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Simulation of Cryogenic Packed Bed Using 1-Dimensional Pseudo Homogeneous Model

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Abstract: The numerical solution of 1-dimensional pseudo homogenous model for cryogenic packed bed is a challenging task due to very steep gradients of temperature and concentration. In this study the simulation of cryogenic packed bed is presented to capture carbon dioxide. The finite difference method, Forward-Time Central Space (FTCS) scheme is used for simultaneous numerical solution of 1-dimensional pseudo homogenous model. A case study is also discussed to validate the numerical solution.

Key words: Cryogenic paked bed, FTCS, 1-D pseudo homogenous model, CO_2

INTRODUCTION

A cryogenic packed bed is an assembly of usually uniformly sized spherical particle, which are randomly arranged and firmly held in position within a vessel or tube. The bulk fluid flows through void spaces of the bed and deposit at the surface of the packing. The temperature of packing is maintained below the freezing temperature of fluid so fluid frost on the surface of packing. Convection of the bulk fluid is connected with heat and mass dispersion. Dispersion effects are largely caused by the complex flow patterns in the bed induced by the presence of the packing. Also, the dispersion effects are caused by transport phenomena like molecular diffusion, thermal conduction in fluid and solid.

Due to the complex phenomena like frosting and sublimation taking place in cryogenic packed bed, the exact description leads to complex mathematical problem. The more detailed mathematical models lead to more parameters. Therefore need of simplified mathematical model is inevitable to overcome these complexities.

A lumped pseudo homogeneous model was first described by Taylor for the species equation only when the transverse diffusion time is much smaller than the advection time with axial mixing (Taylor, 1953). Later McGuire and Leon analyzed the stability of a packed-bed reactor and presented a lumped model for the species and energy equations with the chemical reactions happening on the surface of the pellets, they introduced the porosity term also (McGuire and Lapidus, 1965).

Smit *et al*. (2003) proposed 1-D pseudo homogeneous model to simulate the reverse flow reactor due to presence of very steep gradient of concentration and temperature at different locations of reverse flow reactor. The model was solved by using Weight Essential Non-Oscillatory (WENO) scheme with adaption of very fine grid due to steep gradients. Tuinier *et al.* (2011) used 1-D pseudo homogeneous model for simulation of dynamically operated packed bed for removal of CO_2 from flue gasses. For accumulation term finite volume discretization technique and for convection term fifth order WENO scheme was used. Maqsood *et al.* (2014) developed an experimental setup for cryogenic separation of CO_2 from natural gas. The numerical study was completed using 1-D pseudo homogeneous model for individual component, mass and energy balance equations were solved separately using this model (Mohamad, 2012).

In present study finite difference and Forward-Time Central Space (FTCS) scheme is used to solve simultaneous mass and energy balance equations of 1-D pseudo homogeneous model.

METHODOLOGY

Process descriptions: To study the 1-D pseudo homogenous model in cryogenic packed bed, an experimental setup was constructed. The schematic diagram is shown in Fig. 1. When carbon dioxide is passed through a chilled packing, it frost on the surface of packing. The packing is kept below the freezing point of carbon dioxide.

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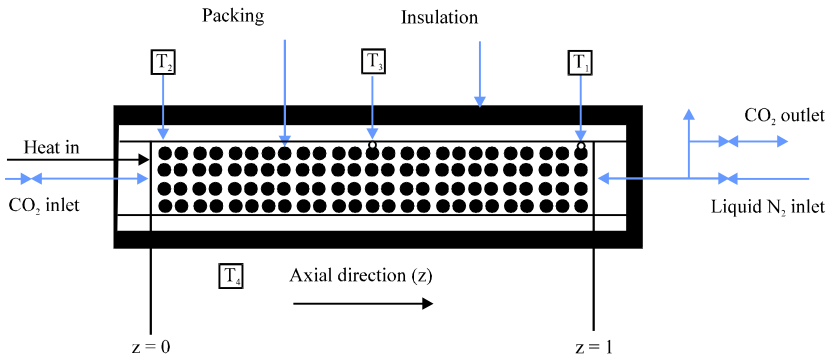

Fig. 1: Schematic diagram of cryogenic packed bed

Mathematical formulation of 1-D pseudo homogenous model: It is important to understand the fundamentals of the pseudo-homogenous one-dimensional model in order to formulate the mass and energy balance equation. When the packed bed under study does not have a significant length in the radial direction, simplification allows efficient modeling in one-dimension (Depcik and Assanis, 2005). As a result, only the mass and energy equations require solution. The pseudo-homogeneous model deals with the properties of the solid (packing) and fluid into a single governing equation while assuming a negligible pressure drop. This allows one equation each for the governing equations of mass and energy, instead of the requirement of modeling both the solid and fluid phases independently.

For the gas flowing through cryogenic packed bad the governing equation for mass balance in one dimension is presented in Eq. 1:

$$\varepsilon_g \rho_g \frac{\partial X_i}{\partial t} + \rho_g u \frac{\partial X_i}{\partial z} = \frac{\partial}{\partial z}\left(\rho_g D_{eff} \frac{\partial X_i}{\partial z}\right) - \dot{m}_i'' a_s \quad (1)$$

The first term on the right hand side describe the change in concentration with respect to time within inertial space. The second term on the left hand side describes time-change concentration due to advection of gas and the first term on right side describes diffusion effect. Since pore structure involve relative small area, diffusion effect becomes significant. Axial or longitudinal mass dispersion was calculated by Edwards and Richardson (1968) (Eq. 2):

$$D_{eff} = 0.73 D_m + \frac{0.5 u d_p}{1 + \frac{9.7 D_m}{u d_p}} \quad (2)$$

At low Reynolds numbers, the dispersion is effected by molecular diffusion but at high Reynolds numbers eddy diffusion predominates.

Energy balance equation for both solid and gas: The energy balance equation for gas flowing within interstitial space in pores is defined in Eq. 3:

$$\varepsilon \rho_g c_p \left(\frac{\partial T_g}{\partial t} + u \frac{\partial T_g}{\partial z}\right) = \frac{\partial}{\partial z}\left(\rho_g \lambda_g \frac{\partial T_g}{\partial z}\right) + q_{g \to S} \quad (3)$$

where, the first term on the left hand side describes the time-change of temperature of the gas within the interstitial space and the second term represents the transfer of energy due to advection of the gas in the pores. The second term on the right hand side is heat transfer from gas to solid phase. This equation only describes the energy transfer due to movement of fluid and it does not include the effective thermal conductivity. So the phase energy equation for the surface of the packing is as follows (Eq. 4):

$$(1-\varepsilon) \rho_s c_{p,s} \left(\frac{\partial T_g}{\partial t}\right) = (1-\varepsilon) \frac{\partial}{\partial z}\left(\lambda_s \frac{\partial T_s}{\partial z}\right) - q_{g \to S} - \sum_{i=1}^{n_r} \dot{m}_i'' a_s \Delta h_i \quad (4)$$

Combining both equations the resultant equation which deals with both solid and gas phases with effective axial thermal conductivity is presented in Eq. 5:

$$(\varepsilon \rho_g c_{p,g} + \rho_s (1-\varepsilon) c_{p,s}) \frac{\partial T}{\partial t} = \rho_g u c_{p,g} \frac{\partial T}{\partial z} + \frac{\partial}{\partial z}\left(\lambda_{eff} \frac{\partial T}{\partial z}\right) - \sum_{i=1}^{n_r} \dot{m}_i'' a_s \Delta h_i \quad (5)$$

The axial thermal conductivity can be calculated according to Zehner and Schlunder (1970). They assumed a point contact of particles in the direction of heat flow e.g., the heat conduction through pellets over large surface contact area is not considered:

$$\lambda_{eff}=\lambda_g\left\{1-(1-\varepsilon)^{\frac{1}{2}}+\frac{2(1-\varepsilon)^{\frac{1}{2}}}{1-BK}\left[\frac{(1-K)B}{(1-BK)^2}\ln\left(\frac{1}{BK}\right)-\left(\frac{B+1}{2}\right)-\left(\frac{B-1}{1-BK}\right)\right]\right\} \quad (6)$$

Where:

$$K=\frac{\lambda_g}{\lambda_s} \quad (7)$$

$$B=1.364\left(\frac{1-\varepsilon_g}{\varepsilon_g}\right)^{1.055} \quad (8)$$

The value of K is calculated by Kulkarni and Doraiswamy (1980) and B is calculated by Opris and Johnson (1998).

RESULTS AND DISCUSSION

In order to understand the behavior of cryogenic packed bed, simulations were performed on the bases of mathematical equations which are discussed in previous section. The physical properties used for that simulations are listed in Table 1 and flow rate of gas was taken 10 L min^{-1}.

The simulation results for concentration and temperature change are shown for Fig. 2 and 3. Concentration change with respect to time and temperature is depicted in figures. Initially bed is kept at very low temperature around -100°C and CO_2 is supplied at 20°C. At Z = 0 the bed temperature is supposed to be 20°C. It is observed that after 25 sec small portion of bed is heated due to CO_2 and there the CO_2 concentration is 100%. After that there is steep concentration gradient where deposition of CO_2 is observed. The remaining portion of the bed is still at low temperature and in that portion concentration of CO_2 is reduced. It is also shown from Fig. 2, with passage of time most of the bed becomes saturated and concentration of CO_2 reached to 100%. After 75 sec it was observed the bed temperature was far above the frosting temperature of CO_2 and meanwhile it was also shown that there was no deposition of CO_2 and concentration was reached to 100% in whole bed.

Table 1: Physical properties of cryogenic packed bed

Properties	Values
Length of bed (m)	0.60
Diameter of bed (m)	0.0418
Diameter of packing (m)	0.01
Density of packing (kg/m^3)	2500
Porosity (dimensionless)	0.60
Heat capacity of packing (J g^{-1} K^{-1})	0.84

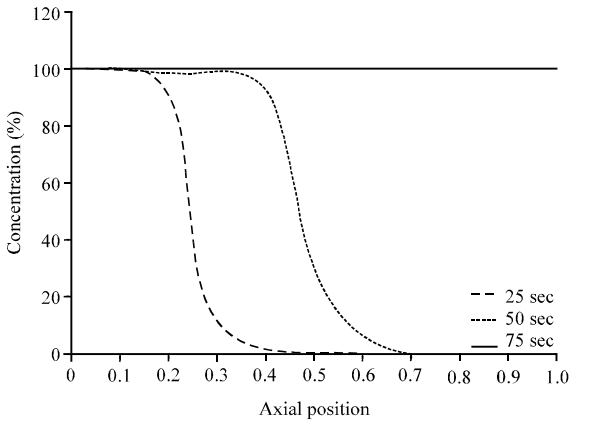

Fig. 2: Concentration profiles in axial position

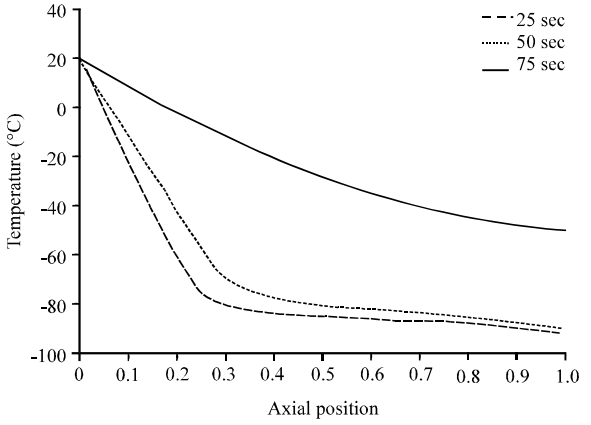

Fig. 3: Temperature profiles in axial position

The result of these simulations show the coupled solution of mass and energy balance using FTCS scheme.

The experimentation was conducted in order to validate the model using pure CO_2. The experimental and simulated temperature profiles are presented in Fig. 4. It is evident from the Fig. 4 that axial temperature profile for both simulated and experimental are similar. To investigate the concentration change the samples were analyzed by using gas chromatography and the saturation point of CO_2 was found similar to simulation.

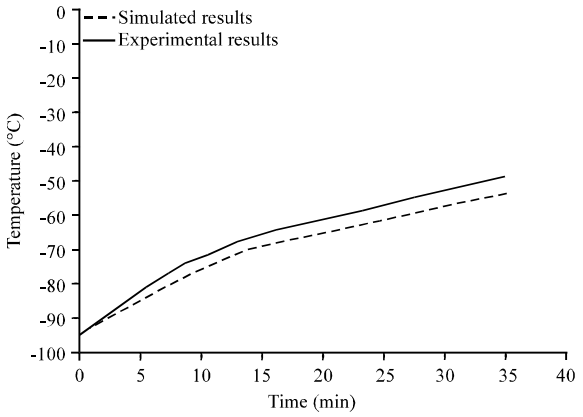

Fig. 4: Comparison between experimental and simulation results

CONCLUSION

In this study, a finite difference FTCS scheme has been used to solve the 1-dimensional pseudo homogeneous model for cryogenic packed bed. It is evident from results that FTCS scheme is efficient for this model. Furthermore simulation results were compared to experimental measurements to validate the model. The interpreted model shows promising potential for use in oil and gas industries.

Notations:

D_m	Molecular diffusion coefficient (m^2 sec^{-1})
u	Superficial velocity (m sec^{-1})
d_p	Particle diameter (m)
T	Temperature (K)
X	Concentration
C_p	Heat capacity (J kg^{-1} K^{-1})
a_s	Specific surface area (m^2 m^{-3})
$\dot{m}''$	Mass deposition rate per unit surface area (kg m^2 sec^{-1})
D_{eff}	Effective diffusion coefficient (m^2 sec^{-1})
Greek letters	
λ	Thermal conductivity (J m^{-1} K^{-1} sec^{-1})
λ_{eff}	Effective thermal conductivity (J m^{-1} K^{-1} sec^{-1})
ρ	Density (kg m^{-3})
ε	Porosity (dimensionless)
Subscripts	
g	Gas
s	Solid

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