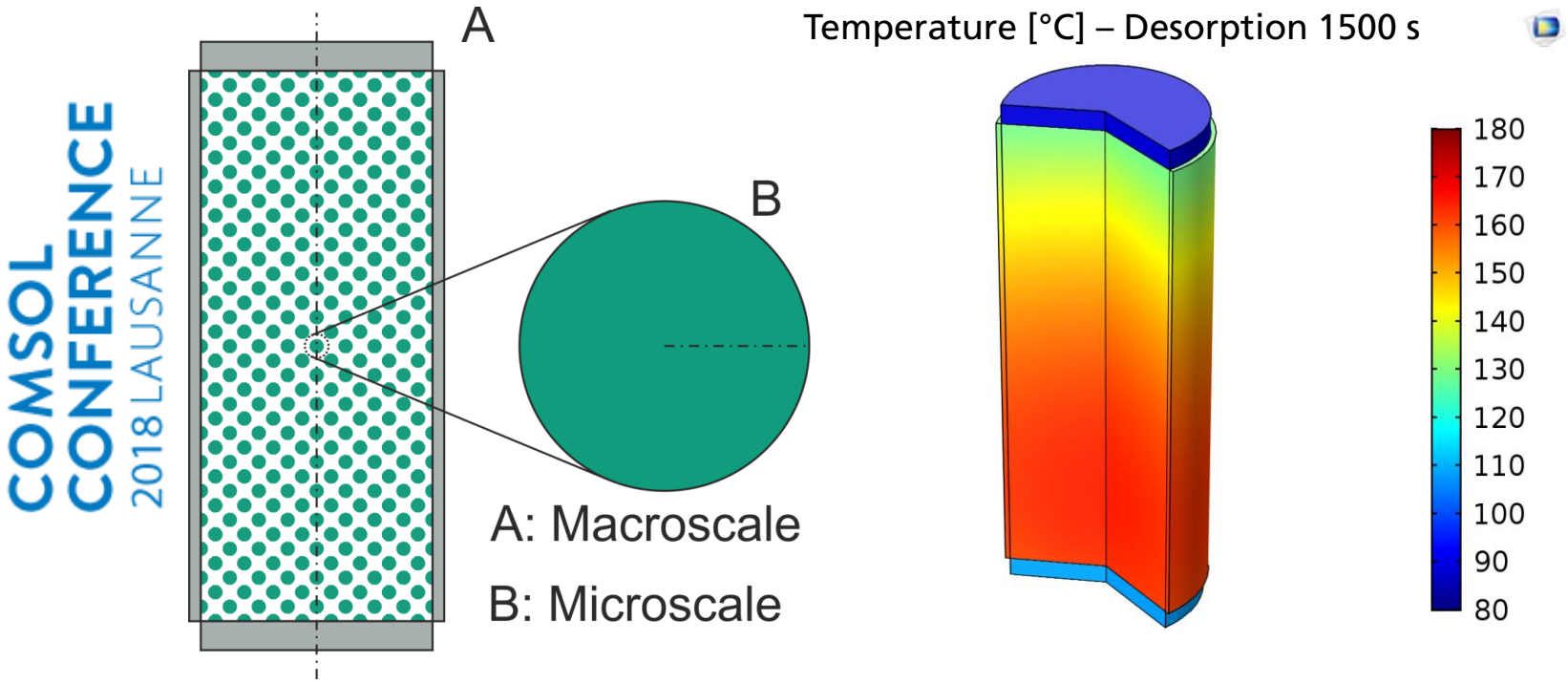
SIMULATION OF A MULTICOMPONENT TRACE GAS ELECTRIC SWING ADSORPTION

Kinetic model of an adsorber within a conductive adsorbent

Fraunhofer UMSICHT – Christian Geitner



Introduction

- Applications:

  gas cleaning, catalysis
- Temperature and pressure swing adsorption
- Multiscale model for the investigation, dimensioning and operation of an adsorber

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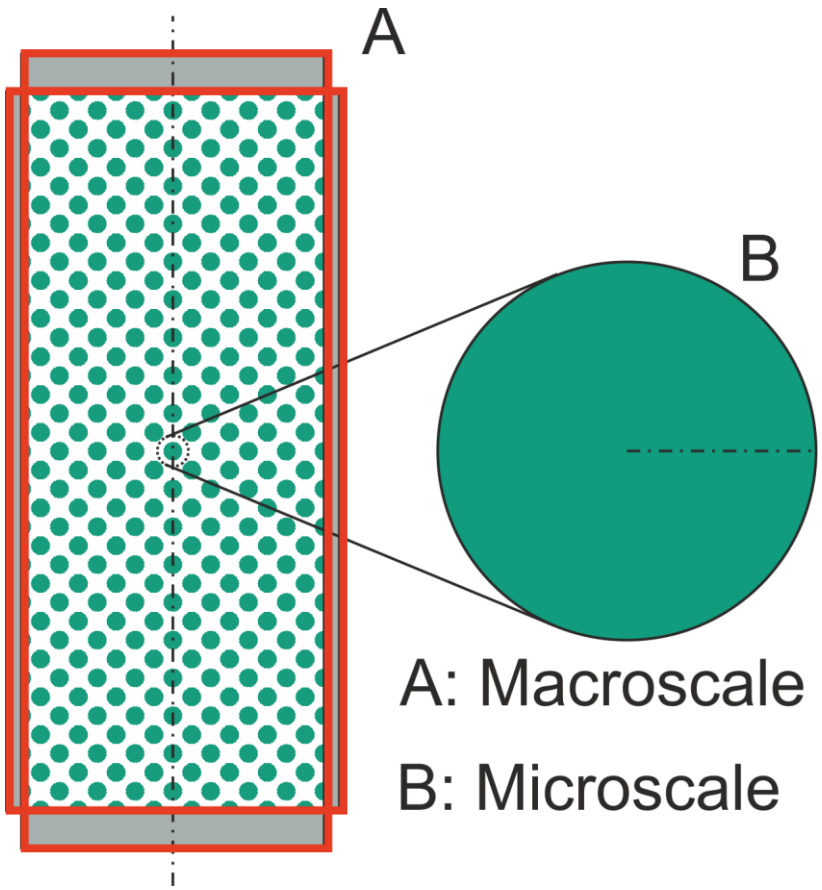
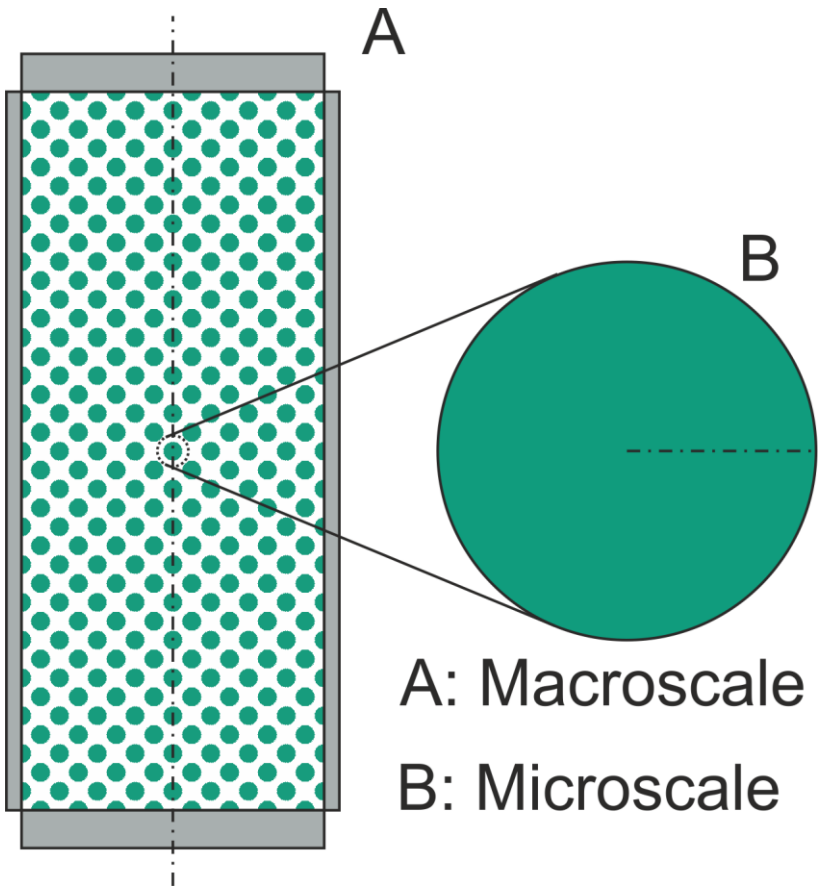


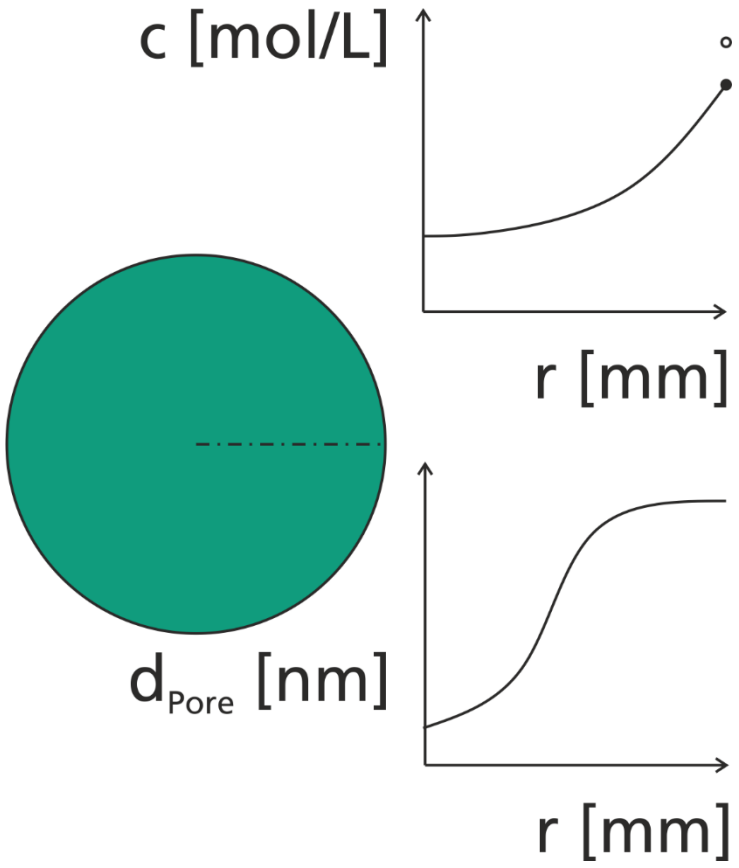
Model Architecture

- Macroscopic model of the apparatus, 2D axissymmetric
- Microscopic model of a particle, 1D axissymmetric
- Differential equation systems are coupled with the mass transfer

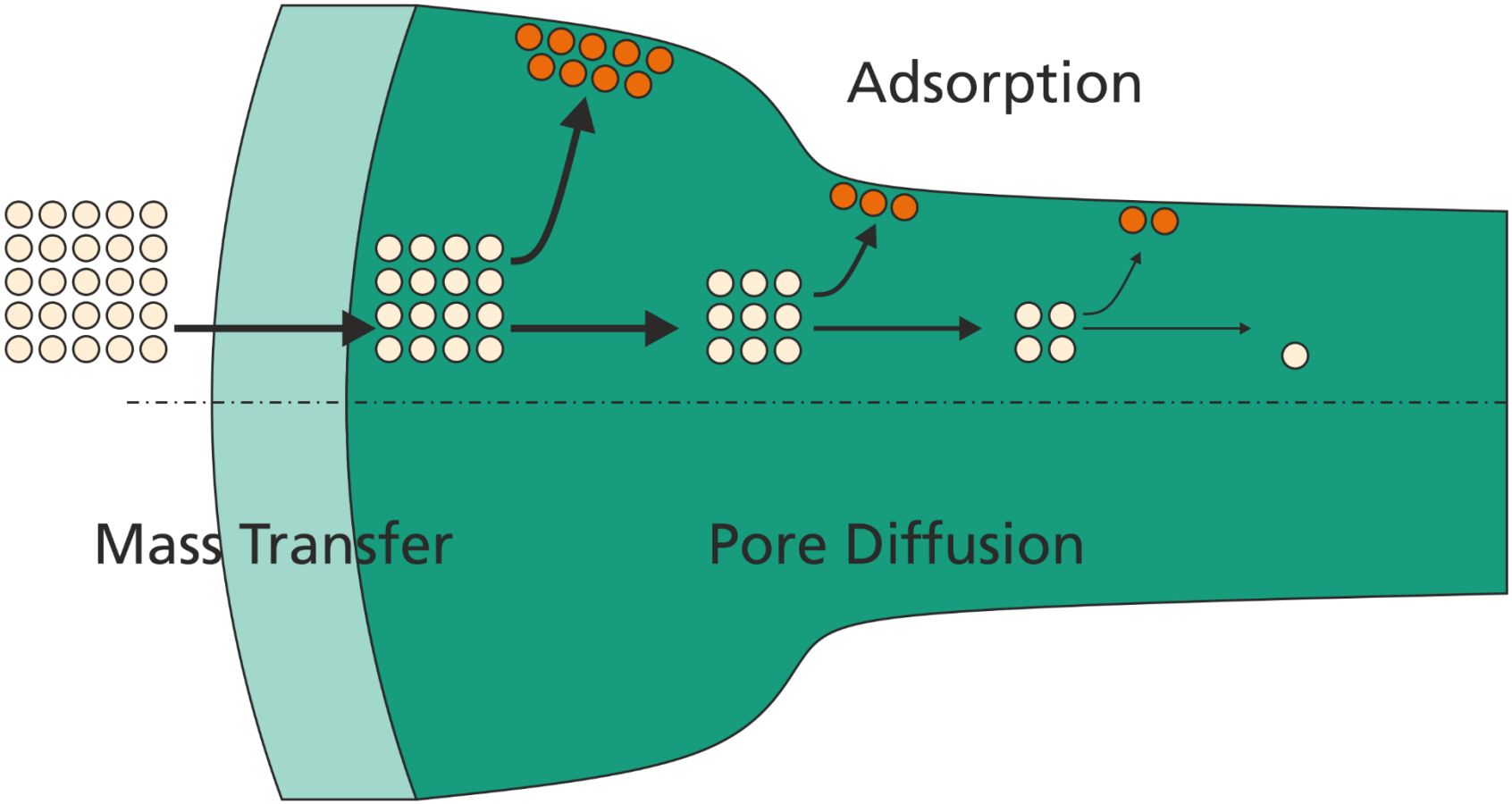


Microscopic Model

- Mass conservation
- Mass transfer
- Source/sink couples micro and macro scale
- Temperature of the macro scale is used in the micro scale



Kinetic Adsorbate Formation



Multicomponent Adsorption Equilibrium (IAST, RAST, GSTA)

- Ideal Adsorbed Solution Theory (IAST)

$$P_T y_i = p_i^0 x_i \gamma_i \quad \gamma_i = 1$$

- Real Adsorbed Solution Theory (RAST)

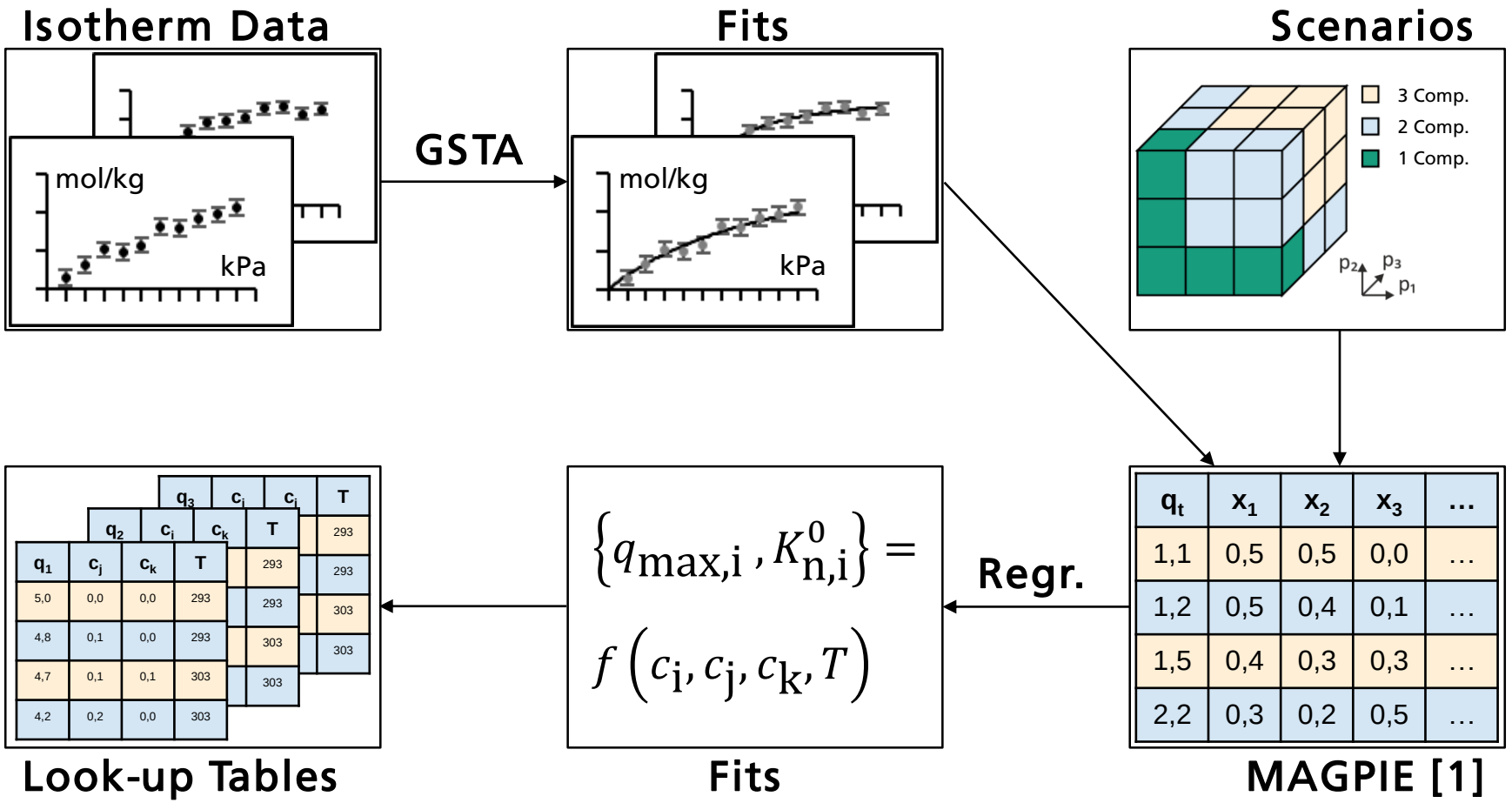
$$P_T y_i = p_i^0 x_i \gamma_i \quad \gamma_i = f(p_i, p_j, \dots) \neq 1$$

- Generalized statistical thermodyn. Adsorption (GSTA)

$$q_i^0 = \frac{q_{max,i}}{m_i} \frac{\sum_{n=1}^{m_i} n K_{n,i}^0 \left(p_i^0 / P^0\right)^n}{1 + \sum_{n=1}^{m_i} K_{n,i}^0 \left(p_i^0 / P^0\right)^n}$$

$$\ln K_{n,i}^0 = -\frac{\Delta H_{n,i}^0}{RT} + \frac{\Delta S_{n,i}^0}{R}$$

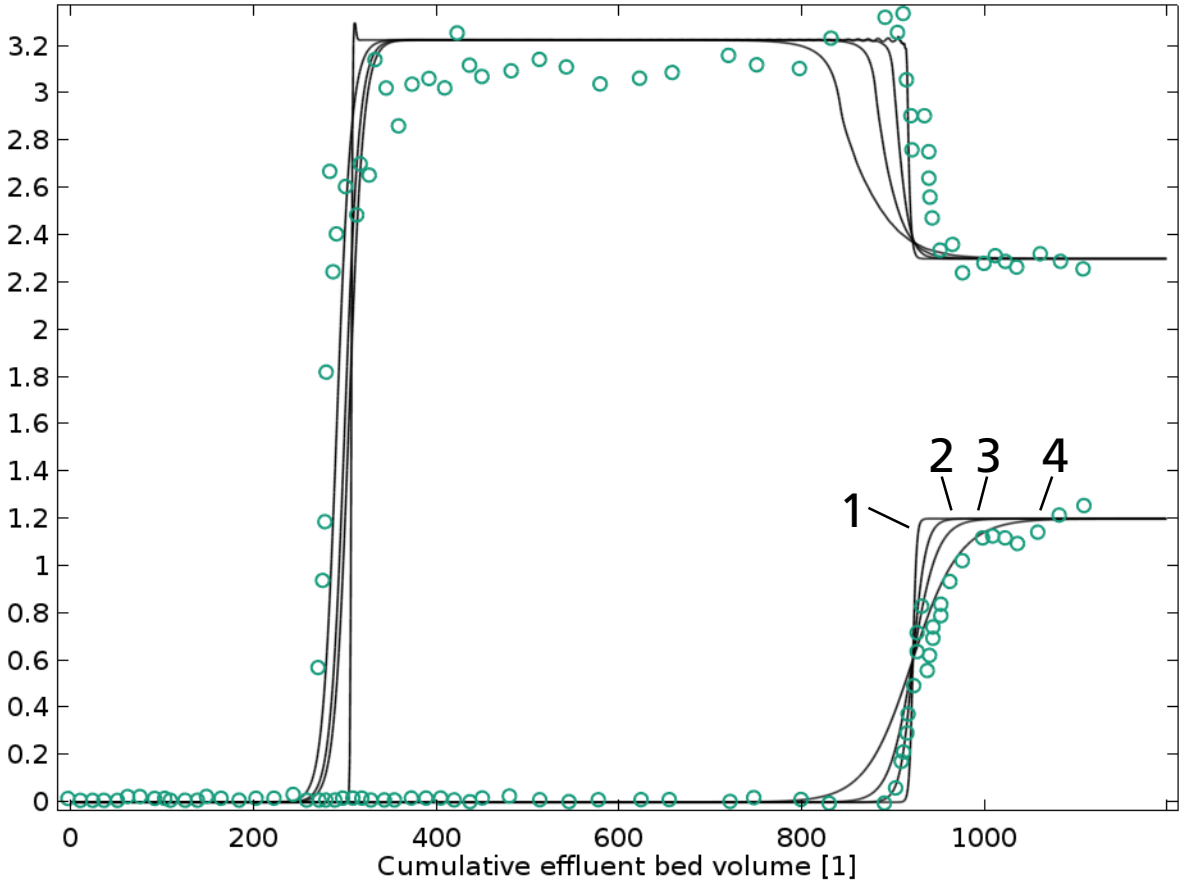
Implementation of Adsorption Data by Look-up Tables



Scenario Discussion [3]

Variation of the mass transfer coefficient

scenario	α / α_0
1	1,0
2	0,2
3	0,1
4	0,05



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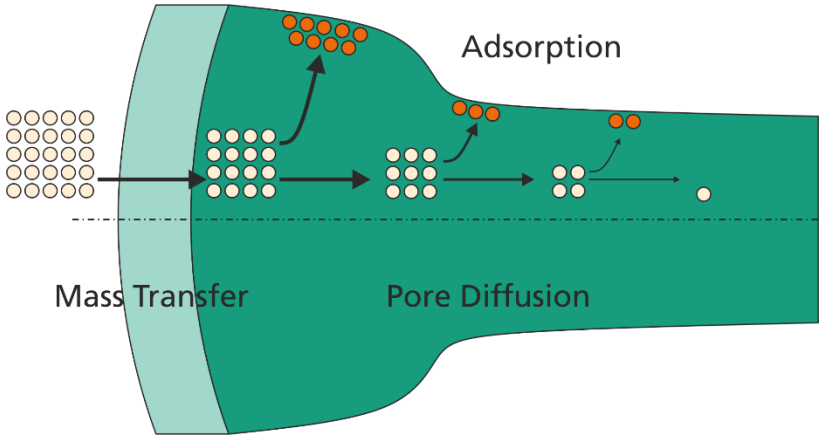
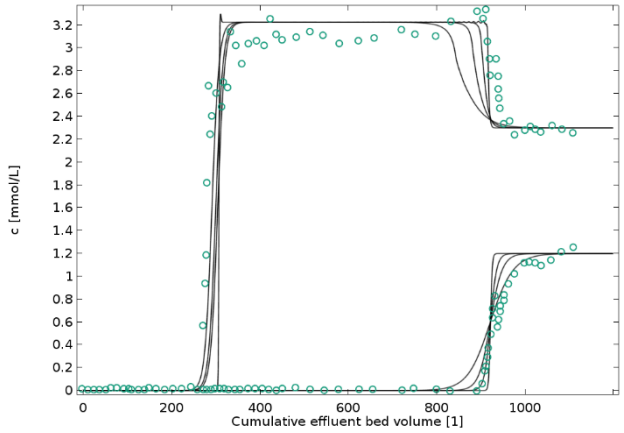
Conclusion

- Multiscale models allow for a more detailed look at intra-particle processes
- Sucessful verification and validation
- Further possible application: catalysis





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REFERENCES

- [1] A. Ladshaw, S. Yiacoumi, C. Tsouris, AIChE J. 2015, 61 (8), 2600 – 2610. DOI: 10.1002/aic.14826.
- [2] H. Dreher, Gleichgewicht und Kinetik bei der Adsorption mehrerer Komponenten aus der Gasphase in einem isothermen Adsorber am Beispiel der Systeme Wasser-Benzol-Methanol-Silicagel, Dissertation, Darmstadt, 1979
- [3] P.-J. Lu, C.-S. Chang, J.-M. Chern, Journal of the Taiwan Institute of Chemical Engineers 2014, 45 (4), 1608 – 1617. DOI: 10.1016/j.jtice.2013.10.018.