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PROSPECTION FOR ADVANCED MATERIALS PROPERTIES FOR CARBON CAPTURE FROM COMBUSTION GASES

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Abstract. *The latest IPCC report shows a scenario in which replacing fossil fuels and improving the efficiency of energy systems may not be enough to ensure an increase in the global average temperature of less than 1.5 °C by 2040. One of the challenges of the 21st century is to reduce emissions and the resulting concentration of CO2 in the atmosphere and, at the same time, carry out the energy transition without major damage to the world economy. Carbon Capture, Use and Storage (CCUS) can be the main route to achieving Greenhouse Gas (GHG) reduction targets. This work presents a computational simulation of the flue gas flow of combustion gases from the burning of fossil fuels such as natural gas and liquefied petroleum gas, which cross pipelines of porous materials in an arrangement with a constructal design. The pipelines are interspersed in constructs which gradually increase in size along the flow to capture carbon. A constructal ratio between the pressure drop and the rate of the capture reaction is also considered. To predict types of hypothetical materials efficient for carbon capture, in this simulation a parametric evaluation is carried out considering the specific mass of the material, its porosity, the average diameter of the pores and the molecular diffusion coefficient. Given that an important objective of this study is the development of carbon capture devices, an analysis of the results obtained when employing advanced carbon capture materials (MACC) is made in this work against those obtained when hypothetical efficient carbon capture materials are being considered. The minimum energy required for the carbon capture process is also evaluated, as well as the capture cost per ton of CO2.*

Keywords: *Carbon Capture, Constructal Design, Pollutants Emission, Advanced Materials, Transport Phenomena, Computational Fluid Dynamics CFD.*

1. INTRODUCTION

The widely known “climate issue” relates to the post-industrial revolution anthropic emissions of greenhouse gases and a rather rapid increase of global average temperature compared to pre-industrial times by affecting the atmosphere´s effective radiative forcing (ERF). Estimates point out an accumulation of about 2,390 (± 240) $GtCO_2$ since 1850, of which 210 ($GtCO_2$) was emitted between 2015 and 2019 (Friedlingstein et al., 2020). The last report of the Intergovernmental Panel on Climate Change (IPCC AR6, 2021) shows the current concentration of carbon dioxide (CO_2) in the atmosphere of 415 ppm, which at the beginning of the industrial era, around 1750, was at the level of 278 ppm. CO_2 emissions caused by the combustion of fossil fuels and industrial processes between 2010 and 2019 represented about 82.4% of the total emitted. The report also presents the consequences of those changes on the planet, current noticeable impacts and future risks. The key message is that the impacts are large and are increasing, and the actions may not be expedient enough to prevent even greater, and perhaps irreversible, impacts.

Therefore, the goal set by the United Nations Framework Convention on Climate Change (UNFCCC) is to reach zero net emissions of greenhouse gases (GHG) by 2050, which mainly requires deep reductions in CO_2, methane, and other emissions. And, it still implies net negative CO_2 emissions. Consequently, carbon dioxide removal (CDR) will be required to achieve net negative emissions. The process of reducing carbon dioxide in the atmosphere consists of biological or geochemical sinks or by capturing from emitting sources or directly sequestering CO_2 from the air. Developed countries accept that proposals for carbon dioxide removal are needed to limit global warming to between 1.5°C and 2°C. CDR projects can be used to reduce emissions in both industry and power generation, with relatively lower costs or energy penalties, otherwise, there would not be a net benefit. Therefore, there is a scientific gap to apply knowledge and develop solutions through devices to capture carbon and mitigate the effects of emissions. (IPCC, 2021).

This work presents a sufficiently simple and low computational cost mathematical model to aid in the search for materials for post-combustion CO_2 capture. The model considers the flow of dry combustion gases from the burning of fossil fuels such as natural gas and liquefied petroleum gas, which cross-tube reactors made of porous materials in an arrangement with a constructive design where the tubes are interspersed in constructions that gradually increase in size along the flow to capture the carbon, where there is a constructive relationship in the pipeline between the pressure drop and the rate of the capture reaction. The exploration of different material characteristics for the construction of porous media is a goal of this simulation that will ultimately be incorporated into a machine-learning algorithm.

2. METHODOLOGY

The method consists of a mathematical modeling of the fluid flow, the dispersion of CO_2 and the chemical reactions through a straight cylindrical packed-bed reactor in both the level of the spherical pellets of a generic capturing material and the level of the packed-bed like shown in the "Figure 1". Then numerical solutions for the overall carbon captured by in the solid and the pressure drop is determined numerically by means of software COMSOL Multiphysics. The gas is a fixed mixture of N_2 and CO_2 representing dry post-combustion exhaust gases.

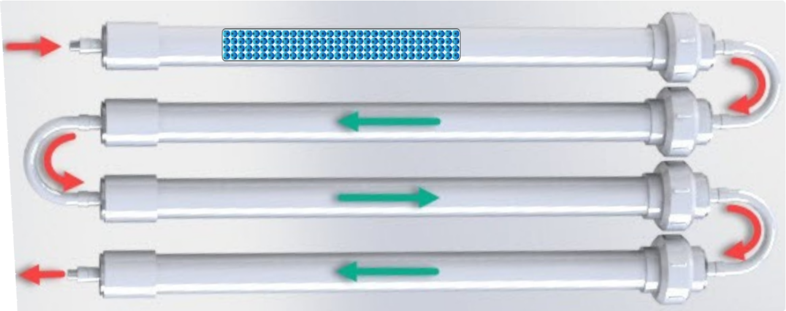


Figure 1: Tubular Packed bed filled with pellets.

In clear regions before or after the tubular reactors, the flow regime is incompressible, Newtonian, laminar and in steady-state and follows a simplified continuity and Navies-Stokes equations. In the packed-bed region, the flow follows the known porous media model, in which the velocity becomes the seepage velocity or the Darcy velocity $v(u, v, w)$. The continuity in the gas phase is given by "Eq.(1)", where φ is the bed porosity and e ρ_f is the gas mixture mean density. And, the flow follows the Darcy regime as given by "Eq. (2)" (Nield and Bejan, 1999), where ∇P is the pressure gradient, μ is the dynamic viscosity, g is the gravity acceleration, K is the permeability of the packed bed.

$$\varphi \frac{\partial \rho_f}{\partial t} + \nabla \cdot (\rho_f \boldsymbol{v}) = 0 \tag{1}$$

$$v = \frac{K}{\mu}\left(-\nabla P + \rho_f g\right) \tag{2}$$

The permeability (also known intrinsic permeability of the medium) does not depend on the fluid properties and can be estimated by simplifying models. Therefore, permeability can be estimated through simplifications of the labyrinth model formed by the pores and the connections between them. Modeling the porous bed as a packet of trapping spheres of diameter d, Kozeny obtained a correlation dependent on pellet diameter and bed porosity. The most applicable version of the relation was obtained considering a bed of pellets of diameter D_p considering the Carman-Kozeny hydraulic radius theory we have the formulation (Nield and Bejan, 1999):

$$K = \frac{D_p^2 \varphi^3}{180(1-\varphi)^2} \tag{3}$$

Considering the processes of transport phenomena in the tubular bed filled with pellets, we can consider the following assumptions: the process is isothermal, the parameters are constant in the bed section, the flow rate of the mobile phase is constant, the diameter of the capturing pellets D_p is constant, the reactor pellet is isotropic, changes in the physicochemical parameters in the radial direction are negligible, dispersion coefficient (D_L) is constant, and inside the porous pellet the only mechanism of mass transport is diffusion (Rodrigues et al., 1984). Based on this, two mass balances can be formulated, the first for the bed and the second for the interior of the pellet, and the model is coupled through the initial boundary conditions (Kaczmarski and Szukiewicz, 2021):

$$\varphi \cdot \frac{\partial C(t,z)}{\partial t} + v\frac{\partial C(t,z)}{\partial z} = \varphi D_L \cdot \frac{\partial^2 C(t,z)}{\partial z^2} - (1-\varphi)k_{ext}\frac{(\alpha+1)}{R_p} \cdot \left[C(t,z) - C_p\left(t, r = R_p, z\right)\right] \tag{4}$$

$$\varepsilon \cdot \frac{\partial C_p(t,r,z)}{\partial t} = D_{eff} \cdot \frac{1}{r^\alpha} \cdot \frac{\partial}{\partial r}\left(r^\alpha \frac{\partial C_p(t,r,z)}{\partial r}\right) - (1-\varepsilon)k_{rea}\left[C_p(t,r,z)\right]^n \tag{5}$$

In the “Eqs. (4) and (5)”, C is the gaseous concentration of CO_2 (considering that nitrogen and other gases are inert in the reaction) (Gasparovic, 2022), C_p is the concentration of CO_2 in the pores of the pellets, v is the Darcy´s velocity, k_{ext} is the external mass transfer coefficient, r is the radial coordinate, z is the axial coordinate, t is time, R_p is the radius of the pellet reactor, D_{eff} is the effective diffusion coefficient, k_{rea} is the kinetic reaction rate in the reactor, n is the apparent order of the reaction, α is the geometry of the pellet which is spherical in this case $\alpha = 2$ and ε is the porosity of the pellet. The initial conditions are: for $0 < z < L$ and $0 < r < R_p$ and when $t = 0$ we have $C(0,z) = C_0$ and $C_p(0,r,z) = C_{p_0}(r,z)$

We denote C_f as the initial concentration at the reactor inlet that comes from the flue exhaust gas, with the conditions $t > 0$ *and* $z = 0$:

$$v \cdot C_f = v \cdot C(t,0) - \varphi D_L \frac{\partial C}{\partial z} \tag{6}$$

and the conditions when the length L is the end of the reactor $t > 0$ *and* $z = L$:

$$\frac{\partial C}{\partial z} = 0 \tag{7}$$

The boundary conditions of “Eqs. (6) and (7)” are the convective and dispersive mass balances at the reactor inlet, that is, the convective flux in position $z = 0^-$ is equal to the sum of the convective flux in position $z = 0^+$, that is crossing the boundary, and the dispersion flux inside the reactor. However, the same convective mass flow for z = L− and z = L+ is assumed at the reactor outlet. The boundary conditions for “Eq. (5)” for $t > 0$ *and* $r = R_p$ (Nauman, 1983), represent that the diffusive flux in the pellet is equal to the mass transfer on the outer surface of the pellet:

$$D_{eff} \cdot \frac{\partial C_p\left(t, R_p, z\right)}{\partial r} = k_{ext} \cdot \left[C - C_p\left(t, R_p, z\right)\right] \tag{8}$$

when $t > 0$ *e* $r = R_d$,where R_d is the radius of the dead zone, the region of the pellet where there are no reagents, we have the following boundary conditions:

$$C_p(t, R_d, z) = 0 \tag{9}$$

when the deadband position, $R_d > 0$ or

$$\frac{\partial C_p(t, R_d, z)}{\partial r} = 0 \tag{10}$$

when the deadband does not exist more, that is, $R_d = 0$.
Thus, we introduce the dimensionless parameters below:

$$Z = \frac{z}{L};\ \tau = \frac{tv}{L\varphi};R = \frac{r - R_d}{R_p - R_d};$$

$$y=\frac{C}{C_r};y_p=\frac{C_p}{C_r};\ D_{eff}=\frac{D_m}{\chi}\varepsilon; \tag{11}$$
$$Pe=\frac{vL}{D_L\varphi};St=\frac{k_{ext}a_pL\varphi}{v};Bi=\frac{k_{ext}R_p}{D_{eff}};\ \Phi^2=\frac{k_0\rho_fR_p^2H_{CO_2}}{D_{eff}C_r}$$

where C_r is a reference concentration, tem que calcular o Cr we will adopt the value $C_r = 0{,}05\ \mathrm{kmol.m^{-3}}$ based on natural gas fuel gases, χ is the tortuosity parameter which is a factor to explain the non-linear nature of the pores, a typical value of 3 was considered (Blamey, 2017), $a_p = \alpha + 1/R_p$ constant for the spherical shape, Bi is the Biot number, Pe is the Peclet number, St is the Stanton number and Φ is the Thiele modulus, which describes the relationship between diffusion and reaction rates in porous catalyst pellets without mass transfer limitations, this value is generally used to measure effectiveness in pellets (Chaudhari and Ramachandran, 1980). The zero-order reaction rate constant is defined by k_0 and its unit is kmol.g^{-1}.s^{-1}, also the solubility coefficient from Henry´s law for the carbon dioxide is $H_{CO_2}$and the unit is defined by m^3 of liquid per m^3 of gas. Finally, D_m is the molecular diffusion coefficient that occurs in the macropores, is unit is m^2/s (Fuller et al., 1966):

$$D_m=\frac{10^{-3}T^{1.75}\left(\frac{1}{M_{CO_2}}+\frac{1}{M_{N_2}}\right)^{\frac{1}{2}}}{p\left[\left(V_{CO_2}\right)^{\frac{1}{3}}+\left(V_{N_2}\right)^{\frac{1}{3}}\right]^2} \tag{12}$$

where T is the temperature of the reaction, p is the total pressure, M_{CO_2} the molar mass of CO_2 (44,01 g/mol), M_{N_2} the molar mass of N_2 (28 g/mol) and V_{CO_2} and V_{N_2} diffusion volume of carbon dioxide and nitrogen molecules respectively. Just that carbon dioxide and nitrogen will be in the diffusion reaction because we are considering stoichiometric combustion for this analysis and water vapor will be removed in a previous process (Gasparovic, 2022).

There are cases in which the axial diffusion cannot be neglected (Peclet number smaller than one) and the plug-flow reactor model no longer holds. Initially, a simplified mass transfer Peclet number (i.e. Pe_{local}) should be calculated based on the equivalent diameter of the carbon capturing pellets d_{eq}, based at the average velocity of the interstitial fluid through the packed bed, v_z (interstitial velocity), and the molecular diffusion of the carbon dioxide in the flue gas mixture D_m and d_{eq} is the equivalent diameter of the pellet when they are spherical. The average velocity of the interstitial fluid is

$$v_z=\frac{q}{\pi R_{PFR}^2\varphi} \tag{13}$$

where q is the volumetric flow rate through the reactor and R_{PFR} is the tube radius in the plug flow tubular reactor (PFR). The porosity φ, is needed to determine the cross section of the actual flow and calculate the average velocity of the reactive mixture between the carbon capturing pellets. The prescription for calculating the simplified mass transfer Peclet number for component A is:

$$Pe_{local}=\frac{v_zd_{eq}}{D_m} \tag{14}$$

the dimensionless quantity ϒ, defined by the “Eq. (15)”:

$$\Upsilon=\frac{D_{eff}}{D_m} \tag{15}$$

Empirical correlations for ϒ are summarized in the “Table 1” below:

Table 1: Empirical and Theoretical Correlations between Effective Axial Dispersion Coefficients and the Interstitial Fluid Velocity in Packed Beds and Porous Media:

$\Upsilon = 0{,}67$	$10^{-3} \leq Pe_{local} < 1$
$\Upsilon = Pe_{local}$	$1 \leq Pe_{local} < 100$
$\Upsilon = 2Pe_{local}$	$100 < Pe_{local} < 3\times10^6$

The following comments on the experimental correlations in Table 1 provide further insight into the fundamental underlying basis for their existence.

1. Pellet size has no explicit effect on correlations. This is obvious because the correlations are not classified in terms of the equivalent diameters of the filler material used to obtain the experimental data.

2. The effective axial dispersion coefficient, D_{eff}, is not expressed as a function of the common molecular diffusion coefficient. In other words, the correlations introduced above for D_{eff}/D_m vs. Pe_{local} are exactly the same as D_{eff} vs. v_z

$$D_{eff} \cong v_z d_{eq} \tag{16}$$

If $\Upsilon \approx 2 \{Pe_{local}\}$ when the simplified Peclet number is greater than 100, then:

$$D_{eff} \cong 2 v_z d_{eq} \tag{17}$$

3. When the simplified mass transfer Peclet number is very small (i.e. <1), $\Upsilon \approx 0{,}67$ instead of unity because the numerator of Υ (i.e. D_{eff}.) is based on pore diffusion in an unstable state without convection, while the denominator of Υ (i.e. D_m) is measured in an unrestricted bulk fluid phase. In other words, the diffusivity in the numerator of Υ is reduced by porosity and tortuosity factors.

The mass transfer Peclet number is:

$$Pe_{MT} = Re \cdot Sc = \frac{L_{PFR} v_z}{D_{interpellet}} \tag{18}$$

which is based on interpellet axial dispersion, reactor length L_{PFR} and mean interstitial fluid velocity. The above discussion outlines the strategy for calculating:

$$D_{interpellet} = D_{eff} = \phi_{correlation} v_z d_{eq} \tag{19}$$

where:

$$\phi_{correlation} \approx \begin{cases} 1, when\ 1 < Pe_{local} \leq 100 \\ 2, when\ Pe_{local} > 100 \end{cases}$$

It is the Peclet mass transfer number that represents the interpellet axial dispersion:

$$Pe_{MT} = Re \cdot Sc = \frac{L_{PFR} v_z}{D_{interpellet}} = \frac{L_{PFR}}{\phi_{correlation} d_{eq}} \tag{20}$$

This dimensionless parameter is necessary to analyze the effects of the residence time distribution in packed tube reactors (Belfiore, 2003). So Eqs. (4) and (5) are rewritten with the dimensionless parameters are:

$$\frac{\partial y(\tau,z)}{\partial \tau} + u\frac{\partial y(\tau,x)}{\partial x} = \frac{1}{Pe} \cdot \frac{\partial^2 y(\tau,x)}{\partial x^2} - \frac{(1-\varphi)}{\varphi} St\left[y(\tau,x) - y_p(\tau, R=1, x)\right] \tag{21}$$

$$\frac{\partial y_p(\tau,r,x)}{\partial \tau} = \frac{1}{\varepsilon} \frac{St R_p^2}{(\alpha+1) Bi \left(R_p - R_d\right)^2} \left(\frac{\alpha\left(R_p - R_d\right)}{R_d + \left(R_p - R_d\right) R} \frac{\partial y_{p(\tau,r,x)}}{\partial R} + \frac{\partial^2 y_p(\tau,r,x)}{\partial R^2} \right) - \frac{(1-\varepsilon)\Phi^2 St\left[y_p(t,r,z)\right]^n}{\varepsilon(\alpha+1) Bi} \tag{22}$$

The initial conditions for $\tau = 0$:

$$y(0,x) = y_0 \tag{23}$$

$$y_p(0,R,x) = y_{p,0}(R,x) \tag{24}$$

For these conditions, the "Eq. (21)" in the bed for $\tau > 0\,; x = 0$ becomes:

$$y_f - y(\tau,0) = -\frac{1}{Pe} \frac{\partial y(\tau,0)}{\partial x} \tag{25}$$

for $\tau > 0\,; x = 1$:

$$\frac{\partial y(\tau,1)}{\partial x} = 0 \tag{26}$$

for the "Eq. (22)" in pellets, we have $\tau > 0\,; R = 1$:

$$\frac{R_p}{\left(R_p - R_d\right)} \frac{\partial y_p(\tau,R)}{\partial R} = Bi\left(y - y_p(\tau,R)\right) \tag{27}$$

for $\tau > 0\,; R = 0$:

$$y_p(\tau,R) = 0 \; e \; \frac{\partial y_p(\tau,R)}{\partial R} = 0 \tag{28}$$

Note that, for the given definition of the dimensionless radius R, the value of R changes between 0 and 1, although the radius of a deadband may change with decreasing substrate concentration along the reactor. Replacing the coordinate r by its dimensionless equivalent R simplifies the numerical solution of the reactor model.

When the mass transfer rate is sufficiently large, another simplification is to consider the lumped reaction model, which is now controlled by the kinetics of the reaction and the amount of calcium hydroxide. To determine the CO_2 capture rate we use the principle of pellet and bed porosity through the formula below (Gasparovic, 2022). The mass flow is fixed and it is considered that the operating time t_{op} is equal to 60 minutes and is enough to reach maximum conversion, the reactor is used completely during the entire reaction; that is, there are no deadbands inside the pellet at any point in the bed. According to the heterogeneous model for the bed, Thiele's modulus is greater than the critical value at all points in the bed (Shih et. al., 1999).

$$\bar{n}_{capt'} = (\pi R_{PFR}^2) \frac{(1-\varphi)(1-\varepsilon)}{V_{CH}} \frac{(1 - exp(-k_1 k_2 t))}{k_2 60 t_{op}} \; (mols.s^{-1}.m^{-1}) \tag{29}$$

where R_{PFR} is the plug flow reactor radius (m), V_{CH} is the molar volume of $Ca(OH)_2$ (m^3/mol), k_1 and k_2 are reaction constants:

$$k_1 = 1.11\, Sg(-lnRH)^{-0{,}96} \exp\left(-\frac{17400}{RT}\right) \; (min^{-1}) \tag{30}$$

$$k_2 = \frac{5.31}{Sg} \exp\left(\frac{0.603}{RH}\right) \exp\left(\frac{2900}{RT}\right) \; (-) \tag{31}$$

where R is the universal gas constant equivalent to 8,314 (J/mol K), RH is the relative humidity of the porous bed, Sg initial specific surface area of solid, (m^2/g).

The heterogeneous model for the porous bed is formulated with the following considerations: 1) Isothermal process; 2) The flow rate of the mobile phase is constant; 3) The bed is loaded with spherical reactive pellets with the same radius R_p; 4) The pellet is isotropic; 5) The radius of the dead zone in a reactive pellet is R_d and can be a function of time and position inside the reactor; 6) Changes in physicochemical parameters in the radial direction are negligible; 7) The D_L dispersion coefficient is constant. 8) According to the classic treatment of transport and reactions in porous catalysts, diffusion is the only mechanism considered inside the pellet (Rodrigues et al., 1984).

Figure 2 shows the mechanics of the reaction that takes place inside the pore and in the water film in the pore of the pellet. For the modeling of the system, the literature presents the steps involved and first the formation of carbonic acid reacting with calcium hydroxide to form calcium carbonate. For modeling purposes, information from the literature is presented on the steps involved in the reaction and the possibility of each one being limiting, for the liquid film system, focusing on calcium hydroxide (Gasparovic, 2022). The overall reaction for CO_2 capture with $Ca(OH)_2$ in water is expressed by:

$$Ca(OH)_2 + CO_2 \rightarrow CaCO_3 + H_2O - 69{,}1 \; (KJ/mol\, CO_2) \tag{32}$$

The carbonation of calcium hydroxide requires the presence of adsorbed water (Shih et al., 1999). Water-CO_2 binary static adsorption data available in the literature show that, for diluted systems, the presence of a small amount of water favors the adsorption of CO_2 at low partial pressures, but with higher concentrations of CO_2 and water, this inhibits the adsorption of CO_2.

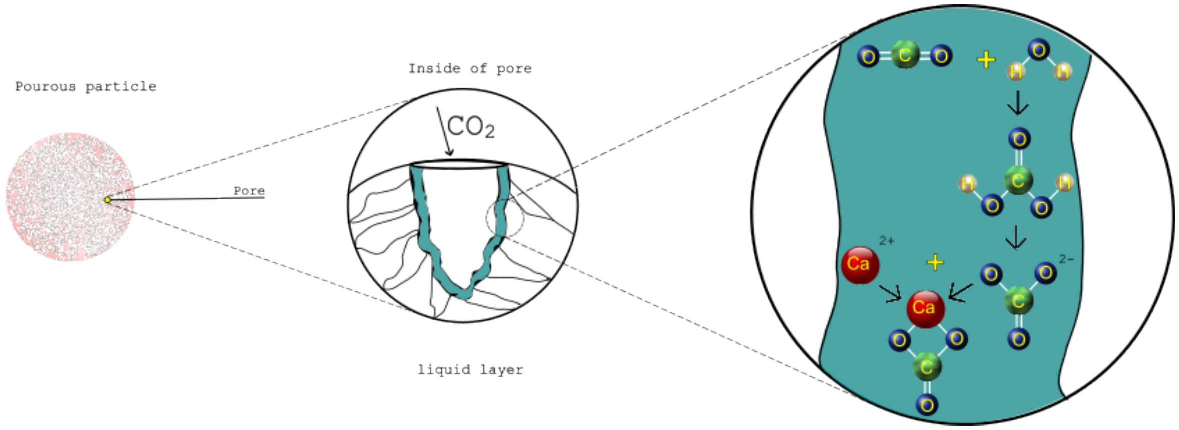


Figure 2 – Indirect carbonation reaction in aqueous base inside the pellet pores.

The constructal design method (Bejan and Lorente, 2008) is used to guide the development of designs for the device, whose operation will be simulated to define the best design among those tested for the construction of prototypes. This method is based on the view that flow configuration (geometry and design) can be understood based on a principle of configuration generation and temporal evolution towards greater global access of flows in systems that are free for transformations, bringing to the final result complexity, organization, and evolution (Bejan and Errera, 2016). Tondeur and Luo, 2004 developed prototypes with stereolithography based on the theory of constructal design with the commitment to reduce costs and space in relation to the minimum pressure drop and viscous dissipation and on the other hand to increase the volume of gas retention in the porous structure.

3. REVIEW OF LITERATURE

According to Directive 2009/31/EC on limiting global climate change to 2 degrees Celsius, the goals set for reducing global emissions of greenhouse gases define what reduction is technically feasible and that the benefits far outweigh the costs, but that, to achieve this, all mitigation options must be taken advantage of. However, carbon capture cannot in itself mean a high penalty for the energy or industrial generation process, that is, the parasitic energy associated with the consumption of the carbon capture and storage system and also the impacts caused in the production plant originally installed without carbon capture. Many processes are studied and developed for carbon capture, absorption is the most mature and most used post-combustion capture process with 57% utilization, 14% use adsorption, 8% use membranes and 21% apply mineralization or biofixation (Dewil et al., 2020). However, even according to Dewil, carbon capture with an efficiency rate of 90% of exhaust gases by absorption with amines consumes about 30% of the energy generated by the plant at a cost of 40-100 US$ per ton of CO_2 captured. According to the US Department of Energy (DOE) for energy sector projects, the current capture cost is estimated at US$60 to US$70 per ton of captured CO_2. DOE's goal is to reduce the cost of capture to $30-$40 to make the operation viable, which can be achieved through research and development.

Indirect capture in aqueous media, on the other hand, proves to be viable in terms of technology, energy level and in economic terms its cost can be found around US$ 22,6 per ton./CO_2. The use of industrial waste or construction raw materials can also reduce costs and still be ecologically correct, an example is the use of carbonated bauxite slurry for a wide range of products such as bricks and tiles, cement production, fertilizer production, water treatment and even in the plastics industry (Yadav and Mehra, 2021).

This article emphasizes the possibility of carbon capture and storage with carbonation as a more economical and viable technology for carbon capture, and also explores other materials, analyzing the properties related to the carbon capture process, which could be even more efficient, such as: Basalt (Based on rock formation), Brines, Brucite (Mg(OH)2), Chrysotile (Mg3(Si2O5)(OH)4), Dunite (90% Olivine). Feldspar (CaAl2Si2O8), Forsterite (Mg2SiO4), Harzburgite (CaMgSi2O6 + (Fe, Al)), Listwanite Carbonated serpentinite, Olivine ((Mg, Fe)2SiO4), Peridotite (Based on rock formation), Pyroxene (CaMgSi2O6 + (Fe, Al)), Pyroxenite (Pyroxene rocks), Serpentine (Mg3Si 2O5(OH)4), Serpentinite (Based on rock formation), Slaked lime (Ca(OH)2), Wollastonite (CaSiO3) as cited by Yadav and Mehra (2021).

The use of 3D-printing technology for prototyping zeolite monoliths for CO_2 capture has proven to be an interesting option for the treatment of flue gases, as it presents itself as a simple strategy for building reactors with high performance for capture (Wang et al., 2019). Regufe et al. (2019) created monoliths for carbon capture from 70% 13X zeolites and 30% activated carbon, a wet mixture was made between these adsorbent materials, carboxymethylcellulose and water, demonstrating high CO_2 capture capacity. A large number of nanomaterials are also being researched to improve carbonation processes and also being applied in carbon capture processes other than carbonation, but mostly only in the testing phase, not yet applied on a large scale (Chen et al., 2021).

Therefore, research and effort from the scientific community are needed to find solutions for these opportunities for technical design improvements with a high kinetic reaction rate, high CO_2 removal efficiency and low energy consumption so that government and industry subsidize the design of equipment (Ben-Mansour et al., 2016).

According to Wilcox (2012) the advantages of mineral carbonation are:

1) The possibility of CCS as a single process,
2) Permanent sequestering with minimal leakage potential,
3) Stabilization of harmful pollutants associated with mineral matter,
4) The potential for energy compensation since the mineral carbonation processes are thermodynamically favorable.

However, the reaction rate, process efficiency and capture percentage do not offer advantages to this technology. Therefore, new application approaches must be studied. Camerini, et al. (2019) studied carbonation kinetics using commercially available dispersed calcium hydroxide ($Ca(OH)_2$) nanoparticles and used the "*Boundary Nucleation and Growth Model*" (BNGM) to analyze the carbonation process in the surface area of molecules. They used the wet route for the experiment with the fastest conversion rate at temperatures of 30 °C, the larger the nanoparticle and the smaller its surface area the lower the rate at which the porosities are filled with the reaction products in this case the carbonates.

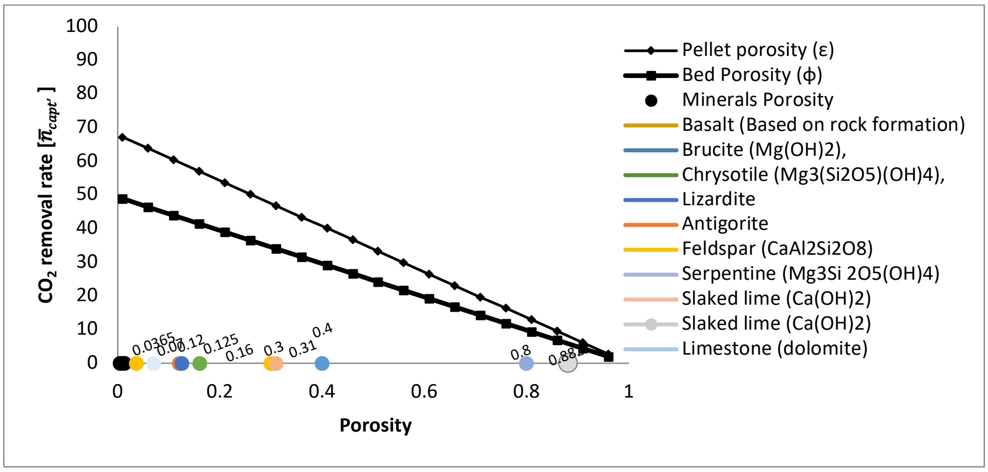
Within a vast amount of possible existing materials and even other materials that can be manufactured in the laboratory and printed in additive manufacturing, it is necessary to find a way to measure and evaluate each of these probable candidates and even create a candidate with the best qualities for carbon capture. The most important properties listed in the review carried out by Farmahini et al. (2021) are: pore volume, porosity, surface area, pore diameter, regenerability, diffusivity, Henry selectivity and density. On the other hand, it is also possible to analyze the functional behavior of materials through metrics appropriate to the process in question, such as: work and recovery capacity, specific energy, productivity, purity, parasitic energy and separation performance parameter.

And it is within this perspective that the present article intends to act in order to evaluate and list the most important properties of materials for carbonation and determine which metrics can determine the materials for CO_2 capture.

4. DISCUSSION AND RESULTS

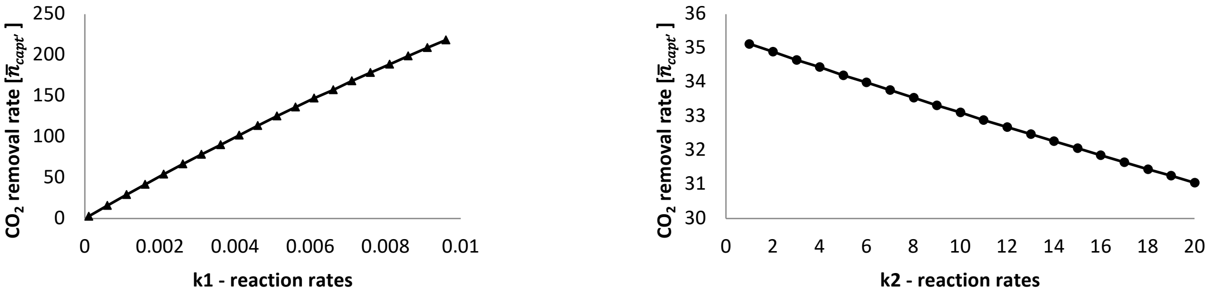
The expected results for the work should include: Obtaining a multiphysics numerical model that adequately describes the CO_2 capture process and validation with experimental data obtained from prototype tests; Obtaining design and design guidelines for a CO_2 capture device, using constructal design theory; Identification, through numerical simulations, of a design, among those proposed, that allows for an improvement in the performance of the device; Development of a methodology for the design/project of reactors to capture CO2 for various exhaust gases, which can help in the expansion of the technology.

The initial values for the graph below demonstrates and proves that as the porosity of the pellet increases, that is, the value of ε is lower , the CO_2 removal rate $\left(\bar{n}'_{capt}\right)$ is higher. Just like the particle porosity, the bed porosity also depends on the type of material, and as the porosity decreases the CO_2 capture rate increases, however the influence of the particle porosity is greater than the bed porosity on the capture capacity. As predicted by Belfiore's statements, pellet size has no explicit effect on correlations. The pellet diameter value was varied from 10 mm to 10 µm, and for all values the CO_2 removal rate was the same $\bar{n}_{capt'} = 34{,}58$, the CO_2 removal rate is constant when the diameter varies.



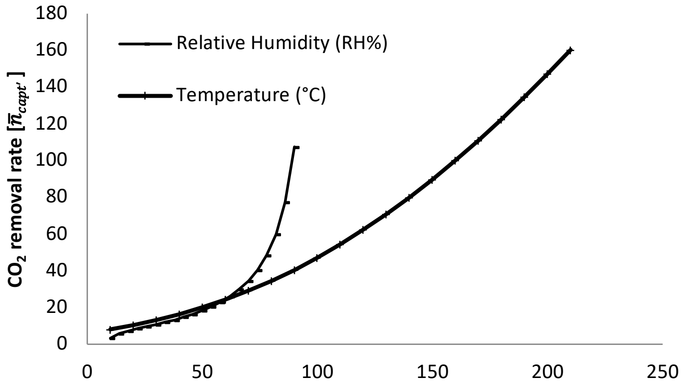
Graph 1: CO_2 removal rate as a function of pellet porosity and bed porosity.

According to the definitions, the reaction rates k1 and k2 are functions of the specific surface area of the solid, temperature, CO_2 concentration and relative humidity in the porous bed. These functions can be derived by analyzing the k1 and k2 data that were obtained by fitting the equation to each set of experimental data. Since the CO_2 concentration in the gas phase has no effect on the reaction in the concentration range of this study, k1 and k2 are independent of the CO_2 concentration in the gas phase. As shown in graph 4 below, as the reaction rate in the pellet increases the CO_2 removal rate also increases when the reaction rate is varied from 1E-4 to 1E-2 with a CO_2 removal rate varying from 2.6 to 218.3. On the other hand, while the reaction rate was varied from 1 to 20, as the reaction rate k2 increases, the CO2 removal rate decreases from 35.1 to 31.05, because K2 is inversely proportional to the CO2 removal rate in the equation.



Graph 2: CO_2 removal rate as a function of reaction rate k_1 and reaction rate k_2.

The reaction takes place in the liquid phase of a porous medium reactor in the film that forms on the outer walls of the pellet. The available humidity mainly influences the extraction of cations from the substrate solid to the solution. The mass transfer rate of the gas phase and the solubility of CO_2 in water are high enough that the chemical reaction is not affected by the increase in the availability of CO_2 molecules in the water present in the pores. Both temperature and relative humidity have an increase in the capture rate as values increase.



Graph 3: CO_2 removal rate as a function of relative humidity and Temperature.

5. CONCLUSION

In this paper we presented a mathematical model and a brief literature review to support that the actions of materials informatics for advanced materials for carbon capture. The mathematical model is simple enough to grasp the basic properties of the materials (ex: for mineral carbonation) and the properties of a packed-bed tubular reactor simple enough to be simulated with low computational cost. The cost must be low because it will be part of a major search algorithm and it will be performed a great number of times. The example showed the basic features of the bed as porosity can be checked with the criterion of carbonic gas captured. As more parameters are considered, more simulations will be carried out to determine “envelopes” of input-output to train the machine learning algorithm that drives the search for the best materials. What we can see is that the pellet porosity and the reaction rate in the CO2 reactor are the items that have the most influence on the CO2 removal rate. Therefore, the search for new porous materials that allow the improvement of the capture rate would be an advantage in the process. As well as materials that allows the reaction rate to be more effective to improve capture capacity

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