Fuel Processing Technology 126 (2014) 504–512

Contents lists available at ScienceDirect

Fuel Processing Technology

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

Simulation of catalytic coal gasification in a pressurized jetting fluidized bed: Effects of operating conditions

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ARTICLE INFO

Article history:
Received 29 December 2013
Received in revised form 4 June 2014
Accepted 4 June 2014
Available online 22 June 2014

Keywords:
Pressurized jetting fluidized bed
Catalytic coal gasification
Numerical simulation
Operating conditions
Gasification scheme
SNG

ABSTRACT

A one-dimensional steady-state model of catalytic coal gasification, which was previously established in a pressurized jetting fluidized bed, is extended to investigate the effects of different operating conditions (catalyst loading, steam/coal ratio and oxygen/coal ratio) on hydrodynamic parameters, particle temperature, gas temperature, gas composition, carbon conversion and methane yield. The results indicate that the steam/coal ratio has significantly associated with hydrodynamic parameters. The maximum particle temperature changes obviously with steam/coal ratio and oxygen/coal ratio. Methane concentration goes up slowly when catalyst loading is above 10 wt.% and reaches maximum point when steam/coal ratio is about 0.5 by weight. Both the total carbon conversion and carbon conversion due to char gasification rise sharply as steam/coal ratio increases, while there are slow increase for both of them as catalyst loading and oxygen/coal ratio increase. The carbon conversion due to char combustion maintains at low level, and the methane yield decreases with the increase of catalyst loading, steam/coal ratio and oxygen/coal ratio. In conclusion, the suitable operating conditions for catalytic coal gasification are as follows: catalyst loading of 10 wt.%, steam/coal ratio of 1 and oxygen/coal ratio of 0.3. The maximum methane yield can be obtained by using the scheme of O_2/H_2O/syngas.

1. Introduction

With rapid economic growth and urbanization, the depletion of nature gas becomes increasingly serious in China. Catalytic coal gasification, as a technology of synthetic natural gas from coal, could satisfy the demand for natural gas together with utilizing the abundant coal resources, which also in turn secures the energy safety by adding the energy supplying source. The aim of catalytic coal gasification is to obtain the high value methane-rich gas. High pressure and alkali metal salt catalyst (mainly potassium carbonate) can enhance endothermic steam gasification and exothermic methanation, which can be coupled in the same reactor, and then offer the possibility for operating the gasifier at relatively lower temperatures but reaching higher thermal efficiency.

The predevelopment of catalytic coal gasification technology was executed by American Exxon Company in seventies of last century [1], and later American GreatPoint Energy developed a 'Blue gas' technology based on Exxon's research [2]. But their research were stuck in stage of an electrically-heated 1 t/d process development unit (PDU). There are three main problems in the previous catalytic coal gasification technology. Firstly, the carbon residue is hard to be gasified due to the low reaction rate at 973 K. Secondly, the particle residence time is too long (about 6 h) to reach a carbon conversion of above 95%, and thus leads to a low capacity of reactor. Thirdly, the heat supply is from superheated steam, which causes high energy consumption. In order to solve these problems, a new catalytic coal gasification process has been developed by ENN-ICC since 2008 [3]. It is a three-stage gasifier: (1) the upper section of the gasifier is the pyrolysis stage which uses the heat of gas produced by catalytic coal gasification to obtain tar; (2) the middle part of the gasifier is catalytic gasification stage, utilizing the heat of gas produced by catalytic combustion and syngas to produce methane, which makes steam gasification, shift reaction and methanation occur in one reactor; (3) the bottom section of the gasifier is the catalytic combustion stage, using gasified carbon residue to produce syngas and heat. The gasifier is expected to obtain high carbon conversion and thermal efficiency by coupling endothermic reactions with exothermic reactions. Owing to the violent movements of complex jetting, particles and bubbles under high pressure, appropriate design procedures are not well established so far, especially for catalytic coal gasification concerning with various gas–solid reaction kinetics, mass and heat transfer. Simulation for catalytic coal gasification in a jetting fluidized bed gasifier is becoming urgent in industrial process.

The simulations of fluidized bed gasifier have been studied extensively. Ma et al. [4] proposed a steady-state two phase model to simulate a pilot-scale fluidized bed coal gasifier and pointed out that high ratio

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http://dx.doi.org/10.1016/j.fuproc.2014.06.006
0378-3820/

of H_2/CO could be obtained through high steam/carbon ratio and low oxygen/carbon ratio. Arastoopour [5] divided the fluidized bed into different sections, considering composition completely mixed and temperature constant in each section. Predications showed that higher air flow rate corresponding to higher feed rate extended the combustion zone to the upper region of the gasifier and caused a deterioration in gas quality at the same char hold-up. Liu et al. [6] simulated a pressurized ash agglomerating fluidized bed gasifier by Aspen plus and suggested that the oxygen/coal ratio should be lower than 0.55 Nm^3/kg. Yan et al. [7] presented a model to simulate bubbling fluidized bed gasifier. The calculated results indicated that water–gas shift reaction had more effects on pilot-scale gasifiers than commercial-scale gasifiers whether it reached equilibrium or not. Kaushal et al. [8] developed a biomass gasification model, capacity of reactor gas releasing and mixing during devolatilization into account, which was capable of predicting the effect of various gasifying media.

But for catalytic coal gasification, the operation of PDU at 3.5 MPa is hard and costly. Hence, a one-dimensional steady-state model of catalytic coal gasification in a pressurized jetting fluidized bed has been established in our previous work and the reliability of the model has also been verified in 0.5 t/d PDU [9].

This model will be used to predict how to obtain higher methane yield and carbon conversion in a 2.4 t/d PDU. The following conditions should be met: (1) the gasifier should be smoothly operated. The maximum particle temperature is chosen to reflect the risk of agglomeration; (2) the bed should be controlled in bubble region to keep enough contact time. The calculated bubble size is accounted for the contact state between particle with catalyst and gas.

In order to further understand the effect of different operating conditions (catalyst loading, steam/coal ratio and oxygen/coal ratio) on hydrodynamic parameters, particle temperature, gas temperature, gas composition, carbon conversion and methane yield, simulations of a catalytic coal gasifier are carried out. In addition, effects of various gasification schemes, including $O_2/H_2O/N_2$, $O_2/H_2O/CO_2$ and O_2/H_2O/syngas, on methane yield are also compared for possible industrial application.

2. Model description and simulated conditions

2.1. Model description

The model of catalytic coal gasification is based on the work of Bi et al. [10], which divided the gasifier into three zones, including grid zone, bubble zone and freeboard zone, as shown in Fig. 1. Moreover, the grid zone was subdivided into jet zone and annulus zone and the bubble zone consisted of bubble and emulsion. More details are available from our previous works [9–11]. The model is made up of hydrodynamic model and catalytic reaction model. The simple features of pressurized hydrodynamic model for catalytic coal gasification are shown below, mainly focusing on minimal fluidization velocity, jet height and bed expansion ratio.

The minimal fluidization velocity is calculated using Wen and Yu correlation [12], and the constant C_1 is taken as 25.25 and C_2 as 0.0651. It is consistent with our PDU (3.5 MPa) experimental data determined by the methods from pressure drop changing.

$$\frac{d_p u_{mf} \rho_g}{\mu} = \left[C_1^2 + C_2 \frac{d_p^3 \rho_g \left(\rho_p - \rho_g\right) g}{\mu^2} \right] - C_1. \tag{1}$$

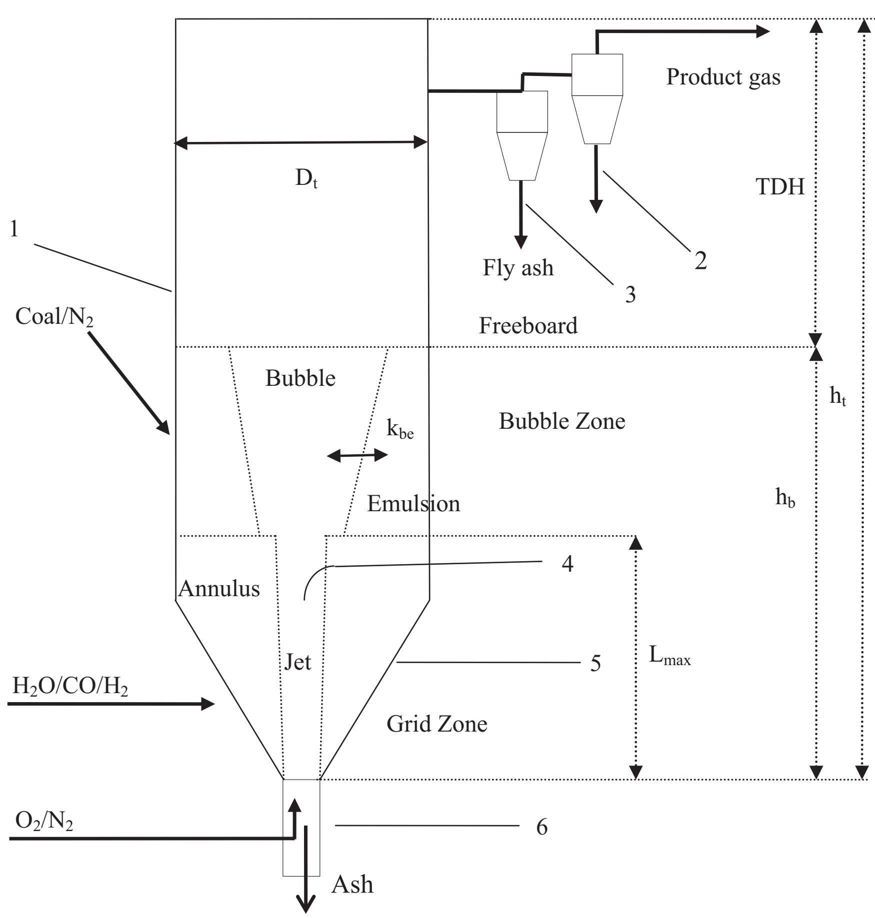

Fig. 1. A schematic diagram of the gasifier and model. 1—gasifier; 2—second cyclone; 3—first cyclone; 4—center thermocouple; 5—cone distribution plate; 6—central tube.