Water–gas shift modeling in coal gasification in an entrained-flow gasifier – Part 2: Gasification application

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HIGHLIGHTS

▶ The calibrated WGS rates in Part 1 is further slowed down to match the data from the Japanese CRIEPI gasifier.
▶ The CFD results match the CRIEPI data reasonably well.
▶ Temperature is within 2%, CO and H_2O within 4 percentage points, and H_2 within 7–9 percent points.
▶ Water vapor data taken right before the syngas cooling section in the gasifier is needed for future calibration study.

ARTICLE INFO

ABSTRACT

Water–gas-shift (WGS) reaction is one of the major reactions in the industrial gasification process. Using an adequate WGS reaction rate is vital to predicting correctly syngas composition in a gasification process. In Part 1, three different WGS reaction rates from Jones, Wade, Sato were modified to match the experimental data of raw syngas undergoing water quench process. It is not clear if these calibrated WGS reaction rates are adequate in a gasification process. Hence, the objective of this study in Part 2 is to apply both the three original published WGS rates and the calibrated rates derived in Part 1 to simulate experiments performed in the Japanese CRIEPI research gasifier. The CFD model incorporates 3-D Navier–Stokes equations and nine species transport equations with seven global gasification reactions (three heterogeneous and four homogeneous,) and a two-step thermal cracking model for volatiles. The Chemical Percolation Devolatilization (CPD) model is used for the devolatilization process. Similar to the result in Part 1 for water quench process, the result in this study further shows that the three originally published rates cannot be directly applied to the simulation of coal gasification process, due to different temperature and pressure range. Even the modified rates obtained from a water quench process in Part 1 also appear faster in the gasification process. The pre-exponential rate constant value (A) of each reaction rate is therefore further slowed down, while the activation energy is kept the same as the original value to match the experimental data. The results show that all three WGS reaction rates can be modified to match the experimental data reasonably well. The exit temperature can be matched within 2% (20 K). The mole fractions of CO and H_2O can be matched fairly well within 4 percentage points (or 10%); however, the simulated H_2 mole fractions are always 7–9 percentage points higher than the experimental data. It needs to be emphasized that the calibrated WGS reaction rates in this study can only be applied in the range of water quench and gasification operating conditions for which they have been validated.

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1. Introduction

1.1. Recent research

Part 1 of this study was mainly focused on investigating WGS reaction rates without involving the gasification process. In this second part of the study, the focus is placed on investigating WGS reaction rates in a coal gasification process. Gasification is an incomplete combustion process, converting various carbon-based feedstock to clean synthetic gas (syngas), which is primarily a mixture of hydrogen (H_2) and carbon-monoxide (CO) as fuels. Feedstock is partially combusted with oxygen and steam at high temperature and pressure with less than 30% of the required oxygen for complete combustion (i.e., the stoichiometric amount) being provided. The syngas produced can be used as a fuel (usually for boilers or gas turbines to generate electricity); it can also be made into a substitute natural gas (SNG), or hydrogen gas and/or

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other chemical products. Gasification technology is applicable to any type of carbon-based feedstock, such as coal, heavy refinery residues, petroleum coke, biomass, and municipal wastes. To help understand the gasification process in gasifiers and subsequently use the learned knowledge to guide designs of more compact, more cost effective, and higher performance gasifiers, computational fluid dynamics (CFD) has been widely employed as a powerful tool to achieve these goals.

Chen et al. developed a three-dimensional simulation model for entrained-flow coal gasifiers, which applied an extended coal–gas mixture fraction model with the Multi Solids Progress Variables (MSPV) method. The model employed four mixture fractions separately track the variable coal off-gases from the coal devolatilization, char–O_2, char–CO_2, and char–H_2O reactions [1]. Bockelie et al. developed a comprehensive CFD modeling tool (GLACIER) to simulate entrained-flow gasifiers, including a single-stage, down-fired system and a two-stage system with multiple feed inlets [2]. The U.S. Department of Energy/National Energy Technology Laboratory (NETL) developed a 3D CFD model of two commercial-sized coal gasifiers [3]. The commercial CFD software, FLUENT, was used to model the first gasifier, which was a two-stage, entrained-flow, slurry-fed coal gasifier. The Eulerian–Lagrangian method was used in conjunction with the discrete phase model to simulate the entrained-flow gasification process. The second gasifier was a scaled-up design of a transport gasifier. The NETL open source MFIX (Multiphase Flow Interphase eXchanges) Eulerian–Eulerian model was used for this dense multiphase transport gasifier. NETL has also developed an Advanced Process Engineering Co-Simulator (APECS) that combines CFD models and plant-wide simulation. APECS enables NETL to couple its CFD models with the steady-state process simulator, Aspen Plus.

From 2005 to 2011, Silaen and Wang have conducted a series of study of entrained-flow gasification process using the commercial CFD solver, FLUENT. Silaen and Wang investigated the effects of several parameters on gasification performance, including the coal input condition (slurry or dry powder), oxidant (oxygen-blown or air-blown), wall cooling, and various coal distributions between the two stages. The simulation results provide the temperature and species distributions inside the gasifier [4]. In 2006, they investigated the effect of flow injection directions on the gasification performance using the same generic two-stage, entrained-flow gasifier [5]. In 2010, they did research that investigated the effects of different parameters on gasification performance, including five turbulence models, four devolatilization models, and three solid coal sizes [6]. With several improvements in the CFD modeling, including updating the finite rates for heterogeneous reactions, adding Chemical Percolation Devolatilization (CPD) devolatilization model, and adding two-stage volatiles cracking reactions, Silaen and Wang again conducted an investigation on the effects of different operation parameters in the gasification process between the two stages [7].

In collaboration with the research team of Industrial Technology Research Institute (ITRI), Wang and Silaen effectively employed the CFD gasification model to investigate gasification process under the influences of different part loads, two different injectors, and three different slagging tap sizes [8–10]. In 2011, Wang et al. performed the simulation on the effects of potential fuel injection techniques on gasification performance in order to help design the top-loaded fuel injection arrangement for an entrained-flow gasifier using a coal-water slurry as the input feedstock. Two specific arrangements were investigated: (a) coaxial, dual-jet impingement with the coal slurry in the center jet and oxygen in the outer jet and (b) four-jet impingement with two single coal-slurry jets and two single oxygen jets [11].

One of the important reactions during the gasification process is the water–gas shift (WGS) reaction ($CO + H_2O \Leftrightarrow CO_2 + H_2$). The WGS has been traditionally used for adjusting the H_2/CO ratio in a syngas to meet the specifications for various final products. The forward WGS reaction favors relatively low temperatures (under 600 °C). When the temperature is higher than 1200 °C, the reverse reaction starts to dominate. This trend has been described and shown in the Table 1 in Part 1.

1.2. Experimental data

In order to get an appropriate WGS reaction rate, detailed and accurate experimental data sets are needed to calibrate the CFD model. However, most of the experimental data available in the public domain was obtained after the syngas cooling or after the gas clean-up process. For limited data taken in the gasifier before the syngas cooling section, typically no information on the water vapor concentration is available. Lack of adequate "raw data" has made calibration of the gasification model and the WGS reaction rate uncertain and difficult. For example, the data of syngas composition published from the Wabash River Coal Gasification Repowering Project (2000) did not show the mole fraction of water vapor at the exit of the gasifier, although the water vapor information was shown for syngas composition after desulfurization [12]. The experimental data provided by the Tampa Electric Polk Power Station IGCC Project (2002) was the cleaned syngas composition, which was taken after the syngas cooler and gas cleanup processes [13]. Hughes et al. provided the syngas data from a two-tonne per day (slurry feed rate) pilot-scale gasifier, and, similarly, no water vapor mole fraction was given [14]. Wained and Whitty performed tests in a 1 ton/day pressurized, slurry-fed, oxygen-blown, entrained-flow coal gasifier. The experimental data also lacked information for the water vapor content at the exit [15]. So far, to the authors' knowledge, the only published experimental syngas data obtained before syngas cooling with water vapor content information is from the CRIEPI research scale coal gasifier presented in the paper by Watanabe and Otaka [16]. Therefore, the CRIEPI data is used for calibrating the WGS reaction rate in this paper.

1.3. Global gasification chemical reactions

This study deals with the global chemical reactions of coal gasification [17] that can be generalized in reactions (R1) through (R10) in Table 1. WGS reaction rates used in this study are presented in Table 2.

In this study, the methanation reactions are not considered since the production of methane is negligible under the studied operating conditions. The volatiles are modeled to go through a two-step thermal cracking process (R7) and gasification processes (R8 and R9) with CH_4 and C_2H_2 as the intermediate products. The coal used in this study is Japanese Black Coal, whose compositions are given in Table 3. The compositions of volatiles are derived from the coal's heating value, proximate analysis, and ultimate analysis. The oxidant is considered to be a continuous flow and the coal particles are considered to be discrete. The discrete phase only includes the fixed carbon and liquid water droplets from the moisture content of coal (5.3 wt%). Other components of the coal, such as N, H, S, O, and ash, are injected as gas, together with the oxidant in the continuous flow. N is treated as N_2, H as H_2, and O as O_2. S and ash are not modeled and their masses are lumped into N_2.

2. Computational model

The governing equations, turbulence models, radiation model, and discrete phases have been stated in Part 1 explicitly, so they are not repeated here, but briefly summarized below. The time-averaged steady-state Navier–Stokes equations as well as the mass and energy conservation equations are solved. Species