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Research paper

Modeling of gasification reaction to produce activated carbon from pistachio shells in a spouted bed

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ABSTRACT

A one-dimensional mathematical model has been developed to predict behavior of a spouted bed reactor during the gasification of char obtained from pyrolysis of pistachio shells leading to the production of activated carbons. The pores overlapping phenomenon is considered in the model with no auxiliary empirical correlation used. This model is capable of the prediction of BET surface area of the produced activated carbons besides the gas-solid hydrodynamics and distribution of gas and solid temperature and concentration in the bed. The results revealed that the one-dimensional model well predicts values for char burn-off, BET surface area, and bed temperature in gasification reactions in spouted bed reactor. This is due to the excellent mixing and high circulation rates of the materials inside a spouted bed which reduces radial distributions.

1. Introduction

Spouted bed reactors (SBRs) have been successfully applied in the study of several processes from experimental as well as theoretical points of view. The studies deal with various processes including drying [1–4], gasification [5–7], oxidation [8], desulfurization [9–11], combustion [12], alkalynation [13], and pyrolysis [14,15]. In each of these processes understanding bed hydrodynamics, coupled heat and mass transfers and chemical reaction phenomena is mandatory for designing, scaling up and optimizing spouted beds [7].

The process of production of activated carbons (ACs) from biomass is an interesting topic consisting of chemical reactions. In the recent years, there is growing interest in the production of ACs from agricultural wastes and residual wastes [16]. This process involves two stages: a pyrolysis stage followed by an activation stage. Each of these two stages, when taking place in a SBR, is a complicated process involving mass, energy and momentum transport phenomena simultaneously. Regarding the pyrolysis stage, SBRs have been proven to be versatile reactors for biomass fast pyrolysis. The good performance of such reactors is for the high heat and mass transfer rates between phases and very short residence times [17]. A number of experimental investigations have been conducted in the field of biomass pyrolysis in SBRs and interesting results have been obtained [18–20]. Alvarez et al. [17] performed fast pyrolysis of rice husk in a conical SBR. They showed the suitability of spouted beds for the fast pyrolysis of rice husk. Amutio et al. [21] performed Pinewood sawdust flash pyrolysis in continuous mode in a conical SBR. The char obtained at 600 °C has a high surface area and was suitable for carbon active production. Aguado et al. [22] studied both the generation of a microporous structure and char formation kinetics in the pyrolysis of sawdust of *Pinus insignis* in a conical SBR. They showed that, the SBR used is suitable for the kinetic study due to the high heating rate and bed isothermicity. Olazar [23] studied the effect of using in-situ catalyst based on a HZSM-5 zeolite in flash pyrolysis of sawdust of *pinus insignis* in a conical SBR. Teo and Watkinson [24] studied rapid pyrolysis of coal in a miniature SBR.

The second stage, namely physical activation of bio-chars in spouted bed is another interesting topic that may result in the production of high quality activated carbons. Physical activation is the partial gasification of a char with an oxidant gas, mainly steam or carbon dioxide (or a mixture of both) [25]. Sue-A-Quan [26] studied experimentally coal gasification in a pressurized spouted bed. Cortazar et al. [27] carried out the steam gasification of sawdust in a bench scale plant fitted with a fountain confined conical SBR and a nonporous draft tube. They used olivine as primary catalyst. Lopez et al. [28] studied the steam gasification of pinewood sawdust derived char in a conical SBR. Lopez et al. [29] carried out the steam gasification of different mixtures of biomass and high density polyethylene in continuous mode in a conical spouted bed gasifier. Bernocco [30] studied the feasibility of building a biomass gasification plant with an innovative SBR for distributed energy production. Erkiaga et al. [31] used Olivine and γ-alumina as primary catalysts for tar elimination in the continuous steam

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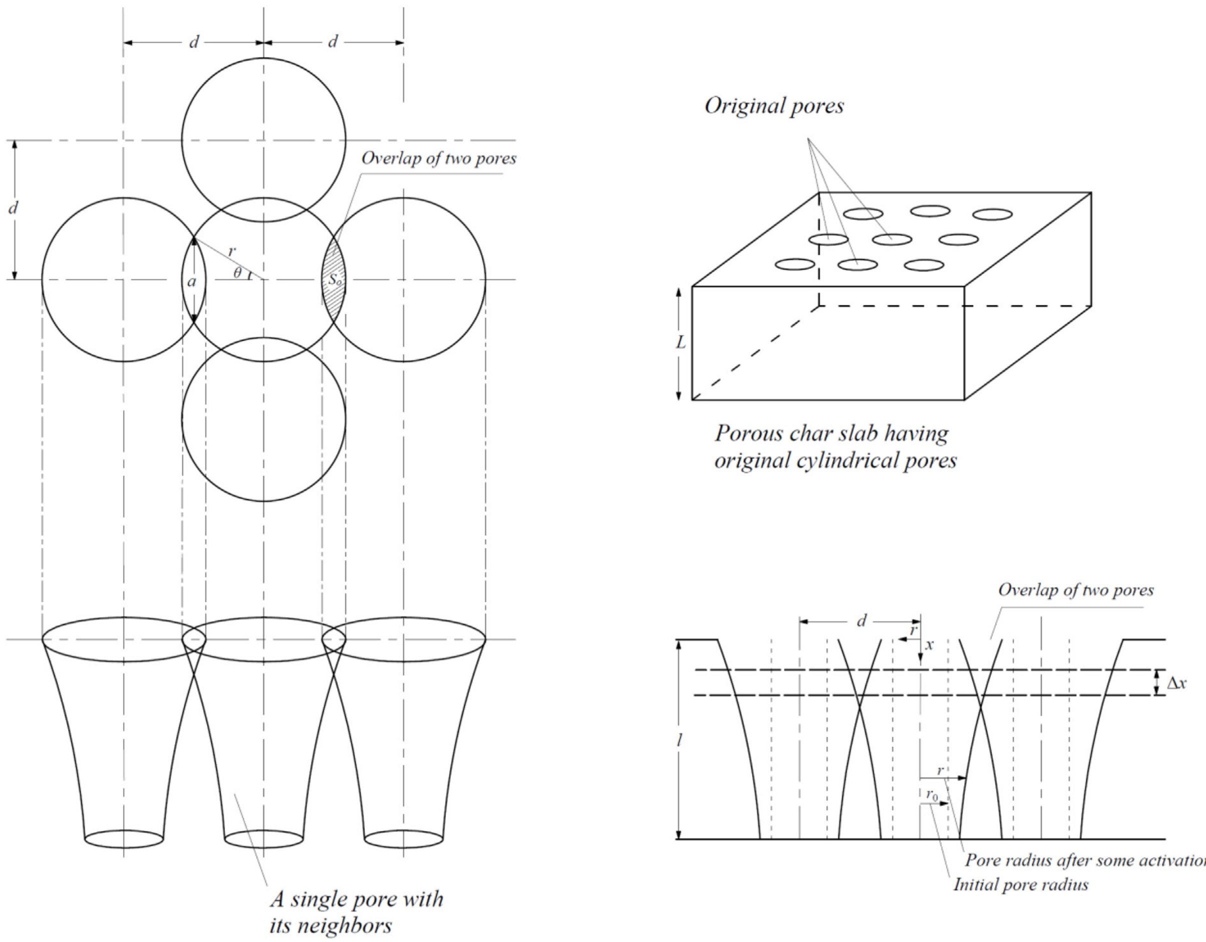

Fig. 1. Schematic diagram of the model representing pore widening in a single slab during activation process.

gasification of pine wood sawdust in a conical SBR.

As a comprehensive study, the authors studied experimentally the production of activated carbons from pistachio nut shells in a SBR for the first time [32]. Both of the pyrolysis and the gasification stages were carried out in the same SBR. The results of this study show that, SBRs are suitable equipment for performing the both carbonization and gasification stages thanks to excellent mixing and high circulation rates of the materials inside a spouted bed.

Besides experimental investigations, a mathematical model could be a useful tool in getting knowledge of the process. Up to now, several computational fluid dynamic (CFD) models have been developed by researchers in order to describe hydrodynamic behavior of spouted beds [33–36]. Nevertheless, when a chemical reaction is involved, available CFD models are scarce. Regardless of the CFD models, a number of researchers have tried to model chemical reactions in spouted bed using simplified assumptions and homemade programming. The presented models in literature deal with various processes including gasification [5–7], oxidation [8], desulfurization [9–11], and pyrolysis [14,15].

Regarding the pyrolysis stage, Niksiar and coworkers developed comprehensive mathematical models for pyrolysis of waste plastics in SBRs [14,15]. The findings of these authors revealed that, due to the excellent mixing and high circulation rates of the materials inside a spouted bed, concentration and temperature gradients inside the reactor are minimized. To our knowledge, no other study has been conducted for modeling pyrolysis reactions in SBRs.

With the aim of modeling the gasification stage in SBRs, some mathematical models have been developed and presented so far by researchers. Most early, Lim et al. [5] developed a mathematical model of the spouted bed gasifier based on streamtube hydrodynamic model of Lim and Mathur [37]. Similarly, Lucas et al. [6] presented a non-isothermal two-region model of a spouted bed gasifier whereas spout was treated as a plug flow reactor of fixed diameter and the annulus region was considered to be a single plug flow reactor. Jarungthammachote and Dutta [38] applied the Gibbs free energy minimization method to predict the composition of the producer gas in a spouted bed gasifier. A SBR undergoing gasification reaction was modelled by Mendes et al. [7] through one-dimensional model in which heat transfer was carefully described at different levels of complexity. Deng et al. [39] presented a three-dimensional CFD model to simulate coal gasification process in a pressurized spout-fluid bed. They obtained the distributions of temperature and gas composition in the spouted bed. Nevertheless, the model was not capable of the predication of solid product characteristics. Literature reviews showed that, no comprehensive model has been proposed yet to predict the performance of spouted beds during activation of chars.

In the present study, a one-dimensional model has been developed to study the behavior of spouted bed during bio-char activation process. This model has been presented based on the previous experiences of Niksiar et al. [14,15] regarding the negligible radial distribution of temperature and concentration inside an experimental scale spouted bed. For the first time, the prediction of BET surface area of the produced activated carbons from a SBR, besides the gas-solid hydrodynamics and distribution of gas and solid temperature and concentration, has been considered by a mathematical model. Pistachio shells, as one of the most common agricultural wastes of the world, have been used to be converted to activated carbons. The results of the presented model have been compared with the experimental data