



Full Length Article

Investigation on co-gasification of coal and biomass in Shell gasifier by using a validated gasification model

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HIGHLIGHTS

- The CO concentration decreased but that of H₂ increased with increasing blend ratio.
- The carbon conversion efficiencies were higher than 99.8% for all blend ratios.
- The cold gas efficiencies ranged between 82.8% and 88.1%.
- 10% of biomass blend ratio was the best case for the oxygen/carbon ratio of 2.51 used in this study.

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ABSTRACT

Co-utilization of coal and biomass in a power plant can reduce the overall CO₂ emission by partly displacing fossil-fuel combustion with near-carbon-neutral combustion of biomass. Computational fluid dynamics (CFD) modeling of co-gasification is conducted using a validated gasification model to examine the effect of biomass amount on the co-gasification process in a Shell gasifier. In the sub-models for coal and biomass char reactions, pore and bulk diffusions are considered using a user-defined function. The coal (Douglas premium coal, South Africa) and biomass (wood pellet treated from sawdust of pine and oak in South Korea) blend ratios (based on calorific value) are 0.0 (coal 100%), 0.05, 0.1, 0.15, and 0.2. The CFD model is validated using the actual operating data of the integrated gasification combined-cycle plant located in Puertollano, Spain. The CO concentration decreases but that of H₂ increases with increasing blend ratio. The cold gas efficiencies range between 82.8% and 88.1%, and the carbon conversion efficiencies are higher than 99.8% for all blend ratios. These efficiencies are similar to those of coal gasification. However, blend ratios of 0.15 and 0.2 are not appropriate for co-gasification because the exit temperatures calculated for these two blend ratios are 1708 and 1621 K, respectively, in which both are lower than the critical slag viscosity temperature (1753 K) of the coal used in this study.

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1. Introduction

In South Korea, a national project to operate an overall power of 380 MWe (net power: 305 MWe) integrated gasification combined-cycle (IGCC) demonstration plant using a Shell gasifier was constructed by the Korea Western Power Company in May 2015. After the first coal firing was successfully performed in September 2015, commercial operation has continued since June 2016.

The Shell gasifier in South Korea is expected to be applied to the co-gasification of coal and biomass in the future because co-utilization of coal and biomass reduces the overall CO₂ emission

by partly displacing fossil-fuel combustion with near-carbon-neutral combustion of biomass. In addition, an important challenge with respect to electricity generation that can be addressed with biomass is the renewable portfolio standards [1]. Therefore, exploring the co-gasification characteristics of a Shell gasifier will be beneficial for future use. A comprehensive validated CFD model is instrumental in ascertaining whether important gasifier performance metrics, such as carbon conversion and cold gas efficiency, are optimized with respect to relevant parameters [2]. In addition, numerical simulation offers an effective technique to predict flow, temperature, and species distributions, and thus, to optimize the operating parameters [3,4].

Several CFD modeling studies of biomass gasification were previously conducted. Fletcher et al. [5] developed a CFD model using CFX4 package to simulate the flow and reaction in an entrained-flow

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biomass gasifier. Their results suggested that simulations to examine the effect of gasifier height and the steam flux in the upper inlets could be beneficial in process optimization. Gao et al. [6] conducted model development for biomass gasification in an entrained-flow gasifier to consider the effects of diffusion rate and kinetic rate on simulation of char gasification. They used an intrinsic reaction rate sub-model with a user defined function in ANSYS FLUENT. Xue and Fox [7] presented a 2-D multi-fluid CFD model of biomass gasification for use in fluidized-bed gasifier simulations. The kinetic model implementation and coupling with a continuously variable particle density was focused. Different air/biomass mass flow ratios, reactor temperatures, and biomass moisture contents were simulated and analyzed to understand their influences on gas compositions and product yields at the gasifier outlet [7]. Xiong and co-workers [8–10] developed an open-source computational framework using OpenFoam. In their studies [8–10], the multi-component, multi-step devolatilization scheme was employed to model the biomass fast pyrolysis reaction in fluidized-bed reactors. Operating parameters including bed temperature, nitrogen velocity, biomass particle diameter, feed rate, sand particle diameter, and initial height of sand bed were varied to investigate their effects on product yields [8–10].

CFD modeling studies of coal gasification were conducted in two different industrial-scale gasifiers. Jeong et al. [11] conducted CFD modeling of an E-Gas™ gasifier by using ANSYS FLUENT to study the effect of coal size (50, 100, 200, and 300 μm) on the gasification performance. Pore and bulk diffusions were considered in the char-gasification model via a user-defined function. Jeong et al. [11] found that the pore and bulk diffusions became important with increasing coal size and the carbon conversion efficiency and cold gas efficiency were maximized with 100 μm of coal size. In the study by Park et al. [12], CFD modeling using ANSYS FLUENT was also carried out in a Shell gasifier. The main goal was to understand the effects of O₂/coal and steam/coal ratios on the gasification performance. Since the coal size was assumed to be uniform as 100 μm, Park et al. [12] did not consider the pore and bulk diffusions in their char-gasification model.

In the current study, coal particles were assumed to have a size distribution. Therefore, pore and bulk diffusions, as well as chemical kinetics, were considered in the char-gasification model, and the effect of co-gasification of coal and biomass on the performance of a Shell gasifier was examined. For 100% coal, the CFD results were compared and verified with the operating data of the Shell gasifier in Puertollano, Spain, where Douglas premium coal (South Africa) was used. After verifying our CFD model, wood pellet, treated from sawdust of pine and oak in South Korea, was used together with the Douglas premium coal for co-gasification in the CFD modeling. The distributions of temperature and species mole fractions, as well as the carbon conversion and cold gas efficiencies at the gasifier exit, were calculated under different blend ratios.

2. CFD modeling

2.1. Numerical models

In the numerical procedure, the 3-D steady-state Navier-Stokes equations were solved in an Eulerian-Lagrangian frame of reference. All of the coal and biomass particles were treated as a discrete, secondary phase dispersed in the continuous phase via the discrete phase model (DPM) with stochastic tracking to consider the turbulent dispersion effect. The discrete ordinate (DO) radiation model, together with the domain-based weighted-sum-of-gray-gases model (WSGGM) for the radiative properties of the gases was applied, and the gravitational force was considered in

the modeling. The realizable *k-ε* model was applied to capture the turbulent flow. The species transport equations were solved through the finite-rate/eddy-dissipation model. Table 1 shows all the gas phase reactions that are included in the model and kinetic parameters of each reaction.

In this study, the two competing rates model was used during devolatilization as provided by ANSYS FLUENT [23]. All of the volatile matter produced during devolatilization was assumed to be CHO compounds [24]. Therefore, it was assumed from the results of ultimate and proximate analyses that the volatile matters produced from the coal and biomass were CH_{1.904}O_{0.352} and CH_{2.377}O_{0.752}, respectively. The proximate analysis, ultimate analysis, and higher heating value results of the coal and biomass used in this study are listed in Table 2.

In order to describe char gasification, the random pore model was applied in this study, as follows [25]:

$$\frac{dm_{c,i}}{dt} = m_{c,0} \eta_i A_{c,i} P_i^{n_i} e^{-E_{c,i}/RT_p} (1-x) \sqrt{1-\psi_i \ln(1-x)} \quad (1)$$

where the subscript *i* represents each gasifying agent, *m_{c,i}* is the mass of char particle (kg), *m_{c,0}* is the mass of char particle at the initial state (kg), *η_i* is the effectiveness factor, *A_{c,i}* is the pre-exponential factor (1/Pa^{*n_i*}/s), *E_{c,i}* is the activation energy (J/kmol), *T_p* is the temperature of the particle (K), *P_i* is the partial pressure (Pa), *ψ_i* is the pore structure parameter, *n_i* is the reaction order, and *x* represents the total carbon conversion of char particle by all gasifying agents. The kinetic parameters used to calculate Eq. (1) are listed in Table 3.

In this study, the effectiveness factor was used to represent the overall reaction rate in three different regimes; regime I (chemical rate control at low temperatures), regime II (pore diffusion and chemical rate control at intermediate to high temperatures), and regime III (bulk diffusion control at high temperatures). In this study, the effectiveness factor, *η_i*, is determined as follows [25]:

$$\eta_i = \frac{3}{\phi_i} \left(\frac{1}{\tanh \phi_i} - \frac{1}{\phi_i} \right) \quad (2)$$

where *φ_i* is the Thiele modulus. The Thiele modulus is expressed as follows [25]:

$$\phi_i = \frac{d_p}{6} \times \sqrt{\frac{n_i + 1}{2} \frac{A_{c,i} e^{-E_{c,i}/RT_p} (1-x) \sqrt{1-\psi_i \ln(1-x)} \rho_p RT_p P_i^{n_i-1} v_{g,i}}{M_c D_{eff,i}}} \quad (3)$$

where *d_p* is the size of char particle (m), *ρ_p* is the density of char particle (kg/m³), *v_{g,i}* is the stoichiometric factor of each gasifying agent for each mole of carbon consumed, *M_c* is the molecular weight of carbon (kg/kmol), and *D_{eff,i}* is the effective diffusivity (m²/s).

Assuming that the pore size distribution is monodisperse and the bulk and Knudsen diffusions proceed in parallel, the effective diffusivity is given as follows [29]:

$$D_{eff,i} = \frac{\theta}{\tau} \left(\frac{1}{D_{KN,i}} + \frac{1}{D_{0,i}} \right)^{-1} \quad (4)$$

where *D_{KN,i}* is the Knudsen diffusion coefficient (m²/s), *D_{0,i}* is the molecular diffusion coefficient (m²/s), *θ* is the porosity of the char particle, and *τ* is the tortuosity of the pores. In this study, the porosity was assumed as 0.5. The tortuosity of 2 was applied in this study, since the tortuosity was assumed to be equal to *τ* = 1/θ [30].

The molecular diffusion coefficient for each gasifying agent is given as follows [31]:

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