Empa
Materials Science and Technology

Multiscale adsorption – outline of research activities
Advanced Colloidal Materials Engineering Group (Empa)

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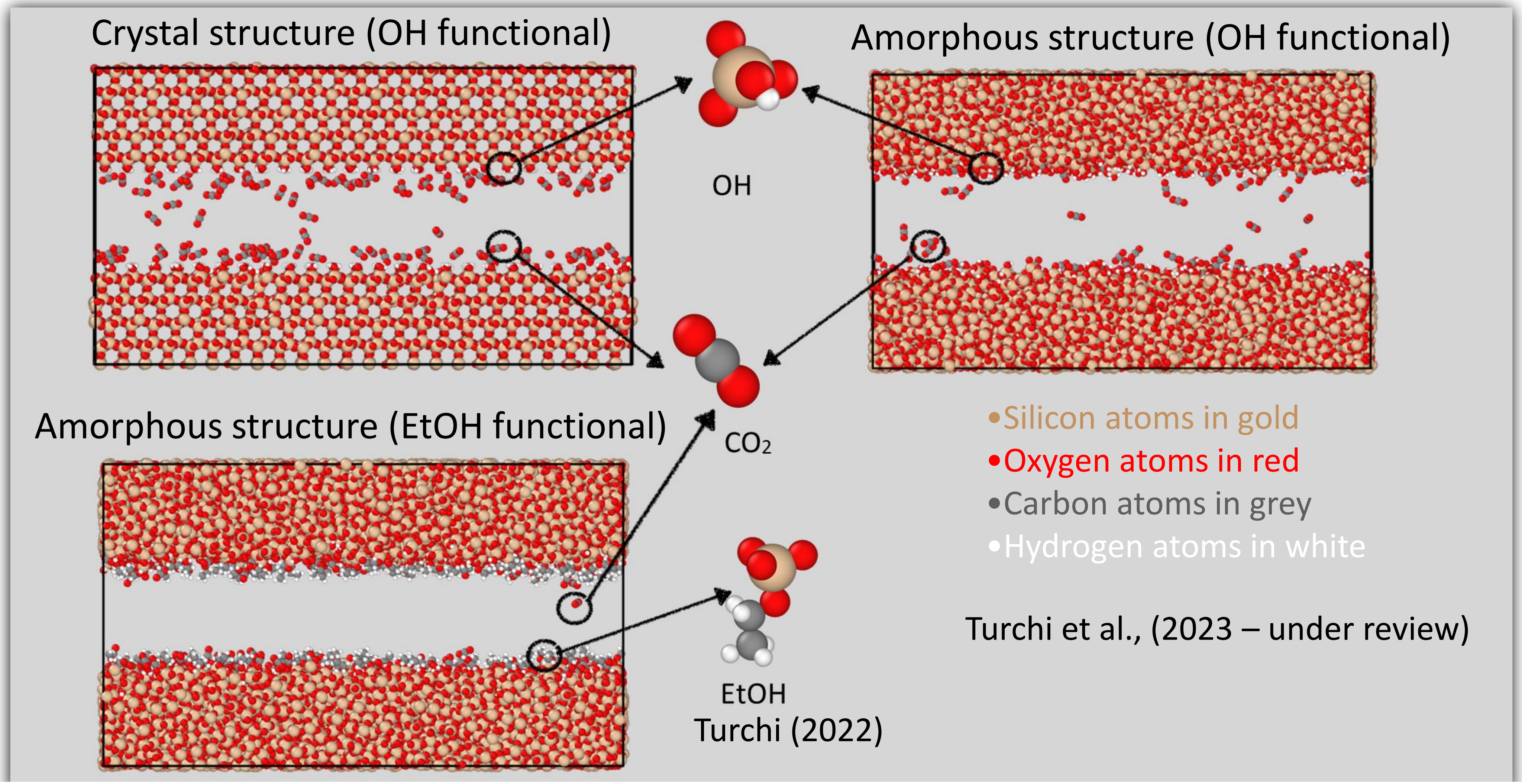
Multiscale aspects of the adsorption process:

1) Molecular dynamics

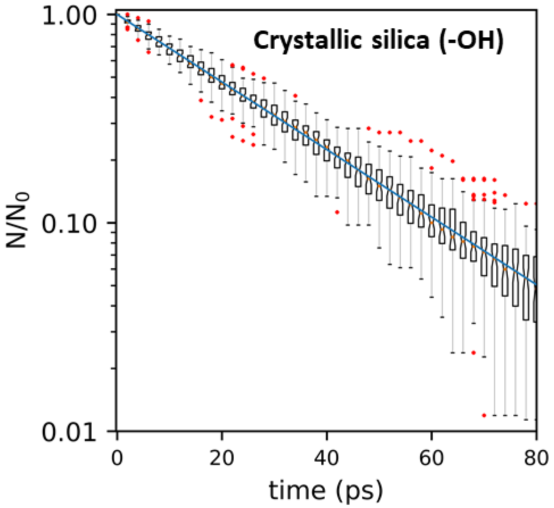
CO_2 physisorption on silica with/without functionalization

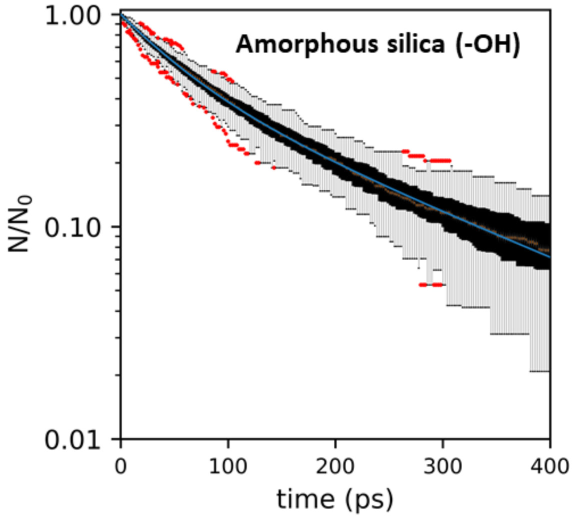


Mattia Turchi* (mattia.turchi@empa.ch) – *in collaboration with Laboratory for Multiscale Studies in Building Physics (Empa)

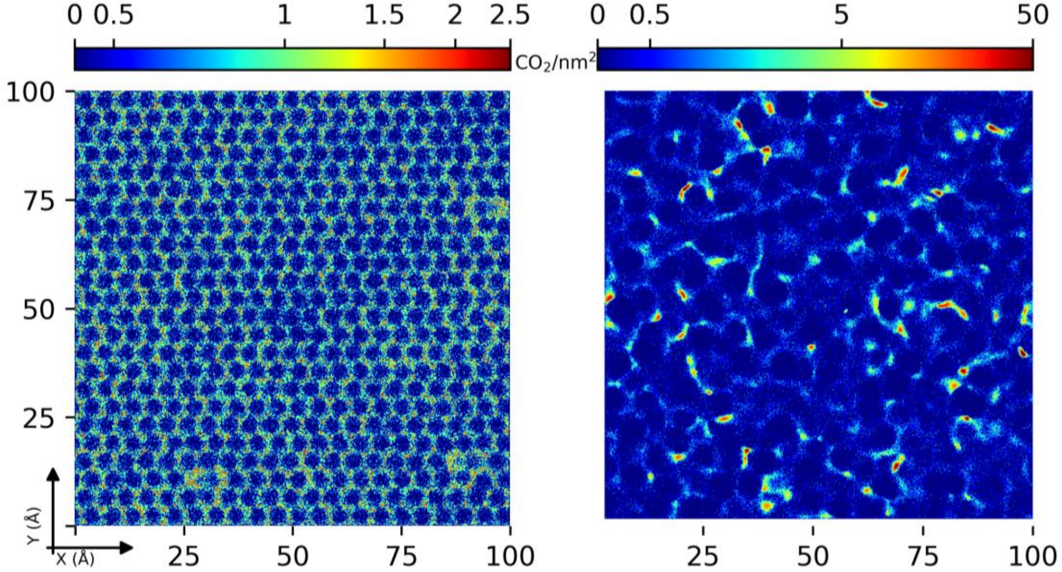
1) Molecular dynamics
CO_2 physisorption on silica with/without functionalization

Desorption rates





Active sites – adsorption density maps



How the underlying structure and functionalization of sorbent affect the sorption and adsorbate mobility

Turchi et al., (2023 – under review)

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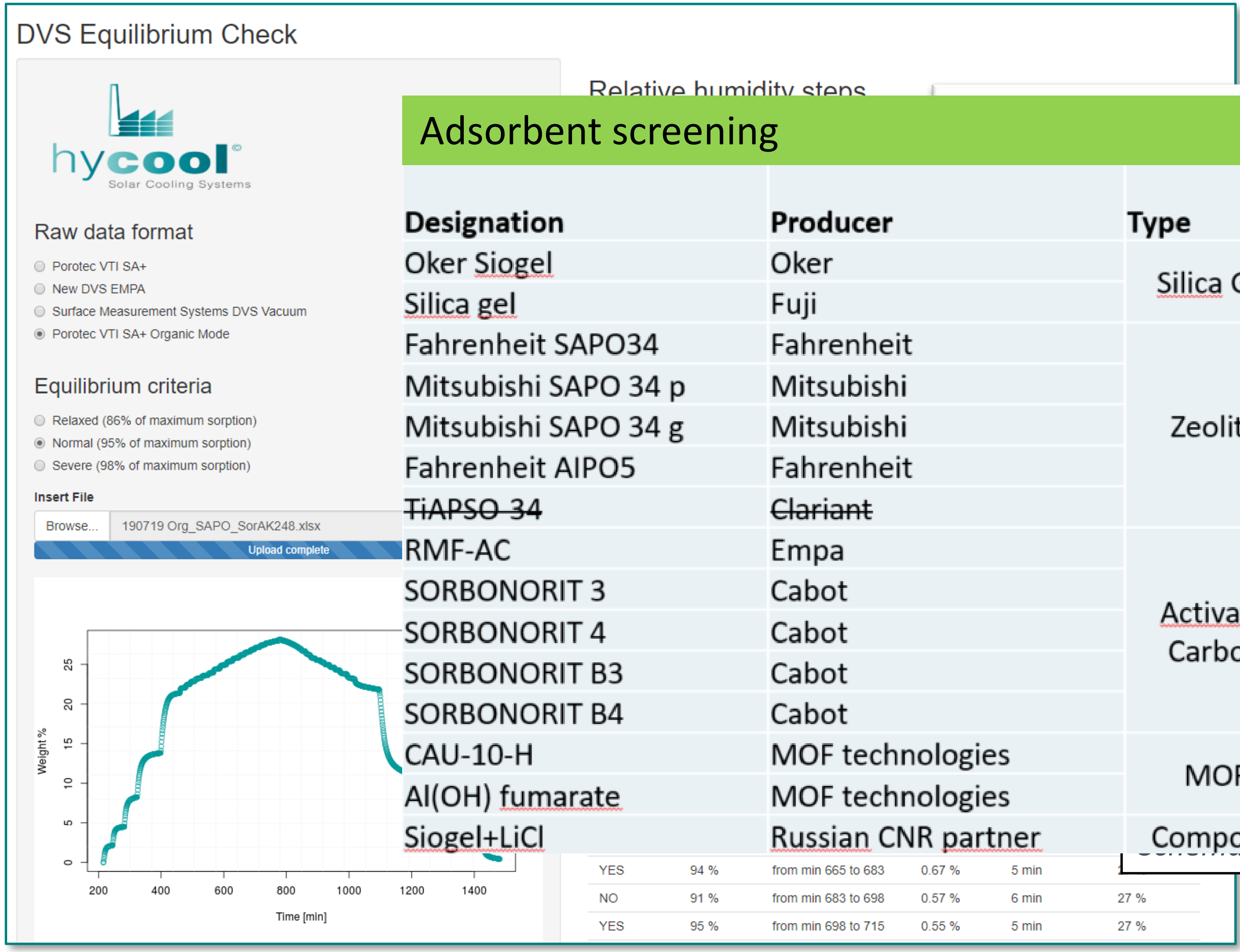
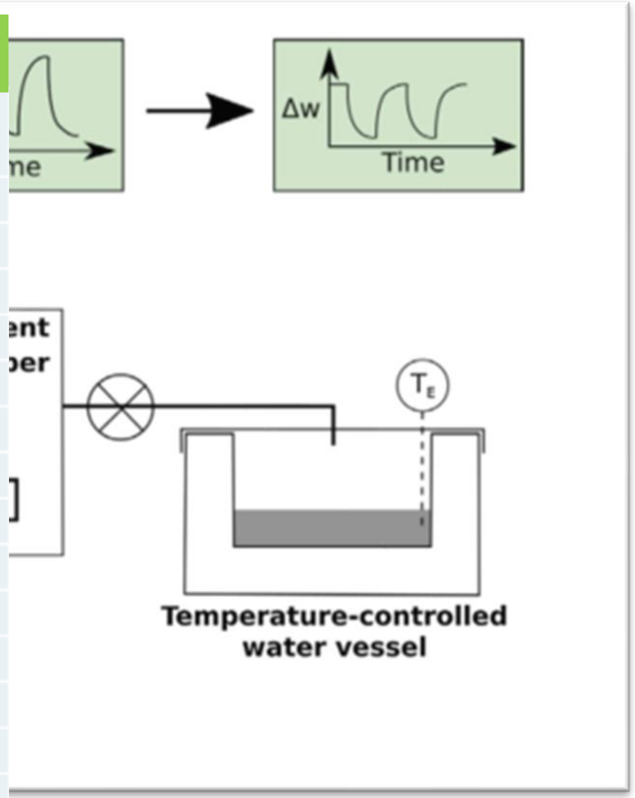
2) Proper characterization of the materials

Workflows, protocols, standardization – then material screening – adsorption heat pumps



Adsorbent screening

Designation	Producer	Type	Full/reduced protocol
Oker Siogel	Oker	Silica Gels	F
Silica gel	Fuji		F
Fahrenheit SAPO34	Fahrenheit	Zeolites	F
Mitsubishi SAPO 34 p	Mitsubishi		R
Mitsubishi SAPO 34 g	Mitsubishi		F
Fahrenheit AlPO5	Fahrenheit		R
~~TiAPSO 34~~	~~Clariant~~		~~F~~
RMF-AC	Empa	Activated Carbons	F
SORBONORIT 3	Cabot		R
SORBONORIT 4	Cabot		F
SORBONORIT B3	Cabot		R
SORBONORIT B4	Cabot		R
CAU-10-H	MOF technologies	MOFs	F
Al(OH) fumarate	MOF technologies		F
Siogel+LiCl	Russian CNR partner	Composite	F



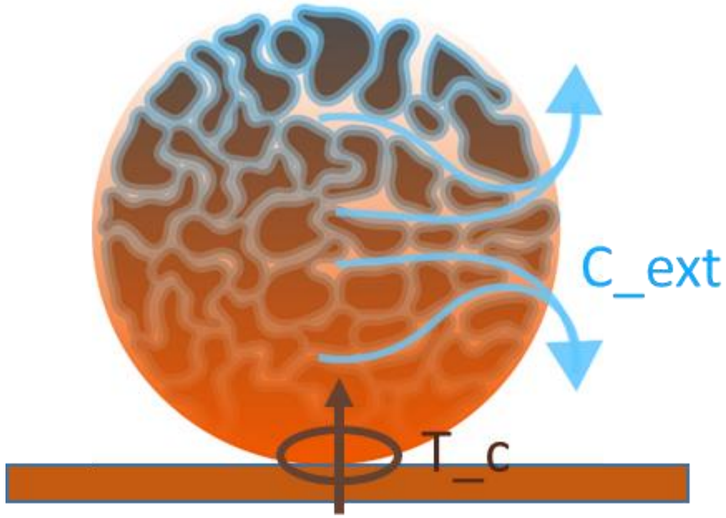
…re swing adsorption analysis set-up

Galmarini et al., 2019 - **10.5281/zenodo.7224978**

Emanuele Piccoli & Sandra Galmarini (sandra.galmarini@empa.ch)

3) Linking the small-scale material properties to the big-scale heat and mass transfer performance
Lumped-parameter model – water adsorption for heat pumps

Simplicity



Lumped parameter material models

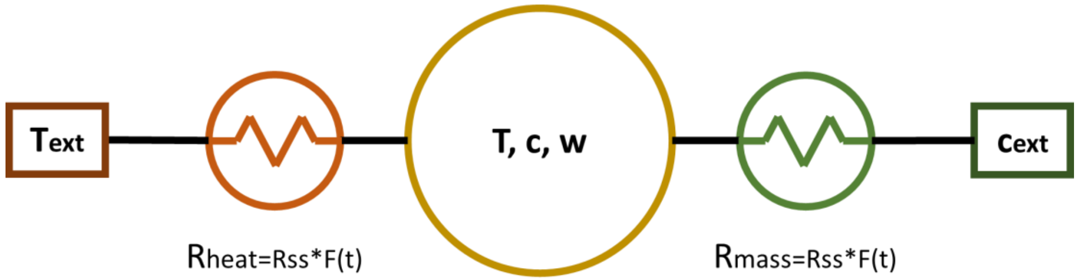
All the part of adsorbent facing similar boundary conditions (temperature, pressure) can be represented as a single object.

Examples

A layer of beads, part or all of a coating, part or all of a monolith, a full packed bed.

Orders of magnitudes faster than numerical (local) models

It describes the heat and mass transfer in the material bits, or monoliths, in scales of millimeters



- Understanding of limiting factors
- Parameter sensitivity studies
- Mitigation strategies

Piccoli et al., 2023, **10.5281/zenodo.7543626**
10.5281/zenodo.7225476

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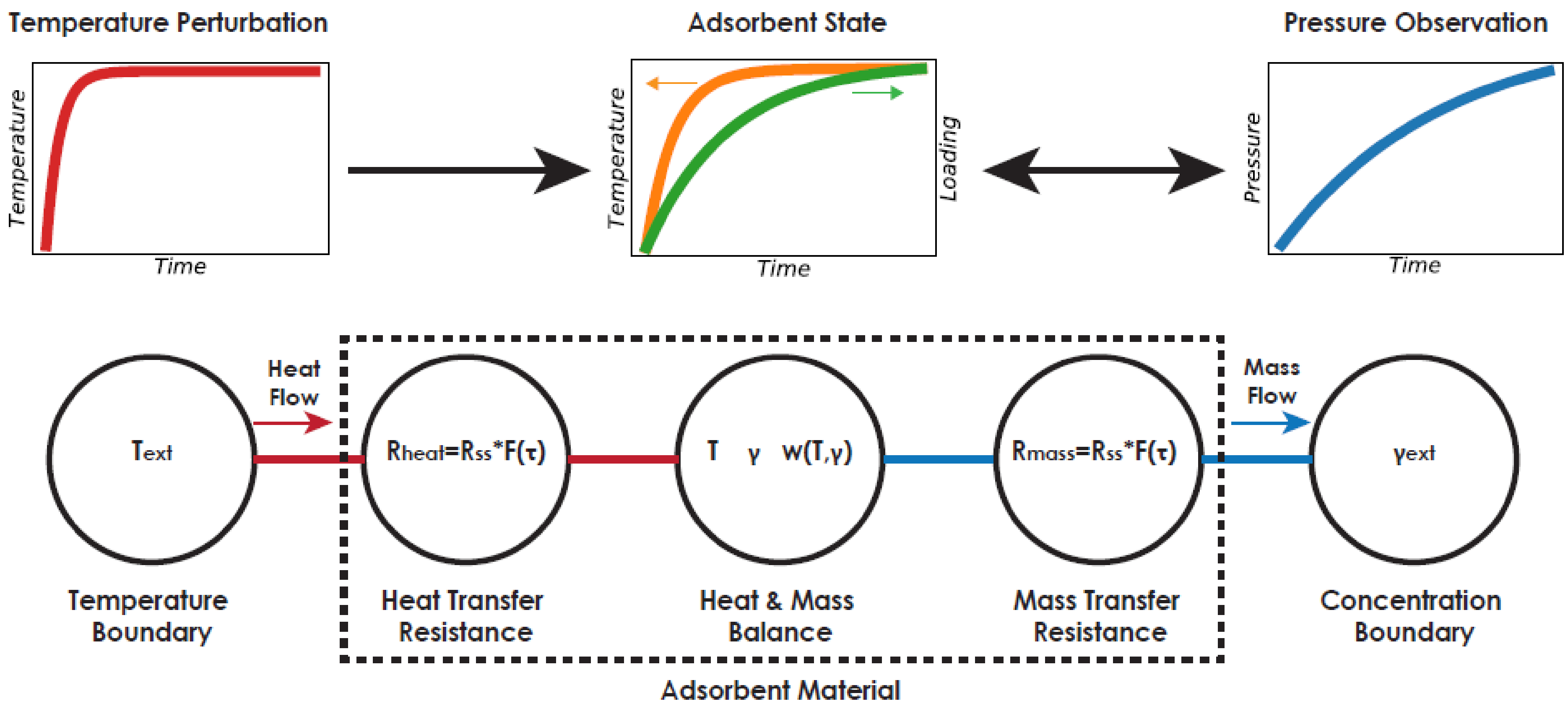
3) Linking the small-scale material properties to the big-scale heat and mass transfer performance

Lumped-parameter model – water adsorption for heat pumps



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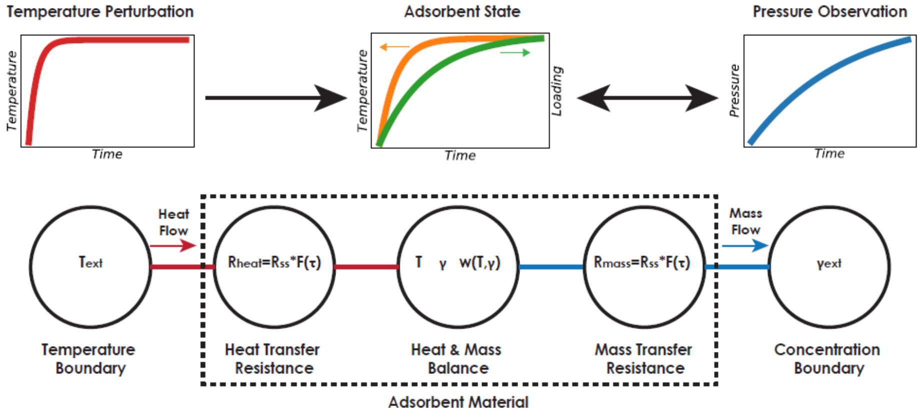


$$R_{heat} = \frac{8/\pi^2}{A\rho_{env}C_p 2\alpha/L} \; \frac{\sum_{n=1,3,5,\ldots}^{\infty} \frac{e^{-n^2\pi^2\tau}}{n^2}}{\sum_{n=1,3,5,\ldots}^{\infty} e^{-n^2\pi^2\tau}}$$

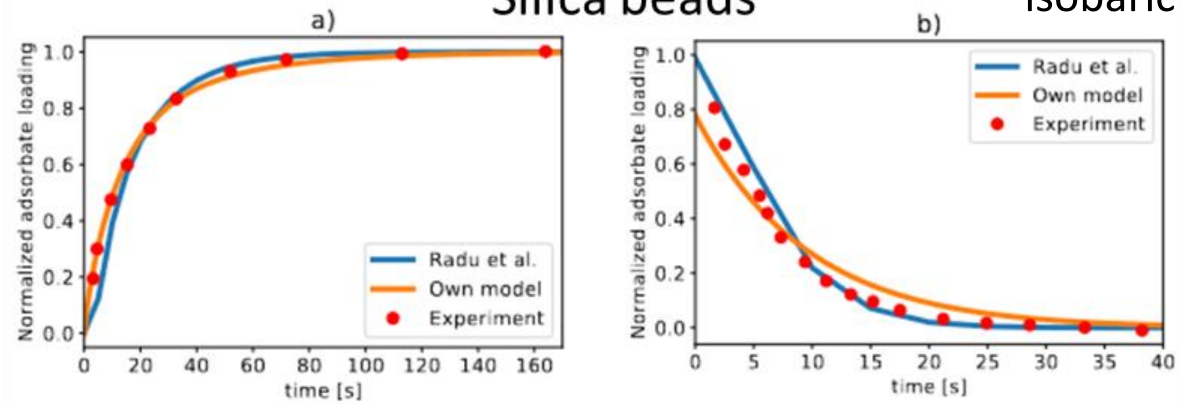
Rsteady

F(τ)

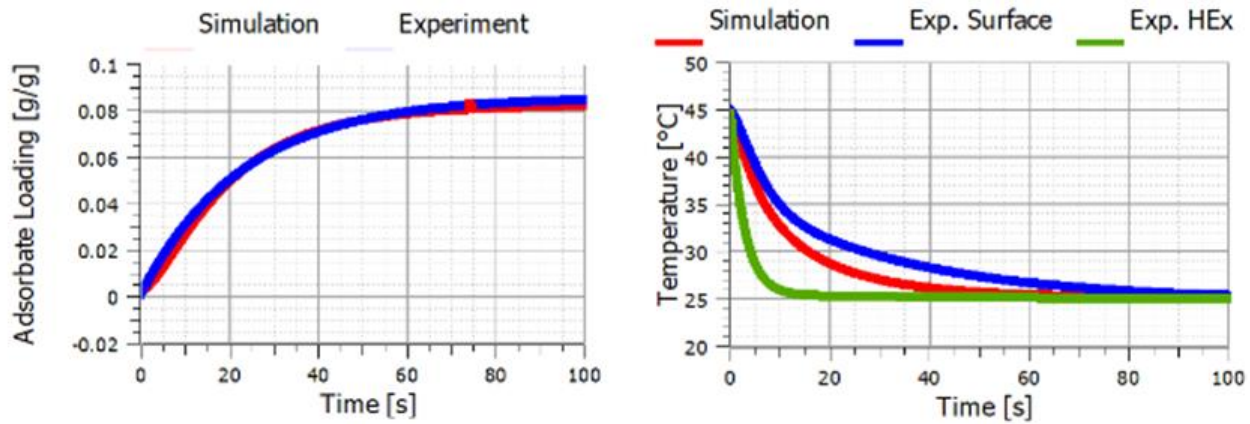
$$\frac{T_{av} - T_{ext}}{T_i - T_{ext}} = \frac{4}{\pi^2} \cdot \sum_{n=1,3,5,\ldots}^{\infty} \frac{e^{-n^2\pi^2\tau}}{n^2} \approx 0.8e^{-\frac{\tau}{0.1}} + 0.2e^{-\frac{\tau}{0.005}}$$

Model Validation

Silica beads — isobaric



Activated Carbon Monolith — isochoric



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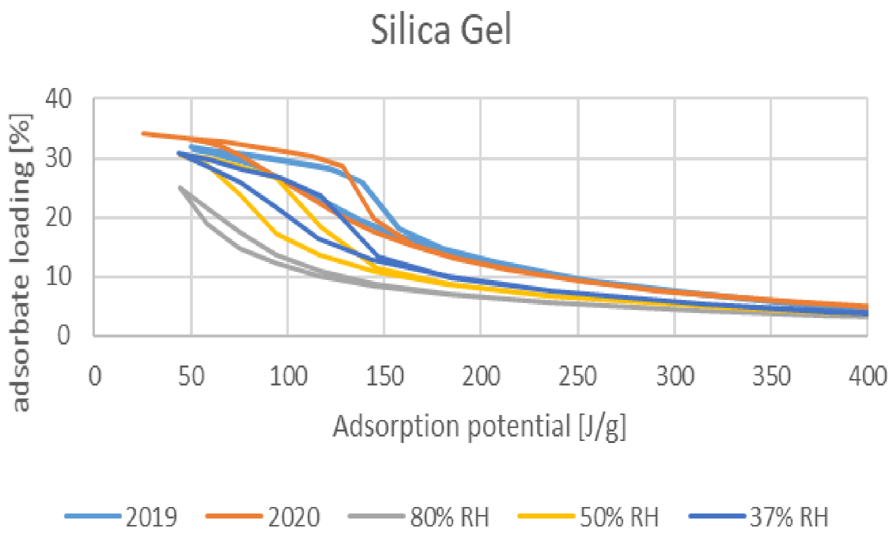
4) Long term stability of adsorbents
Shelf and work life – water adsorption for heat pumps

Do and how porous adsorbents change during their storage and use?



- No evident degradation under operational conditions
- Longer times of exposure and/or extreme conditions should be avoided.
- Accelerated ageing tests for exposure established

Long term storage in controlled humidity environment

Similarities

Saturated steam
2 bar, 120°C
2x2h/cycle

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5) Building on experience from adsorption heat pumps: Research on direct air capture of CO_2

- Improved **understanding of co-sorption** mechanisms
  - By means of atomistic, meso-scale, and multiscale **modelling**.
- Reliable **characterization** of various adsorbent types
  - Quantitative **measurements** of CO_2/H_2O co-sorption
- Reliable **thermodynamic co-sorption models** at different p & T
- Assessment of different sorbents for DAC and subsequent methanation.

Molecular level
Material characterization
Process understanding
Assessment of sorbent suitability

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Thank you for listening!

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References:

Turchi et al., (2023) – under review – preprint - **10.2139/ssrn.4414695**
Turchi (2022) Goldschmidt Conference - Atomistic investigation of functionalized silica pores for CO_2 capture
Galmarini et al., 2019 - **10.5281/zenodo.7224978**
Piccoli et al., 2023 - **10.5281/zenodo.7543626**
HyCool Project Website - **10.5281/zenodo.7225476**