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Reduced order modeling of a short-residence time gasifier

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HIGHLIGHTS

- A reactor network is presented for the modeling of CanmetENERGY's gasifier.
- Axial velocity, molar composition and temperature profiles are presented.
- The model is compared to the results of corresponding CFD simulation.

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ABSTRACT

State-of-the-art gasifiers require rapid mixing of fuel, steam and oxygen to achieve high carbon conversion within a short residence time. This allows reduction of the gasifier's volume and the associated capital costs. CanmetENERGY of Natural Resources Canada has a pilot-scale gasifier that can convert solid fuels to syngas in less than 1 s. This study describes the development of a reduced order model (ROM) for CanmetENERGY's entrained flow short-residence time gasifier. The model consists of a reactor network that represents the gasifier using a set of chemical reactors that are aimed to capture distinct flow zones of the system. The layout of chemical reactors proposed in this work is based on computational fluid dynamics (CFD) simulations of the gasifier that accounted for the detailed gas and particle flows. The ROM implements sub-models for the simulation of drying, devolatilization, chemical reactions, viscous fluid–solid interactions, pollutant formation and heat transfer through the wall of the reactor. The predictions obtained by the ROM are in reasonable agreement with the CFD simulation data for axial temperature, heat flux, conversion and composition. Having established the flow pattern for a given gasifier and range of operating conditions, the proposed ROM is computationally efficient since it only requires 2.5 min to converge whereas CFD simulations require 7–10 days. This attractive feature enables integration of the gasifier ROM to process simulators for further development of integrated gasification combined cycle power plants.

1. Introduction

Integrated gasification combined cycle (IGCC) power plants are considered to be one of the most attractive technologies for clean power production from solid fuels. The key benefits of IGCC over combustion systems are higher efficiency, reduced production of solid wastes, lower SO_x and NO_x emissions, less expensive gas-cleaning equipment and higher fuel flexibility. For IGCC power plants, one of the largest capital expenditures is devoted to the gasifier unit [1]. The purpose of the gasifier in the IGCC plant is to convert carbonaceous feedstocks (e.g. coal, petroleum coke, biomass and/or waste) into synthesis gas, also known as 'syngas', which is mainly composed of hydrogen (H_2) and carbon monoxide (CO). The quality and throughput of the produced raw syngas mainly relies on the operating conditions, oxidation agent, the gasifier's geometric design and the flow jet and recirculation zones established inside the gasifier. Entrained-flow gasifiers are the most common commercial gasifier for IGCC applications, in part due to their high throughput and efficiency when compared to the other types of gasifiers (Monaghan RFD). One of the long-term technologies that can potentially reduce the power production costs of IGCCs is an advanced type of entrained flow gasifier referred to as a short-residence time gasifier [2]. This type of entrained flow gasifier is more compact and applies rapid mixing of fuel and oxygen to obtain a high carbon conversion with

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A	area
A'	pre-exponential factor
C	concentration
C_D	drag coefficient
c_p	heat capacity
d	diameter
D	diffusivity
E	activation energy
f	friction factor
F'	volumetric force
g	gravitational acceleration
h	convection coefficient
H	enthalpy
HS	heat source
k	thermal conductivity
L	length
m	mass
m'	mass flow
MS	mass source
n	reaction order
N	number of particles density
Nu	Nusselt number
P	pressure
Pr	Prandtl number
Q'	heat flux
r	radius
R	reactions
Re	Reynolds number
Sh	Sherwood number
T	temperature
u	velocity
v	volume
x	axial domain

Greek symbols

ϵ	volume fraction
α	recirculation ratio
θ	jet angle
μ	gas viscosity
σ	Stefan–Boltzmann constant
ρ	density
ϑ	conversion decay rate

Subscript

conv	convection
CS	cross section
eff	effective
g	gas
Hetero	heterogeneous reactions
Homo	homogeneous reactions
i	ith gas phase specie
p	particle
rad	radiation
rxn	reaction
slagging	slag transport to wall
w	wall
s	surroundings

residence times of 0.2–0.5 s [3]. According to Fusselman et al. [4], the capital cost of IGCC power plants and electricity costs can be potentially reduced by 14.5% and 18.5% when short-residence time gasifiers are used. Aerojet Rocketdyne is developing a short-residence time gasifier which has been piloted at the Gas Technology Institute in Des Plaines, USA [4]. Testing of some components for this gasifier has been done at CanmetENERGY in Ottawa, Canada. The Aerojet Rocketdyne gasifier is anticipated to accommodate all ranks of coal, including lignite and petroleum coke, while reducing capital costs and improving plant availability.

Increasing IGCC plant availability while using advanced technologies such as short-residence time gasifiers has been identified as one of the key improvements required for obtaining an attractive power cost for near zero emission power plants [5]. Despite the efforts in this area, studies that analyze the performance and availability of short-residence time gasifiers are lacking in the open literature. In order to evaluate the impact of short-residence time gasification on the overall IGCC process, a model that captures the main aspects of gasification is required and needs to be integrated with models of the other units of the power plant such as the combined cycle and CO_2 capture unit [6–8]. Due to the complexity associated with the gasification flows and mixing, gasifier models are often developed using Computational Fluid Dynamics (CFD). Detailed sub-models are often used in CFD simulations to describe the behavior of various mass, energy and momentum transport processes taking place inside the gasifier. However, the integration of CFD models with the overall IGCC process is computationally prohibitive due to the intensive calculations needed by CFD simulations. In addition, convergence issues of the CFD model when integrated with other units of power plants increases the complexity of this integration. To circumvent these issues, the work presented here focuses on the development of a reduced order model (ROM) that captures the fundamental characteristics of a short-residence time gasification unit. Due to their low computational costs, gasifier ROMs are the most widely used models that can be integrated with process simulators such as Aspen® or UniSim® to evaluate the performance of a complete IGCC power plant. ROMs involve the representation of complex reactors by networks of ideal chemical reactors. The reactor network configuration depends on the complex reactor's design and usually requires CFD simulations to determine the flow-regimes and structures inside the gasifier.

The development of a reactor network to design accurate and reliable gasifier models has received continuously increasing attention as it reduces the computational costs compared to CFD-based models. Monaghan et al. presented a comprehensive ROM for a range of entrained-flow gasifiers using Aspen Custom Modeler (ACM) [9]. They showed satisfactory ROM accuracy with the available data for the different gasifier designs [10]. Dynamic simulations of the ROM during start-up, fluxant removal, load following, feed change and feed co-firing were conducted by the same authors to evaluate the transient behavior of the system [11]. Gazzani et al. developed a ROM for a Shell–Prenflo gasifier using ACM [12]. Yang et al. used a similar approach for the modeling of a membrane wall entrained-flow gasifier with two-stage oxygen supply [13]. Kong et al. performed a steady-state simulation in Aspen Plus for an industrial-scale Texaco gasifier by implementing a compartment reactor network [14]. Lee et al. used gPROMS to develop a dynamic ROM for a 300 MW Shell gasifier with slag and membrane wall sub-models [15]. More details regarding recent developments in gasification technology modeling can be found elsewhere [2].

To the knowledge of the authors, details of ROMs for short-residence time gasifiers are not available in the literature. The purpose of this study is to develop a steady-state ROM of a short-residence time gasifier based on CFD modeling of CanmetENERGY's pilot-scale gasifier. The structure of this paper is as follows: Section 2 describes the gasification system used in this