

Mathematical Modelling for the Adsorption Process of CO₂ in Nanopores of Catalytic Particles in a Fixed Bed Reactor Using Numeral Inverse Laplace Transform

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Theoretical analysis on the CO₂ adsorption on NaX has been carried out in fixed bed reactor. In the proposed process, CO₂ was passed through a stationary adsorbent bed allowing continuous operation. A one-dimensional and isothermal model was proposed to describe the adsorption process of CO₂. Attention has been focused on a mathematical model to simulate the transient behavior of dissolved CO₂ within the gas phase and then adsorbed into the nanopores of the solid phase (adsorbent). The simulation results were compared to the one experimental case. After, it was performed a sensibility analysis in relation to CO₂ concentration within of the nanopores of the solid phase as well as accounting for the amount of adsorbed CO₂ in the nanopores of the solid phase.

1. Introduction

It well know that fossil fuel is still the world's primary energy source and its combustion is one of the major sources of the greenhouse gas carbon dioxide. CO₂ has been know as one of the causes of global warming, but the purified and concentrated CO₂ stream can be used as an important carbon source to synthesize clean fuels and fine chemicals. Serious preoccupations have been raised with respect to the impact of the increasing concentration of CO₂ in the atmosphere on the environment. Therefore, it's evident that the strategic importance of pos-combustion capture systems are required to prevent emissions from the existing fleet of power plants when considering the abundant sources of CO₂ emissions (Oliveira and Silva, 2012).

The adsorption process to capture CO₂ on NaX has been widely applied in chemical engineering and environmental engineering. Computer simulation became an increasingly important optimization tool in continuous adsorption-based process such as in the fixed bed reactor. The mathematical explanation for the fixed bed reactor of component systems has been developed. Usually, an analytical solution is not possible for non-linear component model. Although the adsorption process has some restrictions, this technique is attractive since it provides information in relations to concentration dependence of micropore diffusivities.

NaX has presented promising results for separating CO₂ form gas mixtures and can potentially be used in the adsorption processes. Based on the advanced analysis of several important studies with respect to CO₂ adsorption using NaX, it shows that the surface basicity and size of NaX as well as the strength of the electric fields caused by the presence of exchangeable cations in the frameworks and cavities of NaX are the essential factors for the CO₂ adsorption on NaX.

A crucial problem of the adsorption process is CO₂ adsorbent performance (Ding and Alpay, 2000). Based on the capacity of CO₂ adsorption, the adsorbents with high capacity are considered ideal. On the other hand, the adsorbents with low capacity are clearly inappropriate. Therefore, the objective of the present work has been to carry out a sensibility analysis regarding CO₂ concentration within of the nanopores of the solid phase as well as accounting for the adsorbed amount of CO₂ in the nanopores of the solid phase.

$$\frac{\partial q_{CO_2}(r,t)}{\partial t} = k_{ad} \left(C_{CO_2}(r,t) - \frac{q_{CO_2}(r,t)}{\rho_s K_{ed}} \right) \quad (8)$$

The initial condition for the Eq (8) has been described as;

$$\text{for } t \leq 0, q_{CO_2}(t) \Big|_{t=0} = 0 \text{ for all } r \quad (9)$$

2.3 Application of the Laplace transformation on the mathematical model

The Laplace transformation method has been used for transforming partial differential equations (PDEs) in ordinary differential equations (ODEs) according to Silva and Oliveira (2012). PDEs (1) to (9) and their restricted conditions can be transformed easily using the Laplace transformation according to the Equation (10) as follow.

$$\bar{C}_i(z,s) = \int_0^{\infty} C_i(z,s) e^{-st} dt; \bar{C}_i(z,s) = \bar{C}_{CO_2}(z,s), \bar{C}_{CO_2}(r,s) \text{ and } \bar{q}_{CO_2}(r,s) \quad (10)$$

Initially, Eqs (1) to (9) and their initial and boundary conditions were obtained in the Laplace domain using the above Eq (10) as follows.

- Mass balance for the gas phase in the Laplace domain;

$$D_{z,CO_2} \frac{d^2 \bar{C}_{CO_2}(z,s)}{dz^2} - \alpha_1 \frac{d \bar{C}_{CO_2}(z,s)}{dz} - \alpha_2(s) \bar{C}_{CO_2}(z,s) + \alpha_3 \bar{C}_{CO_2}(r,s) \Big|_{r=R} - \bar{C}_{CO_2,0} = 0 \quad (11)$$

- The Eq (11) is restricted the following initial and boundary conditions in the Laplace domain;

$$\text{for } s > 0, \bar{C}_{CO_2}(z,s) = \frac{C_{CO_2,0}}{s} \text{ for all } z \quad (12)$$

$$\text{for } s \geq 0, D_{z,CO_2} \frac{d \bar{C}_{CO_2}(z,s)}{dz} \Big|_{z=0^+} = \frac{4Q_g}{\pi d_c^2} \left[\bar{C}_{CO_2}(z,s) \Big|_{z=0^+} - \frac{C_{CO_2,0}}{s} \right]; \text{ as } z \rightarrow \infty, \frac{d \bar{C}_{CO_2}(z,s)}{dz} = 0 \quad (13)$$

- Mass balance for the solid phase in the Laplace domain;

$$\frac{d^2 \bar{C}_{CO_2}(r,s)}{dr^2} + \frac{2}{r} \frac{d \bar{C}_{CO_2}(r,s)}{dr} - \beta_1(s) \bar{C}_{CO_2}(r,s) = 0 \quad (14)$$

- The Equation(14) is restricted the following initial and boundary conditions in the Laplace domain;

$$\text{for } s \leq 0, \bar{C}_{CO_2}(r,s) \Big|_{s=0} = 0 \text{ for all } r \quad (15)$$

$$\text{for } s \geq 0, D_{e,CO_2} \frac{d \bar{C}_{CO_2}(r,s)}{dr} \Big|_{r=R} = k_{gs} \left[\bar{C}_{CO_2}(z,s) - \bar{C}_{CO_2}(r,s) \Big|_{r=R} \right]; \text{ for } s > 0, \frac{d \bar{C}_{CO_2}(r,s)}{dr} \Big|_{r=0} = 0 \quad (16)$$

- The adsorption rate of CO₂ in the Laplace domain;

$$\bar{q}_{CO_2}(r,s) = \beta_2(s) \bar{C}_{CO_2}(r,s) \quad (17)$$

- The initial condition in the Laplace domain for the Equation (17);

$$\text{for } s \leq 0, \bar{q}_{CO_2}(r,s) \Big|_{s=0} = 0 \text{ for all } r \quad (18)$$

The spatial domain was discretized using centred finite differences of second order over a uniform grip. This approach was found to give a converge solution in which a value of 1.0×10^{-6} for absolute tolerance (Silva, 2012). The coefficients [α_{1g} , $\alpha_{2g}(s)$, α_{3g} , $\beta_1(s)$ and $\beta_2(s)$] of Eqs (11), (14) and (17) are defined in the appendix (A).

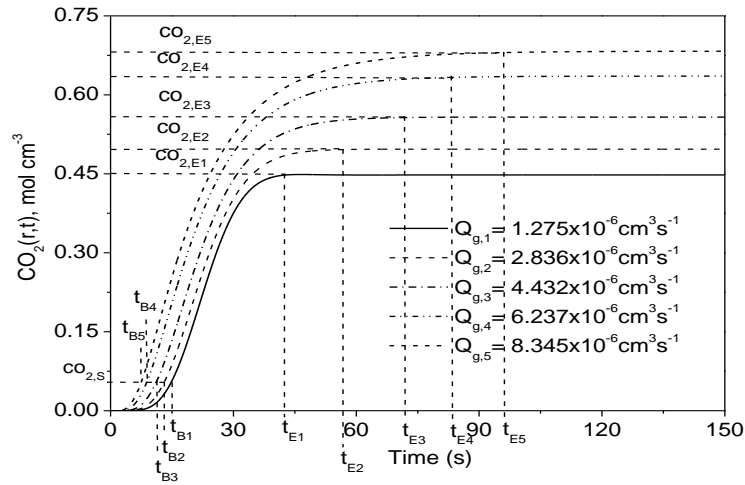


Figure 2: Effect of different flow rates on breakthrough curves at different breakthrough time in the solid phase

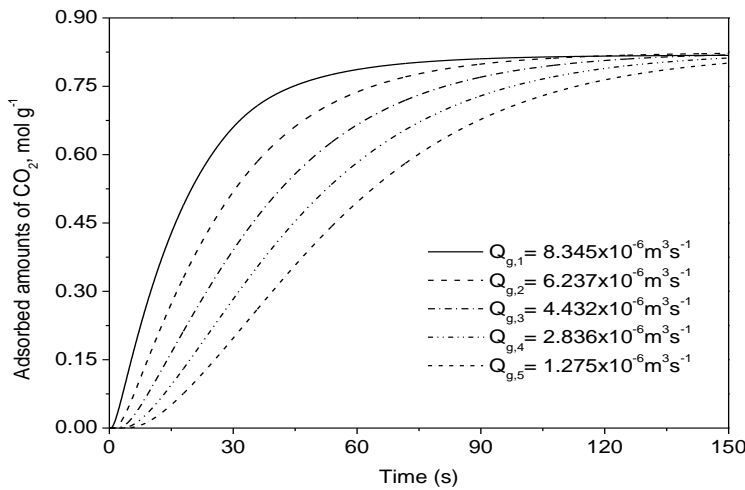


Figure 3: Effect of different flow rates on adsorbed amounts of CO₂ in the solid phase ($CO_{2,0} = 0.56 \text{ kg m}^{-3}$, adsorbent size = 0.156 cm and nanopores diameter = 0.748 ncm)

As can be seen in the Figure 2, the breakthrough curves of CO₂ have shown a growth with the increase in flow rate along the time with the physical properties fixed. Breakthrough time for the curve 1 is t_{B1} ; t_{B2} -breakthrough time for the curve 2, t_{B3} -breakthrough time for the curve 3, t_{B4} -breakthrough time for the curve 4 and t_{B5} -breakthrough time for the curve 5; t_{E1} -exhaustion time for the curve 1, t_{E2} -exhaustion time for the curve 2, t_{E3} -exhaustion time for the curve 3, t_{E4} -exhaustion time for the curve 4 and t_{E5} -exhaustion time for the curve 5; $CO_{2,E1}$ -exhaustion concentration of CO₂ for the curve 1, $CO_{2,E2}$ -exhaustion concentration of CO₂ for the curve 2, $CO_{2,E3}$ -exhaustion concentration of CO₂ for the curve 3, $CO_{2,E4}$ -exhaustion concentration of CO₂ for the curve 4 and $CO_{2,E5}$ -exhaustion concentration of CO₂ for the curve 5). According to Figure 3 the adsorbed amounts of CO₂ increased with growth in flow rate ($1.275\text{--}8.375 \times 10^{-6} \text{ cm}^3 \text{ s}^{-1}$).

