Applied Energy 221 (2018) 437–449

Contents lists available at ScienceDirect

Applied Energy

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

Mathematical modeling and numerical investigation of carbon capture by adsorption: Literature review and case study☆

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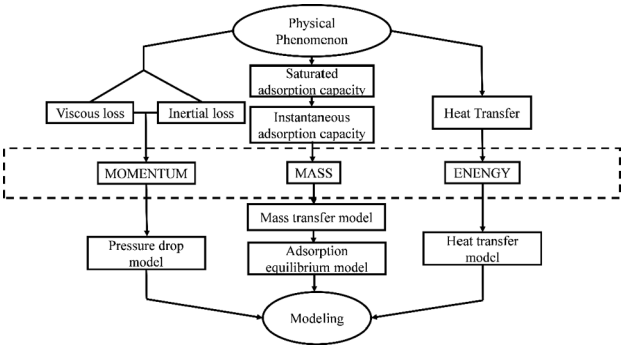
HIGHLIGHTS

- The sub-models screening of CCA is presented with the literature review.
- A pathway map is established through model group forming.
- A case study demonstrates a fluent optimal design based on the pathway map.

GRAPHICAL ABSTRACT



ARTICLE INFO

Keywords:
CCS
Adsorption
Numerical simulation
Mass and heat transfer

ABSTRACT

The carbon capture by adsorption (CCA) is regarded as an available engineering technology because of its low energy-consumption, easy to control, and possible integration with renewable energy. The recent advances in CCA research comprises mainly about the performance improvement of adsorbents, design and optimization of engineering process. However, considering the time-consuming and intensive funding required for experimental investigation, the numerical simulation has been widely applied in CCA. In numerical simulation field of CCA, the adsorption process is commonly simplified into mathematical models group comprised of adsorption kinetics model, the adsorption equilibrium model, pressure drop model and heat transfer model. However, few studies' focus is to provide a detailed review of the research methodology of mathematical modeling in CCA simulation.

This paper presents a pathway map on CCA mathematical modeling through literature review and case study. An overview of model screening and modeling method of CCA is provided in the review part. This part also provides a short guided tour on how to combine the fundamental models about heat and mass transfer together to form a model group for various application scenarios in CCA. Then the pathway map on CCA modeling, which is summarized based on the review, is applied to a case study. In this part, the adsorption of CO_2/N_2 mixtures on activated carbon under the conditions of high temperature and low pressure is numerically investigated based on the established models. The performance indicators comprise gas temperature, mole fraction, and adsorbate amount of the fixed bed, are applied in the evaluation performance of CCA. Based on the proposed methodology, the CCA modeling demonstrates a more fluent design process relative to the real physical scenario, with a possible access to further optimization. Particularly, the simulation results showed that the optimized dimensionless velocity for the highest utilization efficiency of the fixed bed can be obtained and thus is proposed as

☆ The short version of the paper was presented at ICAE2017, Aug 21–24, Cardiff, UK. This paper is a substantial extension of the short version of the conference paper.

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https://doi.org/10.1016/j.apenergy.2018.03.093
Received 27 December 2017; Received in revised form 5 March 2018; Accepted 25 March 2018
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1.2–1.4 for the most suitable feed velocity to fit different size of fixed bed and different types of adsorbents for the engineering design.

1. Introduction

Fossil fuels are still the mainstream of the energy sector in recent years, considering a dominant proportion of the cumulative total amount worldwide. Actually, the annual CO_2 emissions from fossil fuel combustion are still appropriate 30Gt in 2010, and the deforestation of tropical rainforests results in CO_2 emissions increasing at an annual rate of 4Gt [1]. It is obvious that human activity leads to an increase in atmospheric CO_2 concentration, and the increase in CO_2 concentration in the atmosphere would lead to an irreversible climate change. It has been suggested that this tendency will continue for more than 1000 years even after the elimination of CO_2 emissions [2], and it is of practical significance to study CCS technology which can reduce atmospheric CO_2 content.

In the large-scale capture of CO_2 industrial technology, the adsorption method attracts much attention as the equipment is easy to control with a low energy consumption. The CCA is concerned widely also because the low-grade thermal energy can be applied for regeneration, and the method suitable for a large temperature range [3]. However, with the development of adsorbent, design and optimization of process, high investment and large time-consumption features will become a challenge to the experimental investigation.

With such problems and also a rapid development of tools to solve the differential equations, the numerical simulation had played an important role in the research on carbon capture by adsorption (CCA). At the current stage, the solution of CCA numerical investigations could be realized by numerical software. The typical application scenario of these softwares, such as PDECOL, gPROMS, Fluent and their characteristics are listed in the Table 1. Delgado [4], Cavenati [5], Ben-Mansour [6] et al. have conducted a series of work based on these softwares, but the methodology on screening of physical-based models and modeling methods with mathematical equations are still rare in the existing publications and not completely clarified.

In order to solve the problems of the heat and mass transfer in the fixed bed during the capture process, the conservation equations formed by the mass equation, the energy equation and the momentum equation are required at least [11]. In 2016, Ben-Mansour presented a comprehensive review include numerical studies and modeling which covers nearly 200 papers in the existing knowledge pool [12], in which the CCA modeling can be found commonly includes three parts: (1) modeling the mass transfer process to a combination of adsorption kinetics model and the adsorption equilibrium model; (2) modeling the momentum loss to the pressure drop in the fixed bed; (3) modeling the heat transfer between the gas and solid adsorbent. In additional, Cai [13] analyzed the adsorption kinetics model including linear driving force model (LDF) and pore diffusion model. Qu [14] introduced the importance of the study on adsorption equilibrium model for the application of adsorbent. However, their review work did not provide a relationship analysis of these three equations, and thus without a detailed highlight on research methodology on this field.

In this study, the mathematical modeling methodology of CCA is presented. The adsorption kinetics model, the adsorption equilibrium model, pressure drop and heat transfer model with the corresponding physical phenomenon in the fixed bed of carbon dioxide adsorption are reviewed, respectively. Such literature research on specific modeling classifications in CCA was presented for the first time based on the authors' knowledge. Particularly, such review study would guide a more clear tour in this research field. A mathematical modeling pathway map is presented which comprise the correspondence between the real physical scenario and mathematical model. This map can be applied with the combination of sub-models screening, the details of sub-models are presented in the review section. In order to further clarify how to apply the pathway map and screen the reviewed sub-models to form a complete modeling group to assist numerical simulation on CCA, a case study on CO_2 capture by adsorption on activated carbon is demonstrated. The adsorption of CO_2/N_2 mixtures on a commercial activated carbon was numerically measured and the performance evaluation indicator (PEI) variation during the adsorption process is studied as well.

2. Literature review

The appropriate screening of model is important for numerical investigations. Thus, a simulation work with suitable models would agree well with experimental results within an acceptable error range. Commonly, an entire CCA model, or called model group, include 4 sub-models: adsorption kinetics model, the adsorption equilibrium model, pressure drop model and heat transfer model. In this section, the most-applied models are reviewed with pros and cons, based on the existing publications. Such characteristics of those sub-models are helpful for the CCA model screening. A summary of the typical mathematical models in CCA research is shown in Table 2.

Such overview, which was presented in this section, could be used as a guideline to understand the modeling methodology. Particularly, source terms design, which can be considered as the main barrier to a successful solution, was presented in three sub-sections as well, as shown in Fig. 1.

2.1. Adsorption kinetics model

The essence of adsorption separation in CCA is the mass transfer process between the solid adsorbent particles and external gas in the fixed bed, resulting in changes in the gas quality. The adsorption kinetics model describes the amount of variation in the mass of the gas absorbed over time due to the mass transfer between the solid adsorbent particles and the external gas, which are the mass transfer rate of gas adsorption. Models for realization of numerical computation are presented in order to simplify the mass transfer process. The typical adsorption kinetics model includes three types: local equilibrium model, linear driving force model and role diffusion model.

2.1.1. Local equilibrium model

Local equilibrium (LE) model ignore the mass transfer resistance, assume that the mass transfer between solid adsorbent particles and external gas instantaneous completes. It is a common assumption on the effect between the adsorbent material and the strong-adsorbed component. Such assumption means the variation mass amount of the adsorbed gas component during the adsorption time is equal to the variation mass amount of equilibrium. The mathematical expression for the local equilibrium model is shown below:

$$\frac{\partial q_i}{\partial t} = \frac{\partial q_i^*}{\partial t} \tag{1}$$

where q_i is the average amount of component i adsorbed, q_i^* is the amount adsorbed at equilibrium given by the selected adsorption isotherm model.

Due to the neglect of mass transfer resistance, the model has accepted limitation in the practical applications. Only when the simulated conditions are close to ideal state, the simulated results would have a good agreement with the experimental results. Thus, the mechanism of modeling limit the application range of modeling method. Shendalman

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