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Modeling and simulation of co-gasification of coal and petcoke in a bubbling fluidized bed coal gasifier

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ABSTRACT

In this work we discuss the modeling and simulation of a fluidized bed coal gasifier which uses a mixture of coal and petcoke as its feed. A two phase model consisting of the bubble phase and the emulsion phase is used to describe the coal gasification process. We consider a non-isothermal model taking into account the effect of four heterogeneous reactions and four homogeneous reactions. We analyse the effect of various operating parameters such as composition of feed, location of feed point and ash content on the performance of the gasifier. The results of predictions of the simulations have been found to be in good agreement with the experimental results in the literature. It has been found that increase in petcoke content in the feed mixture tends to lower the efficiency and carbon conversion but increases the amount of syngas produced. Also, from the simulations, it has been found that increase in ash content of coal decreases the carbon conversion. We have concluded that the feed point of the solids should be above the point where O₂ that is present in the bed gets exhausted, in order to obtain the maximum carbon conversion and efficiency.

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1. Introduction

The depletion in the reserves of petroleum has encouraged industries to look at coal as an alternative energy source. Traditionally, coal as an energy source involves handling of solids, ash, pollutant emissions etc. and is hence considered as a dirty source. Gasification of coal allows us to convert this to a cleaner energy source. The objectives of coal gasification can be either the production of syngas (a mixture of CO and H_2) or power production as in an IGCC unit. Coal gasification is carried out in three classical reactors moving bed, fluidized bed and entrained bed. The features of these reactors, the different reactions taking place in them are detailed in [1–3]. The advantages and disadvantages of the different types of reactors and guidelines for choosing a reactor for different characteristics of coal are explained there.

Normally the type of reactor is chosen so that the efficiency is optimized. The different types of reactors perform differently with different types of coals and their feed size. It has been reported that fluidized bed reactors in general perform better with coals having high ash content [1,2]. The ash released from coal lowers the temperature of the bed and increases the efficiency of the process.

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Since, Indian coal contains high ash content, fluidized bed reactor has been chosen to carry out the coal gasification study in this paper.

de Souza-Santos [4] developed a comprehensive one-dimensional model of a fluidized bed gasifier which takes into account 24 chemical reactions and the devolatilization reactions. The model consisting of mass and energy balance equations for individual phases was used to predict the gasifier performance. The predictions compared favourably with experimental results. Yan, et al. [5,6] and Ross, et al. [7] have used two phase theory to describe the hydrodynamic behaviour of a fluidized bed and show that a non-isothermal model gives better predictions of a system than an isothermal model. Recently several studies have used CFD to understand the hydrodynamic behaviour in more detail and have included this in the reactor model [8,9].

Several experimental studies on using a mixture of feed stocks have been carried out using coal, petcoke, biomass etc [10–13]. These studies have examined the effects of temperature, pressure, gasifying agent on cold gas efficiency and carbon conversion. It has been reported that as the fraction of petcoke in the feed is increased to 60 wt.%, there is a decrease in carbon conversion and an increase in the production of syngas [12].

A good understanding of the parameters which govern the behaviour of a gasifier can be obtained using a mathematical modeling approach. To our knowledge, detailed models have not been developed and analysed for a co-gasification process of coal and petcoke. Models and their simulations would allow us to identify the role of various parameters and identify optimum conditions for operation.

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In this work, our focus is on developing a mathematical model of gasification of a mixture of coal and petcoke. Petcoke is a by-product from petroleum refinery coker units or other cracking processes and has high carbon content. Consequently co-gasification of coal has relevance in the Indian context where coal has a high ash content, and petcoke which is devoid of ash can be used to effectively decrease the ash content of the feed mixture. We develop a mathematical model for co-gasification of coal and petcoke in a bubbling fluidized bed coal gasifier. This model takes into account the different reaction rates of the two feed components. A non-isothermal model is used which takes into account 8 heterogeneous (4 with coal and 4 with petcoke) and 4 homogeneous reactions. We use the model to determine (i) the optimum composition of the feed mixture (ii) to determine the optimal location of the feed point along the bed and (iii) to analyse the effect of ash content of coal on the gasification efficiency.

2. Model

Since our focus is on understanding the trends in a quantitative manner, a one-dimensional model has been chosen to describe the process. Here the variation of the dependent variables along the axial length alone is considered.

We follow [5] and depict the interactions between the different phases in a bubbling fluidized bed gasifier under consideration schematically in Fig. 1. The reactor has been divided into three phases, bubble phase, gas phase in emulsion and solid phase in emulsion. There is interaction between (i) the gas phase in the emulsion and the solid phase in the emulsion and (ii) between gas in the bubble phase and the gas in the emulsion phase. The heterogeneous reactions take place only in the emulsion phase.

In our system, coal and petcoke are mixed together as a blend and fed into the reactor. Here they undergo co-gasification and produce syngas (H_2 and CO).

2.1. Model assumptions

The model is based on the following important assumptions [1,5]

1. The system is at steady-state. Therefore, the feeding and withdrawal rates of gaseous and solid streams are constant.



Fig. 1. Schematic of flow and interactions in a bubbling fluidized bed coal gasifier (see [5]).

- 2. The bed mainly consists of two phases, the emulsion phase and the bubble phase. The bubble phase is free of solid particles, as confirmed by experimental observation [1]. The emulsion phase is composed of interstitial gas and solid species. Two types of solids have been considered in the present model, carbonaceous matter (coal and petcoke) and inert ash (SiO₂).
- 3. The gases in the bubble and emulsion phases move in a plug flow regime while the solids are assumed to be in a perfectly mixed state.
- 4. Devolatilization of the carbonaceous solids occurs instantaneously at the feed point.

2.2. Reactions

The gasifier sustains several reactions both homogeneous as well as heterogeneous. In this work we consider only a few select reactions which are significant to make the problem tractable and help us obtain a physical insight to interpret the results.

The following reactions are assumed to take place inside the fluidized bed gasifier:

2.2.1. Devolatilization in the emulsion phase

The devolatilization reaction of coal and petcoke in the emulsion phase is represented as:

coal / petcoke
$$\xrightarrow{\text{devolatilization}}$$
 char + volatiles (CO, CO₂, CH₄, H₂, H₂O)

2.2.2. Heterogeneous reactions in the emulsion phase

The following four gas–carbonaceous solid reactions are assumed to take place in the emulsion phase of the fluidized bed:

$$C + \phi O_2 - \frac{\Delta H^0 = -350 \text{ kJ mol}^{-1} \text{C}}{-----} \rightarrow 2(1-\phi)\text{CO} + (2\phi-1)\text{CO}_2$$

$$C + 2H_2 \xrightarrow{\Delta H^0 = -74.9 \text{ kJ mol}^{-1}C} CH_4$$

Here, the value of ϕ in the C combustion reaction is given by [1]

$$\phi = \frac{2+\beta}{2+2\beta}$$

where,

$$\beta = 2500 \exp\left(-\frac{6240}{T_{\rm PE}}\right)$$

Here T_{PE} is the temperature of particles in the emulsion phase. In our work, T_{PE} is around 1400 K and the value of ϕ is approximately 0.55.

2.2.3. Homogeneous reactions in bubble and emulsion phase

The homogeneous gas phase reactions take place in both emulsion and the bubble phases of the fluidized bed. The following four exothermic reactions are considered in this work.

$$H_2 + \frac{1}{2}O_2 \xrightarrow{\Delta H^0 = -241.9 \text{ kJ mol}^{-1}H_2} H_2O$$

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