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Modelling the design of dual functional adsorbents for inductively heated CO_2 TSA

GESP
GRUP D'ENGINYERIA I SIMULACIÓ DE PROCESSOS AMBIENTALS

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Adsorption based CO_2 capture processes

Swing Adsorption (SA) works by alternating conditions between adsorption and desorption:

- Pressure (PSA)
- Vacuum (VSA)

Naturally electric

- Temperature (TSA)

+ High recovery and purity

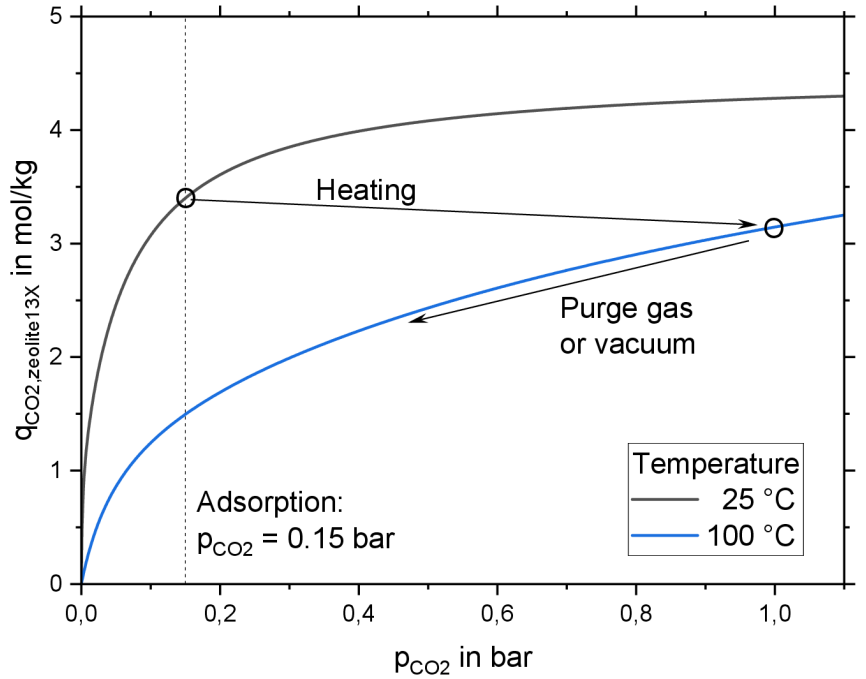
- Waste heat needed, otherwise energy intensive

- Slow heating and cooling

Purge gas or vacuum (VTSA) enhances TSA regeneration

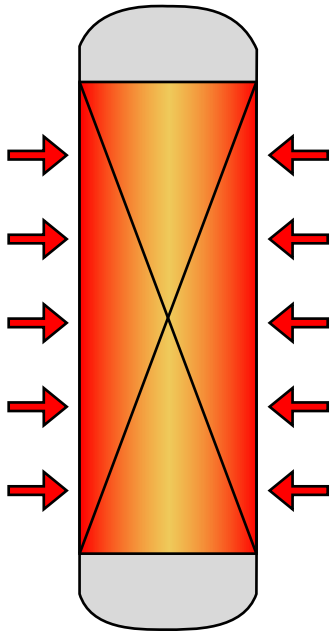
Example:

- CO_2 isotherms on zeolite 13X
- Post-combustion composition: 15% CO_2 in N_2

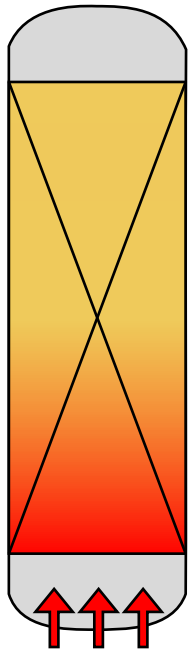


Electrifying TSA

Over reactor wall



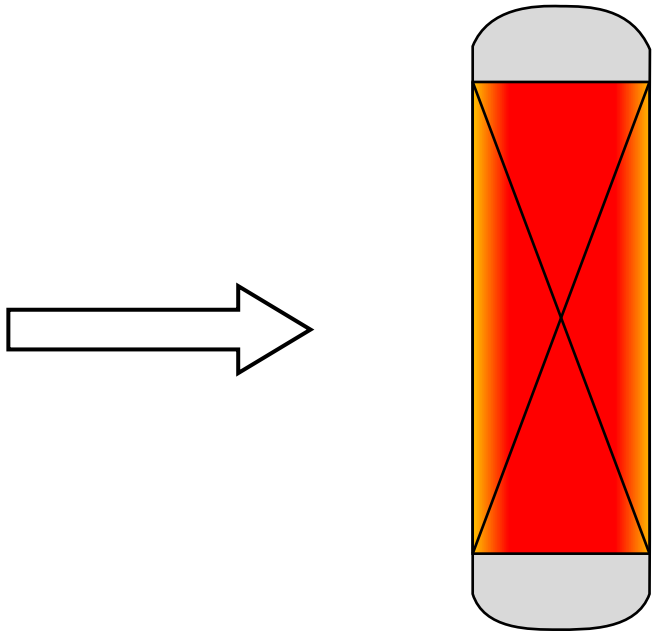
Hot purge gas



- Slow heating ($< 20\ °C/\text{min}$)
- Heating is inhomogeneous
- Parasitic heating

Electric heating methods:

- **Induction heating**
- Resistive heating
- Microwave heating

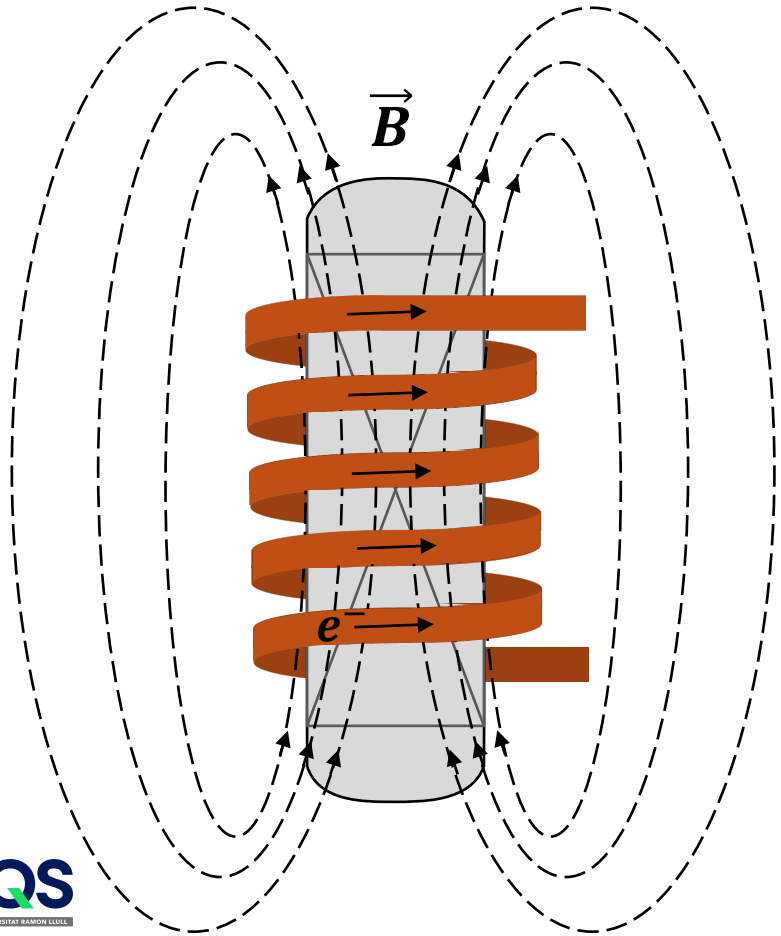


Heat generated inside adsorption bed:

- Faster heating ($50 - 150\ °C/\text{min}$)
- Produces heat on the spot
  - More homogeneous
  - Less parasitic heating

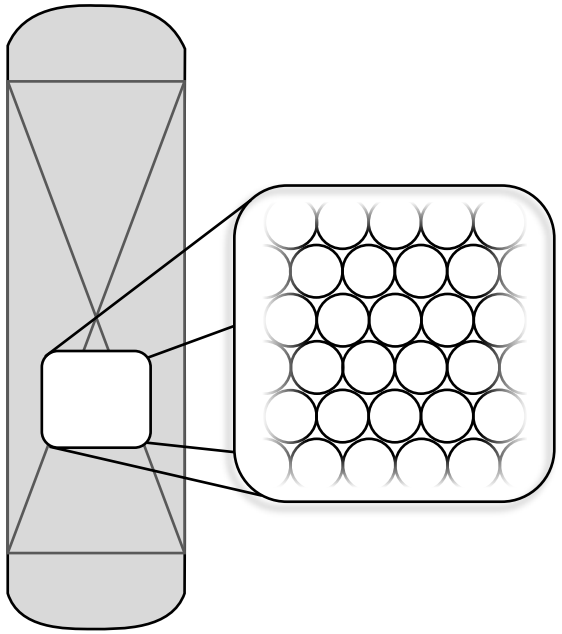
Induction heated TSA

Alternating magnetic field $\vec{B}$



Adsorbent bed filled

with DFM beads



Heating properties:

- (Ferro-) magnetism
- Electric conductivity

Typically, adsorbents are neither of both

→ Create dual functional materials (DFM)

- High adsorption capacity & selectivity
- Induction heating properties

Example:

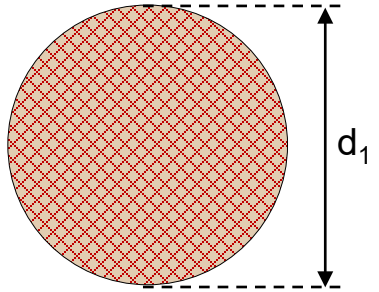
- Zeolite 13X for adsorption
- Fe_3O_4 for heat release

Energy release „*SAR*“ measured:

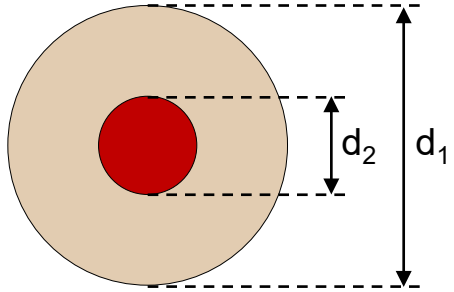
$SAR\ \left(\frac{W}{g}\right)$ at constant $\vec{B}$ and $20°C < T < 100°C$

DFM design model idea

Homogeneous (HM):



Core-shell (CS):



Fe_3O_4 Zeolite 13X

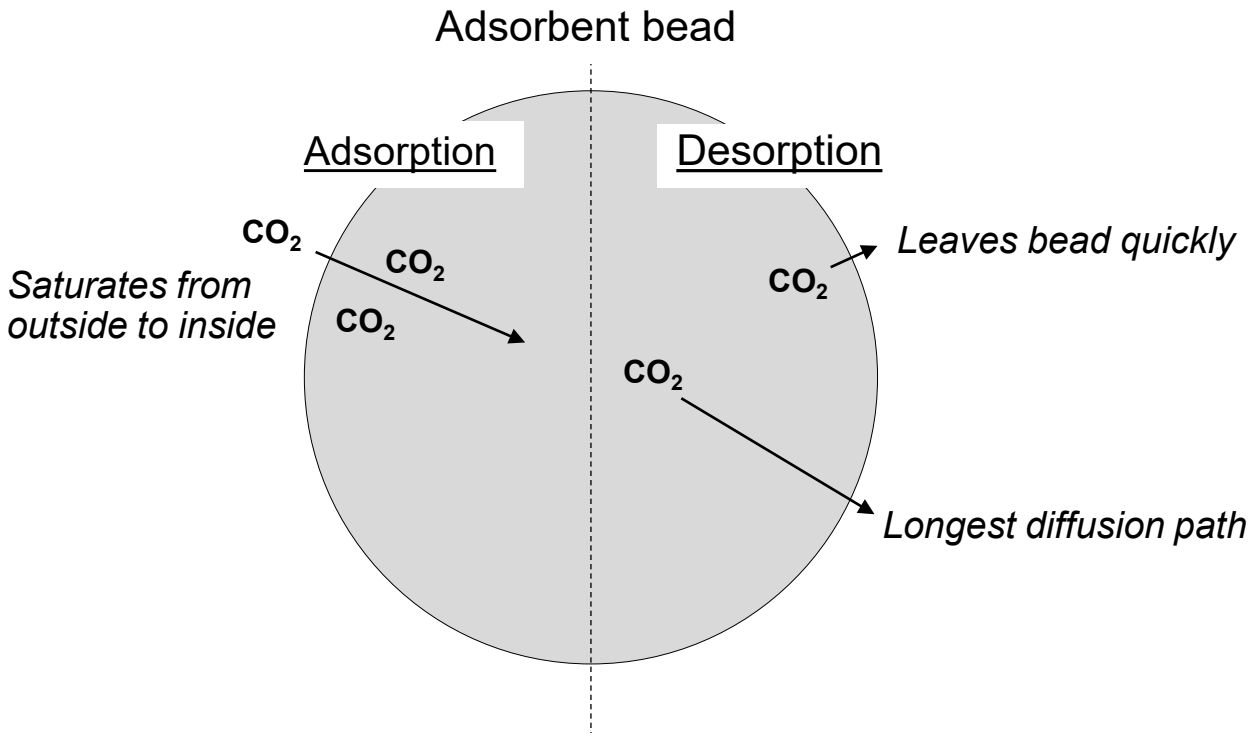
„How does the DFM design affect adsorption and desorption time?“

	Homogeneous (HM)	**Core-Shell (CS)**
Adsorption & Heating properties:	Diluted by mass fraction, but over whole bead	Full properties, but in separated parts
Diffusion path:	Full bead distance in diluted capacity	Shorter diffusion distance in higher capacity
Temperature profile:	More homogeneous heating	Heat accumulation in centre → Diffusion closer to center is accelerated

Idea to model:

- Same bead size and mass fractions, only distributed differently
- Adsorption (15% CO_2 in N_2)
- Desorption (N_2 purge) under the same heating conditions

Expected effects

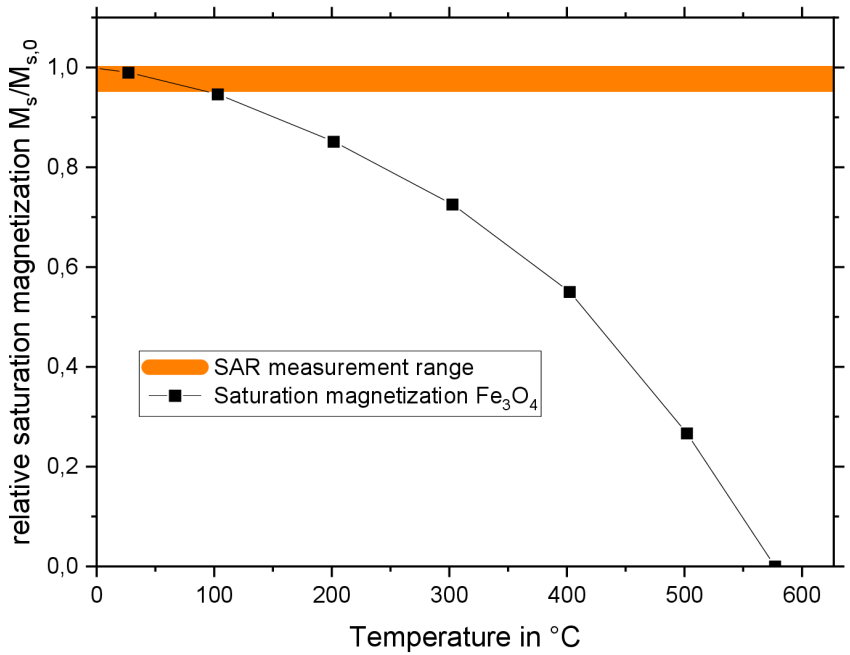


Core-Shell: Reducing diffusion depth and increasing internal temperature gradient

→ *Steeper breakthrough curve at adsorption?*

→ *Faster desorption?*

Magnetic properties drop with temperature*

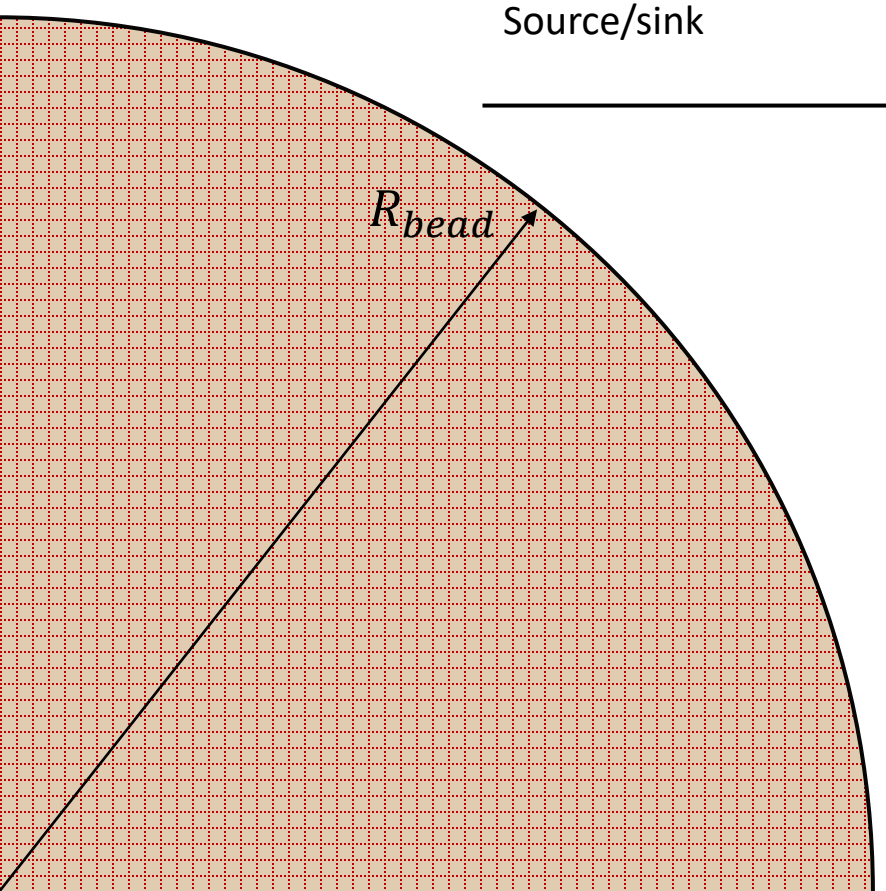


→ *Negative for heat accumulation in CS?*
„The hotter it gets, the less it heats“

*From data of: Levy, D., Giustetto, R., & Hoser, A. (2012). Structure of magnetite (Fe3O4) above the Curie temperature: a cation ordering study. *Physics and Chemistry of Minerals*, *39*(2), 169–176. https://doi.org/10.1007/s00269-011-0472-x

Mathematical model

	Mass balance	Heat balance
External flux	Convective film resistance	Convective film resistance
Internal flux	Fick diffusion (Knudsen & Binary)	Heat conduction
Source/sink	Adsorption equilibrium	Fe_3O_4 energy release Heat of adsorption

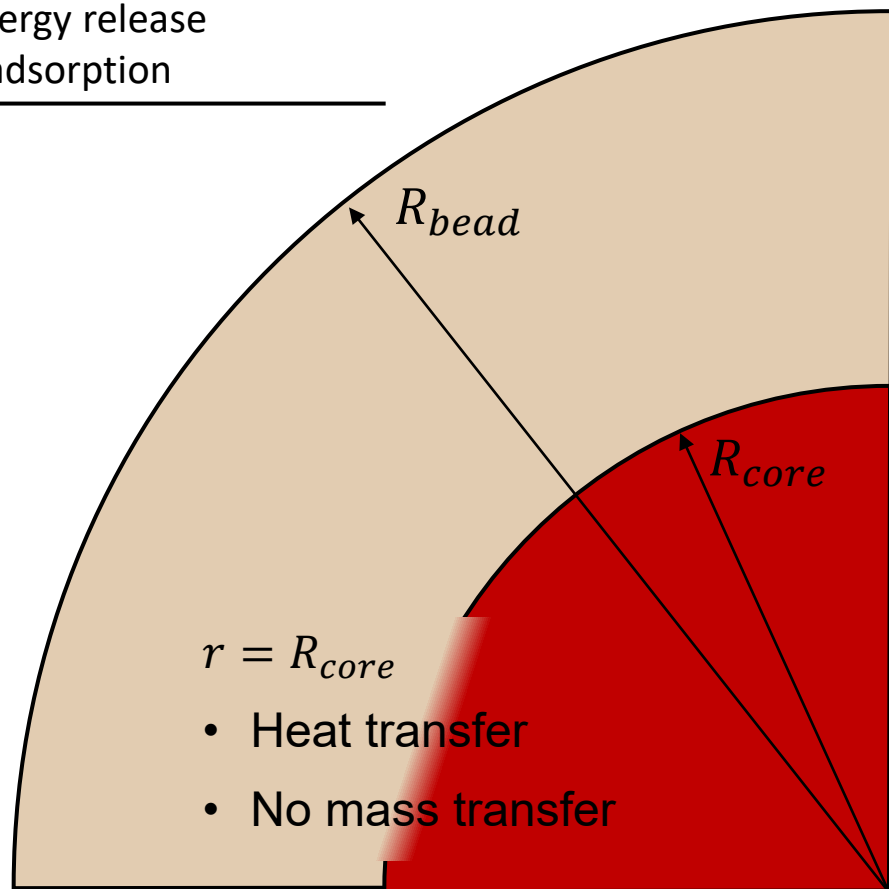


Boundary conditions

- 1D radial flux
- No flux at center
- Constant outer gas concentration
- Flexible outer temperature

Initital conditions

Mass and thermal equilibrium

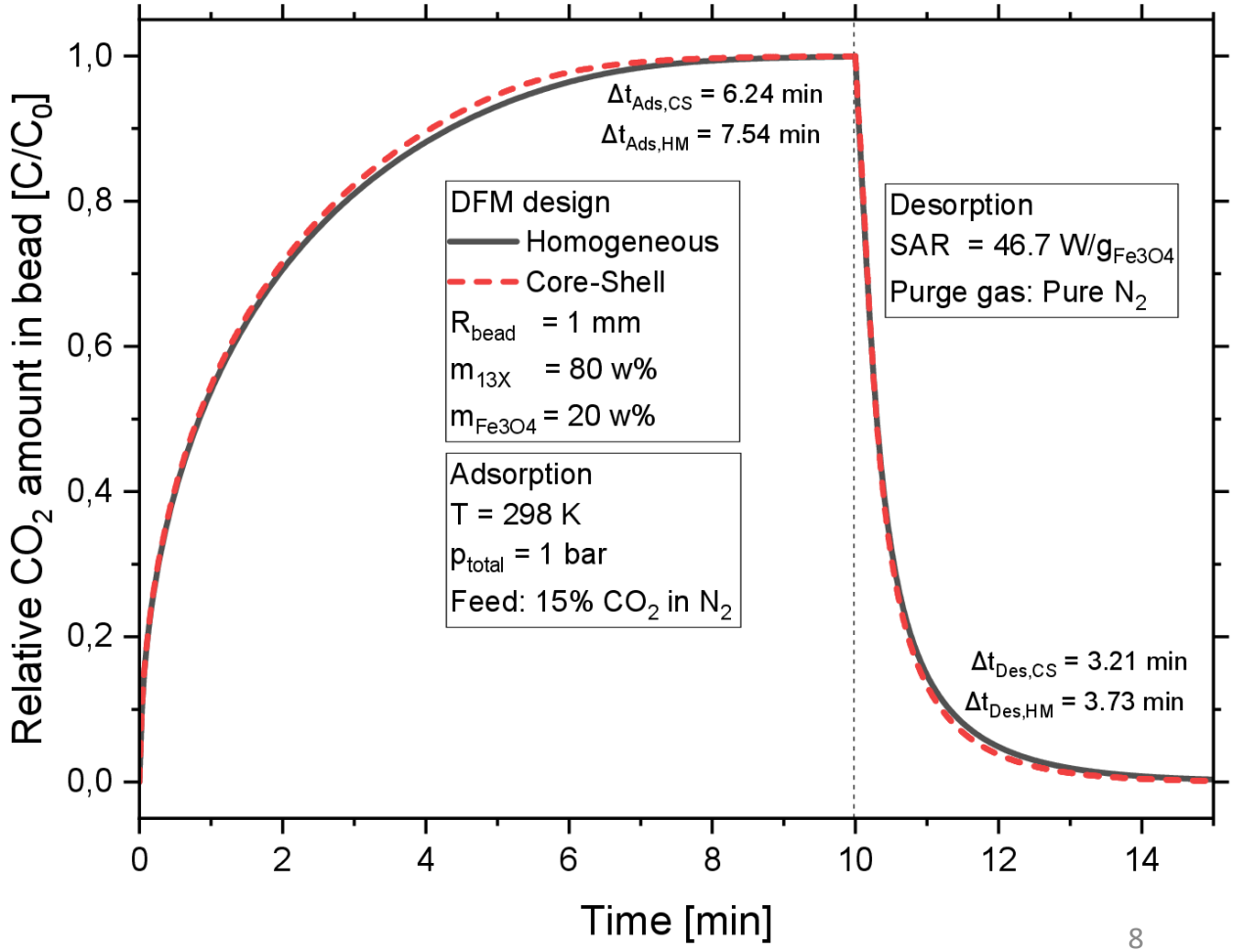


Model verification

Temperature comparison with literature**

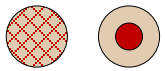
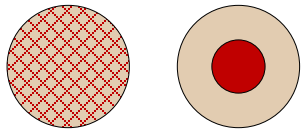
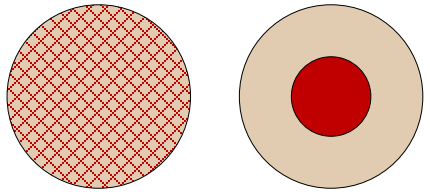
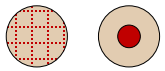
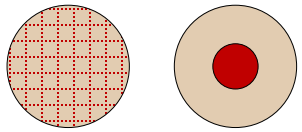
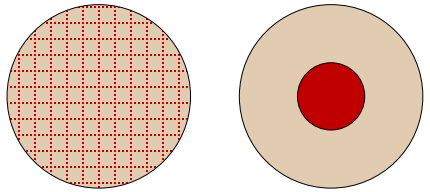
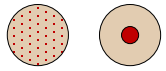
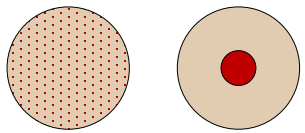
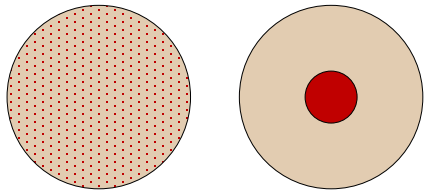
R_{bead}	$x_{Fe_3O_4}$	$SAR\ W/g$	$T_{reference}$	T_{model}
1 mm	10%	58.1	100°C	113°C
1 mm	10%	149.7	200°C	147°C
1 mm	20%	46.7	195°C	170°C
1 mm	20%	137.9	240°C	234°C

**Gholami, M., Verougstraete, B., Vanoudenhoven, R., Baron, G. V., Van Assche, T., & Denayer, J. F. M. (2022). Induction heating as an alternative electrified heating method for carbon capture process. *Chemical Engineering Journal*, *431*. https://doi.org/10.1016/j.cej.2021.133380



Parameter variation

Particle size and composition:

R_{Bead} / 13X : Fe_3O_4	1 mm	2 mm	3 mm
70:30			
80:20			
90:10			

Desorption conditions:

$$SAR = 50 \frac{W}{g_{Fe_3O_4}}$$

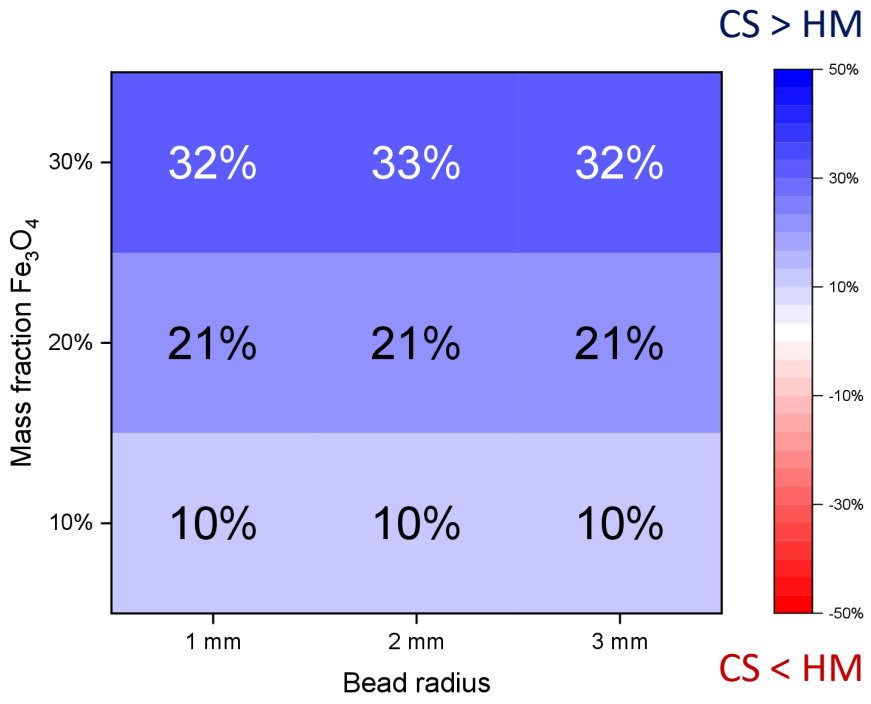
$$= 100 \frac{W}{g_{Fe_3O_4}}$$

$$= 150 \frac{W}{g_{Fe_3O_4}}$$

„Variating of magnetic field strenght $\vec{B}$“

Comparison: Adsorption time CS vs. HM

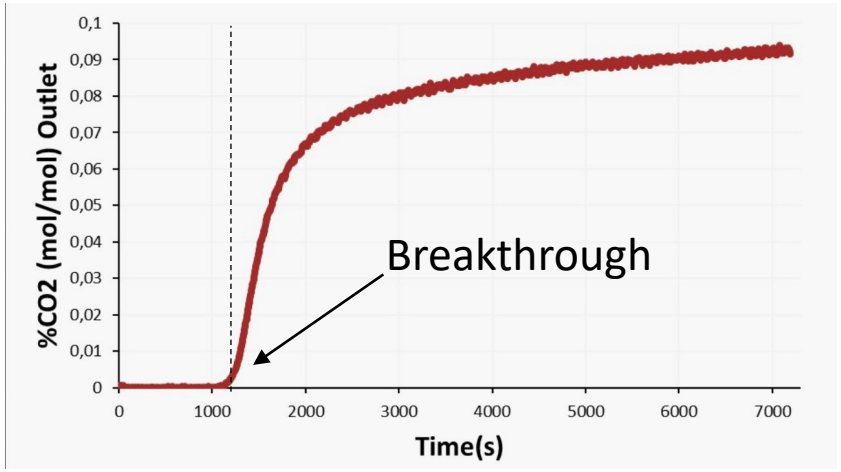
„CS adsorption time is XX% shorter/longer than HM adsorption time“



Shorter diffusion path of CS design affects positively the adsorption time

→ Can be beneficial for breakthrough curve

Example breakthrough curve:



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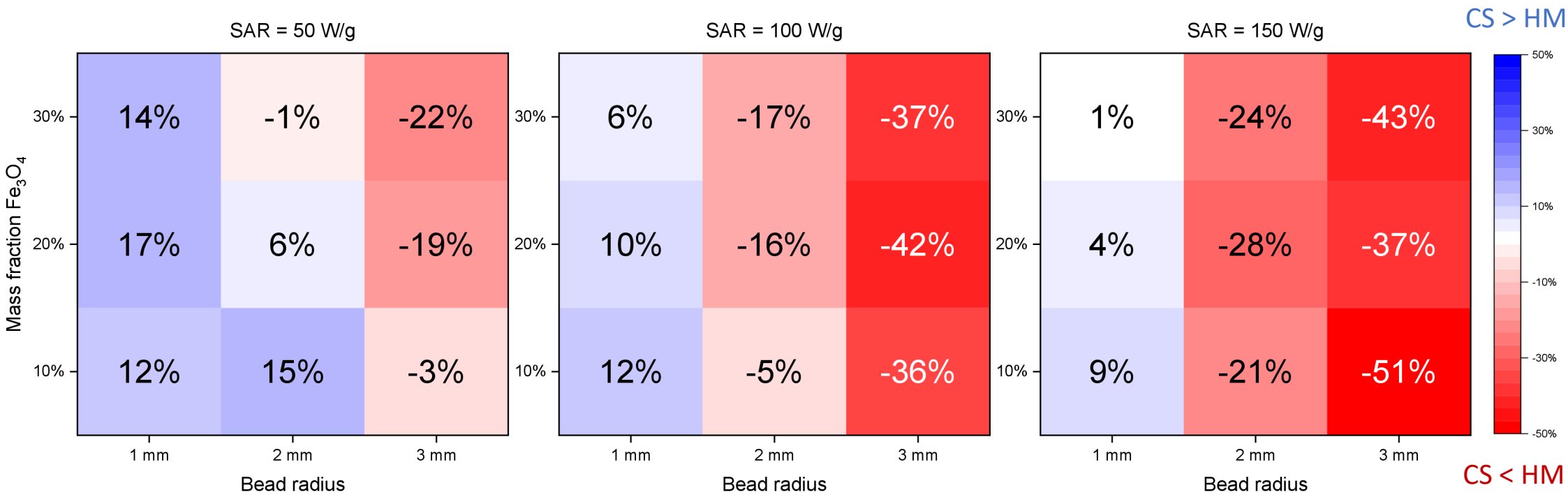
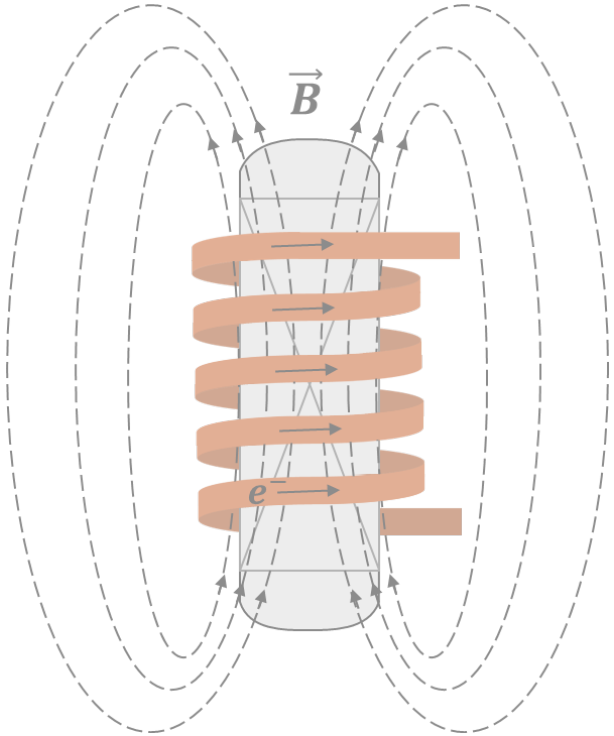


CS design only beneficial in smaller beads with „lower“ SAR

→ Still desorption time fast (few minutes) and not the bottleneck of cycle time



Acknowledgements

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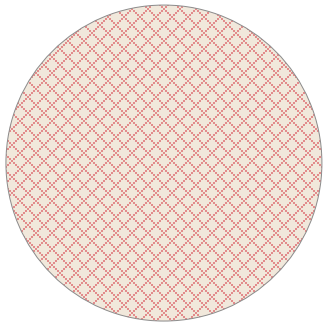

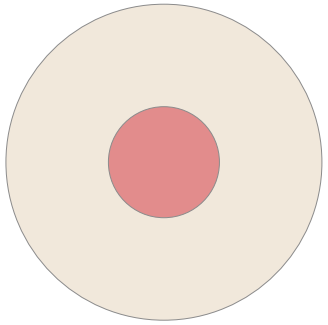

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