Contents lists available at ScienceDirect

Chemical Engineering Research and Design

journal homepage: www.elsevier.com/locate/cherd

A review of mathematical modeling of fixed-bed columns for carbon dioxide adsorption

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ABSTRACT

Carbon dioxide emissions must be stabilized to mitigate the unfettered release of greenhouse gases into the atmosphere. The removal of carbon dioxide from flue gases, an important first step in addressing the problem of CO_2 emissions, can be achieved through adsorption separation technologies. In most adsorption processes, the adsorbent is in contact with fluid in a fixed bed. Fixed-bed column mathematical models are required to predict the performance of the adsorptive separation of carbon dioxide for optimizing design and operating conditions. A comprehensive mathematical model consists of coupled partial differential equations distributed over time and space that describe material, energy, and the momentum balances together with transport rates and equilibrium equations. Due to the complexities associated with the solution of a coupled stiff partial differential equation system, the use of accurate and efficient simplified models is desirable to decrease the required computational time. The simplified model is primarily established based on the description of mass transfer within adsorption systems. This paper presents a review of efforts over the last three decades toward mathematical modeling of the fixed-bed adsorption of carbon dioxide. The nature of various gas–solid equilibrium relationships as well as different descriptions of the mass transfer mechanisms within the adsorbent particle are reviewed. In addition to mass transfer, other aspects of adsorption in a fixed bed, such as heat and momentum transfer, are also studied. Both single- and multi-component CO_2 adsorption systems are discussed in the review.

Keywords: Adsorption; Carbon dioxide; Fixed bed; Modeling; Mass transfer; Linear driving force approximation

Contents

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Received 16 March 2013; Received in revised form 22 July 2013; Accepted 19 August 2013
0263-8762/$ – see front matter
http://dx.doi.org/10.1016/j.cherd.2013.08.018

1. Introduction

Concerns over the gradual increase in the atmospheric concentration of CO_2 and its impact on climate change have prompted a global research effort to capture CO_2 from point source emissions and stabilize its concentration in the atmosphere (Gomes and Yee, 2002; Grande and Rodrigues, 2008; Plaza et al., 2007; Shafeeyan et al., 2010). The most important sources of CO_2 emissions are power plants that generate electricity from fossil fuels (coal, oil, and natural gas) (Dantas et al., 2011a; Grande et al., 2008; Grande and Rodrigues, 2008; Kikkinides et al., 1993; Mulgundmath et al., 2012; Park et al., 2002; Shafeeyan et al., 2012). Therefore, it is critical to separate and recover carbon dioxide from the flue gases emitted by power plants to avoid excess CO_2 emissions (Chou and Chen, 2004; Ko et al., 2005; Mulgundmath et al., 2012). Various separation techniques, such as liquid solvent absorption, membrane separation, cryogenic techniques, and adsorption over solid sorbents, are increasingly used to reduce CO_2 emissions (Gomes and Yee, 2002; Takamura et al., 2001). At present, the most widely used technology for the removal of CO_2 from gaseous mixtures is amine absorption (Delgado et al., 2006b; Leci, 1996). However, this process is energy-intensive during the regeneration of solvent and is also plagued by extensive corrosion of the process equipment (Chue et al., 1995; Gray et al., 2004, 2005; Ko et al., 2005; Shafeeyan et al., 2011). It is therefore important to explore economical and energy-efficient alternative approaches for CO_2 separation (Grande et al., 2008; Xu et al., 2005).

Recently, it was reported that the cost associated with CO_2 capture can be reduced below the cost of conventional absorption with liquid solvents by using adsorption separation technologies (Ho et al., 2008; Radosz et al., 2008). Several technological advances in the field of CO_2 capture by adsorption have been developed around the world, demonstrating the attractiveness of this technique for post-combustion treatment of flue gas (Dantas et al., 2011a,b; Grande et al., 2008). Two main adsorption technologies are viewed as feasible for CO_2 separation and purification on a large scale: pressure/vacuum swing adsorption (PSA/VSA) and temperature swing adsorption (TSA) (Chue et al., 1995; Clausse et al., 2004; Plaza et al., 2009, 2011). Recent developments have demonstrated that PSA is a promising option for separating CO_2 due to its ease of applicability over a relatively wide range of temperature and pressure conditions, its low energy requirements, and its low capital investment costs (Agarwal et al., 2010b; Cen and Yang, 1985; Delgado et al., 2006b; Gomes and Yee, 2002). Many studies concerning CO_2 removal from various flue gas mixtures by means of PSA processes have been addressed in the literature (Agarwal et al., 2010b; Chaffee et al., 2007; Chou and Chen, 2004; Chue et al., 1995; Grande et al., 2008; Ho et al., 2008; Kikkinides et al., 1993; Ko et al., 2003; Mulgundmath et al., 2012; Na et al., 2001; Reynolds et al., 2005; Sircar and Kratz, 1988; Xiao et al., 2008). Prior to the design of an adsorption process, selecting an appropriate adsorbent with high selectivity and working capacity, as well as a strong desorption capability, is key to separating CO_2. As a result, a wide variety of adsorbents, such as activated carbons, synthetic zeolites, carbon molecular sieves, silicas, and metal oxides, have been investigated in recent years for this purpose (Chue et al., 1995; Dantas et al., 2011a,b; Moreira et al., 2006; Plaza et al., 2011; Xu et al., 2005).

The design of an appropriate adsorption process requires the development of a model that can describe the dynamics of adsorption on a fixed bed with the selected adsorbent (Dantas et al., 2011a,b; Delgado et al., 2006a; Lua and Yang, 2009). The absence of an accurate and efficient adsorption cycle simulator necessitates the use of data from experimental units to develop new processes. This empirical design of an adsorption column through extensive experimentation on process development units tends to be expensive and time consuming (Siahpoosh et al., 2009). A predictive model using independently established equilibrium and kinetic parameters may provide, in principle, a method of estimating the column dynamic capacity without extensive experimentation. A fixed-bed column mathematical simulation that considers all relevant transport phenomena is therefore required to obtain a better understanding of the behavior of new adsorbents during the adsorption/desorption cycles and for optimization purposes. Moreover, these models are capable of estimating the breakthrough curve and temperature profile for a certain constituent in the bulk gas at all locations within the packed column. This experimentally verified model is then used to conduct an extensive study to understand the effects of various process parameters on the performance of the PSA cycle. These are the main reasons why the mathematical modeling of adsorption processes has attracted a great deal of attention among researchers.

In general, prediction of column dynamics behavior requires the simultaneous solution of a set of coupled partial differential equations (PDEs) representing material, energy, and momentum balances over a fixed bed with the appropriate boundary conditions (Hwang et al., 1995). Because the simultaneous solution of a system of PDEs is tedious and time consuming, the use of simplified models capable of satisfactorily predicting fixed-bed behavior is desirable. Many attempts have been made to evaluate and develop simplifying assumptions to decrease computational time and facilitate optimization studies. A review of the literature reveals the development of simplifying assumptions mainly on the representation of mass transfer phenomena within the adsorbent particles as an alternative pathway to simplify fixed-bed adsorption calculations. Modeling and optimization of the fixed-bed adsorption of CO_2 has developed over the past three decades and is still of great interest to investigators. This review presents a fairly extensive survey of previous studies on the mathematical modeling of the CO_2 adsorption process in a packed column. Various models for gas–solid adsorption equilibria as well as different descriptions of the mass transfer mechanisms within the adsorbent particle are reviewed. In addition to concentration variation, other aspects of adsorption in a fixed bed, such as temperature and pressure variations, are also studied. The purpose of this study was to investigate the mathematical models capable of simulating the dynamic behavior of the fixed-bed adsorption of carbon dioxide.

2. Overview of the prediction of adsorption column dynamics

In most adsorption processes, the adsorbent is in contact with a fluid in a packed bed. An understanding of the dynamics behavior of such systems is therefore required for rational process design and optimization (Rutherford and Do, 2000a). The dynamics behavior of an adsorption column system can be classified based on the nature of the gas–solid equilibrium relationship of fluid constituents and the complexity of the mathematical model required for describing the mechanism by which the mass transfer from the fluid to the solid phase