temperatures. *Topics in Catalysis* (2016) 1-27.  
<https://dx.doi.org/10.1007/s11244-016-0717-5>

(189) X. Cai, M. Wörner, H. Marschall, O. Deutschmann. Numerical study on the wettability dependent interaction of a rising bubble with a periodic open cellular structure. *Catalysis Today* 273 (2016) 151-160.

<https://dx.doi.org/10.1016/j.cattod.2016.03.053>

(188) C. Karakaya, L. Maier, O. Deutschmann. Surface reaction kinetics of the oxidation and reforming of CH<sub>4</sub> over Rh/Al<sub>2</sub>O<sub>3</sub> catalysts. *Int. J. Chem. Kinetics* 48 (2016) 144-160.

<https://dx.doi.org/10.1002/kin.20980>

(187) J.N. Bär, M.I. Rocha, E. Jesus de Oliveira, O. Deutschmann. Impact of Sulfur on Catalytic Partial Oxidation of Jet Fuel Surrogates over Rh/Al<sub>2</sub>O<sub>3</sub>. *Int. J. Hydrogen Energy* 41 (2016) 3701-3711.

<https://dx.doi.org/10.1016/j.ijhydene.2015.12.015>

(186) W. Brack, B. Heine, F. Birkhold, M. Kruse, O. Deutschmann. Formation of urea-based deposits in an exhaust system: Numerical predictions and experimental observations on a hot gas test bench. *Emission Control Science and Technology* 2 (2016) 115-123.

<https://dx.doi.org/10.1007/s40825-016-0042-2>

(185) M. Hettel, J.A. Denev, O. Deutschmann. Two-Zone Fluidized Bed Reactors for Butadiene Production: A Multiphysical Approach with Solver Coupling for Supercomputing Application. in W. E. Nagel et al. (eds.), *High Performance Computing in Science and Engineering* 16, 269-280, Springer, Cham. (2016).

[https://doi.org/10.1007/978-3-319-47066-5\\_19](https://doi.org/10.1007/978-3-319-47066-5_19)

## 2015

(184) A. Gremminger, J.-D. Grunwaldt, O. Deutschmann, H.-C. Schwarzer. Untersuchung der Wirkmechanismen bei katalytischer Methanreduktion. *Motortechnische Zeitschrift* 76 (2015) 60.

<https://doi.org/10.1007/s35146-014-2043-4>

(183) A. Zellner, R. Suntz, O. Deutschmann. In-situ investigation of the interaction of surface kinetics with transport processes over catalytic surfaces by planar laser-induced fluorescence. Proc. 7<sup>th</sup> European Combustion Meeting, Budapest, Hungary, 30 March - 2 April 2015.

(182) J. Rischard, C. Antinori, L. Maier, O. Deutschmann. Oxidative Dehydrogenation of n-butane to butadiene with Mo-V-MgO Catalysts in a Two-Zone Fluidized Bed Reactor. *Appl. Catal. A: Gen.* 511 (2016) 26-30.

<https://dx.doi.org/10.1016/j.apcata.2015.11.026>

(181) B. Mozaffari, S. Tischer, M. Votsmeier, O. Deutschmann. A one-dimensional modeling approach for dual-layer monolithic catalysts. *Chem. Eng. Sci.* 139 (2016) 196-210.

<https://dx.doi.org/10.1016/j.ces.2015.09.021>

(180) L. Kunz, F.M. Kuhn, O. Deutschmann. Kinetic Monte Carlo Simulations of Surface Reactions on supported nanoparticles: A novel approach and computer code. *Journal of Chemical Physics* 143 (2015) 044108.

<https://dx.doi.org/10.1063/1.4926924>

(179) H. Gossler, O. Deutschmann. Numerical Optimization and Reaction Flow Analysis of Syngas Production via Partial Oxidation of Natural Gas in Internal Combustion Engines. *International Journal of Hydrogen Energy* 40 (2015) 11046-11058.

<https://dx.doi.org/10.1016/j.ijhydene.2015.06.125>

(178) X. Cai, H. Marschall, M. Wörner, O. Deutschmann. Numerical Simulation of Wetting Phenomena with a Phase-field Method using OpenFOAM. *Chemical Engineering & Technology* 38 (2015) 1985-1992.

<https://dx.doi.org/10.1002/ceat.201500089>

(177) K. Herrera Delgado, H. Stotz, L. Maier, S. Tischer, A. Zellner, O. Deutschmann. Surface Reaction Kinetics of Steam- and CO<sub>2</sub>-Reforming as well as Oxidation of Methane over Nickel-based Catalysts. *Catalysts* 5 (2015) 871-904.

<https://dx.doi.org/10.3390/catal5020871>

(176) E. Japke, M. Casapu, V. Trouillet, O. Deutschmann, J.-D. Grunwaldt. Soot and hydrocarbon oxidation over vanadia-based SCR catalysts. *Catal. Today* 258 (2015) 461-469.

<https://dx.doi.org/10.1016/j.cattod.2015.04.020>

(175) L.A. Schulz, L.C.S. Kahle, K. Herrera Delgado, S. Schunk, A. Jentys, O. Deutschmann, J.A. Lercher. On the coke deposition in dry reforming of methane at elevated pressure. *Appl. Catal. A: Gen.* 504 (2015) 599-607.

<https://dx.doi.org/10.1016/j.apcata.2015.03.002>

(174) V. Menon, A. Banerjee, J. Dailly, O. Deutschmann. Numerical analysis of mass and heat transport in proton-conducting SOFCs with direct internal reforming. *Applied Energy* 149 (2015) 161-175.

<https://dx.doi.org/10.1016/j.apenergy.2015.03.037>

(173) A. T. Gremminger, H. W. Pereira de Carvalho, R. Popescu, J.-D. Grunwaldt, O. Deutschmann. Influence of gas composition on activity and durability of bimetallic Pd-Pt/Al<sub>2</sub>O<sub>3</sub> catalysts for total oxidation of methane. *Catalysis Today* 258 (2015) 470-480.

<https://dx.doi.org/10.1016/j.cattod.2015.01.034>

(172) M. Hettel, C. Diehm, O. Deutschmann. Numerical simulation of a structured catalytic methane reformer by DUO: the new computational interface for OpenFOAM® and DETCHEM™. *Catalysis Today* 258 (2015) 230-240.

<https://dx.doi.org/10.1016/j.cattod.2015.02.011>

(171) H. Karadeniz, C. Karakaya, S. Tischer, O. Deutschmann. Mass transfer effects in stagnation flows on a porous catalyst: Water-Gas-Shift reaction over Rh/Al<sub>2</sub>O<sub>3</sub>. *Zeitschrift f. Phys. Chem.* 229 (2015) 709-737.

<https://dx.doi.org/10.1515/zpch-2014-0622>

(170) A. Zellner, R. Suntz, O. Deutschmann. Two-dimensional spatial resolution of concentration profiles in catalytic reactors by planar laser-induced fluorescence: NO reduction over diesel oxidation catalysts. *Angew. Chemie Int. Ed.* 54 (2015) 2653-2655.

<https://dx.doi.org/10.1002/anie.201410324>

(169) O. Deutschmann. Modeling of the interactions between catalytic surfaces and gas-phase. *Catal. Lett.* 145 (2015) 272-289.

<https://dx.doi.org/10.1007/s10562-014-1431-1>

(168) H. Goßler, O. Deutschmann. Syngas production in piston engines - operating conditions proposed by numerical optimization. Proc. 7<sup>th</sup> European Combustion Meeting, Budapest, Hungary, 30 March - 2 April 2015.

## 2014

(167) M. Hettel, C. Diehm, O. Deutschmann. Answer to the Comment from Goguet et al. to the paper "The Critical evaluation of in situ probe techniques for catalytic honeycomb monoliths" by Hettel et al. *Catalysis Today* 236 (2014) 209-213.

<https://dx.doi.org/10.1016/j.cattod.2014.02.033>

(166) V. Menon, Q. Fu, V.M. Janardhanan, O. Deutschmann. A model-based understanding of solid-oxide electrolysis cells (SOECs) for syngas production by H<sub>2</sub>O/CO<sub>2</sub> co-electrolysis. *J. Power Sources* 274 (2015) 768-781.

<https://dx.doi.org/10.1016/j.jpowsour.2014.09.158>

(165) C. Eßmann, L. Maier, A. Li, S. Tischer, O. Deutschmann. Natural Gas Steam Reforming over Rhodium/Alumina Catalysts: Experimental and Numerical Study of the Carbon Deposition from Ethylene and Carbon Monoxide. *Industrial & Engineering Chemistry Research* 53 (2014) 12270-12278.

<https://dx.doi.org/10.1021/ie5015525>

(164) C. Diehm, O. Deutschmann. Hydrogen Production by Catalytic Partial Oxidation of Methane over Staged Pd/Rh Coated Monoliths: Spatially Resolved Concentration and Temperature Profiles. *International Journal of Hydrogen Energy* 39 (2014) 17998-18004.

<https://dx.doi.org/10.1016/j.ijhydene.2014.06.094>

(163) T. Roussi re, L. Schulz, K.M. Schelkle, G. Wasserschaff, A. Milanov, E. Schwab, O. Deutschmann, A. Jentys, J. Lercher, S. A. Schunk. Structure–Activity Relationships of Nickel–Hexaaluminates in Reforming Reactions Part II: Activity and Stability of Nanostructured Nickel–Hexaaluminate-Based Catalysts in the Dry Reforming of Methane. *ChemCatChem* 6 (2014) 1447-1452.

<https://dx.doi.org/10.1002/cctc.201300958>

(162) T. Roussi re, K.M. Schelkle, S. Titlbach, G. Wasserschaff, A. Milanov, G. Cox, E. Schwab, O. Deutschmann, L. Schulz, A. Jentys, J. Lercher, S. A. Schunk. Structure–Activity Relationships of Nickel–Hexaaluminates in Reforming Reactions Part I: Controlling Nickel Nanoparticle Growth and Phase Formation. *ChemCatChem* 6 (2014) 1438-1446.

<https://dx.doi.org/10.1002/cctc.201300960>

(161) C. Hauck, S. Tischer, L. Maier, O. Deutschmann. Estimation and Modeling of Local Aging Effects of Three-Way-Catalysts by Analysis of Their Spatial Temperature and CO Conversion Profiles. *Canadian J. Chem. Eng.* 92 (2014) 1587-1596.

<https://dx.doi.org/10.1002/cjce.22027>

(160) D. Chan, S. Tischer, J. Heck, C. Diehm, O. Deutschmann Correlation between catalytic activity and catalytic surface area of a Pt/Al<sub>2</sub>O<sub>3</sub> DOC: An experimental and microkinetic modeling study. *Applied Catalysis B: Environmental* 156–157 (2014) 153-165.

<https://dx.doi.org/10.1016/j.apcatb.2014.03.009>

(159) A. Zellner, R. Suntz, O. Deutschmann. In-situ investigations of catalytic gas-phase reactions inside an optically accessible channel reactor. *Chemie Ingenieur Technik* 86 (2014) 538-543.

<https://dx.doi.org/10.1002/cite.201300140>

(158) S. Appari, V. Janardhanan, R. Bauri, S. Jayanti, O. Deutschmann. A Detailed Kinetic Model for Biogas Steam Reforming on Ni and Catalyst Deactivation Due to Sulfur Poisoning. *Appl. Catal. A: Gen.* 471 (2014) 118-125.

<https://dx.doi.org/10.1016/j.apcata.2013.12.002>

(157) W. Brack, B. Heine, F. Birkhold, M. Kruse, G. Schoch, S. Tischer, O. Deutschmann. Kinetic modeling of urea decomposition based on systematic thermogravimetric analysis of urea and its most important by-products. *Chem. Eng. Sci.* 106(2014) 1-8.

<https://dx.doi.org/10.1016/j.ces.2013.11.013>

(156) C. Diehm, H. Karadeniz, C. Karakaya, M. Hettel, O. Deutschmann. Spatial resolution of species and temperature profiles in catalytic reactors: In-situ sampling techniques and CFD modeling. In A.G. Dixon (Ed.) *Modeling and Simulation of Heterogeneous Catalytic Processes. Advances in Chemical Engineering* 45, Academic Press, 2194, 41-95.

<https://doi.org/10.1016/B978-0-12-800422-7.00002-9>

(155) O. Deutschmann. Spezialklasse: Eine spezielle DDR-Nische für (ein wenig mehr) freies Denken. *Cantor-Heft* 16 (2014) 23-26.

[https://www.cantor-vereinigung.uni-halle.de/cantor-hefte/cantor-heft\\_16\\_2014/](https://www.cantor-vereinigung.uni-halle.de/cantor-hefte/cantor-heft_16_2014/)

## 2013

(154) C. Karakaya, R. Otterstätter, L. Maier O. Deutschmann. Kinetics of the water-gas shift reaction over Rh/Al<sub>2</sub>O<sub>3</sub> catalysts. *Appl. Catal. A: Gen.* 470 (2014) 31-44.

<https://dx.doi.org/10.1016/j.apcata.2013.10.030>

(153) V. Menon, V.M. Janardhanan, O. Deutschmann. A mathematical model to analyze solid oxide electrolyzer cells (SOECs) for hydrogen production. *Chem. Eng. Sci.* 110 (2014) 83-93.

<https://dx.doi.org/10.1016/j.ces.2013.10.025>

(152) V. Menon, V. M. Janardhanan, O. Deutschmann. Modeling of Solid-Oxide Electrolyser Cells: From H<sub>2</sub>, CO<sub>2</sub> Electrolysis to Co-Electrolysis. *ECS Transactions* 57 (2013) 3207-3216.

<https://dx.doi.org/10.1149/05701.3207ecst>

(151) V. Menon, V. M. Janardhanan, S. Tischer, O. Deutschmann. Internal Multi-Physics Phenomena of SOFC with Direct Internal Reforming. *ECS Transactions* 57 (2013) 2475-2484.

<https://dx.doi.org/10.1149/05701.2475ecst>

(150) H. Karadeniz, C. Karakaya, S. Tischer, O. Deutschmann. Numerical Modeling of stagnation flows on porous catalytic surfaces: CO oxidation on Rh/Al<sub>2</sub>O<sub>3</sub>. *Chem. Eng. Sci.* 104 (2013) 899-907.

<https://dx.doi.org/10.1016/j.ces.2013.09.038>

(149) D. Livio, C. Diehm, A. Donazzi, A. Beretta, O. Deutschmann. Catalytic Partial Oxidation of Ethanol over Rh/Al<sub>2</sub>O<sub>3</sub>: Spatially Resolved Temperature and Concentration Profiles. *Appl. Catal. A: Gen.* 467 (2013) 530-541.

<https://dx.doi.org/10.1016/j.apcata.2013.07.054>

(148) L.C.S. Kahle, T. Roussière, L. Maier, K. Herrera Delgado, G. Wasserschaff, S.A. Schunk, O. Deutschmann. Methane Dry Reforming at High Temperature and Elevated Pressure: Impact of Gas-Phase Reactions. *Industrial & Engineering Chemistry Research* 52 (2013) 11920-11930.

<https://dx.doi.org/10.1021/ie401048w>

(147) M. Hettel, C. Diehm, B. Torkashvand, O. Deutschmann. Critical Evaluation of In-situ Probe Techniques for Catalytic Honeycomb Monoliths. *Catalysis Today* 216 (2013) 2-10.

<https://dx.doi.org/10.1016/j.cattod.2013.05.005>

(146) K. Hauff, W. Boll, D. Chan, S. Tischer, U. Tuttlies, G. Eigenberger, O. Deutschmann, U. Nieken. Macro- and microkinetic simulation of DOC: effect of aging, noble metal loading and platinum oxidation. *Chemie Ingenieur Technik* 85 (2013) 673-685.

<https://dx.doi.org/10.1002/cite.201200158>

(145) D. Chan, A. Gremminger, O. Deutschmann. Effect of thermal aging on physical and chemical properties of a commercial NO<sub>x</sub>-storage catalyst. *Topics in Catal.* 56 (2013) 293-297.

<https://dx.doi.org/10.1007/s11244-013-9969-5>

(144) W. Zhang, A. Li, B. Reznik, O. Deutschmann. Thermal Expansion of Pyrolytic Carbon with Various Textures. *ZAMM Z. Angew. Math. Mech.* 93 (2013) 338-345.

<https://dx.doi.org/10.1002/zamm.201100132>



(143) O. Deutschmann, J.-D. Grunwaldt. Abgasnachbehandlung in mobilen Systemen: Stand der Technik, Herausforderungen und Perspektiven. *Chemie Ingenieur Technik* 85 (2013) 595-617.

<https://dx.doi.org/10.1002/cite.201200188>

(142) D. Chan, K. Hauff, U. Nieken, O. Deutschmann. Faster Model Calibration for Aged Diesel Oxidation Catalysts and NO<sub>x</sub>-Trap Catalysts. *MTZ* 74 (2013) 54-61.

## 2012

(141) O. Deutschmann, S. Tischer. Numerical simulation of catalytic reactors by molecular-based models. In Model Based Parameter Estimation - Theory and Applications. H.G. Bock, T. Carraro, W. Jaeger, S. Koerkel, R. Rannacher, J.P. Schloeder (Eds.), Springer, Heidelberg, 2013, 227-250.  
[https://doi.org/10.1007/978-3-642-30367-8\\_11](https://doi.org/10.1007/978-3-642-30367-8_11)

(140) O. Deutschmann. Catalytic reforming of logistic fuels at high-temperatures. In Catalysis 24 (2012) 48-82, J.J. Spivey (Ed.), Book Series in Catalysis. RCS Publ.  
<https://dx.doi.org/10.1039/9781849734776>

(139) W. Zhang, B. Reznik, O. Deutschmann. Raman microprobe spectrometry of carbon/carbon composites with differently-textured pyrolytic carbon matrices. ZAMM, Z. Angew. Math. Mech. 93 (2013) 329-337.  
<https://dx.doi.org/10.1002/zamm.201200020>

(138) T. Kaltschmitt, O. Deutschmann, Fuel Processing for Fuel Cells. In Kai Sundmacher (ed.), Fuel Cell Engineering. Advances in Chemical Engineering, Vol. 41, Burlington: Academic Press, 2012, 1-64.  
<https://dx.doi.org/10.1016/B978-0-12-386874-9.00001-4>

(137) O. Deutschmann, D. Chatterjee, R.E. Hayes, M. Votsmeier. Modeling of exhaust-gas after-treatment, preface. Catal. Today 188 (2012) 1.  
<https://dx.doi.org/10.1016/j.cattod.2012.05.032>

(136) C. Karakaya, O. Deutschmann. Kinetics of hydrogen oxidation on Rh/Al<sub>2</sub>O<sub>3</sub> catalysts studied in a stagnation-flow reactor. Chemical Engineering Science 89 (2013) 171-184.  
<https://dx.doi.org/10.1016/j.ces.2012.11.004>

(135) C. Karakaya, O. Deutschmann. A Simple Method for CO Chemisorption Studies under Continuous Flow: Adsorption and Desorption Behavior of Pt/Al<sub>2</sub>O<sub>3</sub> Catalysts. Appl. Catal. A: General 445-446 (2012) 221-230.  
<https://dx.doi.org/10.1016/j.apcata.2012.08.022>

(134) J. Bär, C. Karakaya, O. Deutschmann. Catalytic ignition of light hydrocarbons over Rh/Al<sub>2</sub>O<sub>3</sub> studied in a stagnation point flow reactor. Proc. Combust. Inst. 34 (2013) 2313-2320.  
<https://dx.doi.org/10.1016/j.proci.2012.06.115>

(133) C. Diehm, T. Kaltschmitt, O. Deutschmann. Hydrogen production by partial oxidation of ethanol/gasoline blends over Rh/Al<sub>2</sub>O<sub>3</sub>, Catalysis Today 197 (2012) 90-100.  
<https://dx.doi.org/10.1016/j.cattod.2012.06.032>

(132) S. Dietrich, J.-M. Gebert, G. Stasiuk, A. Wanner, K. A. Weidenmann, O. Deutschmann, I. Tsukrov, R. Piat. Microstructure Characterization of CVI-Densified Carbon/Carbon Composites with Various Fiber Distributions. Composite Science and Technology 72 (2012) 1892-1900.  
<https://dx.doi.org/10.1016/j.compscitech.2012.08.009>

(131) H. Zhu, A. Kromp, A. Leonide, E. Ivers-Tiffée, O. Deutschmann, R. J. Kee. The influence of detailed surface chemistry on solid oxide fuel cell electrochemical impedance spectra. J. Electrochem. Soc. 159 (2012) F255-F266.  
<https://dx.doi.org/10.1149/2.046207jes>

(130) T. Kaltschmitt, C. Diehm, O. Deutschmann. Catalytic partial oxidation of isooctane to hydrogen on rhodium catalysts: effect of tail-gas recycling. *Industrial & Engineering Chemistry Research* 51 (2012) 7536-7546.

<https://dx.doi.org/10.1021/ie201712d>

(129) V. Menon, V.M. Janardhanan, S. Tischer, O. Deutschmann. A Novel Approach to Model Solid-Oxide Fuel Cell Stack. *J. Power Sources* 214 (2012) 227-238.

<https://dx.doi.org/10.1016/j.jpowsour.2012.03.114>

(128) O. Deutschmann. High temperature catalysis: role of heterogeneous, homogeneous, and radical chemistry. Chapter 18 in *Catalysis*, Beller, Renken, van Santen (Eds.), Wiley-VCH Verlag, Weinheim, 2012.

<https://onlinelibrary.wiley.com/doi/pdf/10.1002/9783527671380.fmatter>

(127) V.M. Janardhanan, O. Deutschmann. Computational Fluid Dynamics of Catalytic Reactors. In *Modeling of Heterogeneous Catalytic Reactions: From the molecular process to the technical system*. O. Deutschmann (Ed.), Wiley-VCH, Weinheim 2012.

<https://doi.org/10.1002/9783527639878.ch8>

(126) L. Kunz, L. Maier, S. Tischer, O. Deutschmann. Modeling the Rate of Heterogeneous Reactions. In *Modeling of Heterogeneous Catalytic Reactions: From the molecular process to the technical system*. O. Deutschmann (Ed.), Wiley-VCH, Weinheim 2012.

<https://doi.org/10.1002/9783527639878.ch4>

## 2011

(125) C. Essmann, M. Seipenbusch, T. Schimmel, O. Deutschmann. Coke Formation in Steam Reforming of Natural Gas over Rhodium/Alumina Catalysts: An Atomic Force Microscopy Study using the Oscillating Friction Mode. *Z. Phys. Chem.* 225 (2011) 1207-1224.

<https://dx.doi.org/10.1524/zpch.2011.0160>

(124) V.M. Janardhanan, O. Deutschmann. Modeling diffusion limitation in solid-oxide fuel cells. *Electrochim. Acta* (2011) 9975-9782.

<https://dx.doi.org/10.1016/j.electacta.2011.08.038>

(123) O. Deutschmann. Hochtemperaturkatalyse: Effizientes Verfahren zur chemischen Umwandlung logistischer Kraftstoffe. *Chemie Ingenieur Technik* 83 (2011) 1954-1963.

<https://dx.doi.org/10.1002/cite.201100133>

(122) L. Maier, B. Schädel, K. Herrera Delgado, S. Tischer, O. Deutschmann. Steam Reforming of Methane over Nickel: Development of a Multi-Step Surface Reaction Mechanism. *Topics in Catalysis* 54 (2011) 845-858.

<https://dx.doi.org/10.1007/s11244-011-9702-1>

(121) S. Appari, V.M. Janardhanan, S. Jayanti, L. Maier, S. Tischer, O. Deutschmann. Micro-kinetic modeling of NH<sub>3</sub> decomposition on Ni and its application to solid oxide fuel cells. *Chemical Engineering Science* 66 (2011) 5184-5191.

<https://dx.doi.org/10.1016/j.ces.2011.07.007>

(120) N. M. Mladenov, S. Tischer, O. Deutschmann. Estimation of local aging effects of three-way-catalysts by analysis of their spatial temperature profile in operation. *Chemie Ingenieur Technik* 83 (2011) 1688-1696.

<https://dx.doi.org/10.1002/cite.201100136>

(1119) N.E. McGuire, N.P. Sullivan, O. Deutschmann, H. Zhu, R.J. Kee. Dry reforming of methane in a stagnation-flow reactor using Rh supported on strontium-substituted hexaaluminate. *Appl. Catal. A: General* 394 (2011) 257-265.

<https://dx.doi.org/10.1016/j.apcata.2011.01.009>

(118) S. Prangsri-Aroon, P. Viravathana, W. Bangmek, A. Worayingyong, O. Deutschmann, H. Schulz. Promoted and Un-promoted Co/SiO<sub>2</sub> Fischer-Tropsch Catalysts. *Advanced Materials Research* 287 (2011) 3093-3097.

<https://www.scientific.net/AMR.287-290.3093>

(117) R.J. Behm, Y.E. Seidel, R.W. Lindström, Z. Jusys, U. Wiedwald, P. Ziemann, B. Wickman, B. Kasemo, D. Zhang, O. Deutschmann, J. Boneberg, P. Leiderer. Nanostructured Electrodes – A Tool for Studying Mesoscopic Transport Effects in Electrocatalytic Reactions. In *Nanotechnology – Fundamentals and Applications of Functional Nanostructures*. Th. Schimmel, H. v. Löhneysen, M. Barczewski (Eds.) Baden-Württemberg Stiftung „Research“ Series No. 56, Stuttgart, 2011.

[https://www.bwstiftung.de/uploads/tx\\_news/Nanotechnology2-TOC\\_01.pdf](https://www.bwstiftung.de/uploads/tx_news/Nanotechnology2-TOC_01.pdf)

## 2010

(116) L. Maier, M. Hartmann, S. Tischer, O. Deutschmann. Interaction of heterogeneous and homogeneous kinetics with mass and heat transfer in catalytic reforming of logistic fuels. *Combustion and Flame* 158 (2011) 796-808.

<https://dx.doi.org/10.1016/j.combustflame.2010.11.004>

(115) V. Janardhanan, S. Appari, S. Jayanti, O. Deutschmann. Numerical study of on-board fuel reforming in a catalytic plate reactor for solid-oxide fuel cells. *Chemical Engineering Science* 66 (2011) 490-498.

<https://dx.doi.org/10.1016/j.ces.2010.11.023>

(114) D. Zhang, O. Deutschmann, Y. E. Seidel, R. J. Behm. Interaction of Mass Transport and Reaction Kinetics during Electrocatalytic CO Oxidation in a Thin-Layer Flow Cell. *The Journal of Physical Chemistry* 115 (2011) 468-478.

<https://dx.doi.org/10.1021/jp106967s>

(113) M. Hartmann, L. Maier, O. Deutschmann. Hydrogen production by catalytic partial oxidation of iso-octane at varying flow rate and fuel/oxygen ratio: From detailed kinetics to reactor behavior. *Appl. Catalysis A: General* 391 (2011) 144-152.

<https://dx.doi.org/10.1016/j.apcata.2010.08.051>

(112) A. Li, S. Zhang, B. Reznik, S. Lichtenberg, G. Schoch, O. Deutschmann. Chemistry and Kinetics of Chemical Vapor Deposition of Pyrolytic Carbon from Ethanol. *Proceedings of the Combustion Institute* 33 (2011) 1843-1850.

<https://dx.doi.org/10.1016/j.proci.2010.06.037>

(111) T. Kaltschmitt, L. Maier, C. Hauck, O. Deutschmann. Influence of gas-phase reactions on catalytic reforming of isooctane. *Proceedings of the Combustion Institute* 33 (2011) 3177-3183.

<https://dx.doi.org/10.1016/j.proci.2010.05.050>

(110) N. Hebben, C. Diehm, O. Deutschmann. Catalytic partial oxidation of ethanol on alumina-supported Rh catalysts: an experimental study. *Appl. Catalysis A: General* 388 (2010) 225-231.

<https://dx.doi.org/doi:10.1016/j.apcata.2010.08.055>

(109) W. Boll, S. Tischer, O. Deutschmann. Loading and aging effects in exhaust-gas after-treatment catalysts with Pt as active component. *Ind. Eng. Chem. Res.* 49 (2010) 10303-10310.

<https://dx.doi.org/10.1021/ie100516j>

(108) A. Li, S. Zhang, B. Reznik, S. Lichtenberg, O. Deutschmann. Synthesis of pyrolytic carbon composites using ethanol as precursor. *Industrial & Engineering Chemistry Research* 49 (2010) 10421-10427.

<https://dx.doi.org/10.1021/ie100230b>

(107) J.-M. Gebert, B. Reznik, R. Piat, B. Vierung, K. Weidenmann, A. Wanner, O. Deutschmann. Elastic constants of high-texture pyrolytic carbon measured by ultrasound phase spectroscopy. *Carbon* 48 (2010) 3647-3650.

<https://dx.doi.org/10.1016/j.carbon.2010.06.002>

(106) M. Roos, J. Bansmann, D. Zhang, O. Deutschmann, R.J. Behm. Product gas evolution above planar microstructured model catalysts - A combined scanning mass spectrometry, Monte Carlo and CFD study.

J. Chemical Physics, 133 (2010) 094504. **The Journal of Chemical Physics Editors` Choice for 2010**  
<https://dx.doi.org/10.1063/1.3475518>

(105) M. Hartmann, L. Maier, H.D. Minh, O. Deutschmann. Catalytic Partial Oxidation of Iso-Octane over Rhodium Catalysts: An Experimental, Modeling, and Simulation Study. Combustion and Flame 157 (2010) 1771-1782.  
<https://dx.doi.org/10.1016/j.combustflame.2010.03.005>

(104) Ö. Keskin, M. Wörner, H.S. Soyhan, T. Bauer, O. Deutschmann, R. Lange. Viscous co-current downward Taylor flow in a square minichannel. AIChE J. 56 (2010) 1693-1702.  
<https://dx.doi.org/10.1002/aic.12113>

(103) N. Mladenov, J. Koop, S. Tischer, O. Deutschmann. Modeling of transport and chemistry in channel flows of automotive catalytic converters. Chem. Eng. Sci. 65 (2010) 812-826.  
<https://dx.doi.org/10.1016/j.ces.2009.09.034>

(102) M. Votsmeier, O. Deutschmann. Modellierung und Simulation chemischer Reaktoren: Beispiel Autoabgaskatalyse. Chemie Ingenieur Technik 82 (2010) 1308.  
<https://doi.org/10.1002/cite.201050694>

(101) O. Deutschmann, A.G. Konstandopoulos. Catalytic Technology for Soot and Gaseous Pollution Control. Chapter 18 in Handbook of Combustion, M. Lackner, F. Winter, A. Agarwal (Eds.), Vol. 2: Combustion Diagnostics and Pollutants. 465- 510, Wiley-VCH Verlag, Weinheim, 2010.  
<https://doi.org/10.1002/9783527628148.hoc038>

## 2009

(100) J. Koop, O. Deutschmann. Detailed surface reaction mechanism for Pt-catalyzed abatement of automotive exhaust gases. *Appl. Catal.B: Environmental* 91 (2009) 47-58.

<https://dx.doi.org/10.1016/j.apcatb.2009.05.006>

(99) K. Norinaga, O. Deutschmann, N. Saegusa, J. Hayashi. Analysis of pyrolysis products from light hydrocarbons and kinetic modeling for growth of polycyclic aromatic hydrocarbons with detailed chemistry. *Journal of Analytical and Applied Pyrolysis* 86 (2009) 148-160.

<https://dx.doi.org/10.1016/j.jaap.2009.05.001>

(98) M. Hartmann, T. Kaltschmitt, O. Deutschmann. Catalytic partial oxidation of higher hydrocarbon fuel surrogates on Rh/Al<sub>2</sub>O<sub>3</sub> coated honeycomb monoliths. *Catal.Today* 147 (2009) 204-209.

<https://dx.doi.org/10.1016/j.cattod.2009.07.007>

(97) M. Hartmann, S. Lichtenberg, N. Hebben, D. Zhang, O. Deutschmann. Experimentelle Untersuchung der katalytischen Partialoxidation von Modellkraftstoffen unter definierten Randbedingungen. *Chemie Ingenieur Technik* 81 (2009) 909-919.

<https://dx.doi.org/10.1002/cite.200900011>

(96) J. Thormann, L. Maier, P. Pfeifer, U. Kunz, K. Schubert, O. Deutschmann. Steam Reforming of Hexadecane over a Rh/CeO<sub>2</sub> Catalyst in Microchannels: Experimental and Numerical Investigation. *International J. Hydrogen Energy* 34 (2009) 5108-5120.

<https://dx.doi.org/10.1016/j.ijhydene.2009.04.031>

(95) B.T. Schädel, M. Duisberg, O. Deutschmann. Steam-reforming of methane, ethane, propane, butane and natural gas over a rhodium-based catalyst. *Catalysis Today* 142 (2009) 42-51.

<https://dx.doi.org/10.1016/j.cattod.2009.01.008>

(94) O. Deutschmann, E. J. de Oliveira, H. Wirbser, R. Schießl, U. Maas. Numerical and experimental study of auto-ignition characteristics of ethanol doped gasoline fuel. *Boletim Técnico da Petrobras, Rio de Janeiro*, v. 52, n. 1/3, p. 9-19, 2009.

(93) G. Goldin, H. Zhu, K. Katte, A. Dean, R. Braun, R. Kee, D. Zhang, L. Maier, O. Deutschmann. Coupling Complex Reformer Chemical Kinetics with Three-Dimensional Computational Fluid Dynamics. *ECS Transactions* 25, No 2 (2009) 1253-1262.

<https://doi.org/10.1149/1.3205654>

(92) G. Baldea, L. Maier, M. Hartmann, U. Riedel, O. Deutschmann. Automated mechanism generation and kinetic modeling for partial oxidation of iso-octane. *Proceedings of the 4<sup>th</sup> European Combustion Meeting, Vienna/Austria, April 14-17, 2009.*

(91) O. Deutschmann, H. Knözinger, K. Kochloefl, T. Turek. *Heterogeneous Catalysis and Solid Catalysts*. In *Ullmann's Encyclopedia of Industrial Chemistry, Electronic Release, 7<sup>th</sup> ed.*, Wiley-VCH Verlag, Weinheim, 2009.

[https://doi.org/10.1002/14356007.a05\\_313.pub2](https://doi.org/10.1002/14356007.a05_313.pub2)

## 2008

(90) H.D. Minh, H. G. Bock, S.Tischer, O. Deutschmann. Optimization of Two-Dimensional Flows with Homogeneous and Heterogeneously Catalyzed Gas-Phase Reactions. *AIChE J.* 54 (2008) 2432-2440.

<https://dx.doi.org/10.1002/aic.11563>

(89) A. Li, K. Norinaga, W. Zhang, O. Deutschmann. Modeling and simulation of materials synthesis: Chemical vapor deposition and infiltration of pyrolytic carbon. *Composites Science and Technology* 68 (2008) 1097–1104.

<https://dx.doi.org/10.1016/j.compscitech.2007.07.007>

(88) K. Norinaga, V.M Janardhanan, O. Deutschmann. Detailed Chemical Kinetic Modeling of Prolysis of Ethylene, Acetylene and Propylene at 1073-1373 K with a Plug Flow Reactor Model. *International Journal of Chemical Kinetics* 40 (2008) 199-208.

<https://dx.doi.org/10.1002/kin.20302>

(87) V.M. Janardhanan, V. Heuveline, O. Deutschmann. Three-phase Boundary Length in Solid-Oxide Fuel Cells: A mathematical Model. *J. Power Sources* 178 (2008) 368-372.

<https://dx.doi.org/10.1016/j.jpowsour.2007.11.083>

[Correction](#)

(86) R.U. Khan, S. Bajohr, D. Buchholz, R. Reimert, H.D. Minh, K. Norinaga, V.M. Janardhanan, S. Tischer, O. Deutschmann. Pyrolysis of propane under vacuum carburizing conditions: An experimental and modeling study. *Journal of analytical and Applied Pyrolysis* 81 (2008) 148-156.

<https://dx.doi.org/10.1016/j.jaap.2007.09.012>

(85) H.D. Minh, H.G. Bock, S. Tischer, O. Deutschmann. Fast solution for large-scale for large-scale 2-D convection-diffusion, reacting flows. *Computational Science and its Applications - ICCSA 2008. Lecture Notes in Computer Science* 507, Gervasi, B. Murgante (eds.), 1121-1130, Springer, 2008.

[https://dx.doi.org/10.1007/978-3-540-69839-5\\_85](https://dx.doi.org/10.1007/978-3-540-69839-5_85)

(84) O. Deutschmann. Computational Fluid Dynamics Simulation of Catalytic Reactors. Chapter 6.6 in *Handbook of Heterogeneous Catalysis*, 2<sup>nd</sup> Ed., G. Ertl, H. Knözinger, F. Schüth, J. Weitkamp (eds.), 1811-1828, Wiley-VCH, 2008.

ISBN: 978-3-527-31241-2



## 2007

- (83) J. Koop, O. Deutschmann. Modeling and Simulation of NO<sub>x</sub> Abatement with Storage/Reduction Catalysts for Lean Burn and Diesel Engines. SAE Technical paper 2007-01-1142 (2007).  
<https://doi.org/10.4271/2007-01-1142>
- (82) V.M. Janardhanan, V. Heuveline, O. Deutschmann. Performance Analysis of a SOFC under direct internal reforming conditions. J. Power Sources 177 (2007) 296-307.  
<https://dx.doi.org/10.1016/j.jpowsour.2007.07.008>
- (81) A. Li, G. Schoch, S. Lichtenberg, D. Zhang, O. Deutschmann. A novel CVD/ CVI reactor with an in-situ sampling apparatus connected to an online GC/ MS. Surface & Coatings Technology 201 (2007) 8939-8943.  
<https://dx.doi.org/10.1016/j.surfcoat.2007.05.010>
- (80) A. Li, O. Deutschmann. Transient simulation of chemical vapor infiltration of methane using multi-step reaction and deposition models. Chemical Engineering Science 62 (2007) 4976-4982.  
<https://dx.doi.org/10.1016/j.ces.2007.01.069>
- (79) V.M. Janardhanan, O. Deutschmann. Numerical study of mass and heat transport in solid oxide fuel cells running on humidified methane. Chemical Engineering Science 62 (2007) 5473-5486.  
<https://dx.doi.org/10.1016/j.ces.2007.01.043>
- (78) D. Lysenkov, J. Engstler, A. Dangwal, A. Popp, G. Müller, J.J. Schneider, V.M. Janardhanan, O. Deutschmann, V. Ebert, P. Strauch, J. Wolfrum. Carbon nanotubes anchored on porous alumina. An integrated approach towards formation, process modeling, gas phase analysis and field emission properties. SMALL 3 No.6 (2007) 974-985.  
<https://dx.doi.org/10.1002/sml.200600595>
- (77) K. Norinaga, O. Deutschmann. Detailed Kinetic Modeling of Gas-Phase Reactions in the Chemical Vapor Deposition of Carbon from Light Hydrocarbons. Ind. Eng. Chem. Res. 46 (2007) 3547-3557.  
<https://dx.doi.org/10.1021/ie061207p>
- (76) A. Böttcher, F. Hennrich, H. Rösner, S. Malik, M.M. Kappes, S. Lichtenberg, G. Schoch, O. Deutschmann. Growth of novel carbon phases by methane infiltration of free-standing single-walled carbon nanotube films. Carbon 45 (2007) 1085-1096.  
<https://dx.doi.org/10.1016/j.carbon.2006.12.008>
- (75) F. Birkhold, U. Meingast, P. Wassermann, O. Deutschmann.; Modeling and simulation of the injection of urea-water-solution for automotive SCR DeNO<sub>x</sub>-systems. Appl. Catal. B: Environmental 70 (2007) 119-127.  
<https://dx.doi.org/10.1016/j.apcatb.2005.12.035>
- (74) V.M. Janardhanan, O. Deutschmann. Efficiency Analysis of Planar Solid Oxide Fuel Cell at Direct Internal Reforming Conditions. ECS Transactions 7 (1) (2007) 1939-1943.  
<https://dx.doi.org/10.1149/1.2729306>
- (73) H.-H. Carstensen, A.M. Dean, O. Deutschmann. Rate Constants for the H Abstraction from Alkanes (R-H) by R'O<sub>2</sub>• Radicals: A Systematic Study on the Impact of R and R'. Proc. Combust. Inst. 31 (2007)

149-157.

<https://dx.doi.org/10.1016/j.proci.2006.08.091>

(72) V.M. Janardhanan, O. Deutschmann, Modeling of Solid-Oxide Fuel Cells (invited review), *Zeitschrift f. Phys. Chem.* 221 (2007) 443-479.

<https://dx.doi.org/10.1524/zpch.2007.221.4.443>

(71) B. T. Schädel, O. Deutschmann. Steam Reforming of Natural Gas on Noble-metal Based Catalysts: Predictive Modeling. *Natural Gas Conversion VIII, Studies in Surface Science and Catalysis 167*, M. Schmal, F.B. Noronha, E. F. Sousa-Aguiar (eds.), 207-212, Elsevier, 2007.

[https://dx.doi.org/10.1016/S0167-2991\(07\)80133-9](https://dx.doi.org/10.1016/S0167-2991(07)80133-9)

(70) O. Deutschmann. High temperature catalysis: fundamentals and applications (Invited plenary lecture) *Proceedings of the 3<sup>rd</sup> European Combustion Meeting, ECM 2007, Chania/Crete, Greece, April 11-13, 2007.*

(69) O.R. Inderwildi, D. Starukhin, H.-R. Volpp, D. Lebedez, O. Deutschmann, J. Warnatz. Reaction Processes on Catalytically Active Surfaces. In *Reactive Flows, Diffusion and Transport. From Experiment via Mathematical Modeling to Numerical Simulation and Optimization*, W. Jäger, R. Rannacher, J. Warnatz (eds.), 311-340, Springer, 2007.

[https://doi.org/10.1007/978-3-540-28396-6\\_12](https://doi.org/10.1007/978-3-540-28396-6_12)

(68) H.G. Bock, O. Deutschmann, S. Körkel, L. Maier, H.D. Minh, J.P. Schlöder, S. Tischer, J. Warnatz. Optimization of Reactive Flows in a Single Channel of a Catalytic Monolith: Conversion of Ethane to Ethylene. In *Reactive Flows, Diffusion and Transport. From Experiment via Mathematical Modeling to Numerical Simulation and Optimization*, W. Jäger, R. Rannacher, J. Warnatz (eds.), 291-310, Springer, 2007.

[https://doi.org/10.1007/978-3-540-28396-6\\_11](https://doi.org/10.1007/978-3-540-28396-6_11)

## 2006

(67) R. Quiceno, O. Deutschmann, J. Warnatz, J. Pérez-Ramírez. Rational Modeling of the CPO of methane over platinum gauze: Elementary gas-phase and surface mechanisms coupled with flow simulations. *Catalysis Today* 119 (2007) 311-316.

<https://dx.doi.org/10.1016/j.cattod.2006.08.045>

(66) F. Birkhold, U. Meingast, P. Wassermann, O. Deutschmann. Analysis of the Injection of Urea-water-solution for automotive SCR DeNO<sub>x</sub>-Systems: Modeling of Two-phase Flow and Spray/Wall-Interaction. SAE Technical paper 2006-01-0643, SAE 2006 Transactions Journal of Fuels and Lubricants (2006), 252.

<https://doi.org/10.4271/2006-01-0643>

(65) V.M. Janardhanan, O. Deutschmann. CFD analysis of a solid oxide fuel cell with internal reforming: Coupled interactions of transport, heterogeneous catalysis and electrochemical processes. *Journal of Power Sources* 162 (2006), 1192-1202.

<https://dx.doi.org/10.1016/j.jpowsour.2006.08.017>

(64) K. Norinaga, O. Deutschmann, K.J. Hüttinger. Analysis of gas phase compounds in chemical vapor deposition of carbon from light hydrocarbons. *Carbon* 44 (2006) 1790-1800.

<https://dx.doi.org/10.1016/j.carbon.2005.12.050>

(63) B. Reznik, K. Norinaga, D. Gerthsen, O. Deutschmann. The effect of cooling rate on hydrogen release from a pyrolytic carbon coating and its resulting morphology. *Carbon* 44 (2006) 1330-1333.

<https://dx.doi.org/10.1016/j.carbon.2005.12.014>

(62) R. Quiceno, J. Pérez-Ramírez, J. Warnatz, O. Deutschmann. Modeling the High-Temperature Catalytic Partial Oxidation of Methane over Platinum Gauze. Detailed Gas-Phase and Surface Chemistries Coupled With 3D Flow Field Simulations. *Applied Catalysis A: General* 303 (2006) 166-176.

<https://dx.doi.org/10.1016/j.apcata.2006.01.041>

(61) R. Brück, P. Hirth, W. Maus, O. Deutschmann, N. Mladenov. Fundamentals of „Laminar“ and „Turbulent“ Catalysis; „Turbulent“ beats „Laminar“. Proc. 27<sup>th</sup> International Vienna Motor Symposium, April 27 and 28, 2006.

<https://www.osti.gov/etdeweb/biblio/20773655>

(60) J. Koop, O. Deutschmann, V. Schmeißer, U. Tuttlies, G. Eigenberger, U. Nieken. Modellierung und Simulation der NO<sub>x</sub>-Minderung an Speicherkatalysatoren in sauerstoffreichen Abgasen. *Chemie Ingenieur Technik*, Volume 78, Issue 9 (2006) 1247-1247.

<https://doi.org/10.1002/cite.200650229>

## 2005

(59) O.R. Inderwildi, D. Lebiedz, O. Deutschmann, J. Warnatz. Influence of Coadsorbates on the NO Dissociation on a Rhodium(311). *Surface. Chem. Phys. Chem.* 6 (2005) 2513-2521.

<https://dx.doi.org/10.1002/cphc.200500222>

(58) E. Hecht, G.K. Gupta, H. Zhu. A.M. Dean, R.J. Kee, L. Maier, O. Deutschmann. Methane Reforming Kinetics within a Ni-YSZ SOFC Anode Support. *Applied Catalysis A: General* 295 (2005) 40-51.

<https://dx.doi.org/10.1016/j.apcata.2005.08.003>

(57) S. Tischer, O. Deutschmann. Recent Advances in Numerical Modeling of Catalytic Monolith Reactors. *Catalysis Today* 105 (2005) 407-413.

<https://dx.doi.org/10.1016/j.cattod.2005.06.061>

(56) O.R. Inderwildi, D. Lebiedz, O. Deutschmann, J. Warnatz. Influence of initial oxygen coverage and magnetic moment on the NO decomposition on Rhodium (111). *J. Chem. Phys.* 122 (2005) 154702.

<https://dx.doi.org/10.1063/1.1878692>

(55) O.R. Inderwildi, D. Lebiedz, O. Deutschmann, J. Warnatz.; Coverage Dependence of Oxygen Decomposition and Surface Diffusion on Rhodium (111): A DFT Study. *J. Chem. Phys.* 122 (2005) 034710.

<https://dx.doi.org/10.1063/1.1835891>

(54) H. Zhu, R. J. Kee, V.M. Janardhanan, O. Deutschmann, D.G. Goodwin. Modeling Elementary Heterogeneous Chemistry and Electrochemistry in Solid-Oxide Fuel Cells. *J. Electrochemical Soc.* 152 (2005) A2427-A2440.

<https://dx.doi.org/10.1149/1.2116607>

[Correction](#)

## 2004

(53) R. Schwiedernoch, O. Deutschmann, L.D. Schmidt. Wasserstoffherstellung aus Kohlenwasserstoffen durch Hochtemperaturkatalyse. *Chemie Ingenieur Technik* 76 (9) (2004), 1268.

<https://doi.org/10.1002/cite.200490119>

(52) M. Bizzi, R. Schwiedernoch, O. Deutschmann, G. Saracco. Modeling the Partial Oxidation of Methane in a Fixed Bed with Detailed Chemistry. *AIChE J.* 50 (2004) 1289-1299.

<https://dx.doi.org/10.1002/aic.10118>

(51) R. Schwiedernoch, S. Tischer, H.-R. Volpp, O. Deutschmann. Towards a better understanding of transient processes in catalytic oxidation reactors. *Natural Gas Conversion VI, Studies in Surface Science and Catalysis* 147, Xinhe Bao, Yide Xu (eds.), 511-516, Elsevier, 2004.

[https://dx.doi.org/10.1016/S0167-2991\(04\)80103-4](https://dx.doi.org/10.1016/S0167-2991(04)80103-4)

(50) O. Deutschmann. Vom molekularen Prozess zur chemischen Technik: Detaillierte Modellierung komplexer Reaktionssysteme. *DECHEMA Tätigkeitsbericht* 2004, 12-19.

<https://idw-online.de/en/news90382>

## 2003

(49) Z.R. Ismagilov, M.A. Kerzhentsev, V.A. Sazonov, L.T. Tsykoza, N.V. Shikina, V.V. Kuznetsov, V.A. Ushakov, S.V. Mishanin, N.G. Kozhukhar, G. Russo, O.Deutschmann. Study of Catalyts for Catalytic Burners for Fuel Cell Power Plant Reformers. Korean J. Chem. Eng. 20 (2003) 461-467.

<https://dx.doi.org/10.1007/BF02705548>

(48) R. Schwiedernoch, S. Tischer, C. Correa, O. Deutschmann. Experimental and numerical study on the transient behavior of partial oxidation of methane in a catalytic monolith. Chem. Eng. Sci. 58 (2003), 633-642.

[https://dx.doi.org/10.1016/S0009-2509\(02\)00589-4](https://dx.doi.org/10.1016/S0009-2509(02)00589-4)

(47) T. Zech, J. Klein, S.A. Schunk, T. Johann, F. Schüth, S. Kleditzsch, O. Deutschmann. Miniaturized Reactor Concepts and Advanced Analysis for Primary Screening in High-Throughput Experimentation. Chapter 23 in High Throughput Analysis: A Tool for Combinatorial Material Science, Potyrailo, Amis (eds.), 491-523, Kluwer Academic Publisher, 2003.

[https://doi.org/10.1007/978-1-4419-8989-5\\_23](https://doi.org/10.1007/978-1-4419-8989-5_23)

(46) J. Windmann, J. Braun, P. Zacke, D. Chatterjee, O. Deutschmann, J. Warnatz. Impact of the Inlet Flow Distribution on the Light-Off Behavior of a 3-Way Catalytic Converter. SAE Technical paper 2003-01-0937 (2003).

<https://doi.org/10.4271/2003-01-0937>

## 2002

(45) J. Braun, T. Hauber, H. Többen, J. Windmann, P. Zacke, D. Chatterjee, C. Correa, O. Deutschmann, L. Maier, S. Tischer, J. Warnatz. Three-Dimensional Simulation of the Transient Behavior of a Three-Way Catalytic Converter. SAE Technical paper 2002-01-0065 (2002).

<https://doi.org/10.4271/2002-01-0065>

(44) R. P. O'Connor, L.D. Schmidt, O. Deutschmann. Simulating Cyclohexane Millisecond Oxidation: Coupled Chemistry and Fluid Dynamics. AIChE J. 48 (2002) 1241-1256.

<https://dx.doi.org/10.1002/aic.690480611>

(43) R. Schwiedernoch, S. Tischer, C. Correa, O. Deutschmann, J. Warnatz. Experimental and numerical investigation of the ignition of methane combustion in a platinum-coated honeycomb monolith. Proc. Combust. Inst. 29 (2002) 1005-1011.

[https://dx.doi.org/10.1016/S1540-7489\(02\)80127-4](https://dx.doi.org/10.1016/S1540-7489(02)80127-4)

(42) T. Pery, M.G. Schweitzer, H.-R. Volpp, J. Wolfrum, L. Ciossu, O. Deutschmann, J. Warnatz. Sum-Frequency Generation In Situ Study of CO Adsorption and Catalytic CO Oxidation on Rhodium at Elevated Pressures. Proc. Combust. Inst. 29 (2002) 973-980.

[https://dx.doi.org/10.1016/S1540-7489\(02\)80123-7](https://dx.doi.org/10.1016/S1540-7489(02)80123-7)

(41) K. Maruta, K. Takeda, J. Ahn, K. Borer, L. Sitzki, P. D. Ronney, O. Deutschmann. Extinction Limits of Catalytic Combustion in Microchannels. Proc. Combust. Inst. 29 (2002) 957-963.

[https://dx.doi.org/10.1016/S1540-7489\(02\)80121-3](https://dx.doi.org/10.1016/S1540-7489(02)80121-3)

(40) O. Deutschmann, J. Warnatz. Diagnostics for Catalytic Combustion. Chapter 20 in Applied Combustion Diagnostics, K. Kohse-Hoeinghaus, J.B. Jeffries (eds.), 518-533, Taylor and Francis Publ., 2002. ISBN 1-56032-913-0.

## 2001

(39) S. Tischer, C. Correa, O. Deutschmann. Transient three-dimensional simulation of a catalytic combustion monolith using detailed models for heterogeneous and homogeneous reactions and transport phenomena. *Catalysis Today* 69 (2001) 57-62.

[https://dx.doi.org/10.1016/S0920-5861\(01\)00355-8](https://dx.doi.org/10.1016/S0920-5861(01)00355-8)

(38) J. M. Redenius, L.D. Schmidt, O. Deutschmann. Millisecond Catalytic Wall Reactors: I. Radiant Burner. *AIChE J.* 47 (2001) 1177-1184.

<https://dx.doi.org/10.1002/aic.690470523>

(37) G. Miessen, F. Behrendt, O. Deutschmann, J. Warnatz. Numerical Studies of the Heterogeneous Combustion of Char Particles Using Detailed Chemistry. *Chemosphere* 42 (2001) 609-613.

[https://doi.org/10.1016/S0045-6535\(00\)00234-4](https://doi.org/10.1016/S0045-6535(00)00234-4)

(36) D. Chatterjee, O. Deutschmann, J. Warnatz. Detailed surface reaction mechanism in a three-way catalyst. *Faraday Discussions* 119 (2001) 371-384.

<https://dx.doi.org/10.1039/b101968f>

(35) O. Deutschmann, R. Schwiedernoch, L.I. Maier, D. Chatterjee. Natural Gas Conversion in Monolithic Catalysts: Interaction of Chemical Reactions and Transport Phenomena. In *Natural Gas Conversion VI, Studies in Surface Science and Catalysis* 136, E. Iglesia, J.J. Spivey, T.H. Fleisch (eds.), 251-258, Elsevier, 2001.

[https://doi.org/10.1016/S0167-2991\(01\)80312-8](https://doi.org/10.1016/S0167-2991(01)80312-8)



**2000**

(34) D. K. Zerkle, M.D. Allendorf, M. Wolf, O. Deutschmann. Understanding Homogeneous and Heterogeneous Contributions to the Platinum-Catalyzed Partial Oxidation of Ethane in a Short Contact Time Reactor. *J. Catal.* 196 (2000) 18-39.

<https://dx.doi.org/10.1006/jcat.2000.3009>

(33) O. Deutschmann, L. Maier, U. Riedel, A. H. Stroemann, R. W. Dibble. Hydrogen Assisted Catalytic Combustion of Methane on Platinum. *Catalysis Today* 59 (2000) 141-150.

[https://dx.doi.org/10.1016/S0920-5861\(00\)00279-0](https://dx.doi.org/10.1016/S0920-5861(00)00279-0)

(32) L. L. Raja, R. J. Kee, O. Deutschmann, J. Warnatz, L. D. Schmidt. A Critical Evaluation of Navier-Stokes, Boundary-Layer, and Plug-Flow Models for the Simulation of Flow and Chemistry in a Catalytic Combustion Honeycomb Channel. *Catalysis Today* 59 (2000) 47-60.

[https://dx.doi.org/10.1016/S0920-5861\(00\)00271-6](https://dx.doi.org/10.1016/S0920-5861(00)00271-6)

(31) M. von Schwerin, O. Deutschmann, V. Schulz. Process Optimization of Reactive Systems by Partially Reduced SQP Methods. *Computers & Chemical Engineering* 24 (2000) 89-97.

[https://dx.doi.org/10.1016/S0098-1354\(00\)00305-7](https://dx.doi.org/10.1016/S0098-1354(00)00305-7)

(30) C. Taut, C. Correa, O. Deutschmann, J. Warnatz, S. Einicke, C. Schulz, J. Wolfrum.; Three-dimensional Modeling with Monte-Carlo-Probability Density Function Methods and Laser Diagnostics of the Combustion in a Two-Stroke-Engine. *Proc. Combust. Inst.* 28 (2000) 1153-1159.

[https://dx.doi.org/10.1016/S0082-0784\(00\)80325-2](https://dx.doi.org/10.1016/S0082-0784(00)80325-2)

(29) B. Ruf, F. Behrendt, O. Deutschmann, S. Kleditzsch, J. Warnatz. Modeling of Chemical Vapor Deposition of Diamond Films from Acetylene-Oxygen Flames. *Proc. Combust. Inst.* 28 (2000) 1455-1461.

[https://dx.doi.org/10.1016/S0082-0784\(00\)80362-8](https://dx.doi.org/10.1016/S0082-0784(00)80362-8)

(28) D. K. Zerkle, M. D. Allendorf, M. Wolf, O. Deutschmann. Modeling of On-Line Catalyst Addition Effects in a Short Contact Time Reactor. *Proc. Combust. Inst.* 28 (2000) 1365-1372.

[https://dx.doi.org/10.1016/S0082-0784\(00\)80351-3](https://dx.doi.org/10.1016/S0082-0784(00)80351-3)

(27) O. Deutschmann. Nutzung detaillierter chemischer Reaktionsmodelle in CFD-Berechnungen. *Chemie Ingenieur Technik* 72 (2000) 987-988.

(26) J. Braun, T. Hauber, H. Többen, P. Zacke, D. Chatterjee, O. Deutschmann, J. Warnatz. Influence of Physical and Chemical Parameters on the Conversion Rate of a Catalytic Converter: A Numerical Simulation Study. *SAE Technical paper* 2000-01-0211 (2000).

<https://doi.org/10.4271/2000-01-0211>

## 1999 and before

(25) M. Wolf, O. Deutschmann, F. Behrendt, J. Warnatz. Kinetic Model of an Oxygen-free Methane Conversion on a Platinum Catalyst. *Catalysis Letters* 61 (1999) 15-25.

<https://dx.doi.org/10.1023/A:1019039931310>

(24) O. Deutschmann, L.D. Schmidt, J. Warnatz. Simulation of Reactive Flow in a Partial Oxidation Reactor with Detailed Gas Phase and Surface Chemistry Models. In: *Scientific Computing in Chemical Engineering II. Computational Fluid Dynamics, Reaction Engineering, and Molecular Properties*. F. Keil, W. Mackens, H. Voß, J. Werther (eds.), 368-375, Springer, Berlin, Heidelberg, 1999.

ISBN 978-3-642-60185-9.

[https://doi.org/10.1007/978-3-642-60185-9\\_43](https://doi.org/10.1007/978-3-642-60185-9_43)

(23) V. Schulz, O. Deutschmann. Process Optimization of Reactive Systems Modeled by Elementary Reactions. In: *Scientific Computing in Chemical Engineering II. Simulation, Image Processing, Optimization, and Control*. F. Keil, W. Mackens, H. Voß, J. Werther (eds.), 354-361, Springer, Berlin, Heidelberg, 1999.

ISBN 978-3-540-65851-1.

(22) O. Deutschmann, F. Behrendt, and J. Warnatz. Formal Treatment of Catalytic Combustion and Catalytic Conversion of Methane. *Catalysis Today* 46 (1998) 155-163.

[https://dx.doi.org/10.1016/S0920-5861\(98\)00337-X](https://dx.doi.org/10.1016/S0920-5861(98)00337-X)

(21) O. Deutschmann and L. D. Schmidt. Modeling the Partial Oxidation of Methane in a Short Contact Time Reactor. *AIChE J.* 44 (1998) 2465-2476.

<https://dx.doi.org/10.1002/aic.690441114>

(20) M. Wolf, O. Deutschmann, F. Behrendt, J. Warnatz. Simulation of the Oxygen-free Methane Conversion to Higher Hydrocarbon Fuels Using a Platinum Catalyst with a Catalytically Active Carbonaceous Overlayer. *Natural Gas Conversion V, Studies in Surface Science and Catalysis* 119, 271-276, Elsevier, 1998.

(19) L. D. Schmidt, O. Deutschmann, and C. T. Goralski, Jr.. Modeling the Partial Oxidation of Methane to Syngas at Millisecond Contact Times. *Natural Gas Conversion V, Studies in Surface Science and Catalysis* 119, 685-692, Elsevier, 1998.

[https://dx.doi.org/10.1016/S0167-2991\(98\)80511-9](https://dx.doi.org/10.1016/S0167-2991(98)80511-9)

(18) O. Deutschmann and L. D. Schmidt. Two-Dimensional Modeling of Partial Oxidation of Methane on Rhodium in a Short Contact Time Reactor. *Twenty-Seventh Symposium (International) on Combustion*, 2283-2291, Pittsburgh, 1998.

[https://dx.doi.org/10.1016/S0082-0784\(98\)80078-7](https://dx.doi.org/10.1016/S0082-0784(98)80078-7)

(17) O. Deutschmann, J. Warnatz. Modeling of Catalytic Combustion and Conversion of Methane. *Proceedings of the 1998 International Gas Research Conference*, 717-728, Gas Research Institute, Chicago, 1998.

(16) M. Rinnemo, O. Deutschmann, F. Behrendt, B. Kasemo, Experimental and Numerical Investigation of the Catalytic Ignition of Mixtures of Hydrogen and Oxygen on Platinum. *Combust. Flame* 111 (1997) 312-326.

[https://dx.doi.org/10.1016/S0010-2180\(97\)00002-3](https://dx.doi.org/10.1016/S0010-2180(97)00002-3)

- (15) V. Zumbach, J. Schäfer, J. Tobai, M. Ridder, T. Dreier, T. Schaich, J. Wolfrum, B. Ruf, F. Behrendt, O. Deutschmann, and J. Warnatz. Experimental investigation and computational modeling of hot filament diamond chemical vapor deposition. *J. Chem. Phys.* 107 (1997), 5918-5928.  
<https://dx.doi.org/10.1063/1.474317>
- (14) F. Behrendt, R. Schmidt, O. Deutschmann, I. Weber, B. Mewes, P. Kasasl, D. Brüggemann. Vergleichende experimentelle und numerische Untersuchungen zur Oxidation an katalytisch aktiven Oberflächen. *VDI-Berichte* 1313 (1997) 443-448.
- (13) F. Behrendt, O. Deutschmann, B. Ruf, R. Schmidt, J. Warnatz. Simulation of Heterogeneous Reaction Systems. In *Gas phase chemical reaction systems: experiment and models, 100 years after Max Bodenstein*, J. Wolfrum, H.-R. Volpp, R. Rannacher, J. Warnatz (eds.), 265-278, Springer Series in Chemical Physics, 1996.  
[https://doi.org/10.1007/978-3-642-80299-7\\_21](https://doi.org/10.1007/978-3-642-80299-7_21)
- (12) B. Ruf, F. Behrendt, O. Deutschmann, J. Warnatz. Simulation of Homoepitaxial Growth on the Diamond (100)-Surface in a Hot Filament CVD-Reactor using Detailed Reaction Mechanisms. *Surf. Sci.* 352-354 (1996) 602-606.  
[https://dx.doi.org/10.1016/0039-6028\(95\)01210-9](https://dx.doi.org/10.1016/0039-6028(95)01210-9)
- (11) B. Ruf, F. Behrendt, O. Deutschmann, J. Warnatz. Simulation of Reactive Flow in Filament-Assisted Diamond Growth Including Hydrogen Surface Chemistry. *J. Appl. Phys.* 79 (1996) 7256-7263.  
<https://dx.doi.org/10.1063/1.362672>
- (10) F. Behrendt, O. Deutschmann, B. Ruf, J. Warnatz. Numerical study of apparent activation energies of diamond growth rates in hot filament chemical vapor deposition systems. *J. Vac. Sci. Technol. A* 14 (1996) 1604-1608.  
<https://dx.doi.org/10.1116/1.580304>
- (9) F. Behrendt, O. Deutschmann, R. Schmidt, J. Warnatz. Investigation of Ignition and Extinction of Hydrogen-Air and Methane-Air Mixtures over Platinum and Palladium. Chapter 4 in: *Heterogeneous Hydrocarbon Oxidation*, 48-57, ACS Symposium Series, 1996.  
<https://dx.doi.org/10.1021/bk-1996-0638.ch004>
- (8) O. Deutschmann, R. Schmidt, F. Behrendt, J. Warnatz. Numerical Modeling of Catalytic Ignition. *Proc. Combust. Inst.* 26 (1996) 1747-1754.  
[https://dx.doi.org/10.1016/S0082-0784\(96\)80400-0](https://dx.doi.org/10.1016/S0082-0784(96)80400-0)
- (7) O. Deutschmann, R. Schmidt, F. Behrendt. Interaction of Transport and Chemical Kinetics in Catalytic Combustion of H<sub>2</sub>/O<sub>2</sub> Mixtures on Pt. *Proceedings of the 8<sup>th</sup> International Symposium on Transport Phenomena in Combustion*, 166-175, Taylor and Francis Publ., 1996.
- (6) F. Behrendt, O. Deutschmann, U. Maas, J. Warnatz. Simulation and Sensitivity Analysis of the Heterogeneous Oxidation of Methane on a Platinum Foil. *J. Vac. Sci. Technol. A* 13 (1995), 1373-1377.  
<https://dx.doi.org/10.1116/1.579566>
- (5) O. Deutschmann, U. Riedel, J. Warnatz. Modeling of Nitrogen and Oxygen Recombination on Partial Catalytic Surfaces. *ASME Journal of Heat Transfer* 117 (1995), 495-501.  
<https://dx.doi.org/10.1115/1.2822549>

(4) O. Deutschmann, U. Riedel, J. Warnatz. Modelling of Surface Reactions in Hypersonic Re-Entry Flow Fields. Proc. Second European Symposium on Aerothermodynamics for Space Vehicles, ESA SP-367 (1995), 305-310.

<https://adsabs.harvard.edu/full/1995esasp.367..305d>

(3) O. Deutschmann, F. Behrendt, J. Warnatz. Modelling and Simulation of Heterogeneous Oxidation of Methane on a Platinum Foil. Catalysis Today 21 (1994), 461-470.

[https://dx.doi.org/10.1016/0920-5861\(94\)80168-1](https://dx.doi.org/10.1016/0920-5861(94)80168-1)

(2) O. Deutschmann, J. Warnatz, M.D. Allendorf, R.J. Kee, M.E. Coltrin. Modeling and Simulation of Hydrogen-Oxygen Combustion on Platinum Catalyst. Proc. International Conference on Energy Efficiency in Process Technology, P. A. Pilavachi (ed.), 862-871, Elsevier Applied Science, London, 1993.

ISBN: 978-1-858-61019-1.

(1) O. Deutschmann. Turbulence and Chaotic Dynamics in Combustion Theory. Acta Astronautica 28 (1992) 419-424.

[https://dx.doi.org/10.1016/0094-5765\(92\)90046-L](https://dx.doi.org/10.1016/0094-5765(92)90046-L)