Fuel 111 (2013) 461–471

Contents lists available at SciVerse ScienceDirect

Fuel

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

Effects of combustion parameters on reforming performance of a steam–methane reformer

Jae Seong Lee, Juhyeong Seo, Ho Young Kim *, Jin Taek Chung, Sam S. Yoon

School of Mechanical Engineering, Korea University, 5-Ga, Anamdong, Sungbukgu, Seoul 136-701, Republic of Korea

HIGHLIGHTS

- Effects of combustion parameters on the characteristics of a fuel cell reformer.
- Fuel ratio and equivalence ratio as the combustion parameters.
- Optimization of the production rates of H_2 and CO can be achieved by adjusting the combustion parameters.

ARTICLE INFO

Article history:
Received 25 June 2012
Received in revised form 17 April 2013
Accepted 28 April 2013
Available online 14 May 2013

Keywords:
Combustion parameters
Fuel ratio
Equivalence ratio
Fuel cell
Reformer

ABSTRACT

The effects of combustion parameters on the reformer performance were studied in a 1-kW fuel cell reformer. A reformer system was numerically simulated using a simplified two-dimensional axisymmetric model domain with an appropriate user-defined function. The numerical results were compared with experimental data for validation. The fuel ratio, based on the flow rate of methane in the reforming reactor, was varied from 20% to 80%. The equivalence ratio was changed from $\phi = 0.5$ to 1.0. The results indicated that as the fuel ratio increased, the production rates of hydrogen and carbon monoxide increased, although their increase rate reduced. In fact, at the highest heat supply rates, the hydrogen production rate was actually slightly decreased. Simulations showed that the mixture had the highest fuel conversion rates and production rates of reformate gas at certain equivalence ratio and fuel ratio. This finding implies that adjusting the equivalence ratio and fuel ratio can significantly change the reformer characteristics and that the reforming performance can be optimized by adjusting them.

1. Introduction

With the growing world population and energy demand, it is clear that fossil fuels must be offset by sustainable, clean energy sources. Fuel cells are one of the most promising alternatives among new renewable energy sources, especially in the power generation field. For power generation or large-building applications, the Molten Carbonate Fuel Cell (MCFC) and the Solid Oxide Fuel Cell (SOFC) are most often used. MCFC and SOFC consume syngas, which is comprised of hydrogen and carbon monoxide, as fuel. Because syngas is produced in the reforming process, in which hydrocarbon fuels are converted to hydrogen and carbon monoxide, it is important to understand this process as well as the heat transfer process in the reformer, for the design an optimal fuel-cell system. Because the reforming process involves complex chemical reactions, heat-flow and reforming characteristics are difficult to measure experimentally. Computational modeling of the reforming process is also challenging because the reforming process includes both complex combustion and reforming reactions, which must be modeled simultaneously.

Steam reforming is the most common method for producing hydrogen in the chemical process industry. The primary steam reforming reaction is strongly endothermic, and reactor designs are typically limited by heat transfer rather than reaction kinetics [1]. Several numerical approaches have investigated steam reformers [2–14]. Hoang et al. [2] and Lee et al. [3] experimentally and numerically investigated steam reformers, assuming either constant wall temperature or heat flux conditions. They examined the effects of parameters such as furnace temperature and steam-to-carbon ratio on the performance of the reformer. Pina et al. [4] studied the influence of the heat-flux axial profiles on an industrial primary steam reformer with respect to outlet methane conversion, process gas temperature, tube-skin temperature, and equilibrium reactions. Pedenera et al. [5] and de Jong et al. [6] used heat transfer coefficient models to simulate the heat transfer from the flue gas to the reactant gas in reformer tubes. Pedenera et al. [5] examined the effects of reforming tube diameter and catalyst activity distribution on reformer performance. De Jong et al. [6] evaluated the effects of design modifications on the

* Corresponding author. Tel.: +82 2 3290 3356; fax: +82 2 929 3082.
E-mail address: kimhy@korea.ac.kr (H.Y. Kim).

0016-2361/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.fuel.2013.04.078

Nomenclature

A (k_i)	pre-exponential factor of rate coefficient, k_i
A (K_j)	pre-exponential factor of adsorption constant, K_j
c_p	specific heat at constant pressure (J kg^{-1} K^{-1})
D	diffusion coefficient (m^2 s^{-1})
E	energy (J)
$E_{a,1}$, $E_{a,2}$, $E_{a,3}$	activation energy of reaction I, II, III (J kmol^{-1})
F	momentum sources include Reynolds stresses (N m^{-3})
g	gravitational acceleration (m/s^{-2})
h	enthalpy (J)
ΔH	enthalpy change due to reaction or adsorption (J kmol^{-1})
$\vec{J}$	diffusion flux (kg m^{-2})
k	turbulence kinetic energy (m^2 s^{-2})
k_1, k_2, k_3	rate coefficient of reaction I, II, III
K_1, K_3	equilibrium constant of reaction I, III (bar^2)
K_2	equilibrium constant of reaction II
$K_{CH_4}, K_{CO} K_{H_2}$	adsorption constants for CH_4, CO, H_2 (bar^{-1})
K_{H_2O}	adsorption constant for H_2O
M_W	molecular weight (kg kmol^{-1})
p	pressure (Pa)
p_i	partial pressure for component i (Pa)
r_1, r_2, r_3	rates of reaction I, II, III (kmol m^{-3} s^{-1})
R	net rate of production by chemical reaction (kg m^{-3} s^{-1})
R_0	universe gas constant (J kmol^{-1} K^{-1})
S_h	volumetric heat sources (W/m^{-3})
T	absolute temperature (K)
v_x, v_r	velocity components (m s^{-1})
Y	mass fraction

Greek symbols

β	inverse effective Prandtl number
ε_d	turbulence dissipation (m^2 s^{-3})
ε_v	void fraction
η	effectiveness factor
λ	thermal conductivity (W m^{-1} K^{-1})
μ	viscosity (kg m^{-1} s^{-1})
ρ	density (kg m^{-3})

Subscripts

i	species i
j	species j
m	mixture
s	solid

performance of the reformer. Kvamsdal et al. [7] also applied a heat transfer coefficient model, one that accounted for radiation and convection as well, to estimate the heat transfer from the combustion chamber to the reactor. Kvamsdal et al. [7] evaluated several correlations of the wall heat transfer coefficient and effective radial thermal conductivity and the effects of these correlations on the dynamic responses of reformers with reduced feed flows. Murty and Murthy [8], Shayegan et al. [9], and Latham et al. [10] developed heat transfer models that accounted for both convection and reaction. Murty and Murthy [8] investigated the influence of various parameters, such as the steam-to-carbon ratio, system pressures, inlet tube temperatures, flame length, and reformer size, on reformer performance. Shayegan et al. [9] simulated a steam reformer with a low Reynolds number, large tube diameter, and no extra steam in the feed. Latham et al. [10] developed a mathematical model of an industrial steam–methane reformer and estimated important system parameters. Brus and Szmyd [11] used a radiative model to simulate the heat transfer from the furnace to the reactor; they examined the effects of the reformer position in the module chamber and the emissivity of the reformer surfaces on the temperature and methane conversion characteristics of the reformer. Grevskott et al. [12] solved for heat conservation in the furnace and included source terms to represent radiative energy and energy inflow from the burners. They varied the steam-to-carbon ratio, operating pressure, and heat transfer coefficients of the fixed-bed tube. Seo et al. [13] and Park and Bae [14], respectively, used an Eddy-dissipation model and an Eddy breakup model for combustion reaction analyses. Seo et al. [13] and Park and Bae [14] also considered radiative heat transfer in a discrete radiation transfer model. Seo et al. [13] investigated the heat transfer to the catalyst beds and the catalytic reactions of steam–methane reforming as a function of operation parameters. Seo et al. [13] also examined the effects of the cooling heat flux along the outside wall of the system and the steam-to-carbon ratio on the conversion of methane and carbon monoxide. Park and Bae [14] investigated the effects of reactant flow rate and fuel ratio on the performance of two different reformers.

Researchers have primarily examined the reformer system, neglecting the fact that the system really includes both reforming and combustion reactions. They typically considered parameters such as steam-to-carbon ratio, flow rate in the reforming tube, size and shape of the reformer, temperature and pressure at the tube inlet, and so on. Almost universally, they used heat transfer empiricisms without solving rate equations of combustion reactions. This work focuses on the effects of combustion parameters on reformer performance by simultaneous modeling the reforming reactor and the combustion furnace accounting for reaction kinetics. For an industrial steam reformer, the fuel ratio, defined as the ratio of the methane flow rate in the combustor to that in the reactor, was varied from 20 to 80. The equivalence ratio was changed from $\phi = 0.5$ to 1.0. The kinetics of the steam–methane reaction outlined by Xu and Froment [15] was used to represent the reforming reaction, while an Eddy-dissipation model was used to simulate the combustion reaction in the furnace [16]. Both reaction kinetics were built into the model with user-defined functions. The results of this work provide insights into the operating conditions within the combustion furnace of a reformer, specifically 1-kW MCFC and SOFC fuel cells. The steam reformer is simulated as a two-dimensional axisymmetric system, and the simulation results are compared with experimental data for validation. Then, the effects of combustor-to-reactor fuel ratio and the equivalence ratio on the reformer system are simulated and discussed. The overall results are summarized as plots of temperatures, accumulations of wall heat flux, mole fractions of the species along the reactor or at the reactor outlet, and contours of some parameters used to evaluate the reformer performance.

2. Experimental description

As shown in Fig. 1, a mixture of steam and methane gas passes through the reactor filled with a nickel-based catalyst where the mixture is reformed by the heat supplied by the combustion furnace surrounding the reactor. Table 1 presents the experimental specifications including the catalyst properties. Mass-flow controllers quantified the flow rates of methane and air. Distilled (DI) water was delivered by a pump. For the reforming reaction, methane gas and water vapor were supplied to the catalyst via a vapor coil, which heats the reactants. For the combustion reaction,