Applied Energy 131 (2014) 425–440

Contents lists available at ScienceDirect

Applied Energy

journal homepage: www.elsevier.com/locate/apenergy

Dynamic modeling of Shell entrained flow gasifier in an integrated gasification combined cycle process

Hyeon-Hui Lee [a], Jae-Chul Lee [a], Yong-Jin Joo [c], Min Oh [b,*], Chang-Ha Lee [a,*]

[a] Department of Chemical and Biomolecular Engineering, Yonsei University, 50 Yonsei-ro, Seodaemun-gu, Seoul 120-749, Republic of Korea
[b] Department of Chemical Engineering, Hanbat National University, San 16-1 Dukmyung-dong, Yuseong-gu, Daejeon, Republic of Korea
[c] Korea Electric Power Research Institute (KEPRI), 103-16, Munji-dong, Yuseong-gu, Daejeon, Republic of Korea

HIGHLIGHTS

- Detailed dynamic model for the Shell entrained flow gasifier was developed.
- The model included sub-models of reactor, membrane wall, gas quench and slag flow.
- The dynamics of each zone including membrane wall in the gasifier were analyzed.
- Cold gas efficiency (81.82%), gas fraction and temperature agreed with Shell data.
- The model could be used as part of the overall IGCC simulation.

ARTICLE INFO

Article history:
Received 31 December 2013
Received in revised form 17 June 2014
Accepted 18 June 2014
Available online 12 July 2014

Keywords:
Shell gasifier
Entrained flow gasifier
Dynamic modeling
IGCC

ABSTRACT

The Shell coal gasification system is a single-stage, up-flow, oxygen-blown gasifier which utilizes dry pulverized coal with an entrained flow mechanism. Moreover, it has a membrane wall structure and operates in the slagging mode. This work provides a detailed dynamic model of the 300 MW Shell gasifier developed for use as part of an overall IGCC (integrated gasification combined cycle) process simulation. The model consists of several sub-models, such as a volatilization zone, reaction zone, quench zone, slag zone, and membrane wall zone, including heat transfers between the wall layers and steam generation. The dynamic results were illustrated and the validation of the gasifier model was confirmed by comparing the results in the steady state with the reference data. The product gases (H_2 and CO) began to come out from the exit of the reaction zone within 0.5 s, and nucleate boiling heat transfer was dominant in the water zone of the membrane wall due to high heat fluxes. The steady state of the process was reached at nearly $t = 500$ s, and our simulation data for the steady state, such as the temperature and composition of the syngas, the cold gas efficiency (81.82%), and carbon conversion (near 1.0) were in good agreement with the reference data.

1. Introduction

The integrated gasification combined cycle (IGCC) process is a representative power generation technology because of its high efficiency and environmental advantages over the conventional pulverized coal fired process. Since the syngas composition is determined by the gasifier, the gasification process is regarded as one of the most important processes in IGCC. The gasifier operation is characterized by different flow type mechanisms, including moving-bed processes (e.g., Sasol-Lurgi dry bottom process and BGL slagging process), fluid-bed processes (e.g., Wrinkler process, HTW process and CFB processes) and entrained flow processes (e.g., Shell process, GE process and MHI process).

The entrained flow type gasifiers have several advantages over other types: (1) the ability to utilize any type of coal, (2) high coal throughput capacity particularly at high pressures, (3) product gas is free of tars, (4) high carbon utilization due to high reaction rates [1]. On the other hand, since the gasifier requires a high temperature to operate, the wall structure for preventing heat loss or recovering heat becomes complex and expensive, and consequently, the capital cost increases. During operation, high-temperature waste-heat recovery from the produced syngas is crucial to production of HP (high pressure) and MP (medium pressure) steam for use in the combined cycle.

---

* Corresponding authors. Tel.: +82 2 2123 2762; fax: +82 2 312 6401.
E-mail addresses: minoh@hanbat.ac.kr (M. Oh), leech@yonsei.ac.kr (C.-H. Lee).

http://dx.doi.org/10.1016/j.apenergy.2014.06.044
0306-2619/

Nomenclature

Capital letters

A	area (m^2) or area per control volume (m^2/m^3)
C	mole concentration ($mole/m^3$) or mass concentration (kg/m^3)
D	diffusivity (m^2/s)
F	friction ($kg/m^2/s^2$) or multiflier (–)
HS	heat sources ($J/m^3/s$)
$(HS)'$	heat sources per axial length (kg/m/s)
HT	heat transfer rate ($J/m^3/s$)
MS	mass sources ($mole/m^3/s$) or ($kg/m^3/s$)
MT	mass transfer rate ($kg/m^3/s$)
P	pressure (Pa) or perimeters (m)
Q	heat transfer rate ($J/m^3/s$)
Re	Reynolds number
T	temperature (K)
Y	yield (–)
CGE	cold gas efficiency (%)

Lowercase letters

c_p	heat capacity (J/mole/K)
d	diameter (m)
f	friction factor
f_c	correlating factor
g_z	gravitational acceleration (m/s^2)
h	heat transfer coefficient ($W/m^2/K$) or enthalpy (J/kg)
k	thermal conductivity (W/m/K)
m	mass per char particle (kg/#)
$\dot{m}$	mass flow rate (kg/s)
p	pressure (Pa)
q	heat flow rate (J/s)
q_{flux}	heat flux ($J/m^2/s$)
q'	linear heat flowrate (J/m/s)
r	radius (m)
t	time (s)
u	velocity (m/s)
x	mass fraction (–) or vapor fraction (–)
x_l	thickness of slag layer (m)
x_m	thickness of membrane (m)
$\triangle x$	wall layer thickness (m)
y	volume fraction (–)
y_m	width of membrane (m)
$\triangle y$	width of control volume (m)
z	axial position (m)

Greek letters

Δ	arbitrarily small number
ε	volume fraction (m^3/m^3) or porosity (m^3/m^3) or emissivity (–)
μ	viscosity of slag (Pa s)
ρ	density (kg/m^3) or number density ($\#/m^3$)
σ	Stefan–Boltzmann constant (5.67e-11 $kW/m^2/K^4$)
υ	stoichiometric coefficient for reactions
Ω	wall roughness (m)
ψ	particle structural parameter
ϕ	mechanism factor based on the stoichiometric relation of CO and CO_2
β	angle of the wall from the vertical direction

Subscripts and superscripts

0	initial conditions
cb	convective boiling
conv	convective
cs	cross section
daf	dry ash free
dev	devolatilization
g	gas
gw	gas to wall
Hetero	heterogeneous reactions
Homo	homogeneous reactions
i	gas phase component or inner
L	liquid
m	membrane
N	number
nb	nucleate boiling
o	outer
ONB	onset of nucleate boiling
p	char particle
pf	pressure correction factor
pg	particle to gas
pw	particle to wall
r	reduced
rad	radiative
RXN	reactions
sat	saturation
Sur	surface
Tot	total phase (gas + solid) or total gas phase component
tp	two phase
Vap	vapor
VM	volatile matter
w	wall

Computer-based process simulation can help in obtaining insight into the gasification process and in developing a deeper understanding of the optimal operation of the gasifiers. Many researchers have developed mathematical models for entrained flow gasifiers [2–14]. Table 1 shows the literature reviews of modeling work on entrained-type gasifiers. It includes one-dimensional (1-D) process models [3–6] and 3-D computational fluid dynamics models [6,8–10], and ranges from equilibrium models [2] to rate-based models [3–6] of the reaction kinetics.

Rigorous 3-D CFD models [6,8–10] usually consider turbulence and gas recirculation because they employ momentum balances for the turbulent flow and mixing rate of the gas mixture. However, the higher order models are computationally too demanding, so they are generally used for a normal practice as stand-alone models. Furthermore, the gasifier model must be integrated into an overall IGCC process for efficiency evaluation and operability tests.

Hitherto, most of the process models developed have not included momentum balances [2,3,5,7]. Then, a model including a 1-D momentum balance with an interaction between the gas and solid was developed in terms of a 1-D Navier–Stokes equation [4]. Recently, a model considering mixing and recirculation effects using a reactor network model was suggested [11,12]. In addition, a heuristic recirculation model, that considers these effects, has also been reported [14].

The gasifiers in IGCC generally contain a water circulation system to recover heat. The Shell gasifier also has a membrane wall which consists essentially of high-pressure water tubes and a slag flow layer formed at the reactor wall. Gazzani et al. [13] also suggested a reactor model incorporated within the membrane wall model. In this model, the membrane wall model was simplified and changed to analytic forms by using the equivalent extended fin model.