



Technical Note

Mass transfer and reaction in methanol steam reforming reactor with fractal tree-like microchannel network



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ABSTRACT

A three-dimensional model of methanol steam reforming is developed and numerically analyzed to investigate the mass transfer and reaction in a fractal tree-like microchannel network. The effects of temperature, pressure and bifurcation angle on the reaction performance are examined and discussed. The reaction rate and “figure of merit” (FoM) in a tree-like network are evaluated and compared with corresponding serpentine channel. The results indicate that the existence of bifurcation plays an important role in the mass transfer and chemical reaction in a microreactor. The reaction rate and FoM in tree-like network are more superior to serpentine channel. In addition, in a tree-like network, the reaction rates are improved by increasing operating temperature and pressure. Interestingly, the role of branching angle on chemical reaction performance is less significant in a fractal microreactor.

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1. Introduction

The rapid development of proton-exchange membrane fuel cell (PEMFC) in recent years has stimulated great interest in fuel processing for hydrogen production [1]. The methanol is one of the attractive fuels for hydrogen production in mobile application, whether used directly or preprocessed by steam reforming (SR), partial oxidation (POX), or autothermal reforming (ATR) [2]. In particular, the SR is economical and more tuneable than POX and ATR, so it is a preferred method for hydrogen generation industrially [3]. One challenge for the wide utilization of MSR in mobile application is how to miniaturize the systems. Fortunately, the microreaction technology provided a good solution for this challenge [4–6]. Compared with conventional reactors, micro structured systems can be applied with particular success in highly exothermic and fast reactions due to the high heat and mass transfer rates, controllable short residence times, and uniform flow patterns. Until now, several MSR microreactor configuration for hydrogen production, including serpentine, parallel, semi-T-shaped and zigzag, have been numerically and experimentally studied, and these investigations [7–12] have demonstrated that the channel

structure has a significant role in the behaviors of mass transfer and chemical reaction in microreactors.

The fractal tree-like network (including vascular system, leaf venation, river flow network, etc) is a ubiquitous phenomenon in nature, which bring us a good inspiration for the optimization of heat and mass transfer system in practical engineering. Since Bejan firstly proposed tree network in electronics cooling with high conductivity path [13], the tree network has been represented a new trend in the optimization and miniaturization of micro transport devices, including heat sinks, mass exchangers and fuel cells, due to the inherent advantages of great efficiency in heat and mass transfer. Considering these advantages, the tree-like flow architectures have been introduced into the design of methanol steam reforming microreactor [9,10]. However, in this work, the kinetics of the methanol steam reforming is based on empirically correction factors for reforming and decomposition reactions. In this case, it is unable to determine the reaction rate related with operating pressure and temperature, so it is not clear how the operating parameters affects the reforming and decomposition reactions. In addition, the effects of bifurcation angle on the MSR performance in fractal microreactor is less understood. Therefore, based on a complete Langmuir–Hinshelwood (LH) kinetic approach, a three-dimensional MSR model is developed and numerically analyzed to investigate the mass transfer and reaction in a reactor with fractal tree-like network.

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Nomenclature

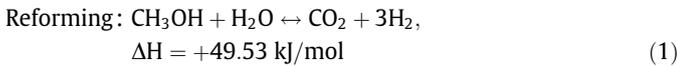
d_{cata}	thickness of catalyst, μm
k_R, k_{rW}	rate constant of MSR and rWGS
K_i	adsorption coefficient for surface species i
P	pressure, Pa
r_R, r_{rW}	rate of MSR and rWGS, $\text{mol s}^{-1} \text{m}^{-2}$
R_u	universal gas constant, $8.315 \text{ J mol}^{-1} \text{ K}^{-1}$
T	temperature, K

Greek symbols	
θ	bifurcation angle, $^\circ$
Subscripts	
cata	catalyst
i	species index
rW	reversed water gas shift
R	reforming

2. MSR reaction in a fractal tree-like microchannel network

A typical fractal tree-like microchannel network can be generated as follows: (1) Every rectangular channel with the same height h is divided into two branches ($N=2$) at the next level, and the bifurcation angle θ is identical for every bifurcation ($\theta=90^\circ$, see Fig. 1); (2) The channel length and hydraulic diameter at the k th branching level obeys $L_k=L_0N^{-k/D}$, $d_k=d_0N^{-k/\Delta}$, where L_0 and d_0 are the initial channel length and hydraulic diameter, D and Δ are the length and diameter exponent; (3) The recursion of branch generation is done m times and then a tree-like network is obtained. Note that the current structure of fractal network could only be viewed as a basic element of a microreactor, i.e. several basic elements are packaged for one reactor. To demonstrate the advantage of tree-like network, a corresponding serpentine reactor is also constructed. The serpentine channel possesses the same reaction area as tree-like network and its cross section is identical to the initial channel of tree-like network. In the simulation, $L_0=10$ and $w_0=2$ mm, $h=1$ mm, $D=2$ and $\Delta=3$.

In this paper, the commercial $\text{CuO}/\text{ZnO}/\text{Al}_2\text{O}_3$ catalyst (BASF F3-01) is uniformly deposited on channel walls with the catalyst thickness of $15 \mu\text{m}$ ($0.471 \text{ mg}/\text{cm}^2$). The reaction occurs only on the wall surfaces since the reactor is considered as the wall-coated. A complete Langmuir–Hinshelwood kinetic model as proposed by Sá et al. [14] is adopted to characterize the reaction at the catalyst surface. The LH kinetic model is a combination of MSR and reversed water gas shift (rWGS) as follows:



The reaction rate expressions for the elementary reaction steps are shown in Table 1. The chemical reaction rates of MSR and rWGS are [14,15]

$$r_R = \frac{k_R K_{\text{CH}_3\text{O}^{(1)}} \frac{P_{\text{CH}_3\text{OH}}}{P_{\text{H}_2}^{0.5}} \left(1 - \frac{P_{\text{H}_2}^3 P_{\text{CO}_2}}{k_R P_{\text{CH}_3\text{OH}} P_{\text{H}_2\text{O}}}\right) \cdot \text{CS}_1 \cdot \text{CS}_{1a} \cdot \text{SC} \cdot \rho_{\text{cata}} \cdot d_{\text{cata}}}{\left(1 + K_{\text{CH}_3\text{O}^{(1)}} \frac{P_{\text{CH}_3\text{OH}}}{P_{\text{H}_2}^{0.5}} + K_{\text{HCOO}^{(1)}} P_{\text{CO}_2} P_{\text{H}_2}^{0.5} + K_{\text{OH}^{(1)}} \frac{P_{\text{H}_2\text{O}}}{P_{\text{H}_2}^{0.5}}\right) \left(1 + K_{\text{H}^{(1a)}}^{0.5} P_{\text{H}_2}^{0.5}\right)} \quad (3)$$

$$r_{rW} = \frac{k_{rW} K_{\text{HCOO}^{(1)}} \cdot P_{\text{CO}_2} P_{\text{H}_2}^{0.5} \cdot \left(1 - \frac{P_{\text{H}_2\text{O}} P_{\text{CO}}}{k_{rW} P_{\text{CO}_2} P_{\text{H}_2}}\right) \cdot \text{CS}_1^2 \cdot \text{SC} \cdot \rho_{\text{cata}} \cdot d_{\text{cata}}}{\left(1 + K_{\text{CH}_3\text{O}^{(1)}} \frac{P_{\text{CH}_3\text{OH}}}{P_{\text{H}_2}^{0.5}} + K_{\text{HCOO}^{(1)}} P_{\text{CO}_2} P_{\text{H}_2}^{0.5} + K_{\text{OH}^{(1)}} \frac{P_{\text{H}_2\text{O}}}{P_{\text{H}_2}^{0.5}}\right)^2} \quad (4)$$

where k_R and k_{rW} are the rate constant of MSR and rWGS, K is the adsorption coefficient for surface species ($\text{CH}_3\text{O}^{(1)}$, $\text{HCOO}^{(1)}$, $\text{OH}^{(1)}$ and $\text{H}^{(1a)}$), and the expressions of these parameters are listed in Table 1. P is partial pressure of reaction species (CH_3OH , H_2O , H_2 , CO , CO_2), CS_1 and CS_{1a} are constants which indicate total surface concentrations as reported by Peppley et al. [15], SC is the specific surface area of catalyst, ρ_{cata} is the density of catalyst which is assumed to be $1300 \text{ kg}/\text{m}^3$, d_{cata} is the thickness of catalyst.

A three-dimensional model of steady heat transfer, fluid flow and multi-component transport reaction are considered. The mixture of the steam and methanol is assumed to behave like ideal gas and is considered as laminar flow. The governing equations of continuity, momentum, chemical species and energy in a micro-reactor are:

$$\nabla \cdot (\rho_{\text{mix}} \vec{V}) = 0 \quad (5)$$

$$\vec{V} \cdot \nabla (\rho_{\text{mix}} \vec{V}) = -\nabla P + \nabla \cdot (\mu_{\text{mix}} \nabla \vec{V}) \quad (6)$$

$$\nabla \cdot (\rho_{\text{mix}} \vec{V} Y_i) = -\nabla \cdot \vec{J}_i + M_i r_i \quad (7)$$

$$\nabla \cdot (\rho_{\text{mix}} C_{p,\text{mix}} \vec{V} T) = \nabla \cdot (\lambda_{\text{mix}} \nabla T) - \nabla \cdot \left(\sum_i h_i \vec{J}_i \right) - \Delta H_R r_R - \Delta H_{rW} r_{rW} \quad (8)$$

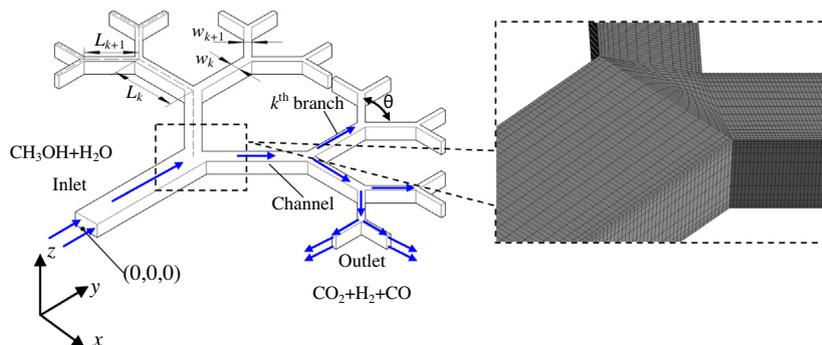


Fig. 1. Schematic of 3-D tree-like flow configuration ($\theta=90^\circ$).

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