TU Clausthal
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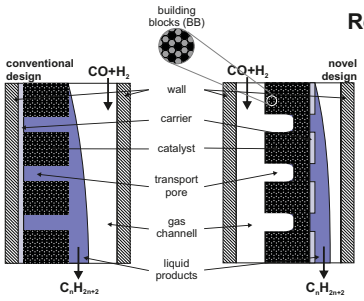
Improving diffusive mass transport in hierarchically structured Fischer-Tropsch catalysts

Motivation and Background

- Mass transport processes in porous catalysts influence selectivity and reaction rate in the Fischer-Tropsch synthesis
- Results indicate that diffusive transport inside the catalyst layers can be enhanced by insertion of transport pores due to increased porosity
- As increased porosity reduces amount of catalyst, optimization of additional porosity is required
- Benefit is strongly dependent on effective diffusion inside transport pores

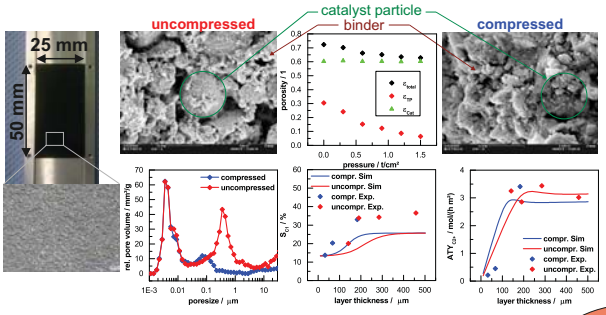


Research Needs and Objectives

- Designing, experimental implementation and iterative optimisation of pore structures
- Improvement of current catalyst and reactor models
- Focus on transport pores under reaction conditions
  - Cylindrical transport pores with smallest possible tortuosity and a diameter of aprrox. 10 µm
  - Transport pores not or only partially filled with liquid
- Omniphobic/oleophobic pore surfaces

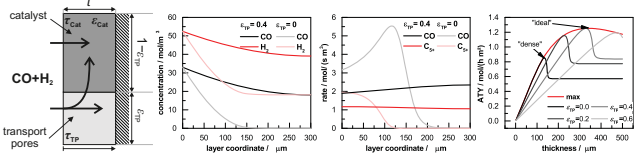
Catalyst Layers for FT Synthesis

- Conventional powder catalyst based on Al_2O_3 (Puralox, 5 µm)
- Mesoporous system impregnated with active material (20% Co, 1% Re)
- Layer preparation: Spraying suspension on metallic carrier
- Subsequent compression enables adjusting of transport pore fraction
- Final calcination to yield mechanically stable layers

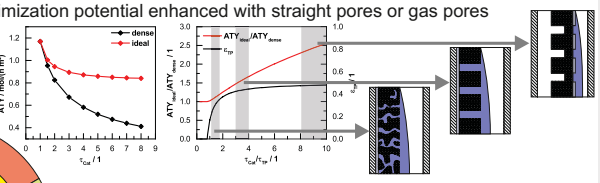


Process Simulation

- Investigation of ideal pore structure for differential reactor
- Optimization of layer thickness and transport pore fraction
- Heat balance shows no influence of temperature profiles

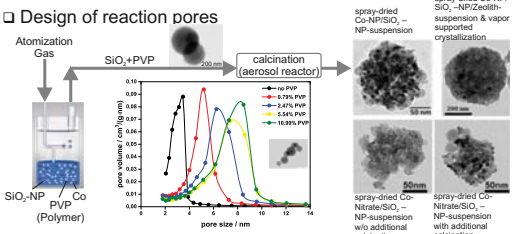


- Integral reactor model for evaluation of external mass transport
- Liquid film formation is negligible
- Parameter estimation: relatively high tortuosity inside transport pores
- Optimization potential enhanced with straight pores or gas pores



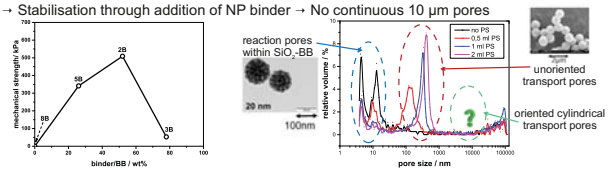
Layer Synthesis

- Design of reaction pores

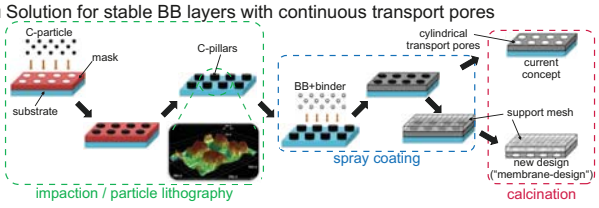


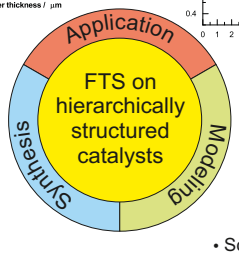
- Problems with the particle layer
  - Mechanical stability of the particle layers
  - Control of pore size distribution of layer systems

→ Stabilisation through addition of NP binder → No continuous 10 µm pores



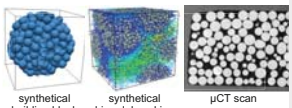
- Solution for stable BB layers with continuous transport pores



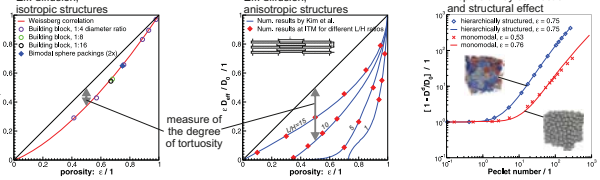


Microscopic Modeling

- Analysis of the transport-morphology relationship:
  - Modeling of porous layer geometry with building blocks



  - Scale resolving calculation of transport in the pore space
  - Determination of efective transport coefficients via local volume averaging (LVA)
- Diffusion: significant tortuosity increasing effect in highly anisotropic media
- Dispersion: significant beneficial effect of transport pores in the presence of convection



- Further approach:
  - Quantification of hindered diffusion in the layer system by further development of the LVA method with respect to reactive flows
  - Quantification of multiphase transport including chemical reactions in partially filled pore space
  - Consideration of Knudsen diffusion in gas phase

Publications

- L. Zeng, A.P. Weber, Aerosol synthesis of nanoporous silica particles with controlled pore size distribution, J. Aerosol Sci. 76, 1-12, 2014
- L. Zeng, A.P. Weber, Synthese von SiO_2-Katalysatorträgern mit einstellbarer Porengröße durch Sprühtrocknung und Kalzinierung, Chem. Ing. Tech. 86, 328-334, 2014
- H. Becker, R. Güttel, T. Turek, Optimization of catalysts for Fischer-Tropsch synthesis by introduction of transport pores, Chem. Ing. Tech. 86, 544-549, 2014
- L. Zeng, A.P. Weber, Herstellung von porösen Nanopartikelschichten auf beliebigen Substraten mittels Niederdruckimpaktion, Chem. Ing. Tech. 86, 238-244, 2014
- E. Monaco, G. Brenner, K.H. Luo, Numerical simulation of the collision of two micro-droplets with a pseudopotential multiple-relaxation-time lattice Boltzmann model, Microfluid. Nanofluid. 16, 329-346, 2014
- E. Dück, S. Sdrenka, Y. Ma, G. Brenner, Numerische Untersuchungen der hydrodynamischen Dispersion in hierarchisch strukturierten porösen Medien, Chem. Ing. Tech., submitted 201502
- H. Becker, R. Güttel, T. Turek, Enhancing internal mass transport in Fischer-Tropsch catalyst layers utilizing transport pores, Catal. Sci. Technol., submitted 201505

Networking in SPP 1570

- Schwieger (FAU Erlangen): one-step synthesis of Co-Zeolith-BB for FTS
- Dittmeyer (KIT): one-step spray drying synthesis of Cu-ZnO for DME synthesis
- Spiecker (FAU Erlangen): TEM tomography and geometrical characterization of building blocks
- Gurlo, Schwarze (TU Berlin): preparation of porous catalyst support, planned

Prof. T. Turek
Prof. A. Weber
Prof. G. Brenner
Chemical and Electrochemical Process Engineering
Particle Technology
Applied Mechanics