Dynamic Sorption Characteristics as Key for Reliable Performance Predictions of Adsorption Chillers

Stefan Graf, Franz Lanzerath, André Bardow
Leipziger Symposium on dynamic sorption 2018
Modelling of Adsorption Systems

SorpLib
- Open Source Modelica Library
  https://git.rwth-aachen.de/ltt_public/SorpLib
- Cells: Adsorbent, Gas, Wall, ...
- Components
  - Adsorber
  - Condenser
  - Evaporator
  - Valves
- Examples
  - Adsorption Chillers
  - Desiccant Systems
Performance Prediction: Simulations

how do I know that my model is reliable?

simulations @ different operating conditions

performance figures: temperatures, heat flows, COP, SCP, …

model

condenser

adsorber

evaporator

I/O

Dynamic Sorption Characteristics as Key for Reliable Performance Predictions of Adsorption Chillers
Leipziger Symposium on dynamic sorption 2018
Model Calibration & Validation

Dynamic Sorption Characteristics as Key for Reliable Performance Predictions of Adsorption Chillers

Leipziger Symposium on Dynamic Sorption 2018

- Many simulations @ different operating conditions
- Adsorption chiller test stand
- Many experiments @ different operating conditions
- Simulation data sets
- Parameter identification + validation
- Reliable performance predictions for the calibrated system
State of the Art Performance Predictions

model calibration and validation with full-size adsorber

- one bed adsorption chiller
- lab scale ~ 1kg sorbent material
- silica gel 123 and zeolite 13X

not transferable to other adsorber configurations (hx design, adsorbent)
State of the Art Performance Predictions

model calibration and validation with full-size adsorber

- one bed adsorption chiller
- lab scale ~ 1kg sorbent material
- silica gel 123 and zeolite 13X

reliable performance predictions, but high effort for a single configuration
How to shrink the sorption lab?

1. What are the important parameters?
2. How do we determine these parameters?
3. How to setup the model?
4. Does it work?
Important Parameters

known
- geometry
  - hx, isolation, volumes, …
- material properties
  - sorption equilibrium, thermal conductivity, heat capacities, …
- evaporator and condenser
  - mass, UA-values, …

unknown / uncertain
- heat and mass transfer coefficients of adsorber
Important Unknown Parameters

Vapor phase
Sorption material
Heat exchanger

Effective heat and mass transfer coefficients
λ: Conductivity in sorbent material
α: Heat transfer coefficient to hx surface
D: Diffusion coefficient

λ: Conductivity in sorbent material
α: Heat transfer coefficient to hx surface
D: Diffusion coefficient
How to shrink the sorption lab?

1. What are the important parameters? \( \lambda, \alpha \) and \( D \)

2. How do we determine these parameters?

3. How to setup the model?

4. Does it work?
Adsorption Chiller Process

Dynamic Sorption Characteristics as Key for Reliable Performance Predictions of Adsorption Chillers

Leipziger Symposium on dynamic sorption 2018
InfraRed - Large Temperature Jump (Adsorption)

measurement of temperatures and pressures during LTJ
Experimental Setup of IR-LTJ
Measurement Cell

- small heat exchanger
  - low heat capacity: fast temperature jumps
  - oil circuit: high temperatures, up to 200°C
IR-LTJ Measurement Conditions

sample material
- Silica Gel 123
- total mass: ~ 450 mg
- pellet size: 0.9 mm

temperatures
- evaporation: 10°C
- condensation: 35°C
- adsorption: 35°C
- desorption: 90°C

results
- temperature and pressure curves
- characteristic times $\tau$
- cannot be used in model directly
- employing dynamic model of IR-LTJ
- determine $\lambda$, $\alpha$ and $D$
Discretized IR-LTJ Model

- simple geometry
- model discretized in z-direction
- no pressure loss in sorbent layer
- measurements with different layer thicknesses → distinguish λ and α
- minimizing RMSD for pressure and temperature → determine λ, α and D by

\[ \text{Discretized IR-LTJ Model} \]

\[ \begin{align*}
\rho_{\text{sim}} & \quad T_v \\
D_{\text{eff}} & \quad \lambda \\
D_{\text{eff}} & \quad ad, i \\
T_{\text{car}} & \quad \alpha
\end{align*} \]
IR-LTJ Results

<table>
<thead>
<tr>
<th></th>
<th>Adsorption</th>
<th>Desorption</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>245 W/m²K</td>
<td>370 W/m²K</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>0.278 W/mK</td>
<td>0.355 W/mK</td>
</tr>
<tr>
<td>$D$</td>
<td>$1.32 \times 10^{-9}$ m/s²</td>
<td>$6.16 \times 10^{-10}$ m/s²</td>
</tr>
</tbody>
</table>

- Good agreement of measurement and simulation
- Deviation smaller than measurement uncertainty
- Coefficients dependent on temperature, pressure and loading
How to shrink the sorption lab?

1. What are the important parameters? $\lambda$, $\alpha$ and $D$ ✔

2. How do we determine these parameters? IR-LTJ measurements ✔

3. How to setup the model?

4. Does it work?
Setup of full-size adsorption chiller model

- geometries, material data, ... are known
- setup component models → e.g. SorpLib
- use heat and mass transfer coefficients from IR-LTJ
- complex adsorber hx → discretized model necessary
Discretized Model of Adsorber

Dynamic Sorption Characteristics as Key for Reliable Performance Predictions of Adsorption Chillers
Leipziger Symposium on dynamic sorption 2018
How to shrink the sorption lab?

1. What are the important parameters? $\lambda$, $\alpha$ and $D$  
2. How do we determine these parameters? IR-LTJ measurements  
3. How to setup the model? Using discretized adsorber model + $\lambda$, $\alpha$ and $D$  
4. Does it work?
Validation with full-size adsorption chiller setup

- silica gel 123
- temperatures 10 / 30 / 95 °C
- cycle times
  - 450 s
  - 900 s
  - 1800 s

Dynamic Sorption Characteristics as Key for Reliable Performance Predictions of Adsorption Chillers
Leipziger Symposium on dynamic sorption 2018
Experiment vs Simulation Ads 450s / Des 300s; 10/30/95°C

- model parameters
  - $\lambda$, $\alpha$ and $D$
  - geometry, …
- model inputs
  - measured inlet temperatures
  - volume flows
- model outputs
  - outlet temperatures
  $\rightarrow$ heat flows, COP, SCP

Prediction almost perfectly describes the characteristics of the full-scale adsorption chiller.
Results of Performance Prediction

- COP and SCP are accurately predicted for various cycle times
- model is based only on coefficients from small and fast IR-LTJ experiments
- accuracy is close to full-scale calibrated model
How to shrink the sorption lab?

1. What are the important parameters? $\lambda$, $\alpha$ and $D$ ✓

2. How do we determine these parameters? IR-LTJ measurements ✓

3. How to setup the model? Using discretized adsorber model + $\lambda$, $\alpha$ and $D$ ✓

4. Does it work? Yes, it does! ✓
LTT’s Guide on how to shrink your sorption lab

1. Determine heat and mass transfer coefficients with IR-LTJ for your specific sorbent – hxc material combination

2. Setup your adsorption chiller model with SorpLib

   https://git.rwth-aachen.de/ltt_public/SorpLib

3. Implement specific adsorber hxc geometry
discretized model for adsorber

4. Carry out simulations for performance prediction and enjoy reliable results

Dynamic Sorption Characteristics as Key for Reliable Performance Predictions of Adsorption Chillers
Leipziger Symposium on dynamic sorption 2018
Vielen Dank
für Ihre Aufmerksamkeit

TailorSorb
Maßgeschneiderte Adsorbentien für
stationäre Wärmetransformatoren
(03SF0515A)