Dieter Bathen, Frederik Berg*

Dynamic Simulation of Gas-Phase Adsorption Processes

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Content

1. Introduction

Facts & Data IUTA (2016):

Employees:	ca. 140
Offices:	2.400 m²
Pilot Plant Area:	5.200 m²
Industrial Cooperations:	ca. 360
R&D-Cooperations:	ca. 150
Turnover:	8,7 (+ 5,1) Mio €

Facts & Data TVT (2017):

Employees:	15 + 5 + (12)
Offices:	160 m²
Laboratory:	200 m²
Third Party Funding:	450 T€

1. Introduction

The Future of Adsorption Technology

Driving Forces for „Classic“ Adsorption Technology

- Worldwide Reduction of Emission Limits
- Growing Market in Energy Production, Storage and Conversion
- Growing Market in Downstream Processing (Biotechnology)
- Growing Demand for Ultra-pure and for Toxic Chemicals

Growing Market for „Hidden“ Adsorption Technology

- New Applications in (High Price) Consumer Sector
- Retarding Pharmaceuticals/Ingredients
- Combination Adsorption + Textiles

High Demand for Research in Adsorption Technology

- Multi-functional and „Cross-over“ Adsorbents
- Efficient Characterisation of Adsorbents
- Adsorption at lowest Concentrations
- Link between Molecular Scale and Process
- Computer-Aided Design of Adsorption Processes (without any Experiments)

1. Introduction





Development of an Adsorption Process

- Choice of Adsorbent
- Adsorption Isotherms (Thermodynamics)
- Breakthrough Curves (Kinetics & Dynamics)
- Desorption Method
- Scale Up



1. Introduction

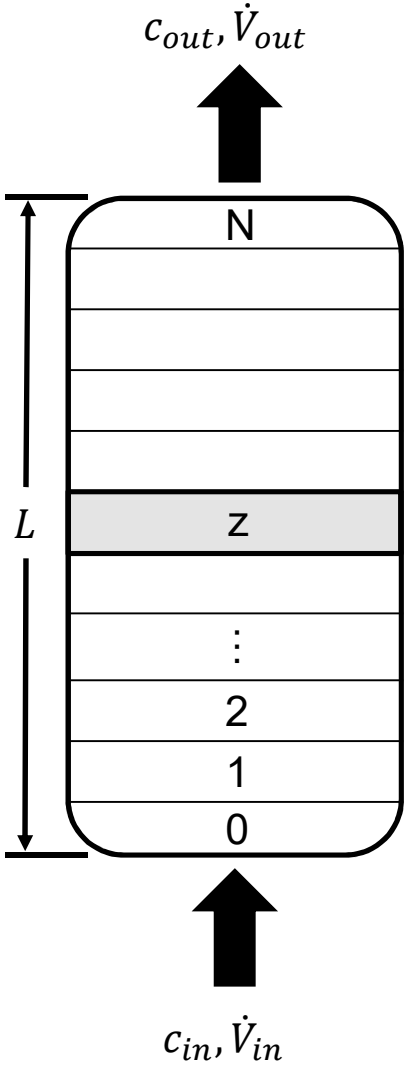
Current research activities (doctorates):

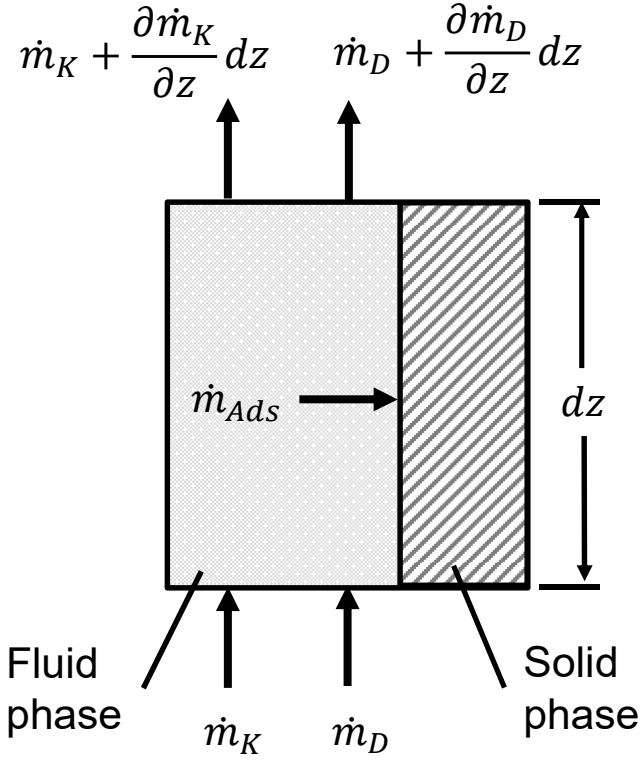
- Coupling of Volumetric and Calorimetric Adsorption Measurements (C. Bläker)
- Characterisation of Adsorbents (J. Treese -> J. Muthmann)
- Adsorptive Purification of Natural Gas (S. Steuten -> V. Chowanietz -> F. Berg)
- Cryogenic Adsorption of Light Hydrocarbons (F. Birkmann -> S. Schmittmann)
- Adsorption of Toxic and Anaesthetising Compounds (R. Ortmann -> D. Bucher)
- Adsorption of Mercury from Batch Processes (M. Ambrosy)
- Development of Adsorptive (Car) Air Conditioning (Bruckner, *Robert Bosch GmbH*)
- Development of a Rapid TSA-Process (Salazar-Duarte, *Linde AG*)
- UV-Spectroscopy of Electrolyte Solutions (C. Cox -> J. Birkmann)
- Raman-Spectrometry in Absorptive Removal of CO2 from Gases (M. Vogt, IUTA)

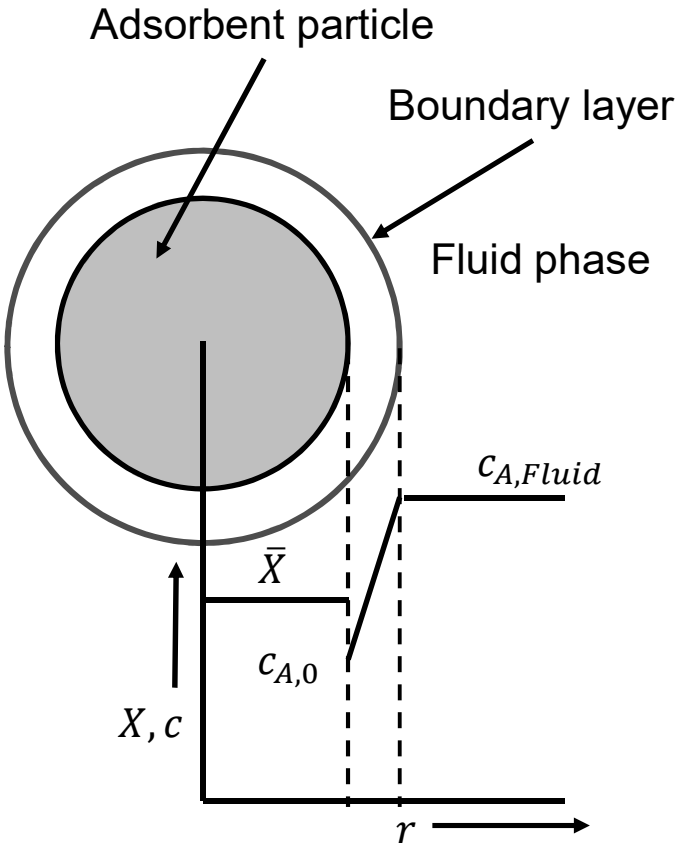


Content

2. Isothermal Adsorption Processes







$$\frac{\partial X}{\partial t} = \frac{k_{eff} \cdot (1 - \epsilon_L) \cdot A_{Sp}}{\epsilon_L} \cdot (X_{eq} - \bar{X})$$

2. Isothermal Adsorption Processes

Often used Assumptions:

- Neglect of radial gradients (T, P, c, X)
- 1D discretization of adsorber column in slices of equal height
- …
- Geometry of particles is approximated by equal spheres
- Fluid phase obeys Ideal gas law
- Thermal conductivity is independent from concentration
- …
- Dispersed Plug Flow-Model
- Axial dispersion calculated by approach of Wakao et al.
- …
- Single component adsorption: no competitive adsorption of carrier gas
- Mass transfer is simplified by the linear driving force (LDF) approach
- External mass transfer resistance taken into account by film diffusion coefficient calculated from Sherwood correlation
- …

2. Isothermal Adsorption Processes

Set of Partial Differential Equations:

- Mass balance of the solid phase:

$$\frac{\partial X}{\partial t} = \frac{k_{eff} \cdot A_{Sp}}{\rho_s} \cdot (X_{GL} - X)$$

- Mass balance of the fluid phase:

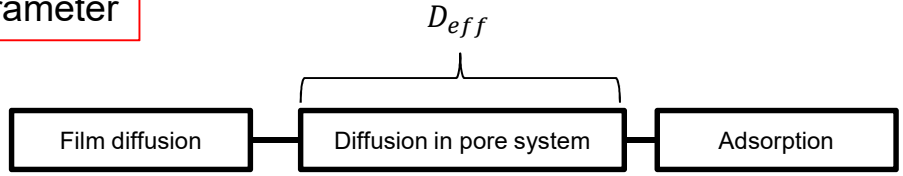
$$\frac{\partial c_A}{\partial t} = D_{ax} \cdot \frac{\partial^2 c_A}{\partial z^2} - \frac{\dot{V}_G}{\epsilon_L \cdot A} \cdot \frac{\partial c_A}{\partial z} - \frac{c_A}{\epsilon_L \cdot A} \cdot \frac{\partial \dot{V}_G}{\partial z} - \frac{k_{eff} \cdot (1-\epsilon_L) \cdot A_{Sp}}{\epsilon_L} \cdot (X_{GL} - X)$$

Kinetic model

- Homogeneous diffusion model

$$k_{eff} = \frac{15}{\mathrm{Rp}^2} * \frac{D_{eff}}{\frac{\rho_p}{\varepsilon_P} * \frac{\partial X}{\partial c_{A,g}}} * \frac{1}{1 + \frac{\varepsilon_P * 15 * D_{eff}}{\mathrm{R_p^2} * \beta_{Film} * A_{Sp}}}$$

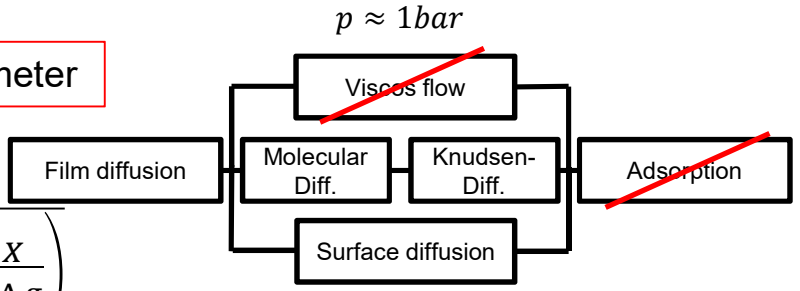
Fit parameter



- Heterogeneous diffusion model

$$k_{eff} = \frac{15}{\mathrm{Rp}^2} * \frac{\frac{D_{Pore}}{\mu_{Pore}} + \frac{D_S}{\mu_S} * \frac{\rho_p}{\varepsilon_P} * \frac{\partial X}{\partial c_{A,g}}}{\frac{\rho_p}{\varepsilon_P} * \frac{\partial X}{\partial c_{A,g}}} * \frac{1}{1 + \frac{15 * \left(\frac{D_{Pore}}{\mu_{Pore}} + \frac{D_S}{\mu_S} * \frac{\rho_p}{\varepsilon_P} * \frac{\partial X}{\partial c_{A,g}} \right)}{\mathrm{R_p^2} * \beta_{Film} * A_{Sp}}}$$

Fit parameter

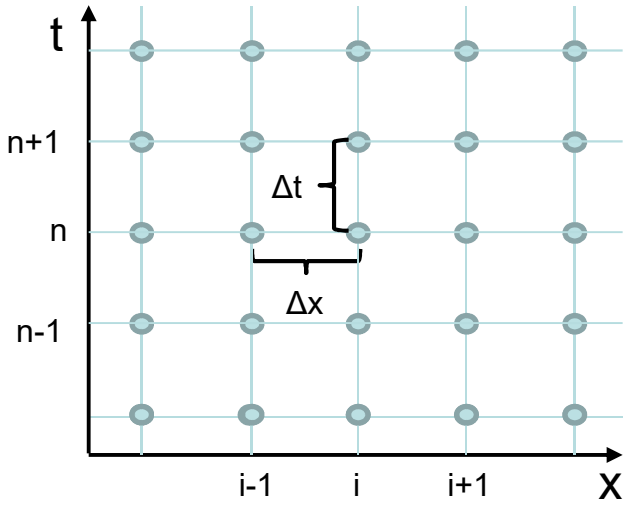


2. Isothermal Adsorption Processes

- Calculation of PDE: Finite differences method
- Transformation of PDE in FDM:

PDE $$\frac{\partial u(x,t)}{\partial t} + \frac{\partial u(x,t)}{\partial x} = 0$$

FDM $$\frac{u_i^{n+1} - u_i^n}{\Delta t} + \frac{u_i^n - u_{i-1}^n}{\Delta x} = 0$$



- Discretization method CFD 2 (central differences 2. order)
- Discretization e.g. (laboratory) column in about 200 slices with height of 1 mm
- Ca. 20 % of overhead increments for numerical stability
- Non linear solver: Mixed-Newton with residual convergence criteria (tolerance 1E-05)
- Integration method: implicit Euler, optionally: Runge Kutta 4. order, explicit Euler…

2. Isothermal Adsorption Processes

Initial and boundary conditions

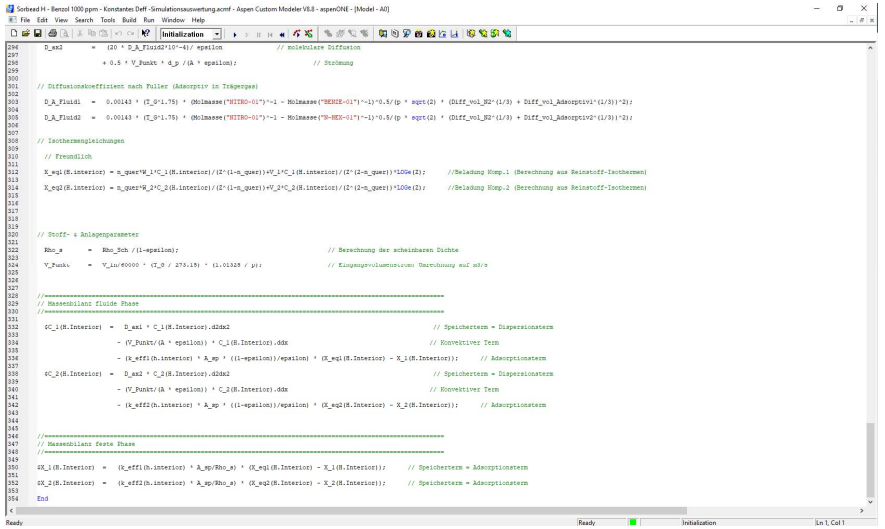
$$X(z,t=0) = X_0 \qquad c_A(z,t=0) = c_{A,0}$$

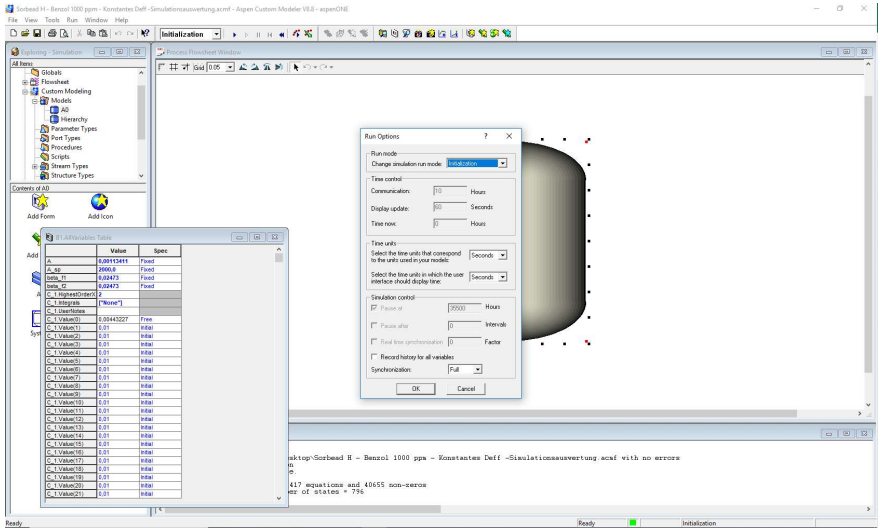
$$\dot{V}_G(z=0,t) = \dot{V}_{G,in} = \text{const};$$

$$c_A(z=0,t) = c_{A,in} \qquad \frac{\partial^2 c_A}{\partial z^2}(z=L,t) = 0$$

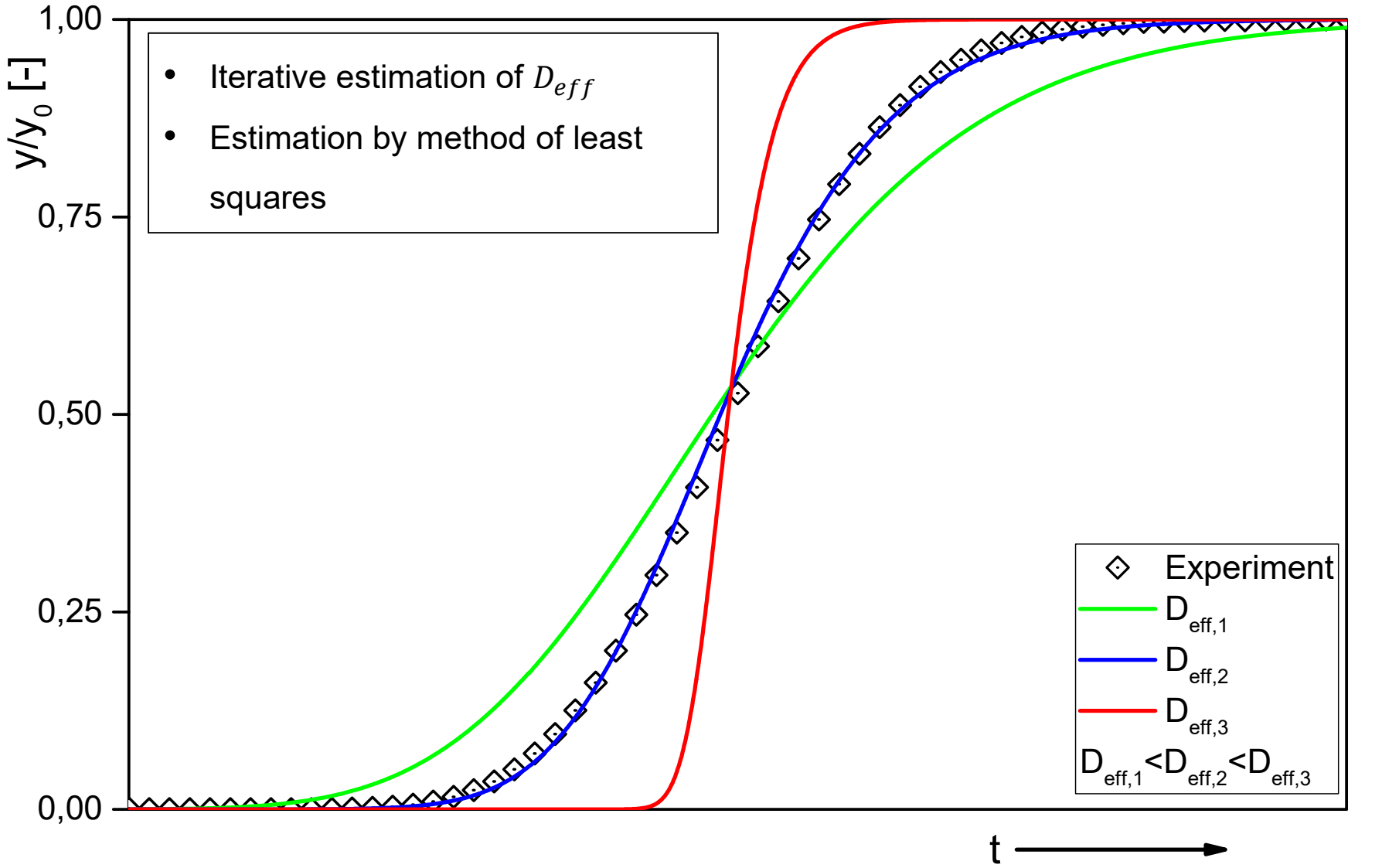
- Specific material and fluid parameters calculated by adjoint equations
- Software for simulation

  PDE-solver:
  - Aspen Custom Modeler® / AdSim®
  - gProms®
  - Speed Up®
  - (Comsol Multiphysics®)
  - AdLin® (Linde Inhouse Software)
  - …



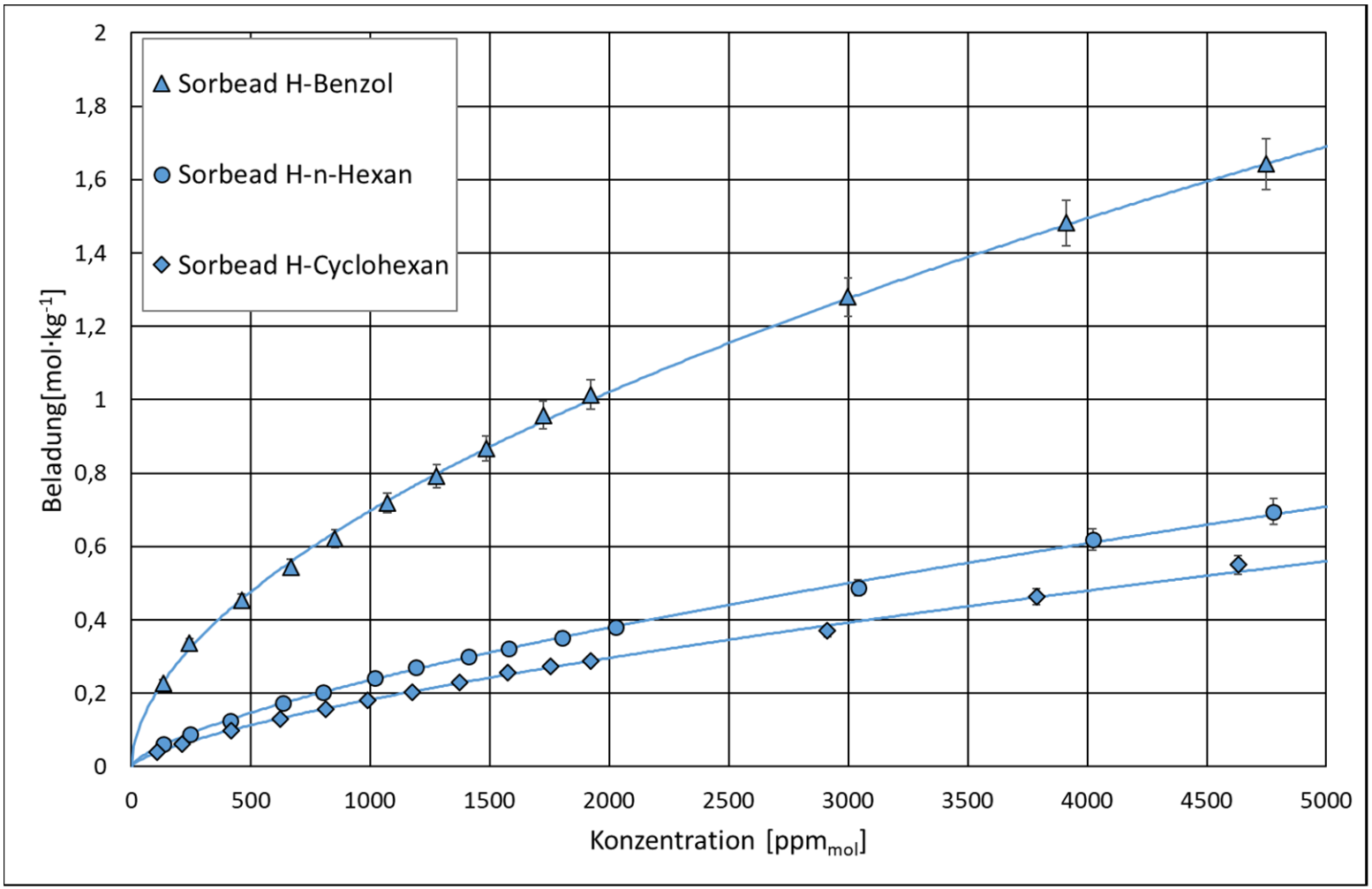


2. Isothermal Adsorption Processes

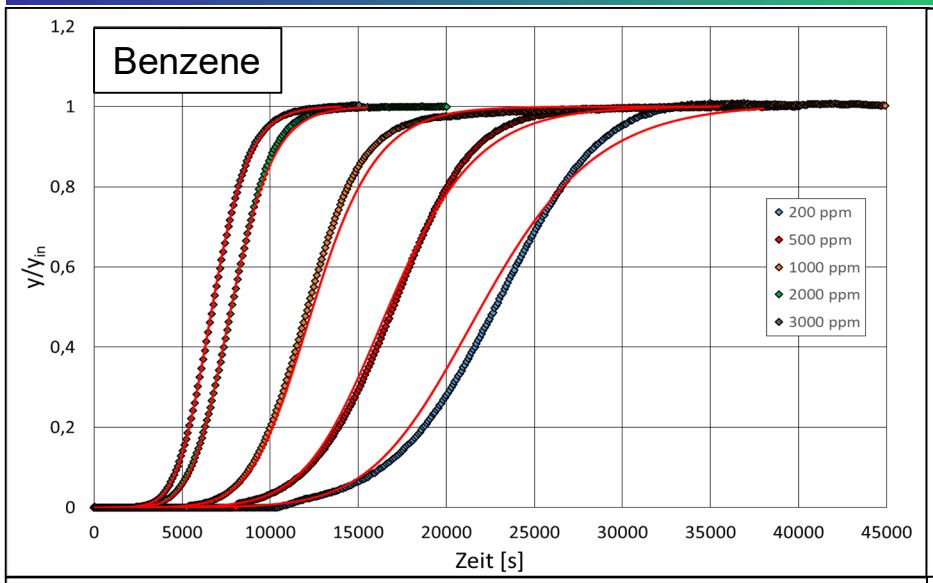


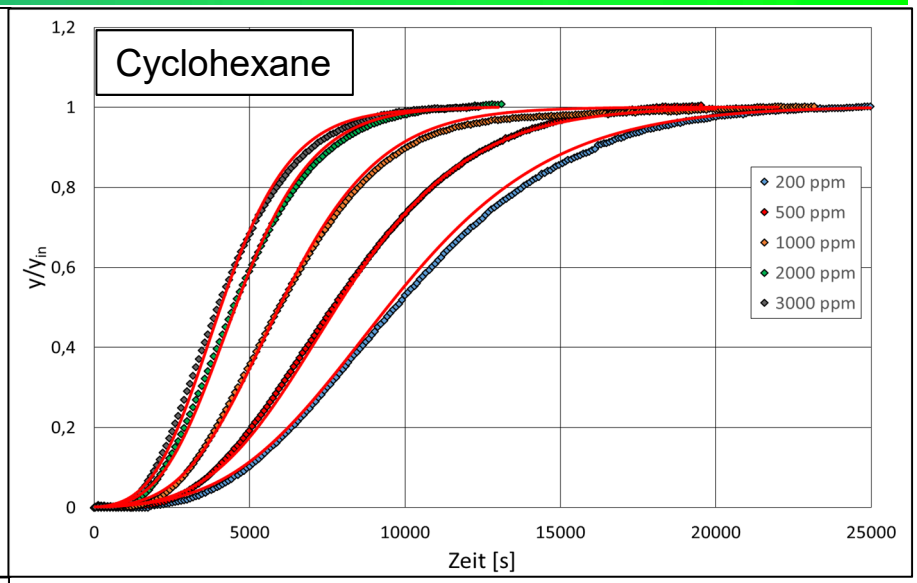
2. Isothermal Adsorption Processes

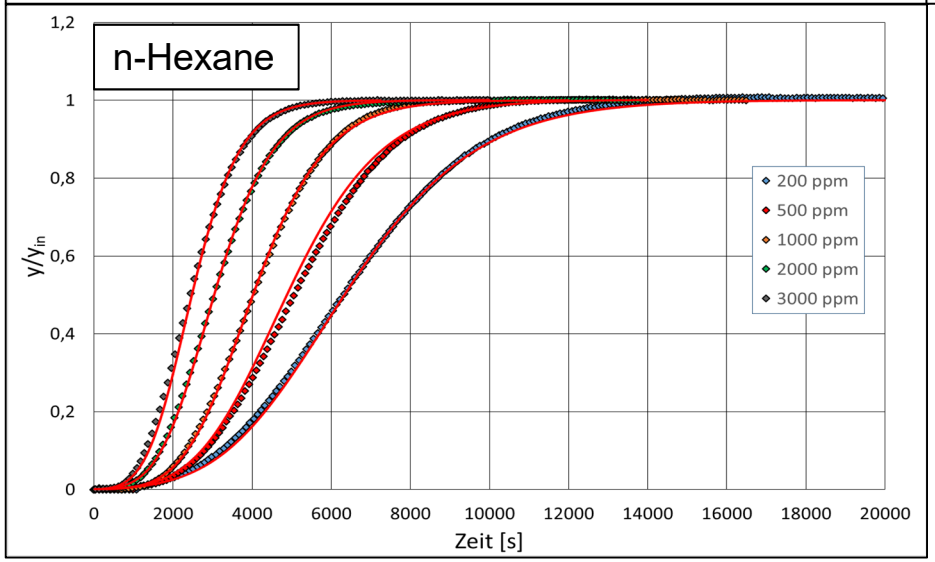
Isotherms of C_6 hydrocarbons on silica alumina gel at 25°C



2. Isothermal Adsorption Processes





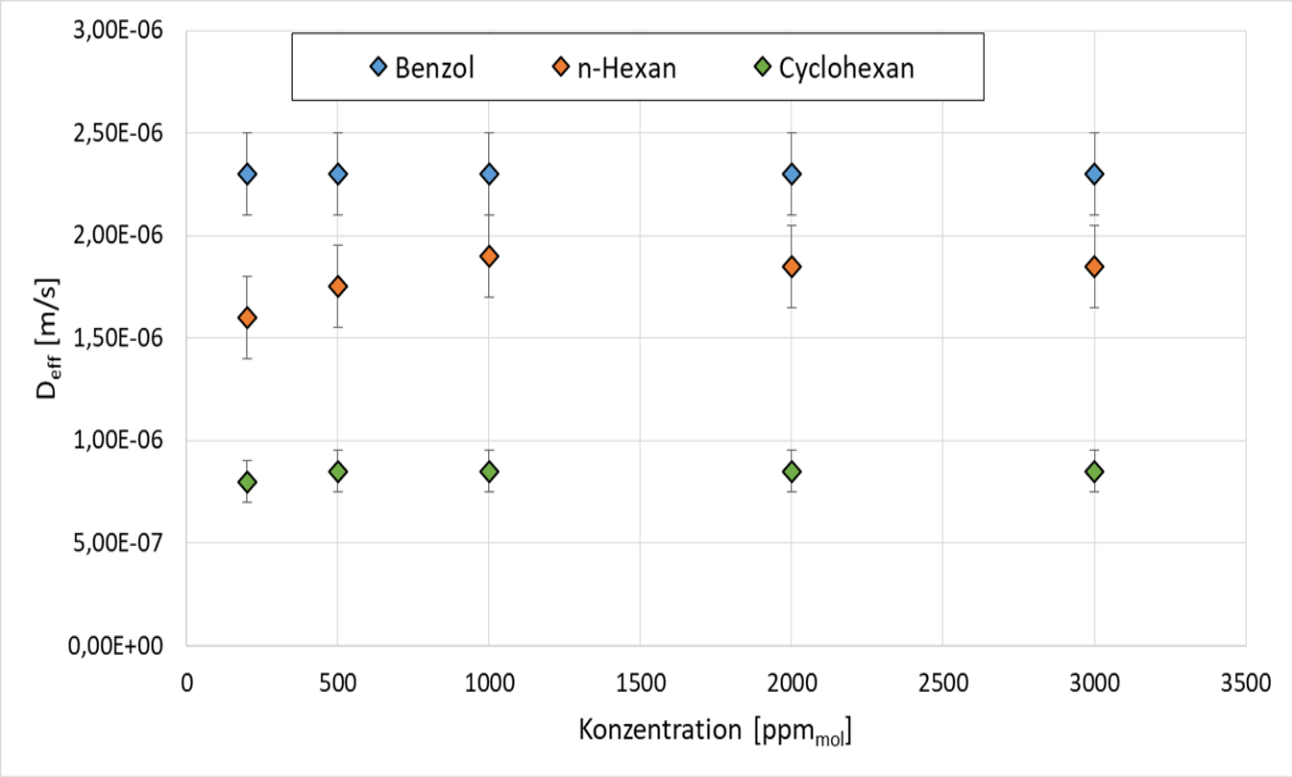


- C_6-BTC (homogeneous model)
- Flattening of BTC at low concentrations
- Individual adjustment of

  $D_{eff}(c_A) \sim 1 * 10^{-6} - 1 * 10^{-7} \frac{m^2}{s}$
- Successful modelling of BTC with constant D_{eff} (R^2 > 99%)

2. Isothermal Adsorption Processes

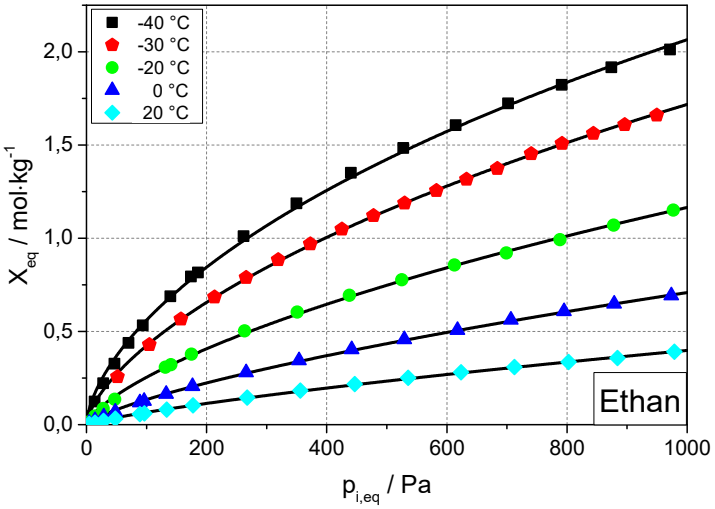
Effective Diffusion coefficients of C_6 hydrocarbons on Silica alumina gel

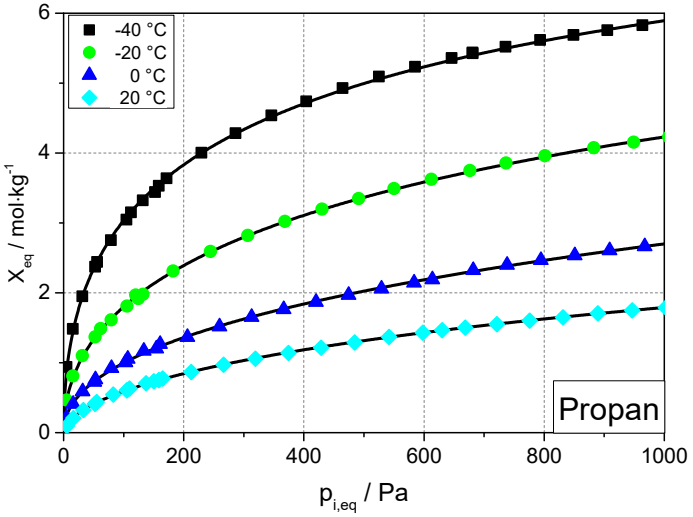


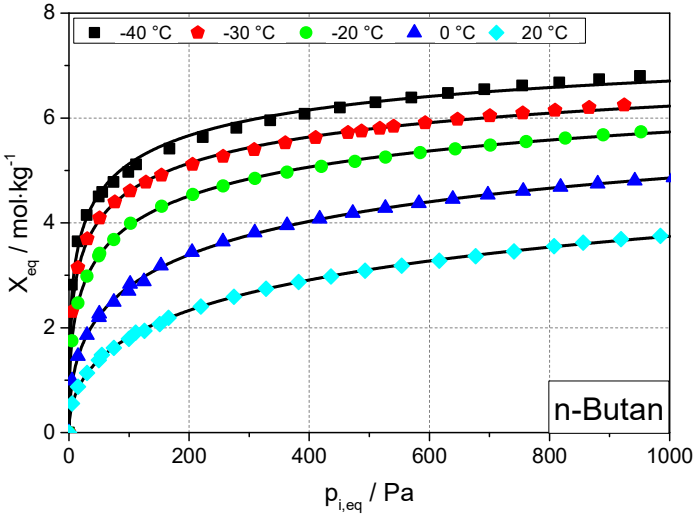
- Constant D_{eff} over whole concentration range
- Simulation with mean D_{eff} possible

2. Isothermal Adsorption Processes

Isotherms of light hydrocarbons on activated carbon



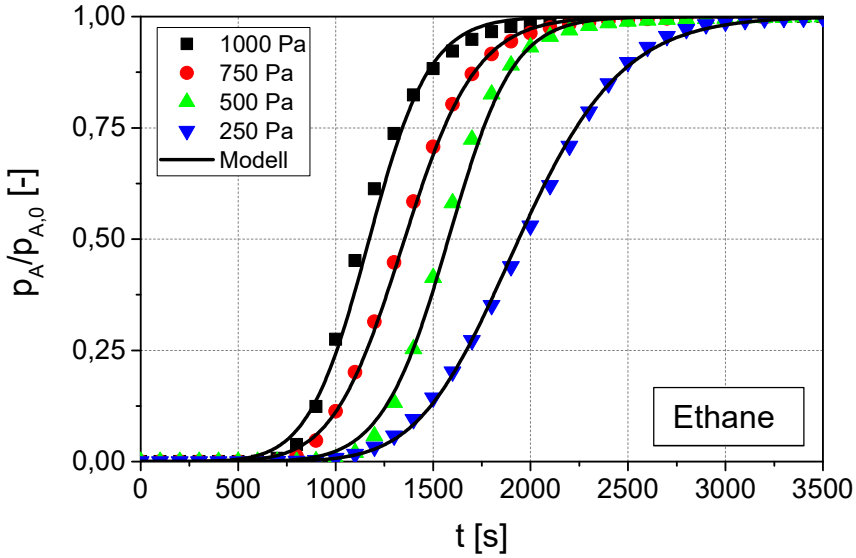


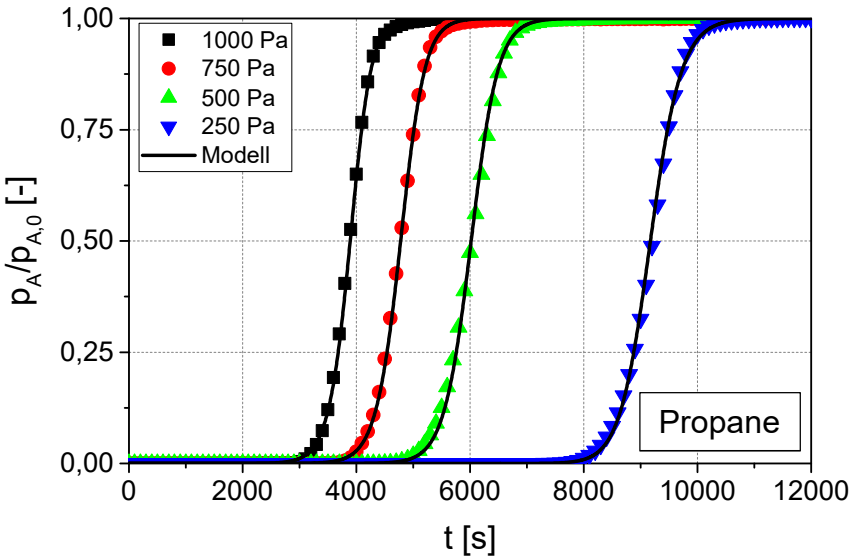


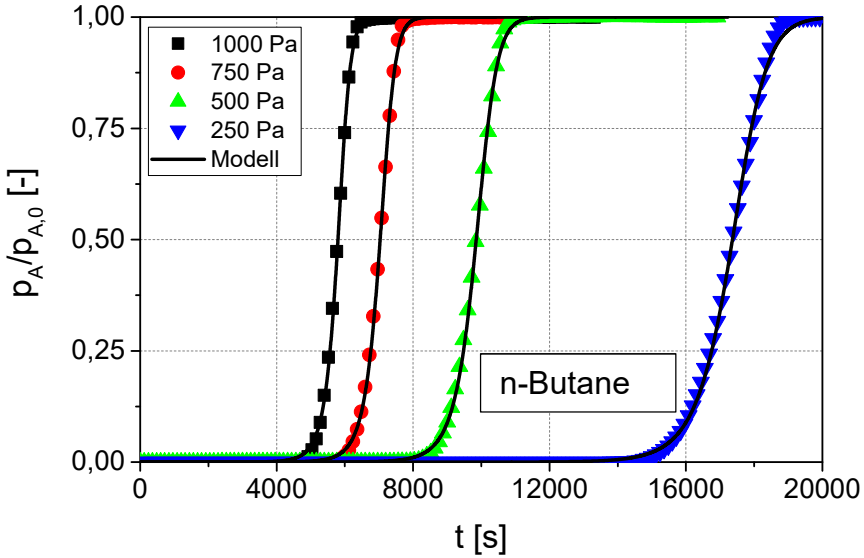
- Isotherms Typ I
- Capacity n-Butane > Propane > Ethane
- Temperature dependency
  Ethane > Propane > n-Butane
- Toth-Isotherm (R^2 > 99,9%)

$$X_{eq}(T, p_{i,eq}) = X_{mon}(T) * \frac{b(T) * p_{i,0}}{\left(1 + (b(T) * p_{i,0})^{n(T)}\right)^{\frac{1}{n(T)}}}$$

2. Isothermal Adsorption Processes

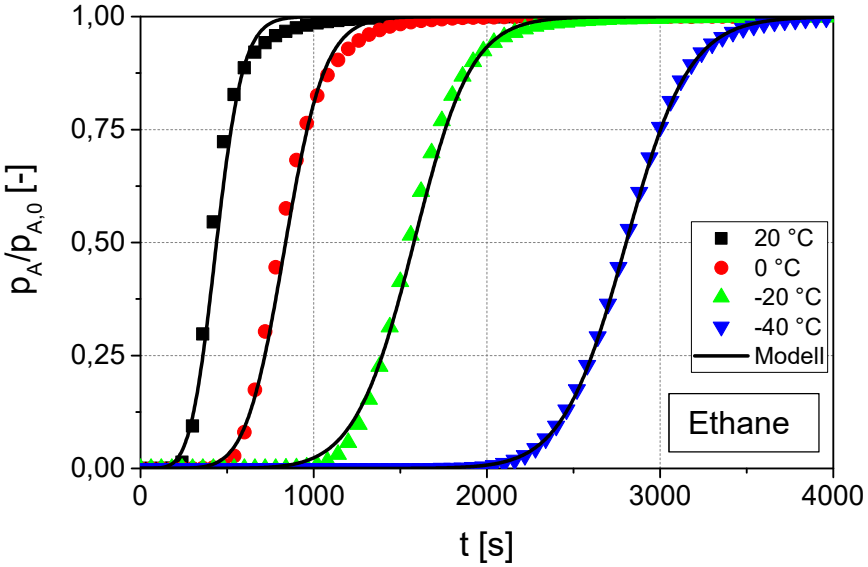


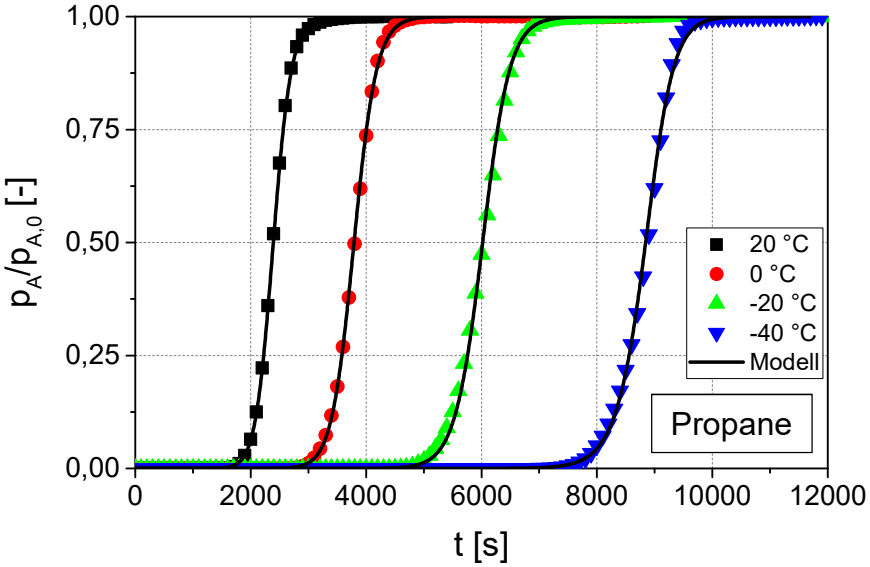


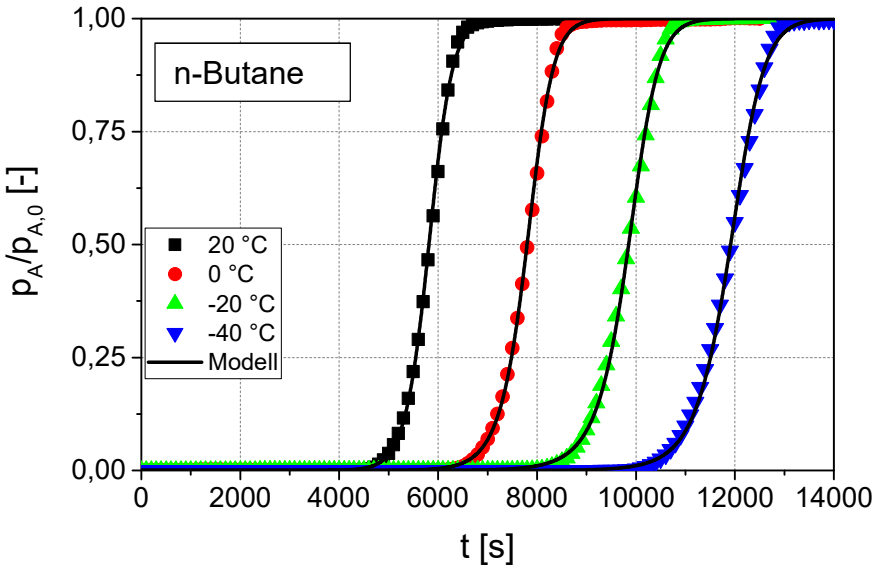


- Light hydrocarbon-BTC at - 20°C (homogeneous model)
- Width of MTZ Ethane > Propane > n-Butane
- Flattening of BTC at low concentrations
- Individual adjustment of $D_{eff}(c_A) \sim 1 * 10^{-5} - 1 * 10^{-6} \frac{m^2}{s}$
- Successful modelling of BTC with constant D_{eff} (R^2 > 99%)

2. Isothermal Adsorption Processes







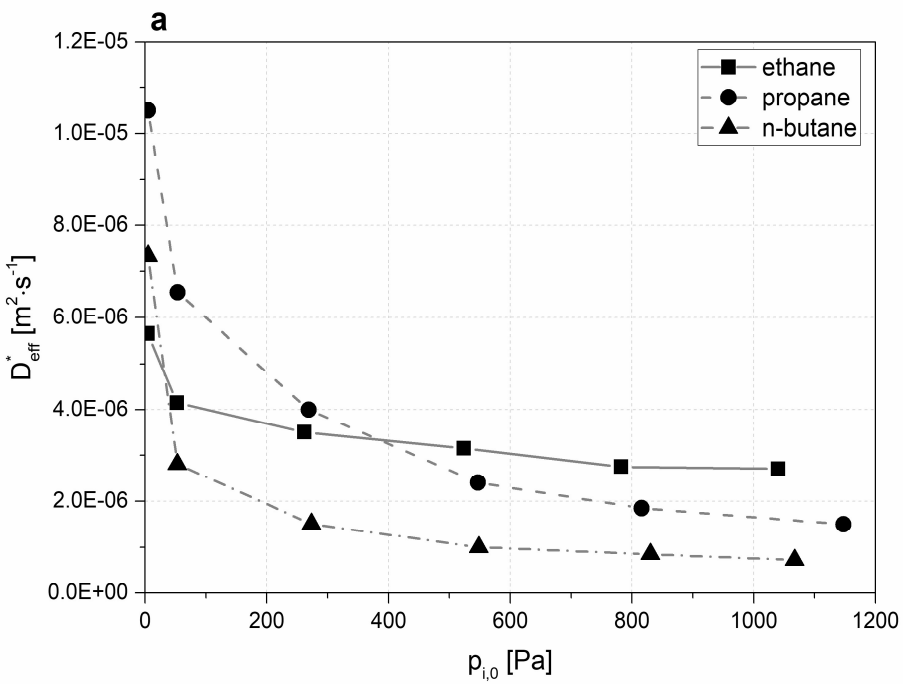
- BTCs at 500 Pa (homogeneous model)
- Flattening of Ethane-BTC by decreasing temperature
- Minor temperature influence on Propane/n-Butane
- Individual adjustment of

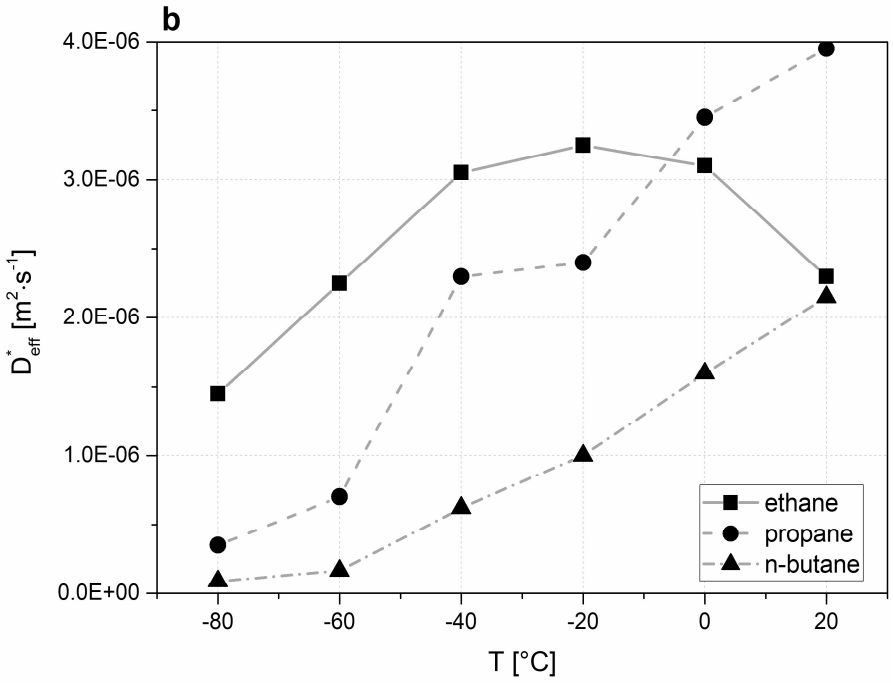
$$D_{eff}(c_A) \sim 1 * 10^{-6} - 1 * 10^{-7} \frac{m^2}{s}$$

- Successful modelling of BTC with constant D_{eff} ($R^2 > 99\%$)

2. Isothermal Adsorption Processes

Effective Diffusion coefficients of light hydrocarbons on activated carbon



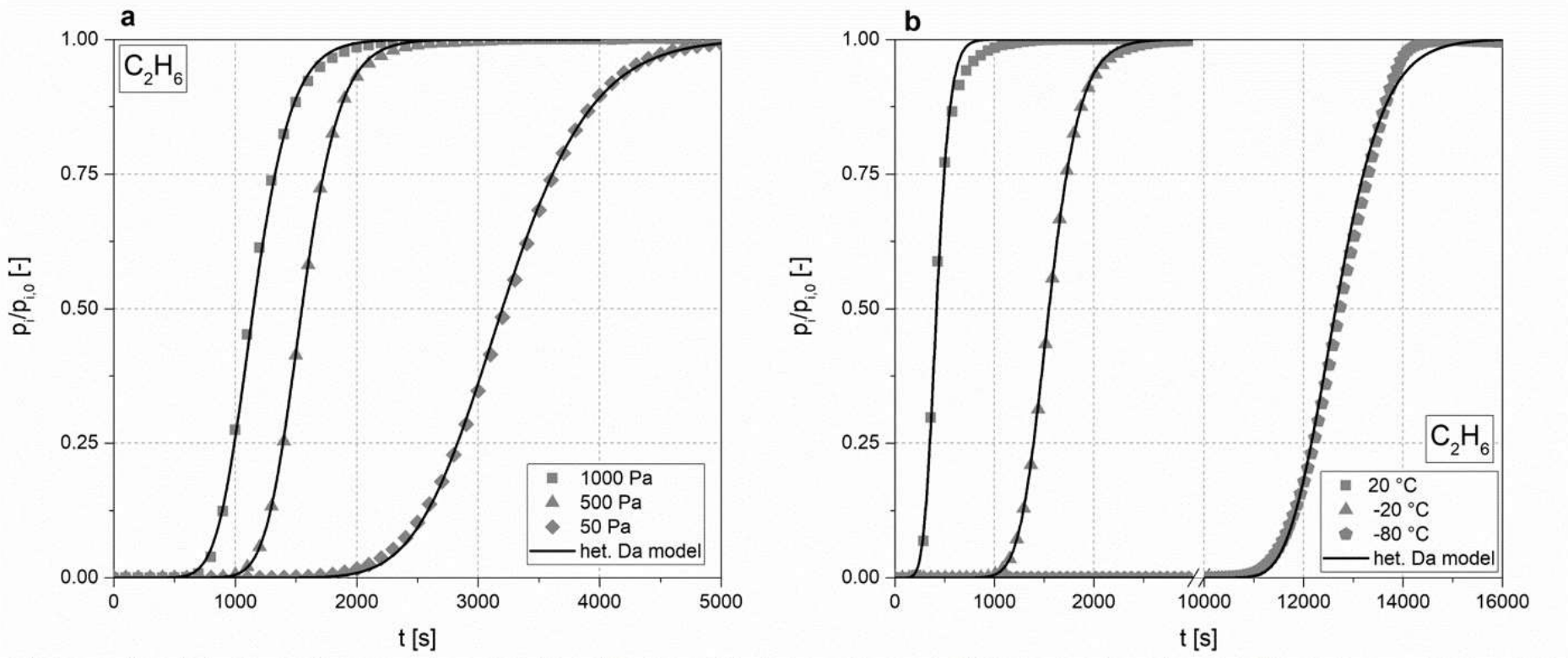


- Decreasing D_{eff} with increasing concentration
- Mathematic approximation by power function $a \cdot x^{-b}$
- Indication of isotherm shape

- No consistent temperature dependency

2. Isothermal Adsorption Processes

Light hydrocarbon-BTC (heterogeneous model)



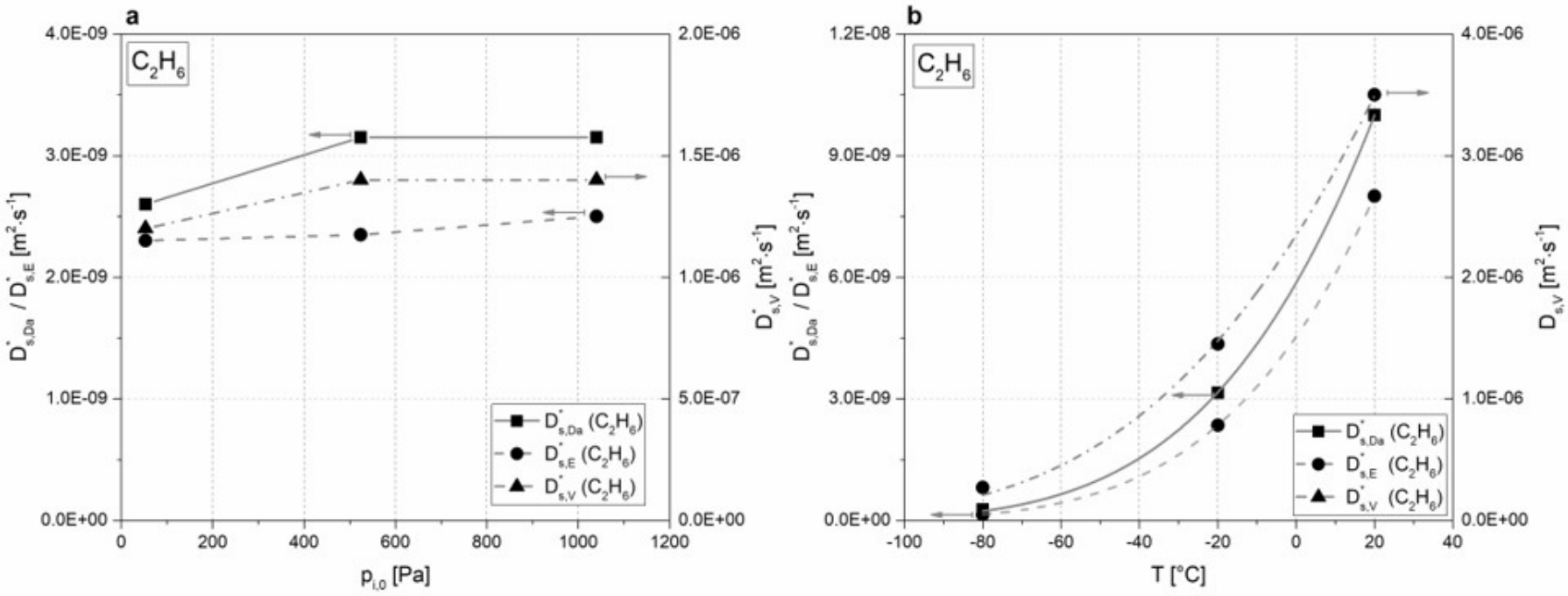
- Surface diffusion by Darken approach:

$$D_{s,Da}(T,X) = D^*_{s,Da}(T) * \frac{\partial\, ln\, c_A}{\partial\, ln\, \bar{X}} = D^*_{s,Da}(T) * \frac{1}{1-\theta^n}$$

- Successful modelling of BTC with heterogeneous model (surface & pore diffusion) (R^2 >99%)

2. Isothermal Adsorption Processes

(Limiting) surface diffusion coefficients of light hydrocarbons on activated carbon



- Constant (limiting) surface diffusion coefficient over whole concentration range
- Exponential temperature dependency of (limiting) surface diffusion coefficient

Content

3. Non-Isothermal Adsorption Processes

Often used Assumptions:

- Neglect of radial gradients (T, P, c, X)
- 1D discretization of adsorber column in slices of equal height
- …
- Geometry of particles is approximated by equal spheres
- Fluid phase obeys Ideal gas law
- Thermal conductivity is independent from concentration
- …
- Dispersed Plug Flow-Model
- Axial dispersion calculated by approach of Wakao et al.
- …
- Single component adsorption: no competitive adsorption of carrier gas
- Mass transfer is simplified by the linear driving force (LDF) approach
- External mass transfer resistance taken into account by film diffusion coefficient calculated from Sherwood correlation
- …
- Heat capacity of bulk phase inside the pore system neglected
- Properties of the adsorbents are constant (independent from temperature)
- …

3. Non-Isothermal Adsorption Processes

Partial differential equation system:

- Mass balance of solid phase:

$$\frac{\partial X}{\partial t} = \frac{k_{eff} \cdot A_{Sp}}{\rho_s} \cdot (X_{GL} - X)$$

- Mass balance of fluid phase:

$$\frac{\partial c_A}{\partial t} = D_{ax} \cdot \frac{\partial^2 c_A}{\partial z^2} - \frac{\dot{V}_G}{\epsilon_L \cdot A} \cdot \frac{\partial c_A}{\partial z} - \frac{c_A}{\epsilon_L \cdot A} \cdot \frac{\partial \dot{V}_G}{\partial z} - \frac{k_{eff} \cdot (1-\epsilon_L) \cdot A_{Sp}}{\epsilon_L} \cdot (X_{GL} - X)$$

- Energy balance of solid phase:

$$\frac{\partial T_F}{\partial t} = \frac{\Delta h_{ads} + c_{p,A} \cdot (T_G - T_F)}{c_{p,S} + X \cdot c_{p,A}} \cdot \frac{\partial X}{\partial t} - \frac{\alpha_P \cdot A_{sp} \cdot (T_F - T_G)}{\rho_S \cdot (c_{p,S} + X \cdot c_{p,A})}$$

- Energy balance of fluid phase:

$$\frac{\partial T_G}{\partial t} = \frac{\lambda_D}{\rho_G \cdot c_{pG}} \cdot \frac{\partial^2 T_G}{\partial z^2} - \frac{T_G}{A \cdot \epsilon_L} \cdot \frac{\partial \dot{V}_G}{\partial z} - \frac{\dot{V}_G \cdot T_G}{A \cdot \epsilon_L \cdot \rho_G} \cdot \frac{\partial \rho_G}{\partial z} - \frac{\dot{V}_G}{A \cdot \epsilon_L} \cdot \frac{\partial T_G}{\partial z} + \frac{\alpha_p \cdot (1-\epsilon_L) \cdot A_{Sp}}{\rho_G \cdot c_{pG} \cdot \epsilon_L} \cdot (T_F - T_G) - \frac{4 \cdot \alpha_{W,i}}{D_i \cdot \epsilon \cdot \rho_f \cdot c_{p,f}} \cdot (T_G - T_W)$$

- Energy balance of adsorber wall:

$$\frac{\partial T_W}{\partial t} = \frac{4}{(D_a^2 - D_i^2) \cdot c_{p,W} \cdot \rho_W} \cdot \left[\alpha_{W,i} \cdot D_i \cdot (T_G - T_W) - \alpha_{W,a} \cdot D_a \cdot (T_W - T_U)\right]$$

Kinetic model:

- Homogeneous diffusion model

$$k_{eff} = \frac{15}{\mathrm{R_p}^2} * \frac{D_{eff}}{\frac{\rho_p}{\varepsilon_P} * \frac{\partial X}{\partial c_{A,g}}} * \frac{1}{1 + \frac{\varepsilon_P * 15 * D_{eff}}{R_p^2 * \beta_{Film} * A_{Sp}}}$$

3. Non-Isothermal Adsorption Processes

Initial and boundary conditions

$$T_F(z,t=0) = T_0 \qquad \dot{V}_G(z=0,t) = \dot{V}_{G,ein}$$

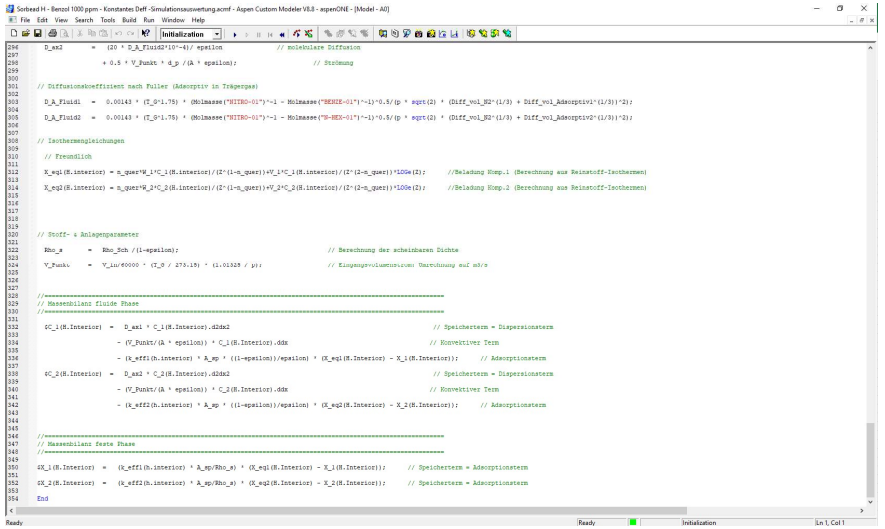
$$T_G(z,t=0) = T_0 \qquad T_G(z=0,t) = T_{G,ein}$$

$$X(z,t=0) = X_0 \qquad \rho_G(z=0,t) = \rho_{G,ein}$$

$$c_A(z,t=0) = c_{A,0} \qquad c_A(z=0,t) = c_{A,ein}$$

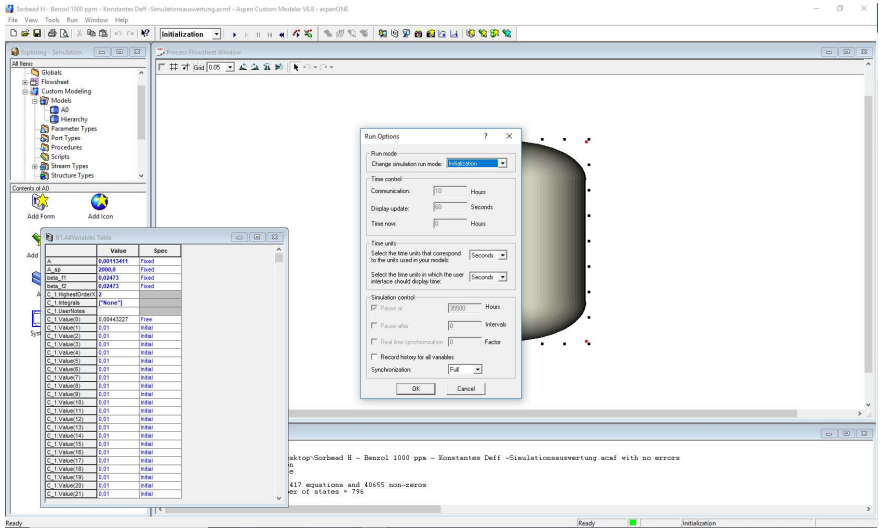
$$\frac{\partial^2 c_A}{\partial z^2}(z=L,t) = 0$$

$$\frac{\partial^2 T_G}{\partial z^2}(z=L,t) = 0$$



- Specific material and fluid parameters calculated by adjoint equations

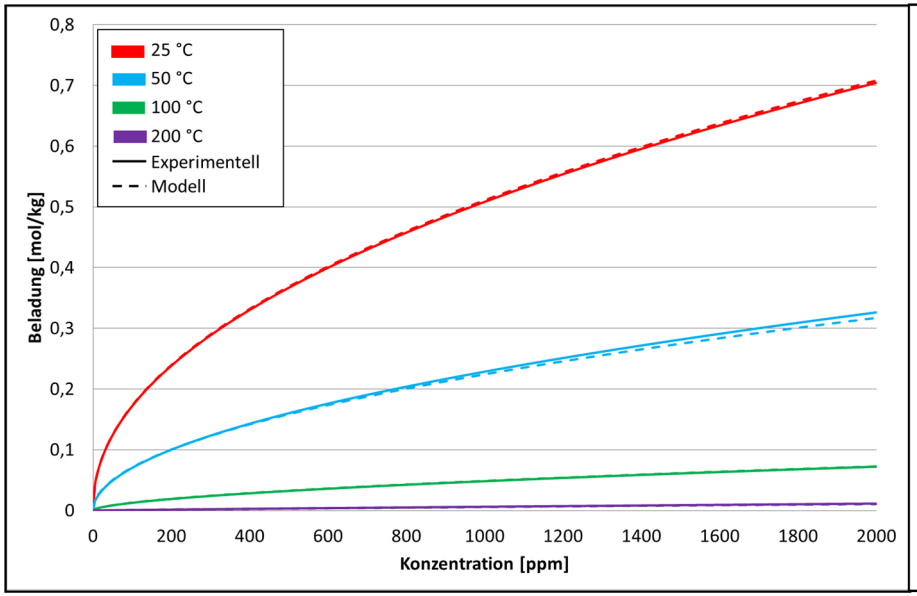
- Software for simulation
  PDE-solver:
  - Aspen Custom Modeler® / AdSim®
  - gProms®
  - Speed Up®
  - (Comsol Multiphysics®)
  - AdLin® (Linde Inhouse Software)
  - …



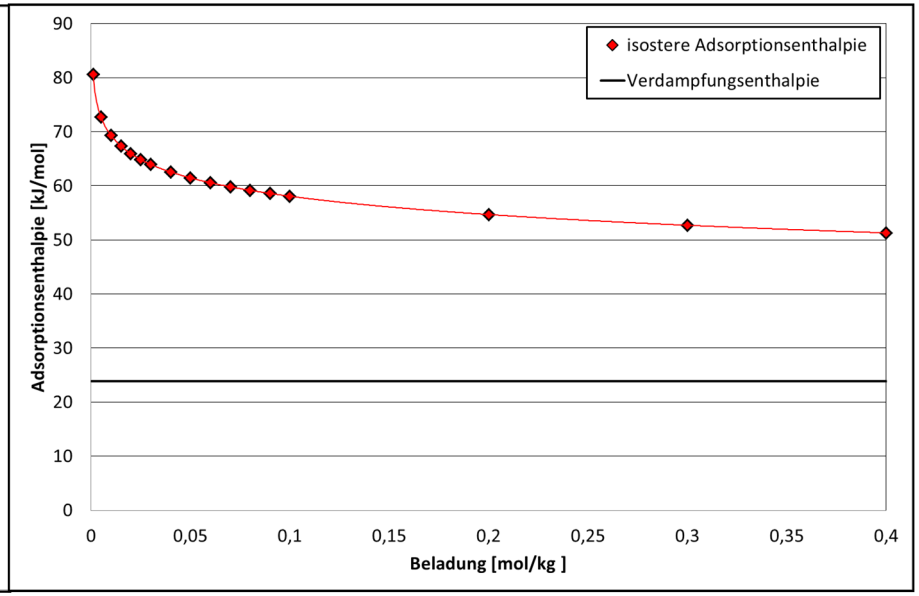
3. Non-Isothermal Adsorption Processes

Necessary data for non-isothermal simulation:

- $X_{eq} = f(T, c)$
- $\Delta h_{ads} = f(X)$
- (have to be determined experimentally)



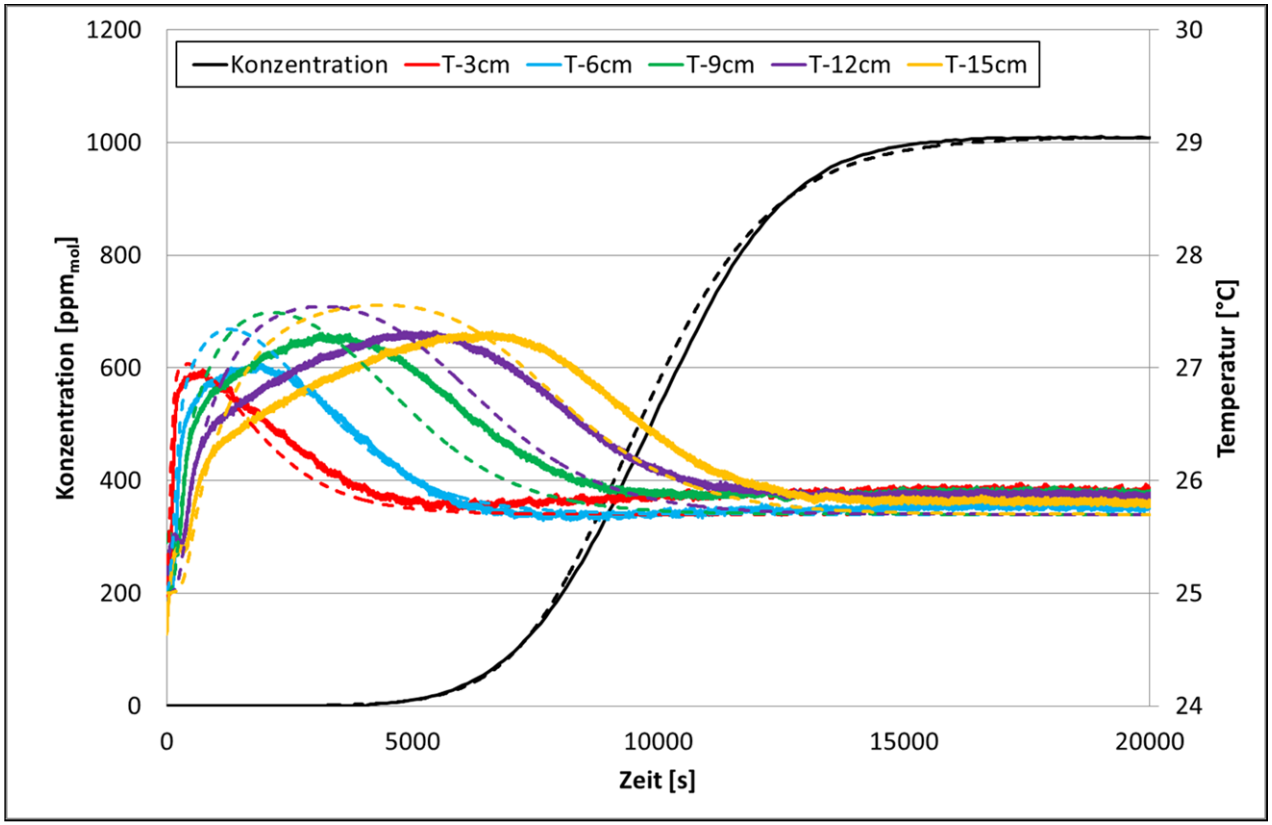
Experimental and calculated field of isotherms of C_2H_5SH on Sorbead H

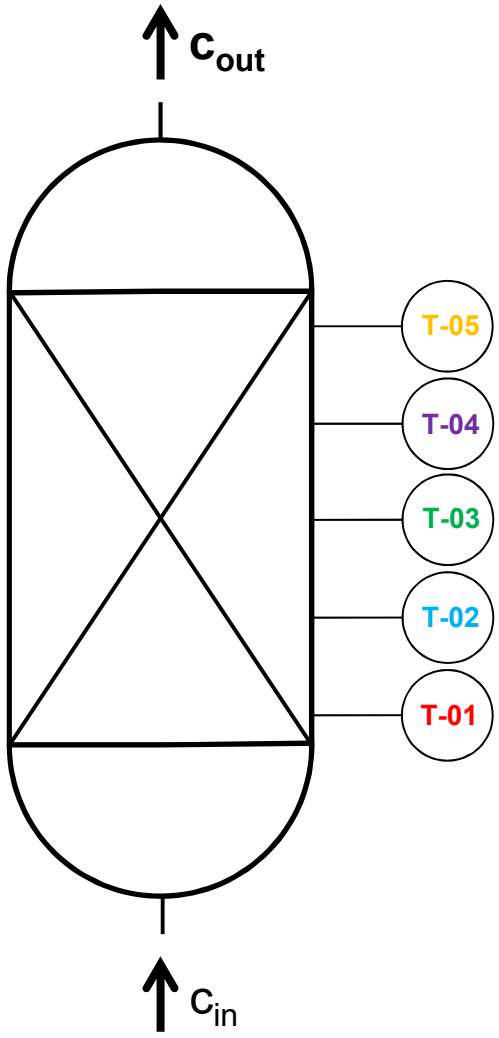


Isosteric heat of adsorption of C_2H_5SH on Sorbead H

3. Non-Isothermal Adsorption Processes

Adsorption Profiles of C_2H_5SH on Sorbead H



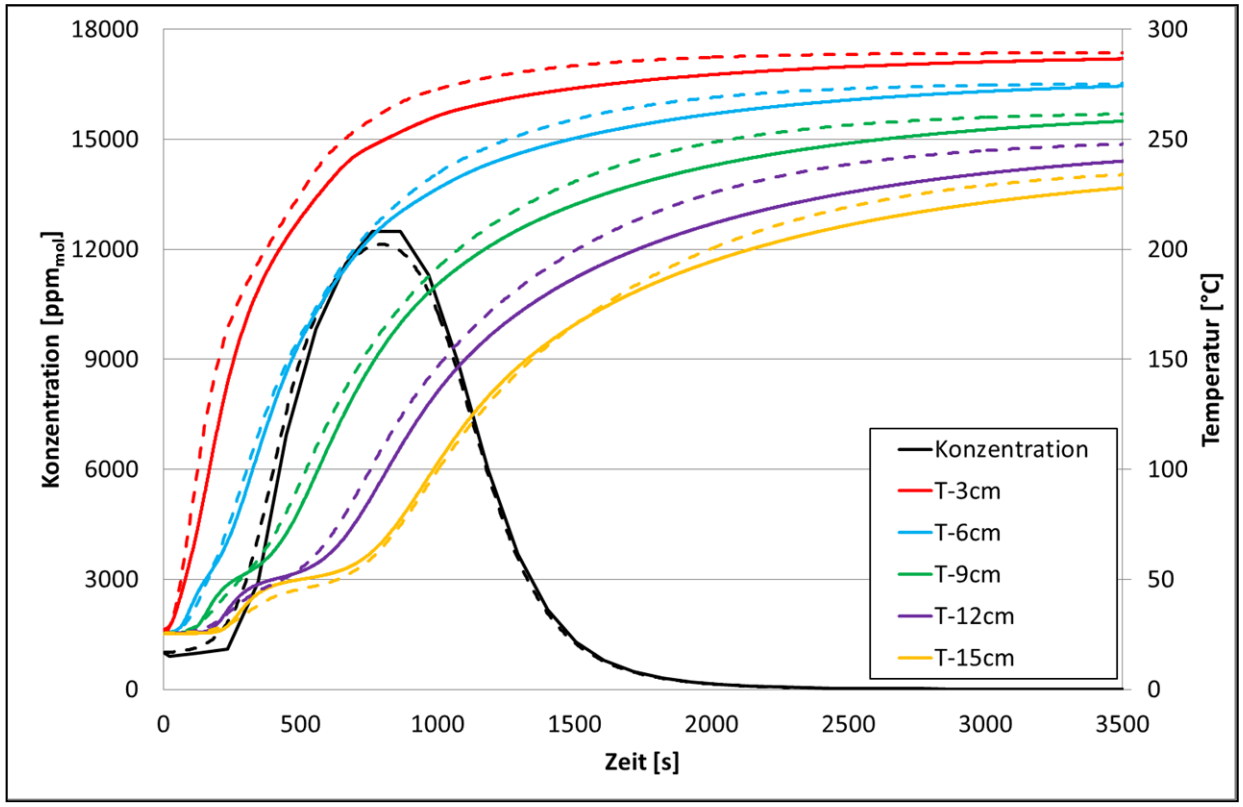


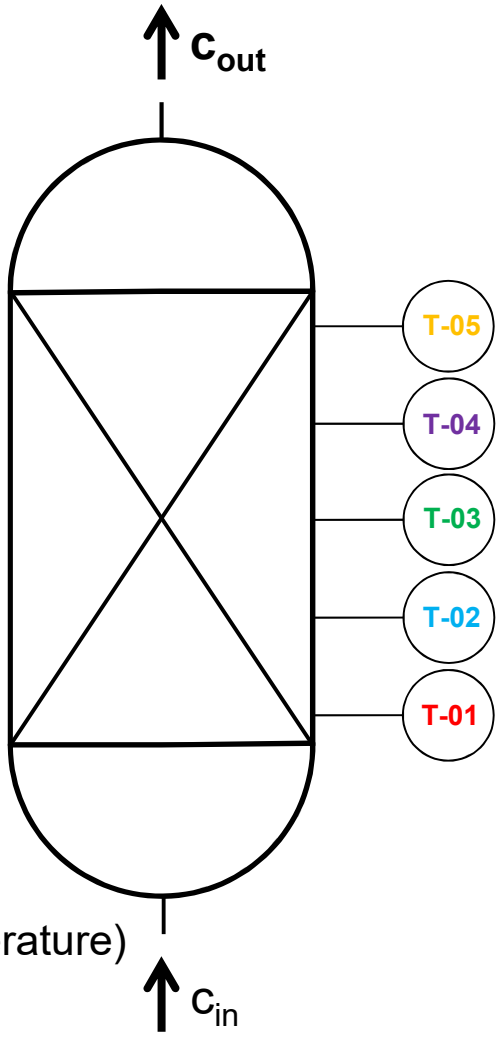
High accuracy of dynamic simulation (concentration and temperature profile)

- Deviation of temperature peak < 0,3 °C
- Slightly faster cooling of fixed bed in the simulated case

3. Non-Isothermal Adsorption Processes

Desorption profiles of C_2H_5SH on Sorbead H





- Simulation with same set of parameters
- High accuracy of dynamic simulation (concentration and temperature)
- Characteristic temperature plateaus with deviation 2 - 5 °C

Content

4. Specific Adsorption Parameters

Dynamic Simulation of Adsorption Processes

⇨ 1. Differential Equation (Mass Balance Fixed Phase):

$$\frac{\partial X}{\partial t} = \frac{k_{eff} \cdot A_{spec}}{\rho_S} \cdot (X_{Gl} - X)$$

⇨ 2. Differential Equation (Mass Balance Fluid Phase):

$$\frac{\partial c_A}{\partial t} = D_{ax} \frac{\partial^2 c_A}{\partial z^2} - \frac{\dot{V}_G}{A \cdot \varepsilon_L} \frac{\partial c_A}{\partial z} - \frac{c_A}{A \cdot \varepsilon_L} \frac{\partial \dot{V}_G}{\partial z} - \frac{k_{eff} \cdot A_{Spec} \cdot (1-\varepsilon_L)}{\varepsilon_L} (X_{Gl} - X)$$

⇨ 3. Differential Equation (Energy Balance Fixed Phase):

$$\frac{\partial T_F}{\partial t} - \frac{\Delta h_{Ads}}{M_A \cdot \left(c_{pS} + X c_{pA} + \frac{m_{Wand} \cdot c_{p\ Wand}}{\rho_S\ A\ L (1-\varepsilon_L)} \right)} \frac{\partial X}{\partial t}$$

$$= - \frac{\alpha_P \cdot A_{Sp}}{\rho_S \cdot (1-\varepsilon_L) \left(c_{pS} + X c_{pA} + \frac{m_{Wand} \cdot c_{p\ Wand}}{\rho_S\ A\ L (1-\varepsilon_L)} \right)} (T_F - T_G)$$

Adsorption Kinetics

MISSING DATA !

Adsorption Thermodynamics

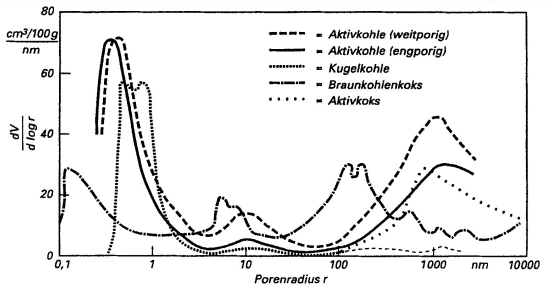
...

4. Specific Adsorption Parameters

Characterisation Methods

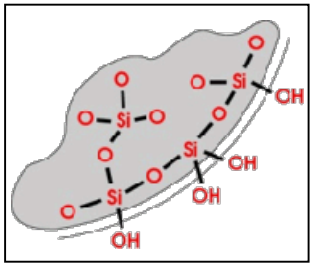
Structural properties:

- ⇨ Nitrogen Adsorption (BET)
- ⇨ Probe Molecule Method (Size Exclusion)
- ⇨ Hg-Porosimetry
- ⇨ Methylene Blue / Iodine Number



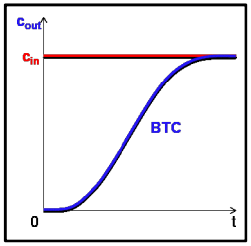
Chemical properties:

- ⇨ Elemental Analysis
- ⇨ IR-Spectroscopy
- ⇨ Boehm Titration
- ⇨ EDX, SAXS, …



Adsorption properties:

- ⇨ Excess Isotherms
- ⇨ Adsorption Enthalpies
- ⇨ Breakthrough Experiments in small Columns
- ⇨ Methylene Blue / Iodine Number

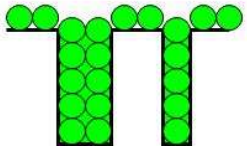


4. Specific Adsorption Parameters

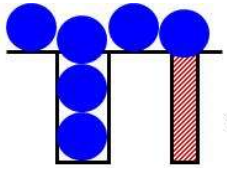
Molecular Probe Method

#	Adsorptive	T_{Ads} [K]	p_0 [kPa]	MIN-1	MIN-2
1	Nitrogen	77	101,35	3,6 Å	
2	n-Hexan	298	20,13	4,2 Å	4,6 Å
3	Cyclohexan	298	13,04	5,1 Å	6,8 Å
4	2,2-Dimethylbutan	298	42,54	5,9 Å	6,0 Å
5	2,2,4-Trimethylpentan	298	6,59	6,2 Å	6,7 Å

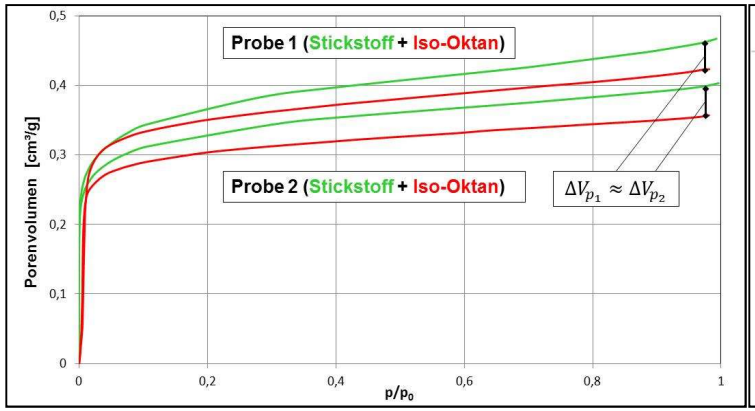
Molecule A:

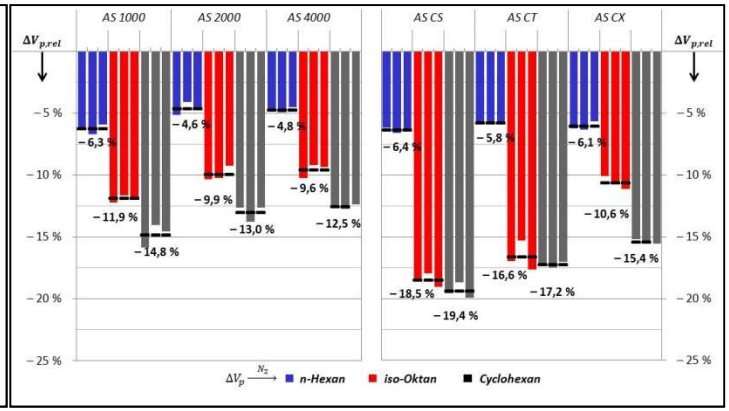


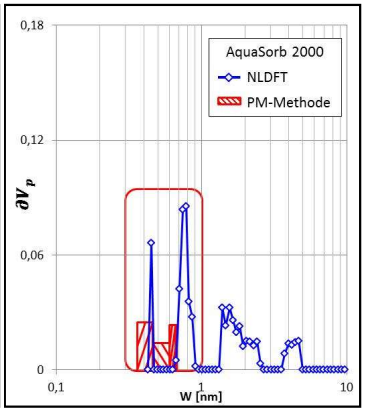
Molecule B:



$$\Delta V_p = V_{p_A} - V_{p_B}$$



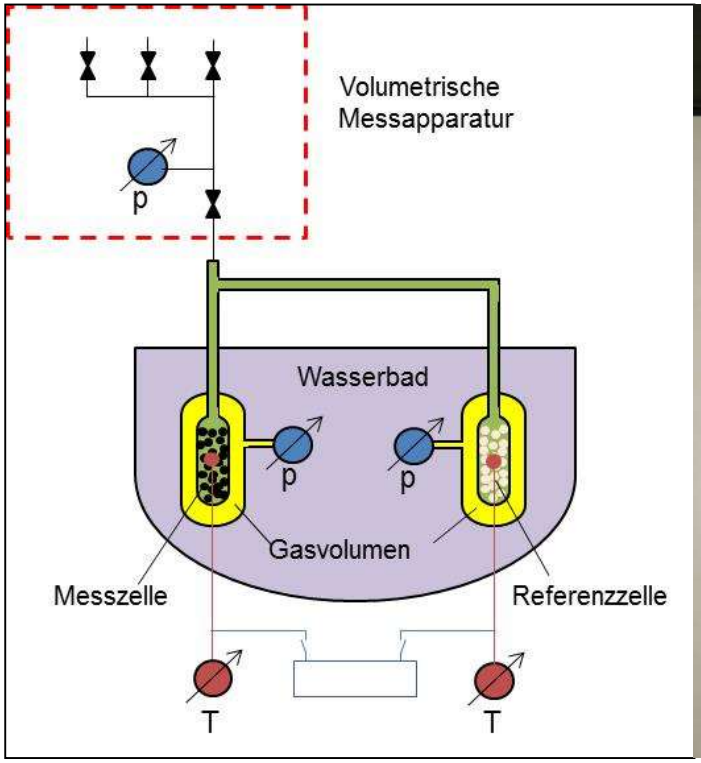


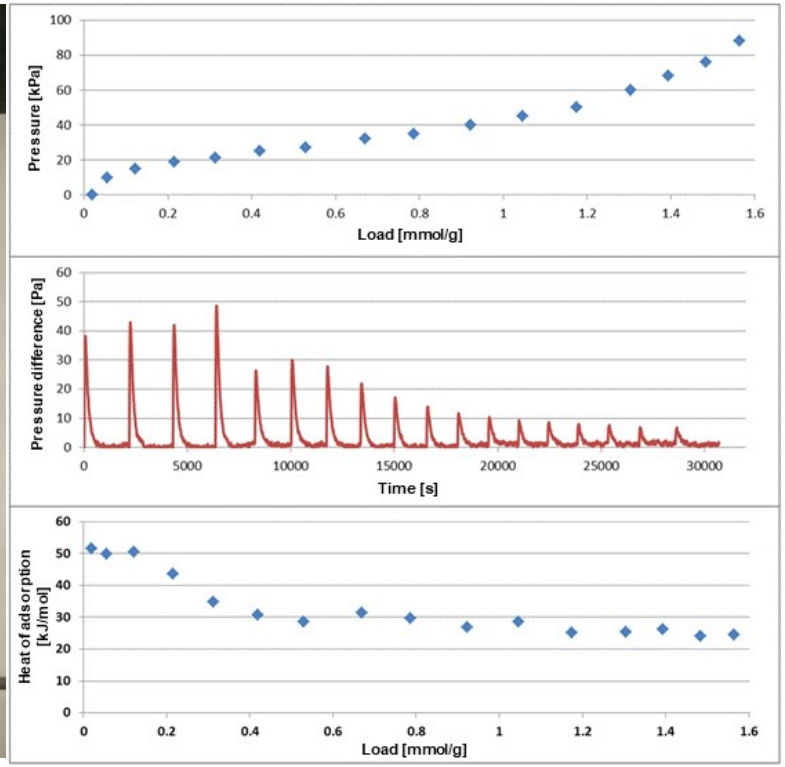


4. Specific Adsorption Parameters

Coupling of Volumetric and Calorimetric Adsorption Measurements

- Extension of Existing Measurement Device (N_2-BET)
- Volumetric Measurement of Adsorption Isotherms
- Simultaneous Measurement of Adsorption Enthalpy by Analysis of Pressure Rise and Decline in Surrounding Gas Volume

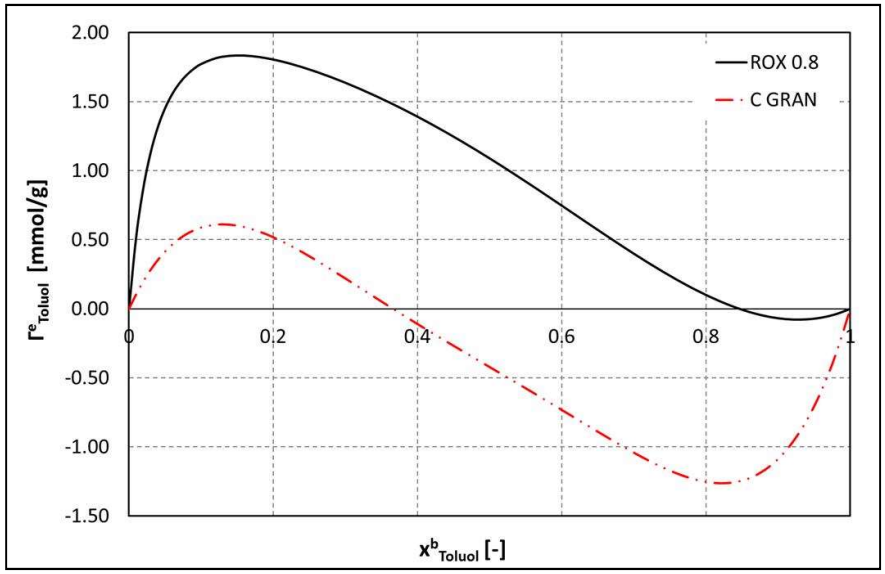




4. Specific Adsorption Parameters

Excess Adsorption Isotherms (in Liquid Phase)

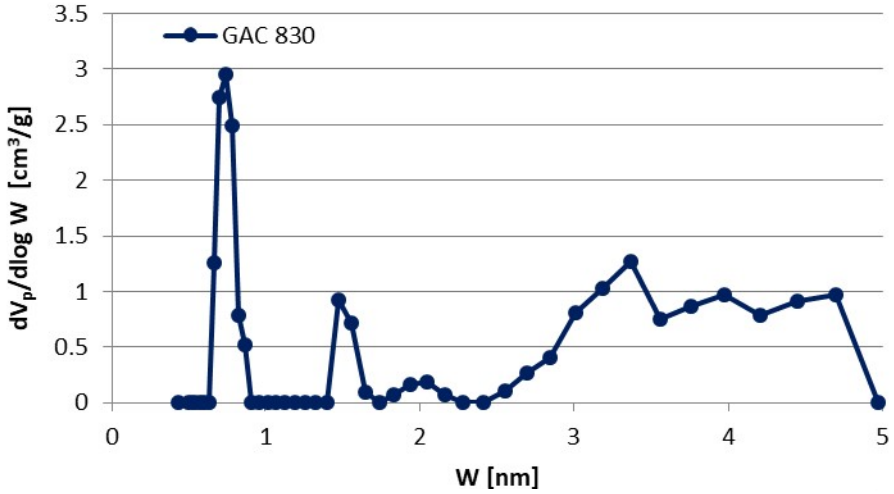
- Interaction Adsorbent ↔ Adsorptive ↔ Solvent
- Group Contribution Model



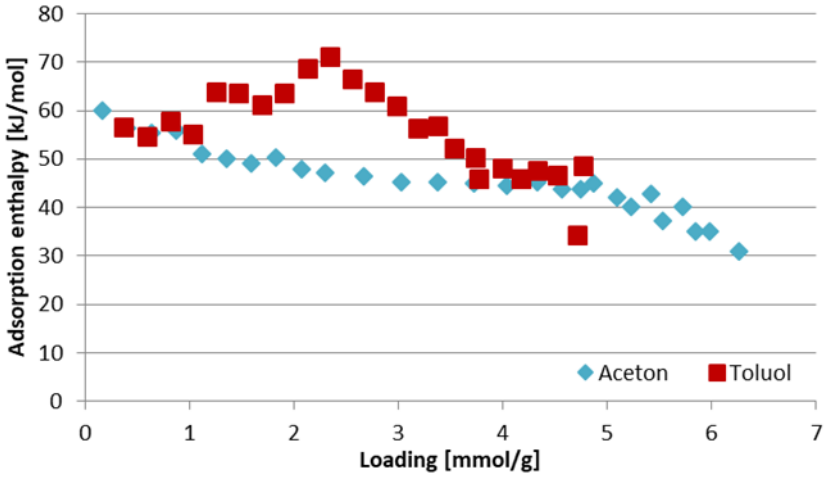
- Characterisation of Activated Carbon by Analysis of Binary Adsorption Isotherms
- Adsorptives:
  - Methyl-Cyclohexane (non-polar)
  - Toluene (aromatic)
  - Acetone (polar)
- Calculation of Adsorptive Sites' Distribution with Layer-Models

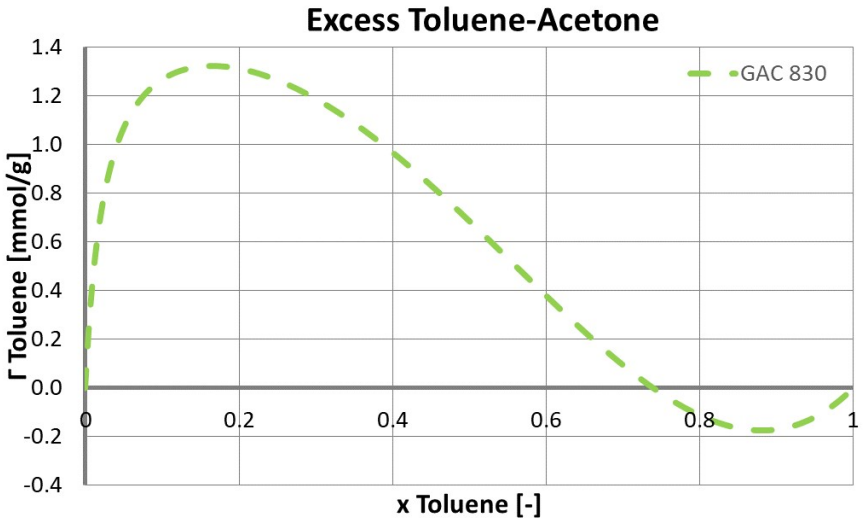
- Calculation of Adsorption Isotherms using the Adsorbate-Solid-Solution-Theory (Ulbig, TU Dortmund)

4. Specific Adsorption Parameters

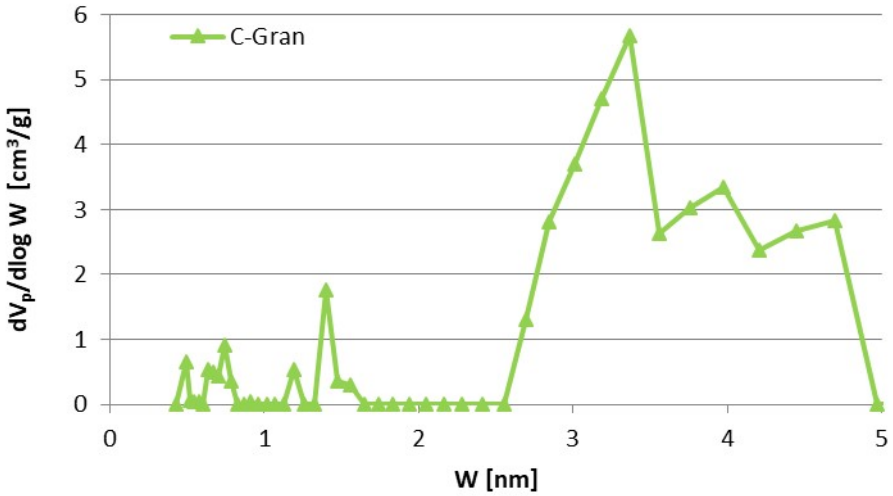


Activated Carbon	A_{BET}	V_p	C	H	O
	$\left[\frac{m^2}{g}\right]$	$\left[\frac{cm^3}{g}\right]$	[wt-%]	[wt-%]	[wt-%]
GAC 830	960	0.57	89.50	0.25	4.32

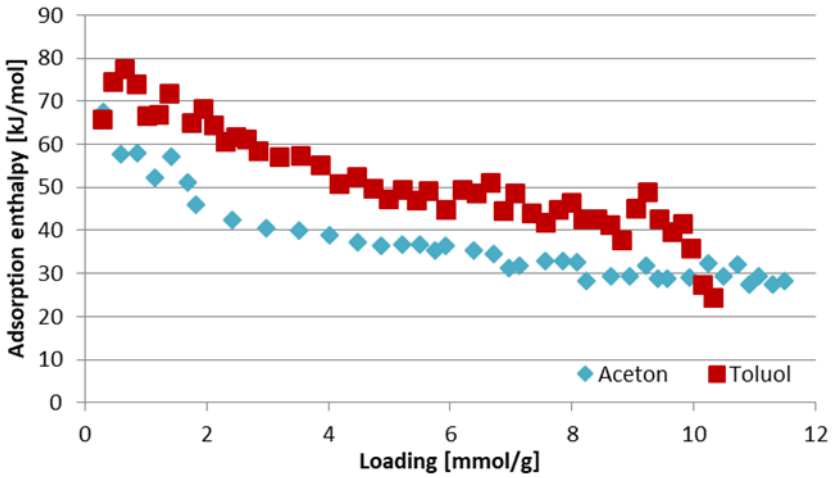


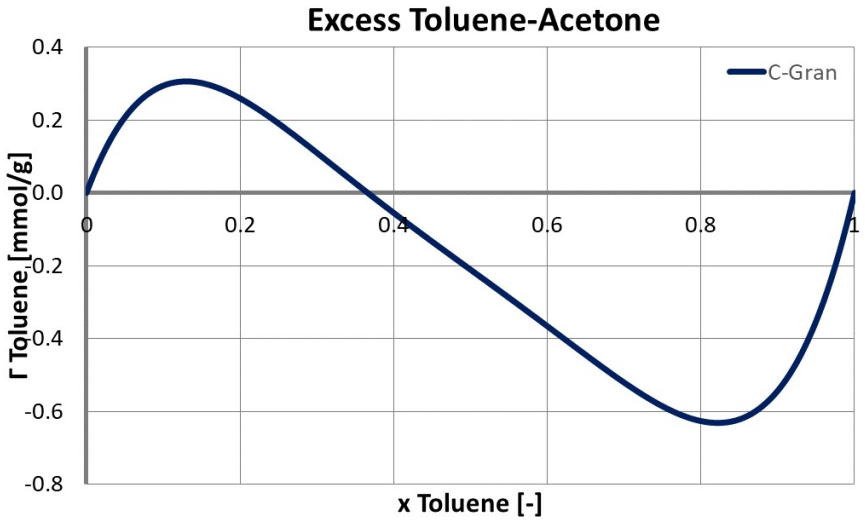


4. Specific Adsorption Parameters



Activated Carbon	A_{BET}	V_p	C	H	O
	$\left[\frac{m^2}{g}\right]$	$\left[\frac{cm^3}{g}\right]$	[wt-%]	[wt-%]	[wt-%]
C Gran	1162	1.02	73.4	1.9	22.0

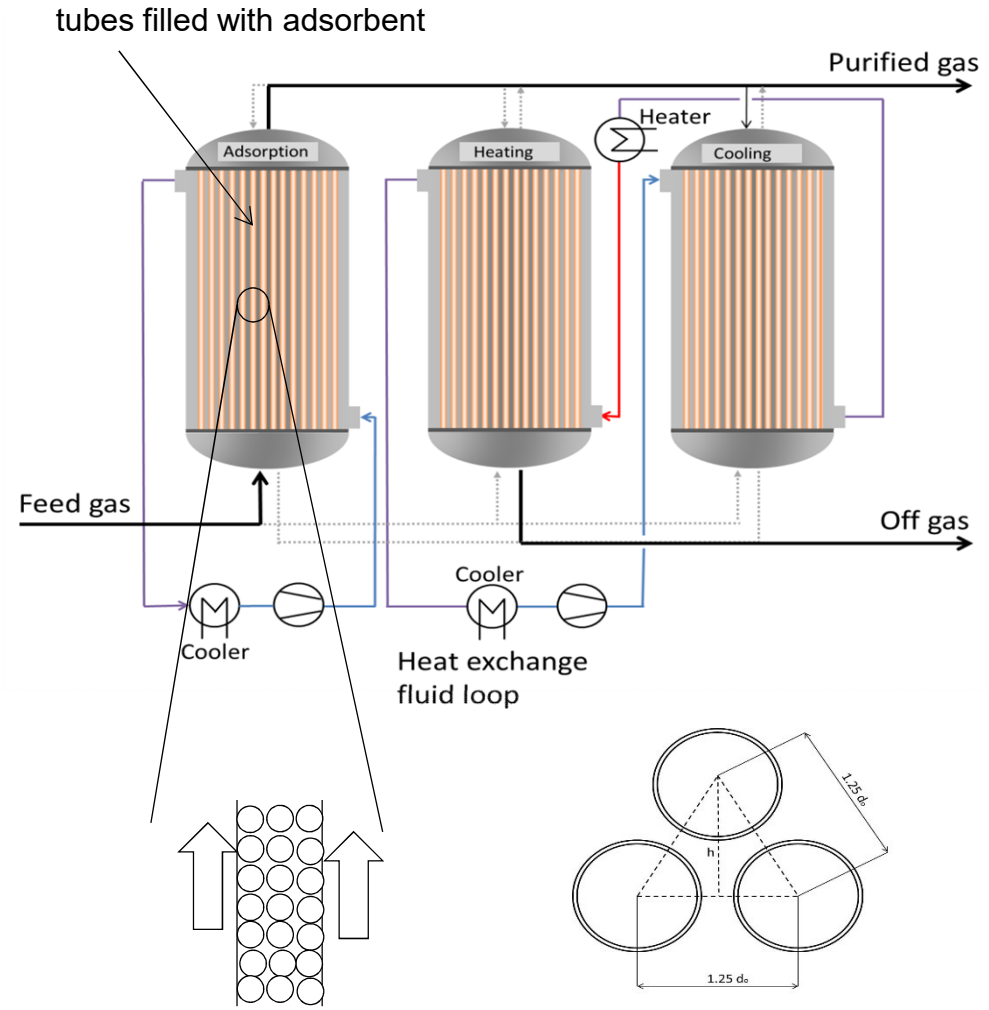




Content

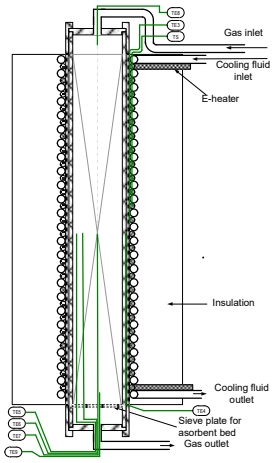
5. Sophisticated Simulations

Rapid TSA-Process (Linde AG)



Concept:

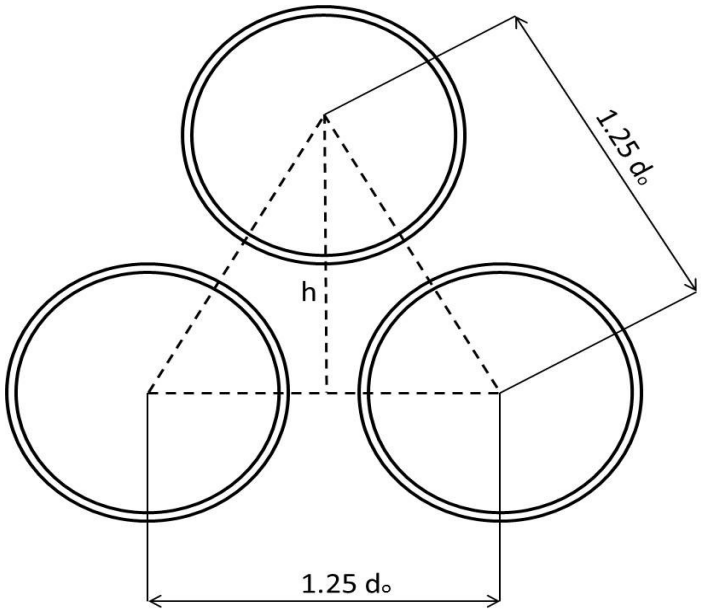
- Two separated flow channels
- Heat exchange between channels
- Cooling/heating fluid in the shell
- Adsorbent in the tubes
- Indirect heating with a utility fluid, e.g. water

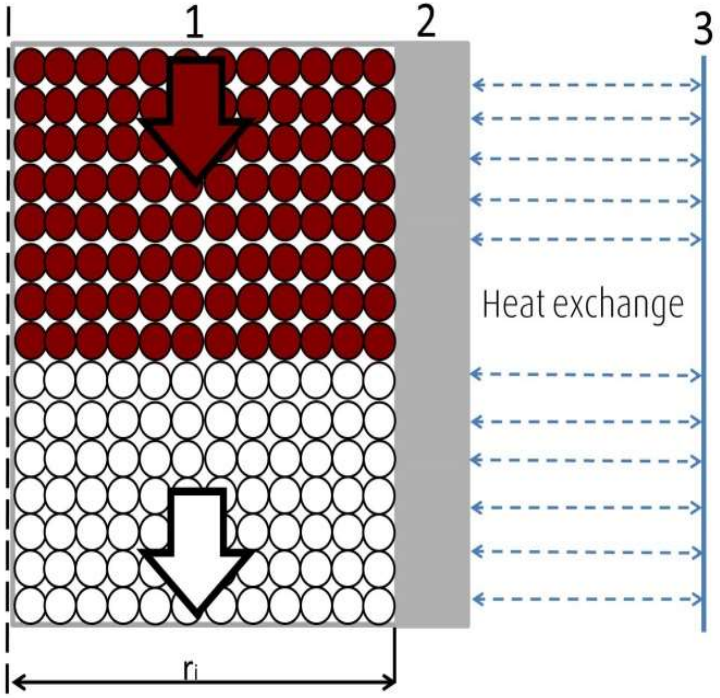


5. Sophisticated Simulations

Simulation of Tube Bundle Adsorber (Linde AG)

- One tube of the tube bundle system
- Numerical study using COMSOL Multiphysics®
- Simulated dry flue gas: 15% CO_2 and 85% N_2
- Geometry: Axial symmetrical 2D model coupled to a 1D model
- Surface to volume ratio ϕ estimated from unit cell





Wall:

$$\frac{\partial T_{wall}}{\partial t} = \nabla\left(\frac{\lambda}{\rho_{wall} c_{p,wall}} \nabla T\right)$$

Adsorbent + gas (local thermal equilibrium and linear driving force):

$$\overbrace{\frac{\partial c_i}{\partial t}}^{Accumulation} = \overbrace{\nabla(D_i \nabla c_i)}^{Dispersion} - \overbrace{\nabla(u_z \cdot c_i)}^{Convection} - \rho_s \overbrace{\frac{1-\epsilon}{\epsilon}\frac{\partial q_i}{\partial t}}^{Adsorption}$$

$$\frac{\partial\left(\left(\rho_g c_{pg}\epsilon + (1-\epsilon)\rho_s c_{ps}\right)T\right)}{\partial t} = \nabla(\lambda_{eff}\nabla T) - \epsilon \cdot \nabla(u \rho_g c_{pg} T) + (1-\epsilon)\,\rho_s \sum \Delta H_{ads,i} \frac{\partial q_i}{\partial t}$$

$$\frac{\partial c}{\partial t} + \nabla(uc) = -\sum \rho_s \frac{1-\epsilon}{\epsilon}\frac{\partial q_i}{\partial t}$$

$$-\nabla p = \left(150\frac{(1-\epsilon)^2}{\epsilon^3}\frac{\eta_g}{d_p^2} + 1.75\frac{1-\epsilon}{\epsilon^3}\frac{\rho_g}{d_p}u_0\right) \cdot \boldsymbol{u}$$

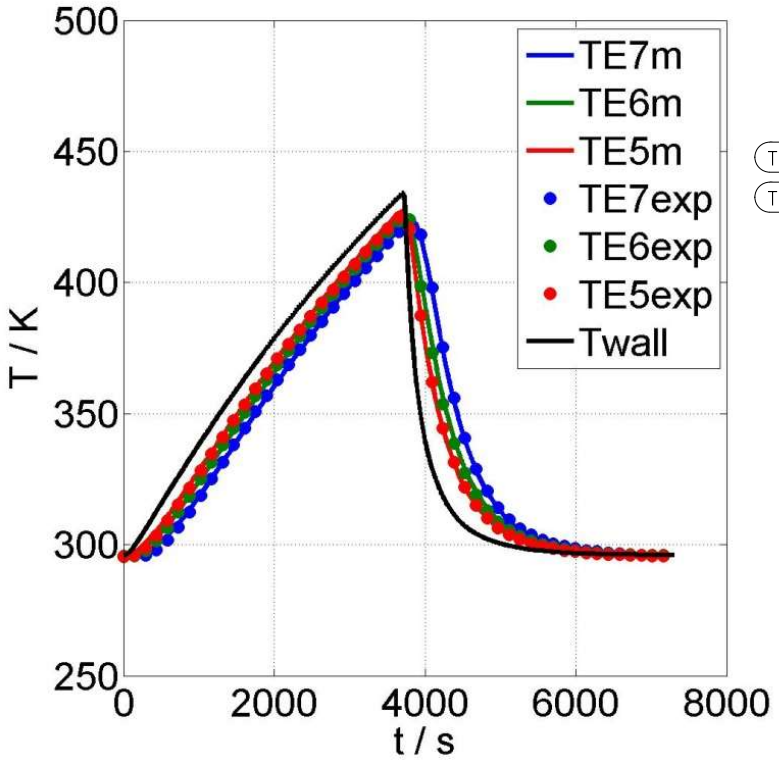
$$\frac{\partial q_i}{\partial t} = k^*_{LDF_{eff}}(q_{eq} - q_i)$$

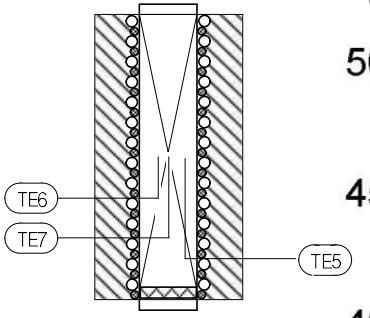
Heat transfer fluid:

$$\frac{\partial T_{\mathrm{Hex}}}{\partial t} + u_{z,\mathrm{Hex}}\frac{\partial T_{\mathrm{Hex}}}{\partial z} = \frac{\partial}{\partial \mathrm{z}}\left(\lambda_{\mathrm{Hex}}\frac{\partial T_{\mathrm{Hex}}}{\partial z}\right) + \phi\alpha_{\mathrm{Hex}}(T_{\mathrm{Hex}} - T_{\mathrm{wall}}(r = r_o))$$

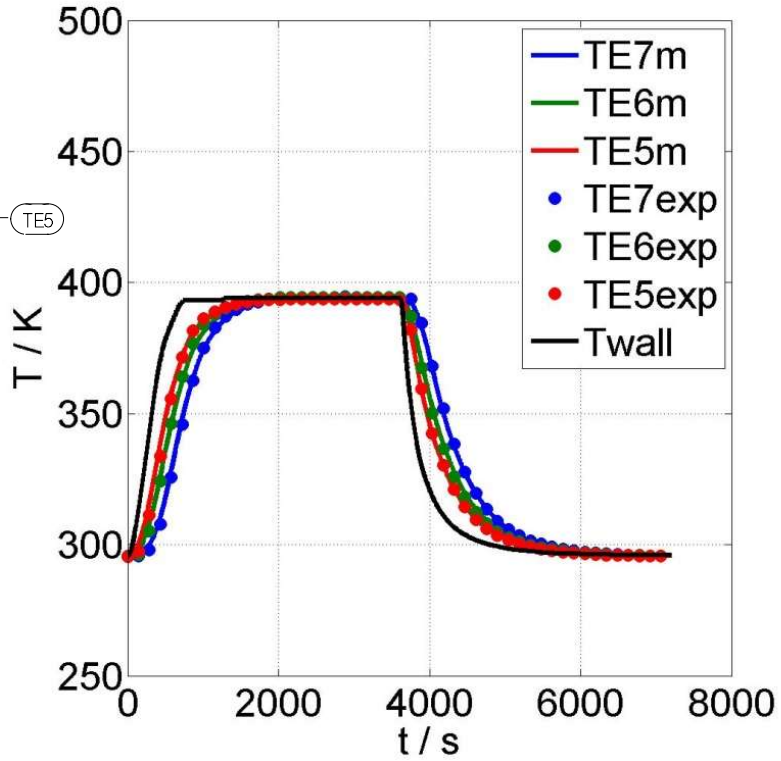
5. Sophisticated Simulations

Constant heat duty (50 W)





Constant wall temperature (120 °C)



$\lambda_p = 0.391 \frac{W}{mK}, Bi = 1.17 \frac{W}{mK}$

$\lambda_p = 0.395 \frac{W}{mK}, Bi = 1.08 \frac{W}{mK}$

→ **Good agreement** between experiments and simulations

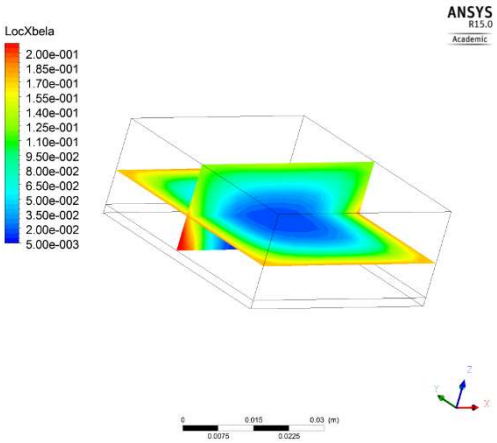
5. Sophisticated Simulations

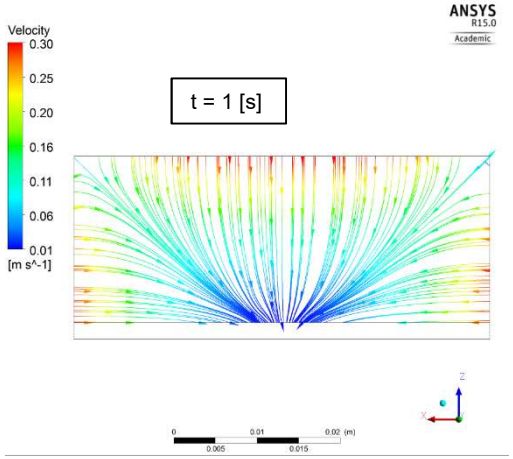
Adsorptive Air Conditioning (Bosch)

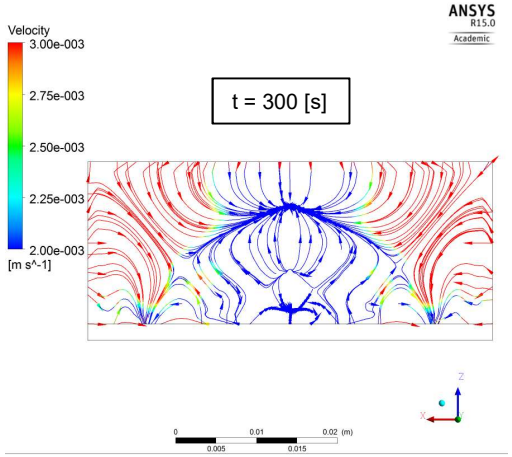
Concept:

- Foam as Basic Structure
- Coating with SAPO 34
- Water as Adsorptive

- CFD-Simulation with Ansys®



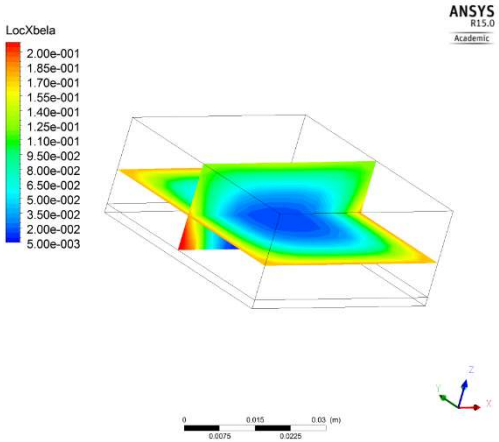


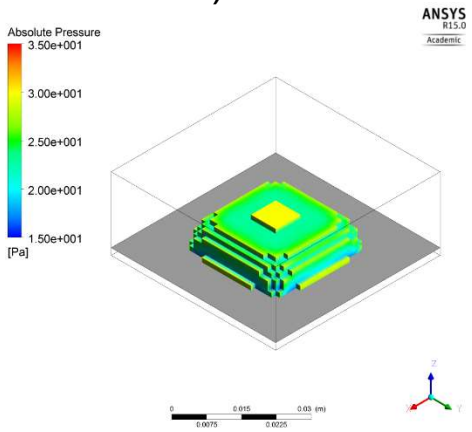


5. Sophisticated Simulations

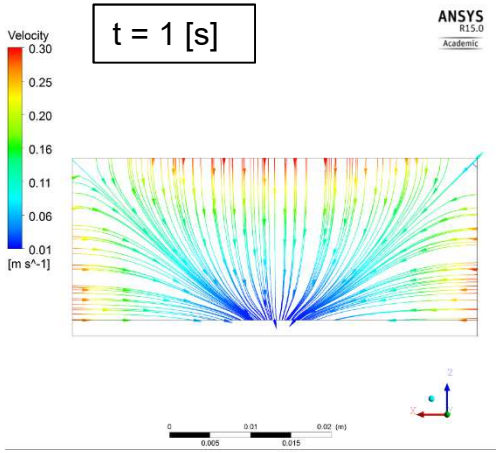
Simulation Results

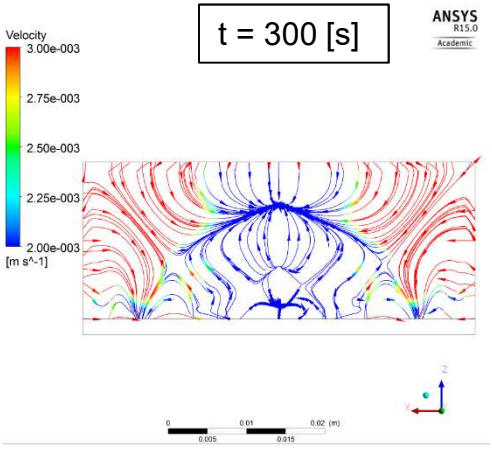
- Loading and pressure profiles (CFD-Simulation)





- Flow profile (CFD-Simulation)





6. Summary

State of the Art in Simulation

- Mathematical Equations are well known
- Performance of Computers is sufficient
- Missing Data on Adsorption-specific Properties
- Missing Data on Multi-component Adsorption
- Missing Data on Adsorption Kinetics

Recent Research Activities

- 2D and 3D Simulations
- Coupling of Adsorption and CFD
- Computer-based Calculation of Adsorption-specific Data
- Simulation of Complete Adsorption Processes (ADS-DES-COOL)

7. Recent Selected Publications

Simulation of Adsorption Processes

- B. Burrichter / C. Pasel / M. Luckas / D. Bathen, Parameter study on the adsorptive drying of isopronanol in a fixed bed adsorber, Sep. & Pur. Tech. 132 (2014), S. 736-743
- B. Burrichter / C. Pasel / M. Luckas / D. Bathen, Experimental and theoretical study on the adsorptive drying of primary alcohols in a fixed bed adsorber, Sep. & Pur. Tech. 145 (2015), S. 39-49
- G. Salazar Duarte / B. Schürer / C. Voss / D. Bathen, Modeling and simulation of a tube bundle adsorber for the capture of CO_2 from flue gases, Chem.Ing.Tech. 88 (2016) 3, S. 336-345
- S. Bruckner / T. Demmer / M. Ganswind / D. Bathen, Modeling of water adsorption in a SAPO 34 coated aluminum foam, Chem.Ing.Tech. 89 (2017) 6, S. 757-764

Characterisation of Adsorbents

- M. Helmich / M. Luckas / C. Pasel / D. Bathen, Characterization of microporous activated carbons using the molecular probe method, Carbon 74 (2014), S. 22-31
- J. Treese / C. Pasel / M. Luckas / D. Bathen, Chemical Surface Characterization of Activated Carbons by Adsorption Excess of Probe Molecules, Chem.Eng.Tech. 39 (2016) 6, S. 1144-1150
- C. Bläker / C. Pasel / M. Luckas / F. Dreisbach / D. Bathen, Investigation of load-dependent heat of adsorption of alkanes and alkenes on zeolites and activated carbons, Microporous and Mesoporous Materials 241 (2017), S. 1-10

Thank you for your attention!

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