Computational Investigation of CO2 Capture using Activated Carbon in a Packed Bed and Optimization of Various Parameters to Improve Efficiency of the Process

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Abstract: ***Greenhouse gas mitigation technology, particularly with respect to CO_2 is assuming increasing importance in the light of climate change fears. In recent times, adsorption using recoverable solid adsorbents is found to be an energy efficient way of capturing carbon dioxide from the flue gas. The adsorbent could be regenerated using Thermal Swing Adsorption or Pressure Swing Adsorption. In this study, Computational fluid dynamics (CFD) simulations are used to investigate post-combustion carbon capture in a packed bed using Activated Carbon as the adsorbent. The paper discusses the laminar flow inside the packed bed (porous media) to describe the flow in adsorption process of CO2 on activated Carbon in a packed bed and focuses on optimization of various parameters in order to improve the efficiency of the process, using CFD.***

Keywords: CO2 Capture, CFD, Modeling and Simulation, Packed Bed, Solid Sorbent modeling

1. INTRODUCTION

Fossil Fuels are currently the major source of energy and would continue to play an important role in the generation of heat and power and for industrial production. In the absence of any viable alternate clean energy source for a foreseeable future, it is extremely important that the CO2 emission from fossil fuel powered power plants and other sources be reduced. In this regard, Carbon capture and Storage (CCS) technologies can effectively reduce CO2 emissions from single point sources like power plants, steel plants, cement plants and other industries.

There are numerous technologies which could be associated with CCS, but only a few have gained acceptance from industrial and economic point of view. Basically, there are three systems for CO2 capture viz. Post Combustion Capture, Oxy fuel Combustion and Pre Combustion capture. Post Combustion capture involves the removal of CO2 from flue gas after the combustion of fuel. The oxidant used for combustion is typically air and hence, the flue gases are diluted significantly with nitrogen. In addition, since the flue gases are at atmospheric pressure, a large volume of gas has to be treated. A number of methods exist for the post-combustion capture of CO2 from flue gas which include Chemical absorption, Physical absorption, Membrane separation, Adsorption, Cryogenic separation etc.

Adsorption of carbon dioxide over solid adsorbents is a promising technology. Physical adsorbents which capture CO2 as a result of their cage like structure could be regenerated using techniques such as Pressure swing or thermal swing. Physical adsorbents such as Activated Carbon, Zeolites have been investigated by many researchers, and have shown high selectivity in their adsorption of CO2 from flue gas stack. Activated Carbon's adsorption capacity and performance depends on surface area and surface chemical characteristics.

2. MATHEMATICAL MODELING

2.1 Model description

The model used to describe the fixed-bed experiments is derived from the mass, energy and momentum balances.

The flow pattern is described with the k-epsilon turbulence model and the mass transfer rate is represented by a Linear Driving Force model – LDF. It was assumed that the gas phase behaves as an ideal gas and the radial concentration and temperature gradients are negligible. The fixed-bed model is described by the equations given below.

The rate of mass transfer to the particle for each component is given by

$$\frac{\partial qi}{\partial t} = Kl(qsat - qi)$$

where, *KL* is the overall mass transfer coefficient of component i and *qsat* is the amount adsorbed at equilibrium, i.e., qsat =*f* (*Ci, Tg*) given by the adsorption isotherm, and *qi* is the average amount adsorbed.

K_L=0.0027s^{-1} at 28°C (Dantas et.al., 2012)
K_L=0.0043 s^{-1} at 50°C(Dantas et.al., 2012)
C_i is given by

$$C_i = \frac{yiP}{RT}$$

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where yi is the molar fraction of each gas in the gas phase, P is the total pressure, *Tg* is the gas temperature and R is the universal gas constant.

Fluid Hydrodynamics

As with pipe flow, the flow through packed beds can also be loosely characterized by the Reynolds number, but this is complicated further by the existence of several forms of Reynolds number, based on different parameters and length scales and each with unique critical values for the onset of turbulence.

In many applications of packed beds the Reynolds number is defined as

$$Re = dp * \varrho * \frac{v}{\mu}$$

Based on this equation and empiricism a new set of values for critical flow are formed, based on the particle Reynolds number where the flow can be characterized as laminar (Re < 10), transitional (10 < Re < 300) or turbulent (Re > 300) (Ziolkowska & Ziolkowska, 1988).

Based on the experiments being carried out by Dantas, Rodrigues and Moriera(2011) for adsorption of a 20% v/v CO2 and 80% N2 mixture in packed bed column of length 0.171 m with porosity 0.52.

Run no.	**Temperature(°C)**	**Re**
1	28	0.36
2	50	0.32
3	100	0.25

At low Reynolds no., a laminar model is suggested to sufficiently model the hydrodynamics associated with the process.

As a function of porosity the velocity may vary throughout the bed due to flow channeling and the changing paths of mainstream velocity, and also because of some part of CO2 being adsorbed on the packing. Due to these effects the bed Reynolds number is likely to vary considerably throughout the media. Based on this assumption, the flow may be laminar in certain areas of the bed but also exhibit true stochastic turbulence in other locations.

The Ergun equation considers the terms for the pressure drop and velocity changes

$$-\frac{\partial P}{\partial z} = 150\frac{\mu_g(1-\varepsilon)^2}{\varepsilon^3 d_p^{\ 2}}u + 1.75\frac{(1-\varepsilon)}{\varepsilon^3 d_p}\rho_g u^2 \quad \ldots \quad (3)$$

where μg is the gas viscosity, $\varrho\ g$ is the gas density, and *dp* is the particle diameter.

Adsorption equilibrium isotherms

The adsorption equilibrium of CO2 and N2 adsorption on activated Carbon is described using the Toth model (Toth, 1971);

$$q = \frac{q_m K_{eq} P}{\left[1+(KP)^n\right]^{1/n}}$$

where *qm* is the maximum adsorbed concentration, i.e., the monolayer capacity; *Keq* is the equilibrium adsorption constant and *n* is the heterogeneity parameter.

The temperature dependence of the equilibrium was described according to the Van't Hoff equation;

K_{eq}=K_0*exp(-Hi/RT)

where *Ko* is the adsorption constant at infinite dilution.

The following values of q^* were obtained at T=28°C and 50°C, using the above model.

q^*=0.743 at 28 °C and 0.466 at 50°C for CO2.

3. COMPUTATIONAL FLUID DYNAMICS

Computational fluid dynamics, as the name suggests, is the use of a computer or computers to solve problems associated with the motion of a fluid. This is achieved in most cases by generating an approximate solution of a partial differential equation (PDE). We know that both ordinary differential (ODE) equations and partial differential equations have unknown variables which are strongly dependent on each other with no obvious, simple mathematical solution. The route of computational fluid dynamics can be traced back to developing numerical techniques for the solution of ODEs and PDEs, ultimately leading to techniques for determining approximate solutions to the Navier-Stokes equations

In this method a grid is created and the derivatives in the PDE are replaced with a finite difference scheme (such as Forward, Backward or central differencing) which then turns the PDE into a linear algebraic description for solution.

4. CFD MODEL SET UP

The CFD analysis was performed using Ansys Fluent 14.0.The geometry was created in Ansys Design Modeler with bed diameter of 0.022 m and 0.171 m length. The domain was then meshed and model was subsequently set up in Ansys Fluent 14.0.

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Since, the flow rate is very low, it could be modeled as Laminar Flow and turbulence effects could be neglected. Also, Navier Stokes energy equation is invoked in order to account for the Energy balance, while the packed bed is modeled as a porous media

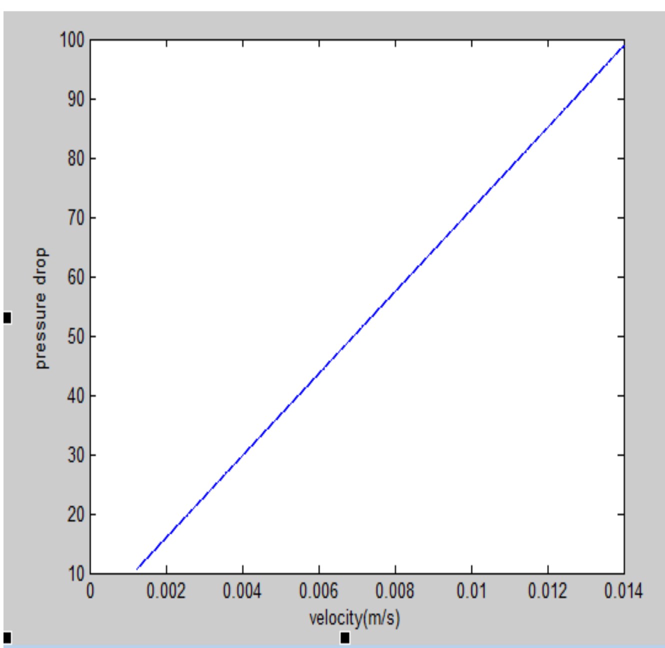
The adsorption of CO2 is an unsteady state time dependent phenomenon; however, since the study is aimed primarily to evaluate it from hydrodynamic point of view, the transient nature of adsorption is not taken into account. To account for adsorption, a mean source term is rather used, which models the adsorption process and hence as a result mass flow rate decreases as the flue gas passes through the packed bed.

The laminar flow model using an averaged sink term was found to have produced results with moderate accuracy, but a better model needs to be proposed to provide better accuracy.

5. OPTIMIZATION STUDY

The major problem in CO2 adsorption in a packed bed is the availability of Pressure drop. As the flue gas is almost at atmospheric pressure(~10mm water), the available pressure drop is very less(~100 Pa).

In order to process large quantities of gas needs to be processed so that the process could be economical .As the pressure drop is directly related to fluid velocity (Ergun Equation), the gas velocity and hence the flow rate has to be optimized with respect to pressure drop.



The pressure drop increases as the velocity is increased and since the available pressure drop is approximately 100 Pa for flue gas, the cutoff value of velocity for this process is 0.014 m/s .Beyond this value of velocity, compressor would be required to perform work on the gas so that its pressure could be increased, which would increase the power requirements of the process and hence again contribute to CO2 emissions.

6. CONCLUSION

Anthropogenic activities are immensely contributing to the emission of CO2 and other greenhouse gases in the atmosphere, primarily through the unchecked combustion of fossil fuels. Because of cost, high selectivity and other operation advantages it won’t be imprudent to say that adsorption of CO2 using Activated carbon is the technology available closest to the commercialization.

Computational study of CO2 adsorption on commercial activated carbon was performed and it was found that Laminar model alone is fairly accurate enough to model the process(Re_p =0.36)as the flow rate was very low.

Computational study was performed to optimize the mass flow rate and the available pressure drop and it was found out that for this particular packed bed(dia.0.022m, length 0.171m), the maximum velocity that could be achieved was 0.014 m/s, therefore the highest particle Reynolds no. which could be achieved was Re_p=4.01, which is well within the laminar range and hence the laminar flow should be able to model the flow behavior accurately.

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