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# Modelling the design of dual functional adsorbents for inductively heated CO<sub>2</sub> TSA

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### Abstract

The decarbonization of industrial processes requires efficient and sustainable carbon capture technologies. While post-combustion carbon capture with adsorption-based technologies is a well-established approach, its widespread implementation is hindered by the high energy demand for adsorbent regeneration [1]. Conventional thermal regeneration methods, often reliant on steam or externally supplied heat, pose challenges for integrating carbon capture with renewable energy sources. To address this, electrification of carbon capture adsorption processes has emerged as a promising strategy, enabling direct coupling with renewable electricity and allowing for more precise, rapid, and efficient energy delivery [2].

Among electrified regeneration methods, Induction-Heated Temperature Swing Adsorption (IH-TSA) offers a faster alternative to conventional TSA by generating heat directly within the adsorbent bed. This is achieved by creating Dual Functional Materials (DFMs), which serve then both as CO<sub>2</sub> adsorbents and induction heat susceptors. However, the introduction of a non-adsorbing magnetic susceptor, such as Fe<sub>3</sub>O<sub>4</sub>, reduces the effective adsorbent capacity, making DFM design a critical factor in optimizing performance.

To understand the impact of DFM design on adsorption and desorption performance, a mathematical model for CO<sub>2</sub> capture using zeolite 13X as the adsorbent and Fe<sub>3</sub>O<sub>4</sub> as the magnetic susceptor was developed. Two DFM configurations were compared with identical bead radius, mass fractions, and energy input during desorption: (1) a homogeneous DFM (H-DFM) where zeolite 13X and Fe<sub>3</sub>O<sub>4</sub> are uniformly mixed, and (2) a core-shell DFM (CS-DFM) where an Fe<sub>3</sub>O<sub>4</sub> core is surrounded by a zeolite 13X shell.



Figure 1: Modelled adsorption and desorption of a single bead of dual functional material (DFM) for induction heated  $CO_2$  temperature swing adsorption. Two DFM designs are compared where the same masses of adsorbent (zeolite 13X) and the magnetic susceptor (Fe<sub>3</sub>O<sub>4</sub>) are either homogeneously distributed among each other (H-DFM) or separated in core-shell structure (CS-DFM) with a heating core and an adsorbing shell.

The results show that both configurations exhibit the same  $CO_2$  adsorption time. This finding is based on the assumption that  $Fe_3O_4$  does not interfere with zeolite 13X through pore blockage or similar, making the longer penetration depth in the H-DFM compared to CS-DFM a not-critical factor. However, during desorption, the CS-DFM achieves 95% desorption in just 3,44 minutes, whereas the H-DFM requires 5,65 minutes to reach the same level.

#### References:

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