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Reduced order modeling of the Shell–Prenflo entrained flow gasifier

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HIGHLIGHTS

- ROM of the Shell gasifier enables the integration of gasifier and overall IGCC simulation.
- Detailed model of the reactor, the membrane wall and the gas quench is developed.
- Calculated cold gas efficiency is 82.5%, outlet temperature is 1588 °C.
- Carbon conversion is sensitive towards O/coal ratio.
- CGE increases to 83.5% when coal is charged with CO_2 instead of N_2.

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ABSTRACT

Pre-combustion capture applied to an integrated gasification combined cycle is a promising solution for greenhouse gas emission's mitigation. For optimal design and operation of this cycle, detailed simulation of entrained flow gasifiers and their integration in the flowsheet analysis is required. This paper describes the development of a reduced order model (ROM) for the Shell–Prenflo gasifier family, used for chemicals and power production because of its high efficiency and compatibility with a wide range of coal quality. Different from CFD analysis, ROM is computationally very efficient, taking around 1 min in a typical desktop or laptop computer, hence enabling the integration of the gasifier model and the overall power plant flowsheet simulation. Because of the gasifier complexity, which includes several gas recirculation loops and a membrane wall, particular attention is paid to: (i) the two-phase heat exchange process in the gasifier wall; and, (ii) the syngas quench process. Computed temperature, composition, velocity and reaction rate profiles inside the gasifier show good agreement with available data. The calculated cold gas efficiency is 82.5%, close to the given value of 82.8%. Results and several sensitivity analyses describe the implementation of the model to explore the potential for operating gasifiers beyond the design point.

1. Introduction

Rising world energy demand has mostly been met by expanding the use of fossil fuels, resulting in higher concentrations of carbon dioxide in the atmosphere. The possible consequences of these trends, in particular global warming, have driven the search for alternative electricity generation technologies capable of limiting CO_2 emissions. It is very likely that carbon dioxide reduction will have to be achieved while fossil fuels continue to be the major source of primary energy for several decades to come. CO_2 reduction must be pursued using a portfolio of different approaches. One of these, carbon dioxide capture and storage, is recognized as one of the most promising options because it addresses the impact of the largest primary energy sources and the largest source of CO_2. Among the three main routes for CO_2 capture in electric energy production, pre-combustion capture, which is compatible with efficient integrated gasification combined cycle power plants adds, in some estimates, the least cost penalty to the price of electricity. This process employs entrained flow gasifiers (EFGs). Among commercially available EFGs are Shell (Prenflo as well as other name brands), GE (former Texaco) and Mitsubishi gasifiers. To design and operate optimal IGCC plants, there is a need for detailed process simulation, which would ideally be based on computational fluid dynamics coupled with high fidelity physical–chemical submodels for coal conversion. However, comprehensive CFD simulation of gasification is nearly impossible to perform as part of an overall IGCC plant flowsheet model, even for simple gasifier designs let alone one as complex as the Shell process which involves several syngas recirculation and steam production inside the gasifier battery unit. The reduced order model (ROM) developed in [1] has been proposed as an alternative to

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Nomenclature

ACM	Aspen Custom Modeler
IP	intermediate pressure
ASU	air separation unit
IRZ	internal recirculation zone
CFD	computational fluid dynamic
JEZ	Jet Expansion Zone
CGE	cold gas efficiency
LH	lock hopper
COS	carbonyl sulfide
LHV	lower heating value
DSZ	downstream zone
LP	low pressure
ERZ	external recirculation zone
PFR	plug flow reactor
GT	gas turbine
ROM	reduced order model
HHV	higher heating value
RNM	reactor network model
HP	high pressure
WGS	water gas shift
HPHT	high pressure high temperature
WSR	well stirred reactor
IGCC	integrated gasification combined cycle

Subscripts

Th	thermal
El	electrical

allow for a reasonably accurate prediction of the gasification process as part of a plant simulation model. In this study, the ROM is modified and implemented in order to predict the performance of the Shell–Prenflo gasifier. Model features, results for a particular reactor size, and sensitivity analysis are presented in this paper.

In Section 2, we describe the Shell gasifier and its integration with the rest of the plant. In Section 3, the Shell ROM is introduced in detail. In Section 4, the geometry and components of the gasifier are presented. Sections 5 and 6 describe two important features of this family of gasifiers, the membrane wall and the syngas quench, respectively. Assumptions and methodology are reported in Section 7. In Section 8, we present the simulation results while sensitivity analyses are presented in Section 9. Finally, Section 10 is dedicated to the conclusions.

2. Shell–Prenflo gasification process

The Shell gasifier is an upflow entrained flow reactor fed with pulverized coal through a number of diametrically opposed burners (4–6) placed in the bottom part of the reactor. The Shell process provides almost separate outlets for the syngas and the ash, with the gas leaving from the top and the larger amount of ash flowing out at the bottom side in the form slag. More than 70% of the ash content in the feed leaves as slag while the remaining stays with the syngas as flyash. The adoption of a dry feed gasifier with high carbon conversion (>99%) leads to higher gasifier efficiency (measured in terms of cold gas efficiency) and higher plant efficiency, when compared to slurry fed gasifiers. Another advantage of the Shell process is the wide variety of coal that can be gasified in this dry-fed system. By using dry gases to pressurize the pulverized coal, there is no limitation on coal composition and the operating conditions. Moreover, the amount of oxygen required for gasification is lower than in slurry fed gasifiers. On the other hand, the gain in cold gas efficiency comes at the cost of higher plant complexity and cost; the higher operating temperature inside the gasifier results in more waste heat and a larger syngas cooler, and requires a water cooled reactor jacket. Even though the reliability of the dry coal feeding system has been one of the main issues during the initial stages of development, the issue has addressed and it no longer contributes significantly to the total downtime [2].

According to Shell, the gasification pressure is set up to 44 bar; there is a trade-off between the efficiency, which is higher at lower pressures, and the vessel size. Oxygen is produced in an ASU which is partially integrated with the gas turbine (GT) compressor: 50% of the air at the ASU distillation column comes from the GT compressor. Oxygen is fed to the gasifier at 180 °C [3]. Coal is dried before feeding it to the gasifier, limiting its moisture content to 2% by mass, to improve the flow through the lock hoppers and lower the amount of oxidant. The coal carrier is typically nitrogen, produced in the ASU, although it may be replaced by CO_2 for carbon-capture plants. Of the N_2 used for coal feeding, only part flows into the gasifier (around 40–50%), while the remaining is vented during the cyclic operation of the feeding process [4]. Finally a small amount of N_2 is used to regenerate the candle filters for the syngas purification after the convective coolers. The hot syngas exiting the gasifier is quenched to 900 °C with cold recycled syngas (at around 200 °C). Molten slag entrained by the gas stream solidifies during the quench process while the syngas is cooled to 300 °C in the syngas coolers, producing saturated HP and IP steam. The last syngas purification step inside the gasifier train is the wet scrubbing, where the remaining solids and soluble contaminants are removed. Syngas exits the scrubber at about 170 °C and, after the regenerative heat exchangers, is sent to a catalytic bed for COS hydrolysis. The latter step is not required in case of pre-combustion CO_2 capture as COS is converted inside the WGS reactor.

Fig. 1 shows a detailed representation of the Shell gasification process as described above. Data reported in Table 1 were obtained at the Politecnico di Milano by calibrating the property 0-D code (GS) in order to reproduce the Shell experimental data at the scrubber exit; this simulation is based on chemical equilibrium, adopting the approach-to-equilibrium method. The overall gasification process for a specific coal was reproduced and validated, and it was used to support the kinetic simulation developed in this work, and in assigning the values of oxidant, coal and moderator at the reactor inlet. Different Shell plant configurations based on chemical equilibrium are reported in [5].

3. Reduced order model

The structure, development and implementation of the reduced order model (ROM) are reported in [1,7–9]. Only the basic concepts of the ROM are briefly described here. In the ROM the gasifier is represented by a reactor network model (RNM). The RNM is based on using idealized chemical reactors (0-D WSR or 1-D PFR) to model different parts of the gasifier. For this reason, the ROM simulation may require some input from CFD. For modeling the current gasifier, the RNM model developed in [7] is chosen, which is based on work in [10,11]. The original model was set up for the GE or MHI gasifiers, which are different in several aspects from the Shell process [12]: (i) the wall design (a refractory lining in GE, a membrane wall in Shell and MHI), (ii) the flow direction (downward in GE, upward in Shell and MHI), (iii) the number of burners (1 in GE, 4/6 in Shell,>4 in MHI), iii) the coal feeding system (wet in GE, dry in Shell and MHI) and iv) the number of stages (one in GE and Shell, two in