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CONSTRUCTAL DESIGN APPROACH FOR CARBON DIOXIDE ADSORPTION SYSTEMS

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Current carbon capture and storage (CCS) benchmark technologies and materials are both energy and economically costly. Therefore, it hopes to rely on uncovering combinations of designs or materials to provide the performance leap to scale up the CCS deployment to meet the most optimistic Intergovernmental Panel on Climate Change (IPCC) projections and socioeconomic shared pathways to mitigate global warming. While the search for advanced materials for carbon capture has drawn much of the efforts to enhance the so-called productivity (CCPr), *i.e.*, CO_2 mols per volume of CC material per cycle for high levels of purity for CO_2 recovery, there is an opportunity to investigate before-hand how those materials would fare energy wise (PE) (total energy expenditure by total amount of CO_2 mols captured) in the reactor. This work presents a formulation based on the Constructal Theory to explore how the features of the materials themselves (absorptivity, molecular diffusivity, density), the packing (pellets shape and size, effective diffusivity, specific capturing rate, porosity), and the configuration of a column packed-bed reactor affects the energy penalty (PE). The investigation is theoretical and numerical by modeling the CO_2 mass balance in a prescribed and constant mobile phase flow rate (initially CO2-rich exhaust gases) isothermal 1d tubular packed-bed reactor and the coupling with CO_2 mass balance at the pellet level with linear driving force model – both are saturated porous media. The simulations were performed using newly developed Python code and commercial software. The model was turned nondimensional, and the influence of the adapted Peclet and Damkhöler numbers was explored, which showed reverse trends in the indices CCPR and PE. It showed the trade-off between the resistances to adsorb CO_2 and the other features of the reactor's design, providing insights into how those systems may evolve.

Keywords: Carbon capture; Constructal design; Carbon capture and storage (CCS); Energy efficiency.

1. INTRODUCTION

According to the IPCC, the demand for carbon capture and storage (CCS) increases as the so-called energy transition from fossil hydrocarbons to low greenhouse gas energy pathways progresses slower than expected [1]. Current CCS benchmark technologies and materials are energy- and economically costly [2]. Recently, Gasparovic *et al.* [3] addressed the design of CCS reactors for mineral capture using Constructal Design approach to explore low-energy expenditure possibilities. In this work, we now explore the comparative influence of the macroscopic and the microscopic CO_2 transport and adsorption (capture) on the two metrics that drives the evolution of CCS systems, namely, the so-called productivity

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(*CCPr*) given in CO_2 mols per volume of carbon-capturing material per cycle and the energy penalty (*PE*) (total energy expenditure in kJ by the total amount of CO_2 mols captured) in a adsorption/desorption reactor.

2. **MATERIALS AND METHODS**

The investigation is theoretical and numerical by modelling the CO_2 mass balance in a prescribed and constant mobile phase flow rate (CO_2-rich exhaust emissions) isothermal 1D tubular plug-flow spheroidal-pellets-packed-bed reactor and the coupling with CO_2 mass balance at the pellet level for linear driving force (LDF) and Langmuir adsorption regime (*e.g.*, [5]):

$$\varepsilon_{\mathrm{b}} \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = \varepsilon_{\mathrm{b}} D_{\mathrm{b}} \frac{\partial^2 C}{\partial x^2} - (1 - \varepsilon_{\mathrm{b}}) \rho_{\mathrm{p}} \frac{\partial q}{\partial t}, \tag{1}$$

$$\frac{\partial q}{\partial t} = K_{\mathrm{L}}\left(q_{\mathrm{p}}^{*} - q\right),\ q_{\mathrm{p}}^{*} = \frac{q_{\mathrm{pm}} b C}{1 + bC}, \tag{2}$$

$$C(x,t) = C_0,\ x = 0, t = 0, \tag{3}$$

$$C(z,t) = 0 \text{ and } q(z,t) = 0,\ 0 < x \leq L, t = 0, \tag{4}$$

$$u \cdot C_0 = u \cdot C(x,t) - \varepsilon_b D_{\mathrm{b}} \frac{\partial C}{\partial x},\ x = 0,\ t > 0, \tag{5}$$

$$\frac{\partial C(x,t)}{\partial x} = 0,\ x = L,\ t > 0, \tag{6}$$

where, $C(x,t)$ is the concentration of the free CO_2 in the mobile phase (mol kg^{-1}) along the axial direction, x (m) in time, t (s); u is the given uniform surface velocity along the axial direction (m s^{-1}); $q(x, t)$ is the average concentration of CO_2 in the pellets of the capturing material (mol kg^{-1}); ε_{b} is the bed porosity (−); D_{b} is the uniform, constant, axial dispersion coefficient (m^2 s^{-1}), ρ_p is the adsorbent pellet density (kg m^{-3}); q_{p}^{*} is the amount adsorbed at equilibrium (mol kg^{-1}); K_{L} is the LDF overall mass transfer and adsorption coefficient (s^{-1}); q_{pm} is maximum adsorption capacity of the pellets (kg$_{\text{adsorbed}}$ kg$_{\text{adsorbent}}^{-1}$); and b is Langmuir isotherm constant (m^3 kg^{-1}).

The ratio between the macroscopic and the microscopic CO_2 transport and adsorption (capture) is seen by the Peclet number, $\mathrm{Pe} = uL/(\varepsilon_{\mathrm{b}} D_{\mathrm{b}})$ and the Damköhler number, $\mathrm{Da} = K_{\mathrm{L}} L \varepsilon_{\mathrm{b}} / u$. The cycle time (s), t_{cycle}, was given when the rate of variation of $C(L, t)$ in time at the exit of the reactor ($x = L$) is negligible. The volume of adsorbent material (pellets) is given by the macroscopic non-void portion of the reactor, V_{ads}, and the CC in each cycle by the time-cumulated CO_2 by the balance between the known constant feed and the exit (mol). The energy expenditure is computed by constant feed flow rate, near constant pressure flow, and the pressure drop, calculated by the known Ergun formula (*e.g.*, [4]). The model was turned nondimensional, and the influence of the adapted Peclet and

Damkhöler numbers on *CCPr* and *PE* was explored. The simulations were performed in newly developed Python code and commercial software.

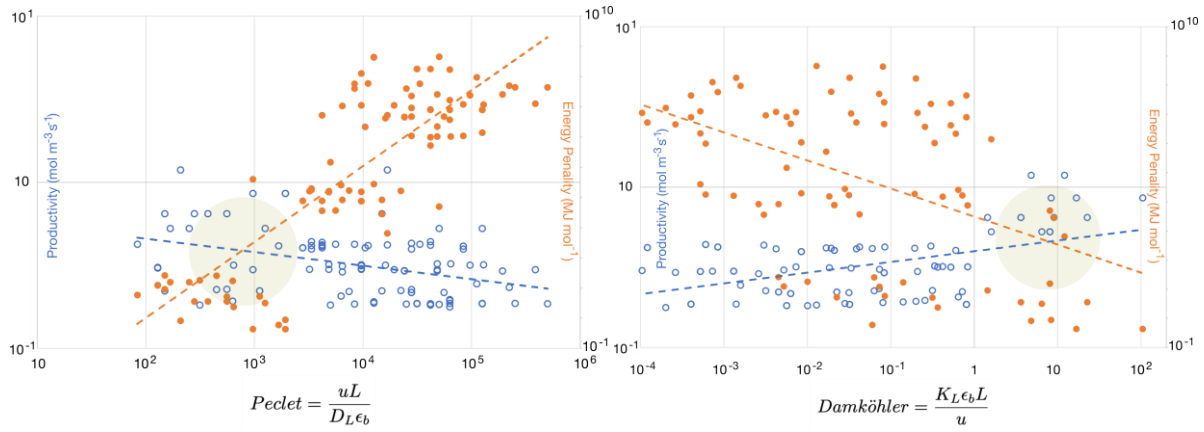
3. **RESULTS**

We explored 101 random consistent combinations of reasonable ranges for L, u, ε_b, D_b, and K_L, with fixed q_p^* and b, then expressed *CCPr* and *PE* concerning Peclet and Damköhler (Fig. 1).

4. **DISCUSSION AND CONCLUSIONS**

In this brief report, we showed that the two main design criteria for CCSs, namely, the Carbon Capture Productivity itself and the Energy Penalty (*PE*), respond in a reverse way concerning Peclet and Damköhler number, showing there is an opportunity to find a matching balance between the macroscopic transport of CO_2 and the microscopic, local, transport in the capturing pellets up to the adsorption of the CO_2. The most promising combinations are Pe ~ 10^3 and Da ~ 10.

Further investigations will show the sensitivity of the maximum adsorption material, the rate in which it reaches such plateau on the balance of transport and the internal structure of the adsorbents.



(a) (b)

Fig. 1 – Variation of the Carbon Capture productivity (*CCPr*) and the Energy Penalty (*PE*) *vs* the (a)Peclet and (b)Damköhler numbers of 101 random simulations (log-log).

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