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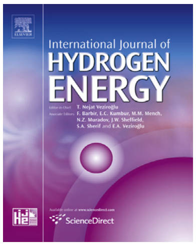

Hydrogen production by compact combined dimethyl ether reformer/combustor for automotive applications

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ABSTRACT

A computational study of hydrogen production by a dimethyl ether reformer combined with a catalytic combustor is conducted to investigate its feasibility for on-board automotive applications. The combined reactor has a stacked channel structure consisting of alternating reformer monoliths and catalytic combustor monoliths on a heat-conducting substrate. The inner surfaces of the walls of each monolith are coated with reforming and combusting catalysts, respectively. The effects of the feeding flow rate, thermal conductivity of the substrate, and porosity of the catalyst layer on the hydrogen production efficiency of the proposed combined reactor are investigated to determine the optimal design and operating conditions.

Introduction

Hydrogen fuel cell vehicles are thought to be the ultimate clean cars and represent the hydrogen economy of the future. Great effort has been made to commercialize and introduce hydrogen fuel cell vehicles worldwide for the last 20 years. It is, however, unusual to find fuel cell vehicles running on streets. In addition to the high cost of fuel cell vehicles, hydrogen supply is the most important challenge in moving toward the hydrogen economy. Building hydrogen infrastructure such as hydrogen production plants, pipelines, and stations is extremely costly and is not viable in the near future, although ultimately it must be constructed. However, fuel cell vehicles should be introduced concurrently with the construction of a hydrogen infrastructure to promote a smooth transition to the hydrogen economy. Alazemi and Andrews conducted a comprehensive review of hydrogen stations for automotive applications [1], which reported that the number of hydrogen stations operating worldwide to date is less than 200. Until the hydrogen infrastructure becomes mature, on-board fuel reforming can be a feasible and reasonable technology, serving as a solid stepping stone for automotive applications. Although several types of hydrogen production technologies have been investigated, as listed in Table 1, only some of them are suitable for on-board applications, which require fast start-up and high energy density.

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Table 1 – Hydrogen production technologies.

Technology	Advantages	Disadvantages
Thermal cracking of methane	Low initial investment Low fuel cost	High temperature (>1600 °C) [1]
Methane steam reforming	Low fuel cost	High temperature (700–1000 °C) [1] Low hydrogen purity
Water electrolysis	Pure hydrogen	High production cost (electricity required) (6.3–25.4 $ kg^{-1})
Coal gasification	Low fuel cost	High temperature (>900 °C) Air pollution
Diesel reforming	Easy to handle (liquid) Conventional fuel station	Fossil fuel [2]
Methanol reforming	Easy to handle (liquid) Low reforming temperature	Toxic

Liquid fossil fuels such as diesel and gasoline have good usability because they have a broad distribution network worldwide. However, most liquid fossil fuels possess long carbon chains, which lead to the production of CO_x and particulate matter (see Fig. 1). In addition, these carbon chains are difficult to break in reforming processes, which implies that hydrogen production from these materials would require considerable energy. For these reasons, methanol has received much attention from various researchers as a hydrogen source. Instead of strong C–C bonds, methanol is rich in hydrogen and oxygen, which facilitates clean combustion. Amphlett et al. [3] conducted a fundamental study of hydrogen production by methanol reforming for fuel cell vehicles. They simplified the reforming kinetics of methanol into three elementary steps: methanol steam reforming, methanol decomposition, and water–gas shift. In addition, optimization of the reactor design to achieve high hydrogen throughput is an important issue [4–7]. Instead of conventional catalytic reactors, which require expensive noble metal catalysts, membrane reactors using inexpensive inorganic material can be applied for methanol reforming. A comprehensive review of methanol reforming technologies, including membrane reactors, was conducted by Iulianelli et al. [8].

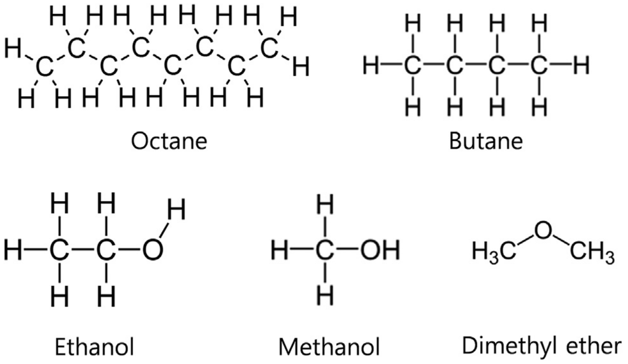

Fig. 1 – Molecular structures of hydrocarbon fuels.

Although methanol has several benefits, including economic advantages, it is toxic in the liquid or vapor phase. Dimethyl ether (DME) is a relatively non-toxic, eco-friendly synthetic fuel that can be inexpensively produced by recycling fossil fuels. A comprehensive review of DME production technologies was conducted by Azizi et al. [9]. Semelsberger et al. [10] discussed the possibility of using DME as an alternative fuel for internal combustion engines. In terms of hydrogen production, because DME has more hydrogen atoms than methanol, it produces more hydrogen than methanol through steam reforming, as follows:

$$\text{DME steam reforming} \quad (CH_3)_2O + 3H_2O \rightarrow 6H_2 + 2CO_2 \tag{1}$$

$$\text{Methanol steam reforming} \quad CH_3OH + H_2O \rightarrow 3H_2 + CO_2 \tag{2}$$

Although the overall reaction is expressed by Eq. (1), the following process will actually occur depending on the temperature and DME/H_2O ratio.

$$(CH_3)_2O + xH_2O \rightarrow a(CH_3)_2O + bH_2O + cH_2 + dCO_2 + eCO \tag{3}$$

For example, the thermodynamic equilibrium values of the coefficients in Eq. (3) are $a = 4.0\%$, $b = 4.4\%$, $c = 66.4\%$, $d = 16.1\%$, and $e = 8.9\%$ when x is 2.0 at 400 K and 1 atm. This result implies that a postprocessing apparatus is necessary to remove carbon monoxide at the channel outlet, because CO typically leads to catastrophic catalyst contamination. The calculation of thermodynamic equilibrium in DME reforming was discussed by Semelsberger and Borup [11].

Most research on DME reforming focuses on the development of new catalyst [12–15] and theoretical studies on the kinetics [16–23]. DME is easy to handle because it can be liquefied under relatively low pressure (~8 bar), in contrast to the high pressure (~700 bar) required for hydrogen. In addition, DME can be easily reformed to hydrogen and carbon dioxide through a catalytic reaction with water at relatively low temperatures (<400 °C), which enables miniaturization of the reforming system to a size appropriate for vehicle installation. It is, however, an endothermic reaction that requires external thermal energy to sustain a steady reforming process. To provide a DME reformer with the required heat, DME combustion can be used, because DME has a relatively high energy content, as shown in Eq. (4).

$$(CH_3)_2O + 3O_2 \rightarrow 3H_2O + 2CO_2 \quad \left(\Delta\overline{H}^0 = -1,460\ \text{kJ mol}^{-1}\right) \tag{4}$$

By using Table 2 under adiabatic combustion conditions at 700 K, the enthalpy of combustion through DME combustion is 9 times greater than the endothermic heat consumption through DME reforming, as follows:

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