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Compartment modeling of coal gasification in an entrained flow gasifier: A study on the influence of operating conditions

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A B S T R A C T

Coal gasifiers are core components of coal-based polygeneration systems for power and chemical production. To study the effects of operational parameters on the performance of entrained flow coal gasifiers, this paper presents an equivalent compartment model (CM) using the Aspen Plus process simulator. The CM blocking is established based on gasifier flow field analysis, using a number of compartments. A simple configuration of these compartments involving material recirculation should be able to simulate the main flow and provide the temperature and gas component distributions. The model predictions exhibit good agreement with industrial data in the model validation. The influences of the oxygen-to-carbon ratio (ROC) and the coal slurry concentration on the gasification performance are discussed. Within the calculation range, the increase in the coal slurry concentration enhances the yield of the effective compositions in product gas. For a given slurry concentration of 62%, the efficient gas yield is a maximum for ROC of 1.43 kg/kg, whereas the oxygen consumption is a minimum for ROC of 1.37 kg/kg. According to the intended final use, however, choosing a reasonable ROC to obtain a higher efficient syngas yield and lower oxygen consumption can be flexible.

1. Introduction

Gasification is a highly efficient and clean conversion process that transforms different feed stocks to a wide array of products for various applications [1]. In comparison to combustion, gasification has higher power production efficiency and an effective and better controlled heating [2]. Gasification technology is being extensively developed in the energy and chemical synthesis process. Efficient syngas ($CO + H_2$) is the target product of gasification, and can be converted into pure hydrogen, methanol, combined heat and power (CHP), Fisher–Tropsch diesel, synthetic natural gas (SNG), dimethyl ether (DME), and so on [3,4]. The core component in a coal-based energy and chemical syntheses plant is coal gasifier. The reactors can be catalogued into fixed bed, fluidized bed and entrained flow gasifiers. By virtue of higher syngas yield, processing capacity, and tar-free product gas, entrained flow gasifiers have been widely utilized [5].

To compare the efficiency and selectivity of different gasification processes and investigate the effects of operating conditions on gasifier performance, numerous research on developing mathematical models have been conducted. Among these mathematical models, process simulators such as Aspen Plus [6–8], gPROMS [9], ChemCAD [10,11], and Simulink [12] are used for a variety of gasifiers (fixed bed, entrained flow, fluidized bed, etc.), based on the sequential modular and the equation oriented methods. Modeling the coal gasification processes using such software provides a powerful tool to evaluate mass and energy flows, realize process optimization, and conduct environmental assessment. Aspen Plus, a sophisticated process simulation software developed by Aspen technology, has been widely accepted in the simulation of coal gasification. Numerous instances have notably proven that Aspen Plus can be successfully applied to simulate the steady state process of an entrained flow gasifier [13–15]. A typical feature of these models is that the major gasification reactions are calculated by approaching minimization of Gibbs free energy in a Gibbs reactor block. The gasifier is assumed to reach chemical and phase equilibria. However, the simple method of Gibbs free energy minimization is not suitable for process analysis and optimization procedures of an entrained flow gasifier, wherein the gas–solid hydrodynamics, heat and mass transfer, and reaction kinetics over the complex gasifier geometry should be considered. Unlike these equilibrium gasification models, a "gasifier" model has been developed by Biagini et al. [16] using a more detailed approach that interconnects each step of gasification (preheating, devolatilization, combustion, gasification, and quench) according to the reactor configuration. The model removes the

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Nomenclature

A	pre-exponential index
B	temperature exponent
C_p	specific heat ($kJ\ kg^{-1}\ K^{-1}$)
D	diameter (m)
E_a	activate energy ($J\ kmol^{-1}$)
f	multiplier factor
f_{IRZ}	mass fraction of flow leaving ERZ to enter IRZ directly
H_{LOSS}	heat loss ($MJ\ s^{-1}$)
k_i	reaction rate constant for *i*th reaction
k_{eqi}	reaction rate constant for *i*th equilibrium reaction
K_i	equilibrium constant for *i*th reaction
L	length (m)
m	mass flow ($kg\ s^{-1}$)
P	pressure (Pa)
R	gas constant ($J\ kmol^{-1}\ K^{-1}$)
R_i	reaction rate of species *i* due to the chemical reactions ($kmol\ m^{-3}\ s^{-1}$)
T	temperature (K)

Greek symbols

α_i	mole fraction of *i*th species after devolatilization
β	oxygen consumption, $m^3/1000\ m^3$ ($CO + H_2$)
θ	jet angle (°)
γ	recirculation ratio (kg/kg)
φ	efficient syngas yield (Nm^3/t)
ω_v	mass fraction of the volatile matter in coal on a dry ash free basis
ω_i	mass fraction of species *i* in coal pyrolysis

Subscripts

i	the *i*th reaction or the *i*th specie
eq	reaction equilibrium

Acronyms

CHP	combined heat and power
CSTR	continuous stirred tank reactor
CWS	coal water slurry
DSZ	downstream zone
ERZ	external recirculation zone
FZ	flame zone
IRZ	internal recirculation zone
JZ	jet zone
PFR	plug flow reactor
CM	compartment model
ROC	oxygen-to-carbon ratio
SNG	synthesis natural gas
WSR	well stirred reactor

hypothesis of the equilibrium by introducing the kinetics of all steps. The gasifier is simulated by two cascade ideal plug flow reactors (PFRs). However, the division of the gasifier into two PFRs cannot reasonably account for hydrodynamic characteristics [17] such as the lack of material recirculation, which has a significant impact on gasification performance. Recently, numerous advanced models [17–19] have been developed for comprehensive simulation, which incorporate reaction kinetics and hydrodynamics. These models can provide detailed information on the gasifier. However, the employment of computational fluid dynamics (CFD) and the highly detailed sub-models occurring inside the gasifier make the integration of these generation plant model difficult and impractical. To overcome this problem, obtain the distribution of parameters in the reactor, and reduce the computational expense compared with the CFD based models, compartment model [20–23], also called Reactor network model wherein a combination of plug flow and well stirred reactors is used to represent the flow field in the gasifiers. This model cannot fully reflect the effect of turbulent mixing on the flow field and gas–solid reactions in the way that the CFD model can; nevertheless, it can still obtain a reasonable distribution of parameters in the furnace. The compartment model can handle complex chemical mechanisms and can be implemented into the process simulation software, through which the gasifier model can be easily integrated into plant-wide optimization and design.

In this article, an equivalent entrained flow coal gasifier CM has been developed and used as a tool for the analysis of an industrial Texaco (GE) gasifier by coupling Aspen Plus with dedicated Fortran files. The CM developed by Pedersen et al. [24,25] was chosen and improved upon. The model consists of three well stirred reactors (WSRs, also called continuous stirred tank reactor, CSTR) and two PFRs to model the CM blocking, including internal and external recirculation zones (IRZ and ERZ), flame zone (FZ), jet zone (JZ), and downstream zone (DSZ). These compartments are modeled using the Aspen Plus Version 2006.5 [26]. In light of this model, analysis about the variations of gasification performance indicators including efficient syngas yield and oxygen consumption has been carried out to investigate how the operating parameters influence the characteristics of the coal gasification system. Finally, optimal operation conditions are suggested by considering the highest efficient syngas yield and lowest oxygen consumption.

2. Methodology

The Texaco (GE) gasifier equipped with a quench chamber is schematically shown in Fig. 1. The coal water slurry (CWS) is

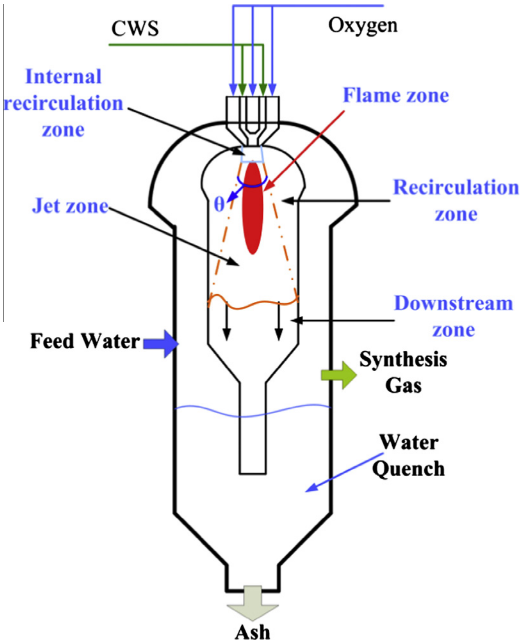

Fig. 1. Schematic diagram of an industrial Texaco (GE) gasifier with quench cooler.