Model-based parameter estimation of heat and mass transfer coefficients using small-scale experiments

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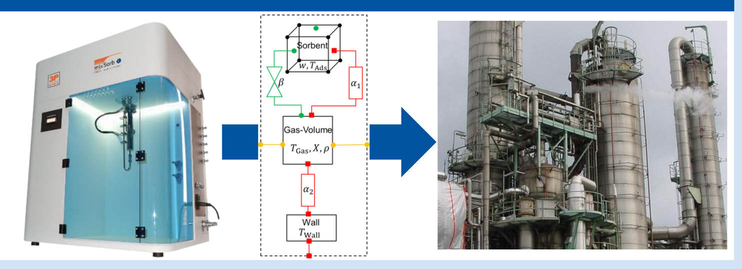
Motivation

- Steady-state design of adsorption columns leads to over-sized systems → causing high investment and operating costs
- Dynamic design requires detailed knowledge of heat and mass transfer coefficients → high effort for large-scale experiments

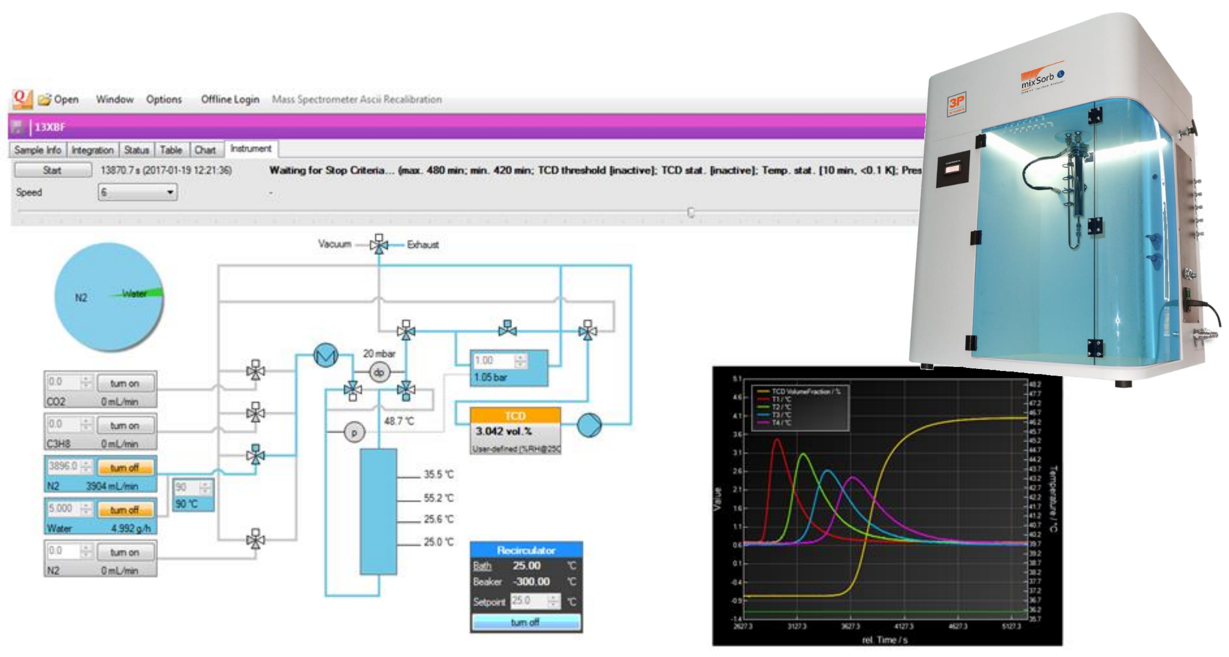
→ Model-based identification of coefficients from small-scale experiments saves time and money



Experimental setup

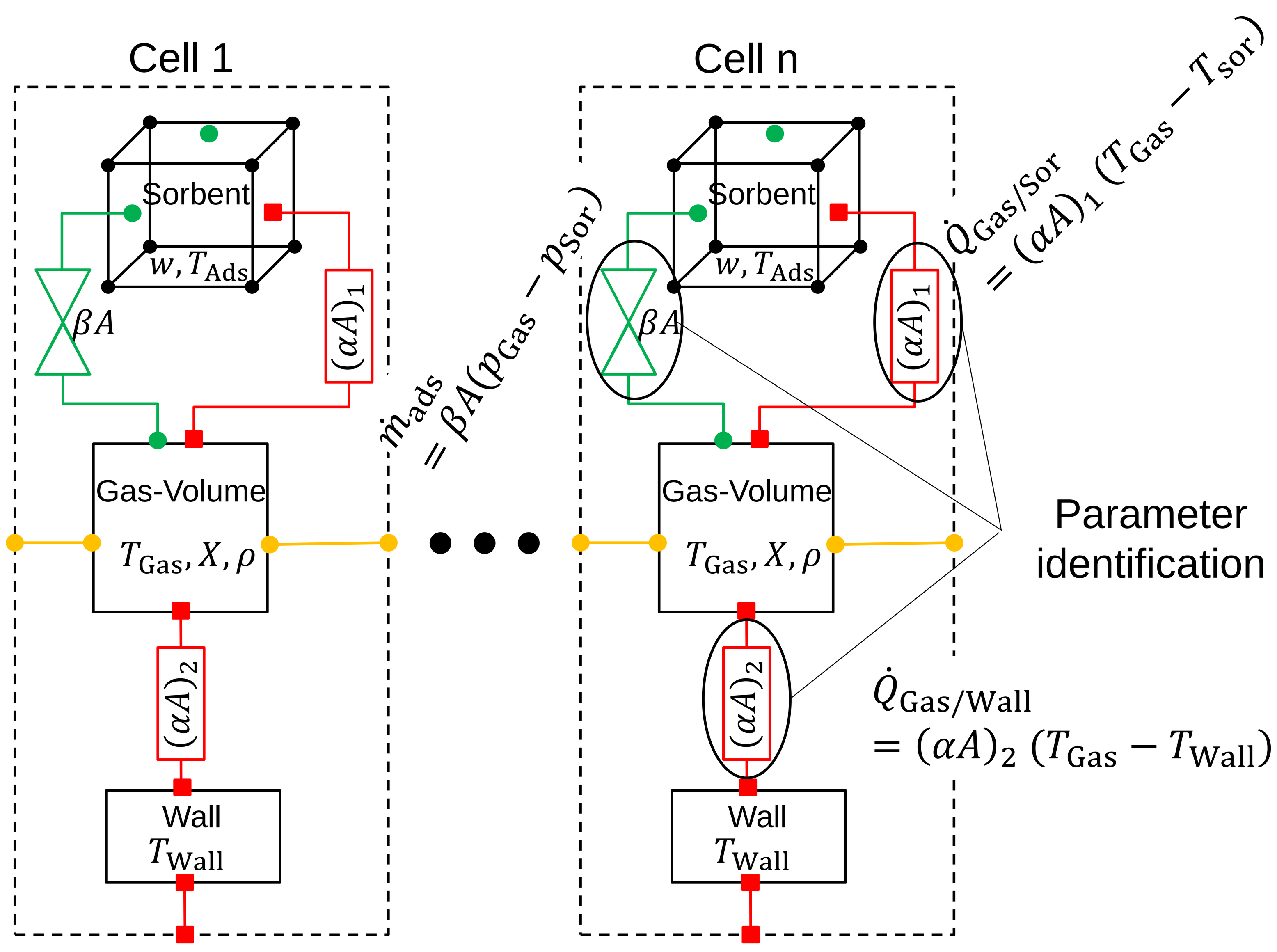
- Dynamic operated test-stand for investigations of packed-bed adsorbers
- Dosing up to 4 gases and up to 2 vapors by evaporation
- Adsorber equipped with 4 temperature sensors in flow direction
- Analysis of effluent gas by heat conductivity and optional MS
- Fully automated sequences and routines for:
  - Down-scaling of technical processes
  - Identification of coadsorption and displacement effects
  - Cycle stability and regeneration characteristics
  - Investigation of sorption dynamics

Output: time resolved data of temperature profiles along adsorber



Dynamic process model

- Dynamic model in Modelica based on our SorpLib[1]
- 1D discretized adsorber: finite-volume model
- Transient energy and mass balances for sorbent, gas and wall cells
- Modelling of mass transfer with linear driving force approach (LDF)
- Calculation of fluid properties with TILMedia[2]



Identification of heat and mass transfer coefficients

Input from experiments

- Experimental conditions:
  gas flow: 4 l/min
  inlet temperature: 25.5 °C
  Inlet pressure: 1.04 bar
  3 different relative humidities (RH):
  30 %, 50 % and 80 %

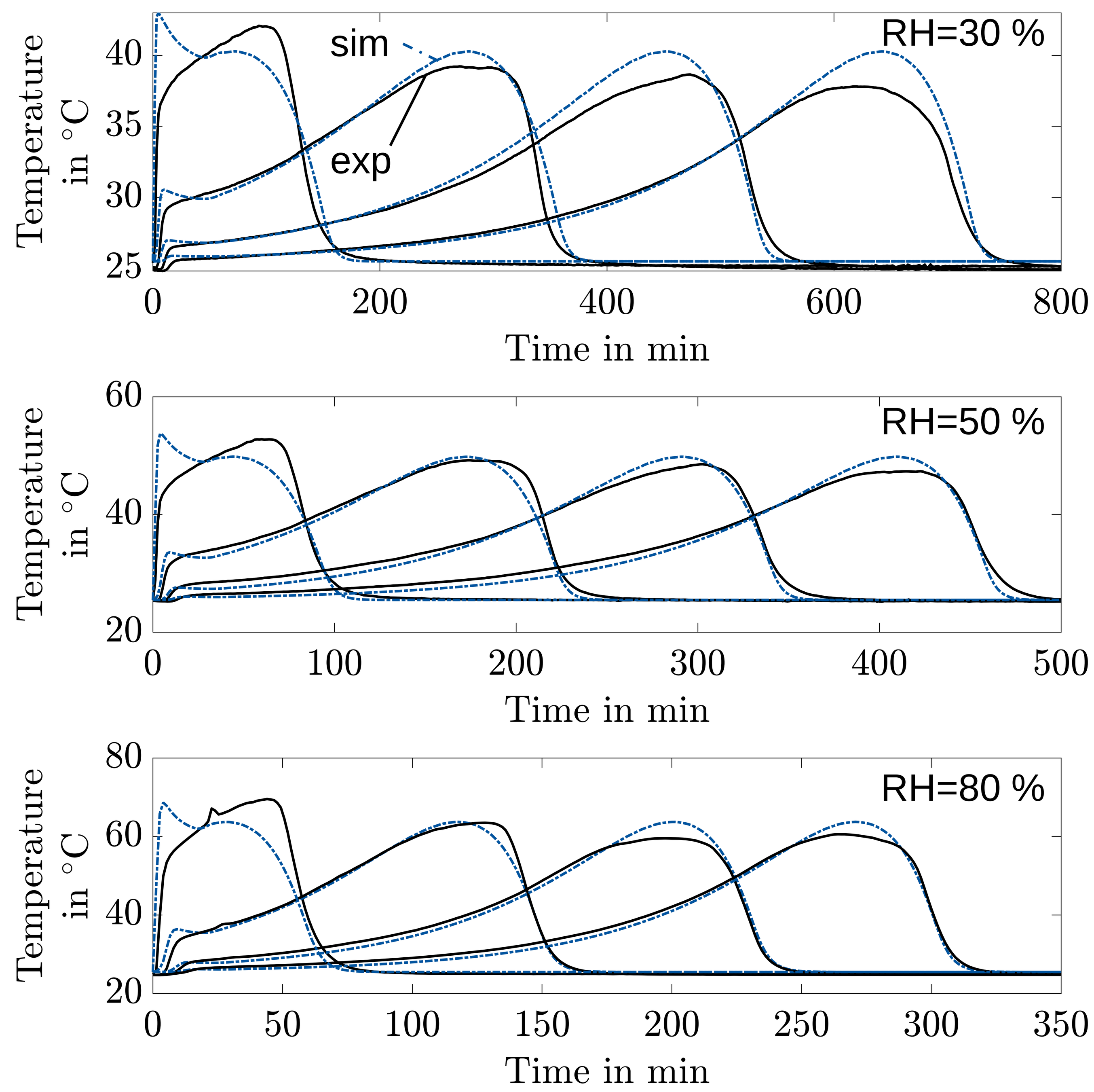
→Time-resolved temperature profiles along adsorber bed T_1-T_4 for 3 experiments

Model-based parameter identification

- Variation of $(\alpha A)_1$, $(\alpha A)_2$ and βA to minimize the root-mean-square deviation (RMSD) between experiment (exp) and simulation (sim)
- $\mathrm{RMSD} = \sqrt{\frac{1}{\Delta\tau}\int \left(T_{exp} - T_{sim}\right)^2 \mathrm{d}\tau}$

→Identified coefficients $(\alpha A)_1$, $(\alpha A)_2$ and βA

Results: $(\alpha A)_1 = 4.5\,\mathrm{W/K}$, $(\alpha A)_2 = 0.01\,\mathrm{W/K}$, $\beta A = 2 \cdot 10^{-10}\,\mathrm{m} \cdot s$



Conclusions and outlook

- Good agreement between experiments and simulation
- Identified coefficients valid for various operating conditions
- Physically-motivated model allows for prediction

→Up-scaling to predict large-scale adsorption columns

→Design optimisation of large-scale adsorptions columns for specific applications

Further Information

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References

[1]SorpLib - Adsorption Energy Systems Library: https://git.rwth-aachen.de/ltt_public/SorpLib

[2]TILMedia Suite – Software package for thermo-physical properties https://www.tlk-thermo.com/index.php/de/tilmedia-suite