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# Numerical study of effect of operating and design parameters for design of steam reforming reactor

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ABSTRACT

A numerical study on the design of a steam reforming reactor consisting of several reforming tubes and one burner is conducted with respect to various operating and design parameters such as GHSV (gas hourly space velocity), input heat capacity, catalyst layer length, and number of tubes. The calculation of the reforming reaction rate is coupled with a three-dimensional heat and mass transfer calculation. It is shown that a large temperature gradient exists in the reforming reactor, resulting in significant variation of the gas temperature and reaction rate along the reforming tube. The reduction of the catalyst layer length induces a decrease in $H_2$ (hydrogen) concentration as well as pressure loss. An increased number of tubes leads to better system efficiency owing to the enhanced heat transfer to the reforming tube. Consequently, to improve the system efficiency and reduce the pressure loss, an increase in heat transfer area and decrease in catalyst layer length should be essential design considerations.



## 1. Introduction

Owing to concerns such as global warming, environmental regulations worldwide have become more stringent in recent years. Among other things, this has led to increasing interest in the use of $H_2$ (hydrogen) as an alternative fuel. Accordingly, the reforming process for $H_2$ production has attracted increased attention. Reforming can be performed by various approaches such as steam reforming, partial oxidation reforming, and auto-thermal reforming. Among these, steam reforming is used most widely owing to the fact that its $H_2$ yield is the highest and that it shows long-term stability [1–4].

Numerical simulations are considered as a useful tool in the development of an efficient steam reforming reactor. They can be used to inexpensively investigate the effects of operating and design parameters, and the obtained results can provide basic data for designing and experimentally testing such systems. Therefore, numerous approaches have been widely applied to the study of steam reforming systems. Rajesh et al. [5] used a mathematical model for simulating a steam reformer and demonstrated the possibility of enhancing the productivity of the steam reformer by performing a multiobjective optimization. Hsieh and Lu [6] investigated the heat-transfer process in the thermally developing region of a porous medium for simulating chemical catalytic beds. Seo et al. [7] numerically investigated a compact steam reforming system integrated with a water–gas shift reactor. They examined the effect of the cooling heat flux at the outside wall of the system and the SCR (steam to carbon ratio). It was confirmed that methane conversion and carbon dioxide reduction increase with SCR. Lee et al. [8] carried out parametric studies of the furnace temperature, SCR, and configuration of a packed bed by using a heterogeneous 2-D model. They showed that an appropriate SCR should be selected in order to maximize the hydrogen production rate and a bed packed repeatedly with inert and active catalysts should be an efficient means to achieve the better hydrogen production with small amounts of the active catalysts compared with a typical steam reformer. Park et al. [9] suggested a modified convective heat transfer coefficient considering a heat sink caused by the endothermic reaction in the steam reformer. They analyzed the effects of wall temperature, and showed that high wall temperature induces high fuel conversion rate. Hofmann et al. [10] simulated a steam reforming reactor by using two different models such as a heterogeneous reaction mechanism model and a global kinetic model. It

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was found that the predicted reforming rates differ according to the model approach. Iwai et al. [11] modeled the steam reforming reaction in a DIR (direct-internal-reforming) planar SOFC (solid oxide fuel cell). They showed that an endothermic DIR reaction actively proceeds near the inlet region and reduces the local temperature in the total SOFC system. These studies focused on a simplified 2-D reactor configuration in order to mainly investigate the effect of specific parameters on the steam reforming characteristics. Therefore, the complicated reactor including the combustion chamber as a heat source is not considered, but the heat transfer to catalytic beds is simplified, such as the assumption of constant heat flux at the wall of the catalytic beds except in one study [7].

Recently, studies on 3-D numerical calculations have been published for considering a complicated reactor configuration. Arzamendi et al. [12] conducted a numerical study of the thermal integration of steam reforming and combustion of methanol in a catalytic micro-channel reactor. They presented the fuel conversion rate and the temperature distribution in the reactor according to different channel reactor size and configurations. Hao et al. [13] numerically investigated the effects of the micro-reactor structure and catalyst-coated method on the conversion rate. The optimal micro-reactor structure and catalyst thickness are proposed based on the simulation results. Behnam et al. [14] showed that trends in methane conversion were well represented by CFD (computational fluid dynamics) simulations for a very small single-pellet-string reactor. These studies focused on a micro-sized reactor under low temperature operation of 200–300 °C or simulations using the simplified heat source instead of combustion. Hence, it is limited to obtain information about the design of a medium-sized reactor operated under high temperatures exceeding 800–900 °C and having a combustion chamber.

Few studies have focused on 3-D calculations of a medium-sized reactor for application to an onsite hydrogen station ($H_2$ production: 30–300 $Nm^3\ h^{-1}$) [15]; such calculations are required for determining the various operating and design parameters of a medium-sized reactor. This study aims to bridge this gap through a numerical investigation of a medium-sized reactor considering combustion (target $H_2$ production: 30 $Nm^3\ h^{-1}$) for various operating and design parameters such as GHSV (gas hourly space velocity), input heat capacity, catalyst layer length, and number of tubes. A numerical model applicable to the steam reforming system is established and validated through a comparison of the numerical results with previous experimental data. The steam reforming reactor is analyzed with respect to various operating and design parameters to realize an optimized design for the medium-sized reactor of an onsite hydrogen station.

## 2. Numerical models

### 2.1. Calculation domain

Fig. 1 shows a schematic diagram of the steam reforming reactor. The reactor consists of several reforming tubes and one burner. For an endothermic process, the supplied fuel ($CH_4$) and air are burned in the reactor. The produced combustion gas provides heat to the reforming tube and then exhausts out through an exit in the bottom region. Each reforming tube has an annular tube structure in which the reactant gases ($CH_4$, $H_2O$) enter from the outer side and the reforming gases ($H_2$, CO, $CO_2$, etc.) exit from the inner side as shown in Fig. 1. Table 1 lists the geometrical parameters of the reactor.

### 2.2. Governing equation

The governing equations for the three-dimensional domain are given by Eqs. (1)–(5).

Continuity equation:

$$\nabla\cdot(\rho\vec{u}) = 0 \tag{1}$$

Momentum equation:

$$\nabla\cdot(\rho\vec{u}\,\vec{u}) = -\nabla p + \nabla\cdot(\vec{\tau}) + \rho\vec{g} \tag{2}$$

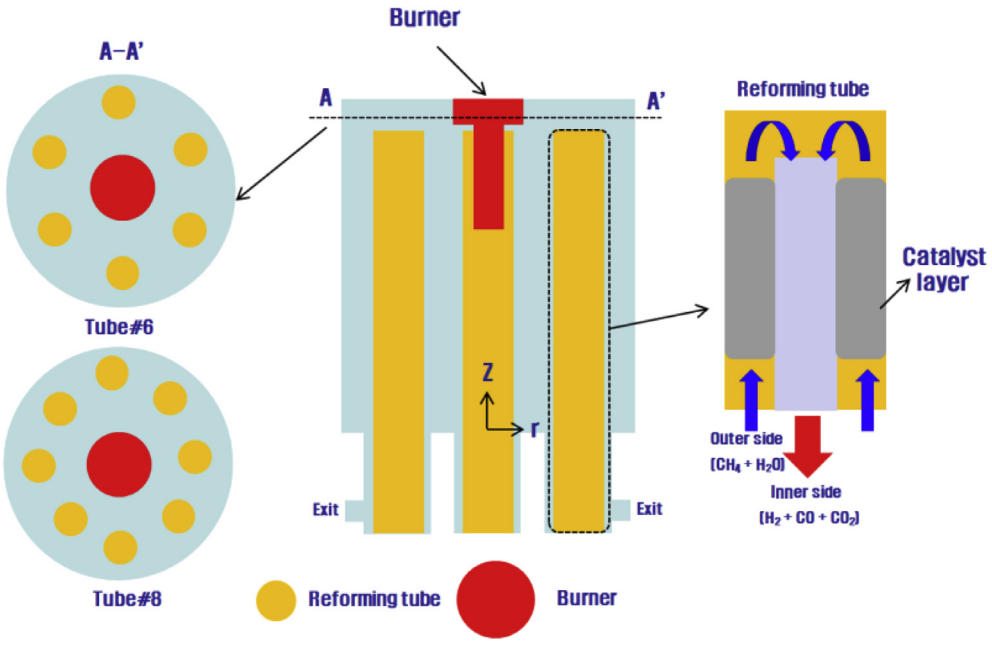


**Fig. 1.** Schematic diagram of steam reforming reactor.