

Development of an unified surface reaction mechanism of oxidation and reforming reactions of light hydrocarbons over platinum

 Lea Burger¹, Lubov Maier², Olaf Deutschmann^{1,2}

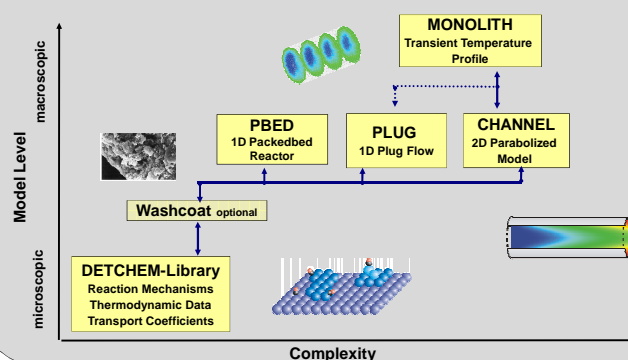
lea.burger@kit.edu

Introduction

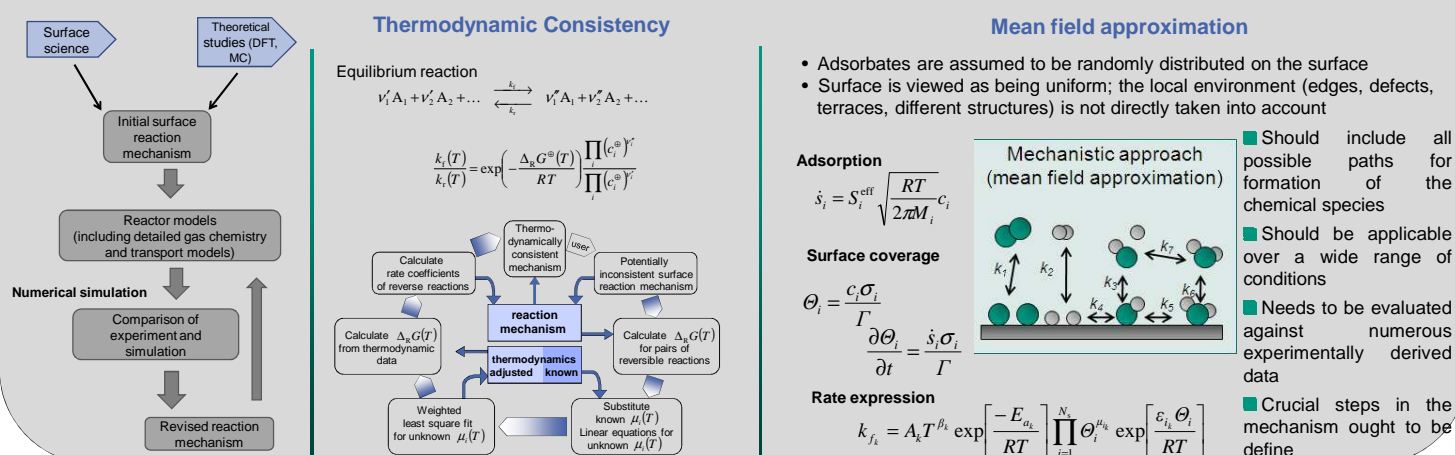
Reforming and partial oxidation of hydrocarbons [1,2], combustion of natural gas [3,4], and the reduction of pollutant emissions from automobiles [5] are important examples for catalytic reactions over platinum.

The application of reliable and predictive modeling of technical reactors used by CFD simulations calls for a better understanding of the kinetics and elementary-step reactions. A detailed surface mechanism is developed against numerous experimentally derived data. The software DETCHEM [6] was applied for numerical simulation. Steady state and transient models of packed bed, channel and monolithic reactors have been evaluated concerning their ability to describe laboratory experiments specific.

Numerical Model, DETCHEM Package

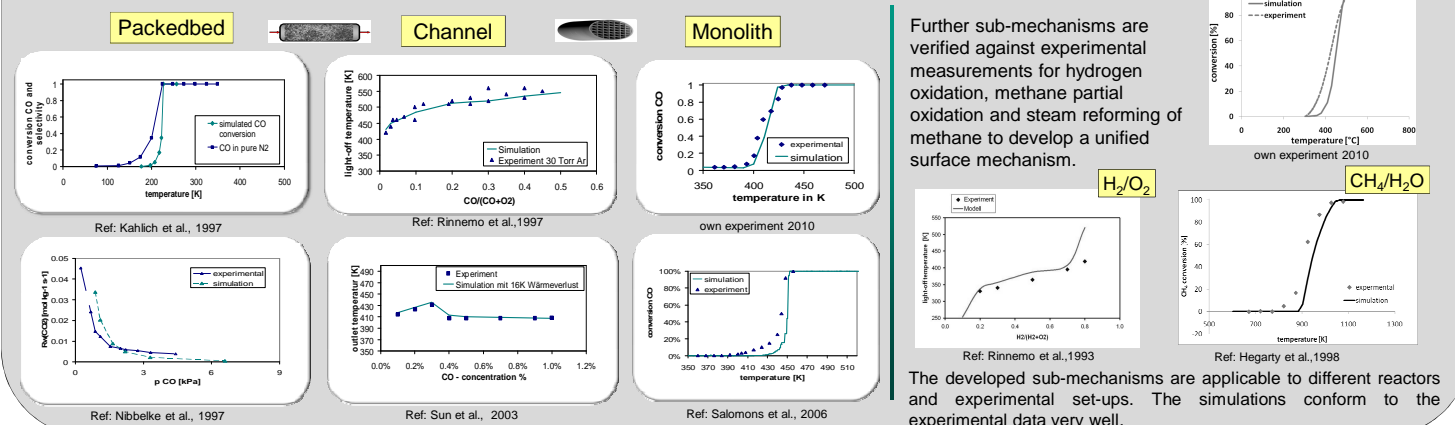


Modeling approach

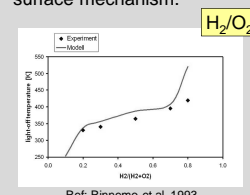


Experimental CO oxidation results (dots) of different reactor systems were simulated (solid line) by corresponding DETCHEM software tools.

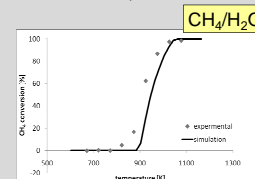
Simulation Results



Further sub-mechanisms are verified against experimental measurements for hydrogen oxidation, methane partial oxidation and steam reforming of methane to develop a unified surface mechanism.



Ref: Rinnemo et al., 1993



Ref: Hegarty et al., 1998

The developed sub-mechanisms are applicable to different reactors and experimental set-ups. The simulations conform to the experimental data very well.

References:

- [1] R. Schwidernoch, S. Fischer, C. Correa, O. Deutschmann, J. Warnatz, *Proc Combust. Inst.* **29**, 2002, 1005
- [2] R. Quiceno, O. Deutschmann, J. Warnatz, J. Pérez-Ramírez, *Catalysis Today* **119**, 2006, 311
- [3] O. Deutschmann, O. Maier, L. I. Riedel, U. Stroemman, A. H. Dibble, R. W. Catalysis Today **59**, 2000, 141
- [4] M. Rinnemo, D. Kulginov, S. Johansson, K. L. Wong, V. P. Zhdanov, B. Kasemo, *Surface Science*, Vol. 376, **1997**, 297
- [5] J. Koop, O. Deutschmann, *Appl. Catal. B: Environmental* **91**, 2009, 47-58
- [6] O. Deutschmann et al., DETCHEM version 2.3, 2010, www.DETCHEM.com
- [7] S. Salomons, M. Votsmeier, R.E. Hayes, A. Drochner, H. Vogel, J. Grieshof, *Catalysis Today*, Vol. 117, **2006**, 491-497
- [8] M. J. Kahlich, H. A. Gasteiger, R.J. Behm, *Journal of Catalysis*, Vol. 171, **1997**, 93-105
- [9] R. H. Nibbelke, M. A. J. Campman, J. H. B. J. Hoebink, G. B. Marin, *Journal of Catalysis*, Vol 171, **1997**, 358-373
- [10] M. Sun, E. B. Croiset, R. R. Hudgins, P. L. Silvestro, M. Menzinger, *Ind. Eng. Chem. Res.*, Vol. 42, **2003**, 37-45
- [11] Rinnemo M., Fasshi M., Kasemo B. *chem. phys. letters* **211**, 1993, 60
- [12] Hegarty, M.E.S. et al. *Catalysis Today* **42**, 1998, 225

Acknowledgement:

Florian Schott for the experimental results.