

Design and optimization of segmented reformer based on NSGA-II optimization algorithms[#]

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ABSTRACT

The reformer is a key component in MRFC for on-site H₂ production and operation of HT-PEMFC. In this study, a segmented reformer was designed using heat transfer structure optimization to control the temperature segmentation of the reaction zone, achieving high conversion rate and low CO outlet molar fraction. The multi-objective optimization of methanol conversion rate and CO output molar fraction was conducted to determine the optimal structures with the NSGA-II optimization algorithm. Under the optimal structure, the methanol conversion rate of the segmented reformer reaches 99.6%, with a CO outlet mole fraction of 1.3%. For the output power, the MRFC with the segmented reformer can generate output power of 302 W, which provides reference significance for the commercialization of MRFC.

Keywords: reformer, HT-PEMFC, methanol, waste heat utilization

1. INTRODUCTION

The energy crisis and the deterioration of the ecological environment have forced people to focus on the development of green and renewable energy. In recent years, with the continuous maturity of hydrogen fuel cell technology on mobile devices, the development and use of hydrogen energy have quickly become a research hotspot. Hydrogen (H₂), as a clean renewable energy carrier, is considered the most promising alternative to fossil fuels [1]. However, the difficulties in H₂ storage and transportation have become one of the main obstacles limiting its further development. In this context, the method of on-site hydrogen production from hydrogen rich fuels through reforming reactions has quickly attracted people's attention due to its simple and convenient advantages. Methanol, as a liquid fuel from a wide range of sources, can be used to produce hydrogen on-site using reforming technology, with a high H₂ yield, low reforming temperature and low CO content,

as well as cheap catalyst [2-4]. Methanol reforming fuel cell (MRFC) is a combination of methanol steam reforming and high temperature fuel cell and it can provide solutions for portable energy or distributed energy. The HT-PEMFC is directly fueled by the reformed gas and does not require CO removal because the HT-PEMFC is highly tolerant to CO and unconverted methanol in the reformed gas [5]. In addition, the hydrogen-containing tail gas is fed to the combustion chamber to provide the heat required for reforming.

In MRFC systems, utilizing methanol or exhaust gas from the anode of fuel cell stacks to provide heat for reforming reactions can significantly improve system energy efficiency [6]. The structural design of the reformer is crucial for increasing the internal temperature and achieving high methanol conversion rates. Microchannel reactors have received widespread attention due to their high heat transfer efficiency. Zhou et al. [7] designed and manufactured microchannel structures using laser micro milling method, and used microchannels as catalyst carriers for methanol steam reforming. Mei et al. [8,9] designed and manufactured a new type of microreactor based on micro triggering technology, which uses a micro needle fin array to improve the compactness of hydrogen production microreactors. Chen et al. [10] proposed and designed a methanol steam microreactor with a tree like network structure, and numerically optimized its flow structure. However, the high cost and cumbersome manufacturing process limit the industrial application of microchannel reactors. At present, packed fixed bed reactors are still the main structure for practical applications. Yao et al. [11] enhanced convective heat transfer by arranging wavy fins, thereby improving reactor performance. Chein et al. [12] improved the temperature field inside the reformer by installing baffles in the reforming chamber. Zhang et al. [13] used spiral finned tubes for heating in tubular reactors to improve the performance of methanol reforming reactors. Ha et al. [14] investigated the effects of temperature, feed, and geometric

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dimensions on the conversion performance of tubular converters, and proposed the influence of residence time on CO selectivity.

The aim of this study lies in the segmented strengthening strategy in the methanol reformer that can ensure high conversion rates while achieving lower CO molar fractions in the MRFC system. The innovation of this study lies in the application of the multi-objective NSGA-II optimization algorithm to structural design. In this study, in the framework of an MRFC system with waste heat recovery, a combination structure of sine fins and flat fins was used in the combustion exhaust gas channel to achieve segmented heat transfer enhancement. The MRFC with the segmented reformer can generate an output power of 306 W, with a system efficiency of 49.3% and a CO outlet molar fraction of 1.1%, which provides reference significance for the commercialization of MRFC.

2. PHYSICAL AND MATHEMATICAL MODEL

2.1 Physical model of reformer

The structural model of the segmented reformer is shown in Fig.1. The reformer consists of a methanol water fuel overhear channel, a superheat chamber, a reforming chamber, and a combustion exhaust channel. The methanol water fuel superheat chamber adopts a plate fin structure. The combustion exhaust channel refers to the outermost fin channel of the reactor, with a fin spacing of 3 mm and a fin height of 8 mm. Methanol water fuel is preheated in the external superheat chamber and superheat chamber before entering the reforming chamber. Install 7 equally spaced baffles in the reforming chamber to increase the residence time of the reactants. The length of the reformer reaction zone is 150 mm. In the design of the reformer, a segmented

strengthening strategy was applied, which designs the fin channel of the combustion exhaust gas as a combination of flat fins and sine wave shaped fins. The sinusoidal fins at the entrance can improve the heat transfer effect and move the reforming reaction towards the front section of the reaction chamber.

2.2 Mathematical model of reformer

The following assumptions were conducted to simulate the numerical model:

- (1) MSR catalysts were considered as isotropic porous media.
- (2) The heat transfer between the reactor and the environment is natural heat convection.

Based on the above assumptions, the conservation of mass, momentum, energy, and component transport equations are established sequentially.

Continuity equation is

$$\rho(u \frac{\partial u}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial w}{\partial z}) = 0 \quad (1)$$

ρ is the fluid density, $\text{kg}\cdot\text{m}^{-3}$; u , v , and w are the fluid velocities in the x , y , and z directions, respectively.

Momentum equation is

x-direction

$$\epsilon \rho (u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z}) = -\epsilon \frac{\partial P}{\partial x} + \epsilon \mu_{\text{mix}} (u \frac{\partial^2 u}{\partial x^2} + v \frac{\partial^2 u}{\partial y^2} + w \frac{\partial^2 u}{\partial z^2}) + S_u \quad (2)$$

y-direction

$$\epsilon \rho (u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z}) = -\epsilon \frac{\partial P}{\partial y} + \epsilon \mu_{\text{mix}} (u \frac{\partial^2 v}{\partial x^2} + v \frac{\partial^2 v}{\partial y^2} + w \frac{\partial^2 v}{\partial z^2}) + S_v \quad (3)$$

z-direction

$$\epsilon \rho (u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z}) = -\epsilon \frac{\partial P}{\partial z} + \epsilon \mu_{\text{mix}} (u \frac{\partial^2 w}{\partial x^2} + v \frac{\partial^2 w}{\partial y^2} + w \frac{\partial^2 w}{\partial z^2}) + S_w \quad (4)$$

where ϵ is the porosity of the catalyst bed, μ_{mix} is the dynamic viscosity, $\text{Pa}\cdot\text{s}^{-1}$; P is operating pressure of the fluid, Pa.

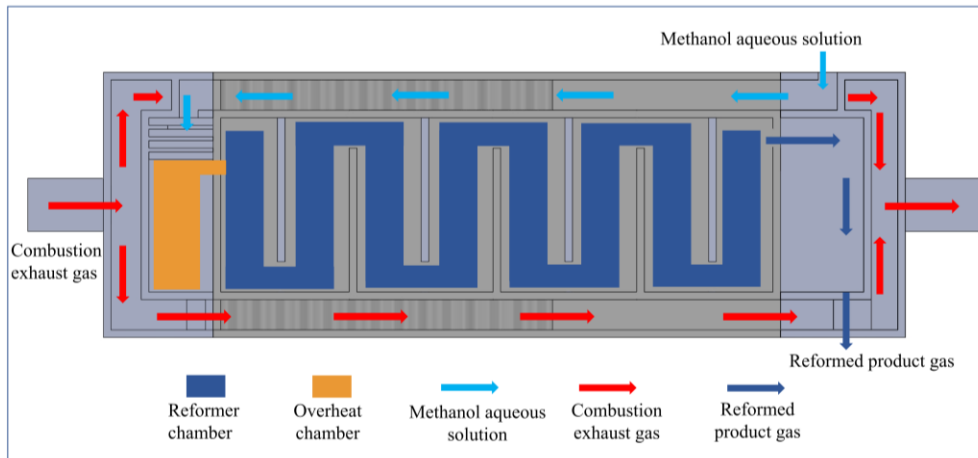


Fig. 1 Structure of a segmented reformer

Energy equation

$$\rho_f C_p \left(u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} + w \frac{\partial T}{\partial z} \right) = \lambda_{\text{eff}} \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + \epsilon S_t \quad (5)$$

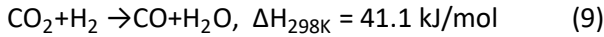
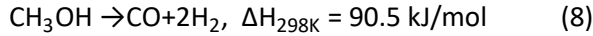
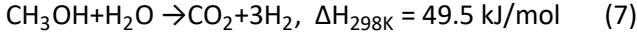
Component transport equation

$$\epsilon \left(u \frac{\partial m_i}{\partial x} + v \frac{\partial m_i}{\partial y} + w \frac{\partial m_i}{\partial z} \right) = D_{\text{eff}} \left(\frac{\partial^2 m_i}{\partial x^2} + \frac{\partial^2 m_i}{\partial y^2} + \frac{\partial^2 m_i}{\partial z^2} \right) + \epsilon \sum_{r=1}^N M_{w,i} R_r \quad (6)$$

where m_i is the mass fraction of component i , D_{eff} is the effective mass diffusion coefficient.

Methanol reforming kinetic

The material changes in the reforming chamber can be described by methanol water vapor reforming (MSR), methanol cracking (MD) and inverse water gas shift (rWGS) [15], as shown in Eq.(7)-(9).



According to the literature on kinetic models [16], the dual-rate MSR-rWGS was determined in the experimental system. The dual-rate MSR-rWGS kinetic model is as follows:

$$r_{\text{MSR}} = k_1 P_{\text{CH}_3\text{OH}}^{0.60} P_{\text{H}_2\text{O}}^{9.56} \left(1 - \frac{P_{\text{H}_2}^3 P_{\text{CO}_2}}{K_{\text{MSR}} P_{\text{CH}_3\text{OH}} P_{\text{H}_2\text{O}}} \right) \exp\left(-\frac{E_{\text{MSR}}}{RT_R}\right) \quad (10)$$

$$r_{\text{rWGS}} = k_3 P_{\text{H}_2}^{-6.0} P_{\text{CO}_2}^{0.78} \left(1 - \frac{P_{\text{H}_2\text{O}} P_{\text{CO}}}{K_{\text{rWGS}} P_{\text{H}_2} P_{\text{CO}_2}} \right) \exp\left(-\frac{E_{\text{rWGS}}}{RT_R}\right) \quad (11)$$

where E_{MSR} is MSR activation energy, 101440 J·mol⁻¹, E_{rWGS} is rWGS activation energy, 100887 J·mol⁻¹, k_1 , k_2 are the response finger prefactors, which are 6.14478×10^{-4} , 5.52158×10^9 , respectively.

2.3 HT-PEMFC

The theoretical open-circuit voltage E_{cell} of a single cell can be expressed by the Nernst equation [14], as shown in Eq.12.

$$E_{\text{Nernst}} = 1.229 - (8.5 \times 10^{-4})(T_{\text{FC}} - 298.15) + (4.308 \times 10^{-5}) T (\ln p_{\text{H}_2} + 1/2 \ln p_{\text{O}_2}) \quad (12)$$

Output voltage of single cell E_{cell} is:

$$E_{\text{cell}} = E_{\text{Nernst}} + \eta_{\text{act}} + \eta_{\text{ohm}} + \eta_{\text{con}} \quad (13)$$

where η_{act} is the activation polarization voltage [17], η_{ohm} is the Ohmic polarization voltage [18], η_{con} is the differential concentration polarization voltage [19].

The output power is:

$$W_{\text{FC}} = n E_{\text{cell}} I \quad (14)$$

2.4 NSGA-II optimization algorithm

NSGA-II has the advantages of fast running speed and good convergence, and has made progress in the field of energy optimization [20]. The NSGA-II algorithm was utilized to perform dual-objective optimization of the CO outlet molar fraction (f_{CO}) and methanol conversion rate ($\eta_{\text{CH}_3\text{OH}}$). The steps of NSGA-II optimization algorithm are shown in Fig.2.

The optimization model is

$$\begin{cases} \max F(x) = \max [f_{\text{CO}}, \eta_{\text{CH}_3\text{OH}}] \\ x_k = (a, b) \end{cases} \quad (35)$$

Optimization objectives $F(x)$ contains f_{CO} (CO outlet molar fraction) and $\eta_{\text{CH}_3\text{OH}}$ (methanol conversion rate).

Variable x_k contains a (the sinusoidal fin amplitude) and b (the length of wavy fins).

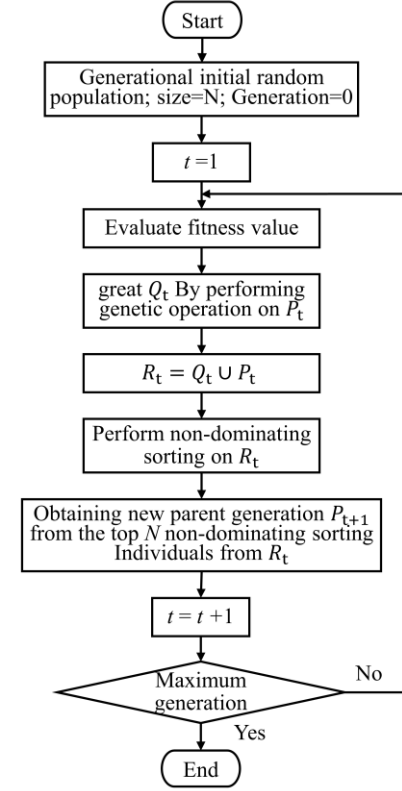


Fig. 2 Steps of NSGA-II optimization.

3. MATERIAL AND METHODS

3.1 Performance analysis

Fig.3 shows the effect of the segmented strengthening strategy on the methanol conversion rate and CO molar fraction at the outlet of the reformer. The high temperature in the latter half of the reforming chamber will promote the endothermic reaction of rWGS, resulting in an increase in CO mole fraction. The components in the reformed gas are crucial for extending the service life of HT-PEMFC. By adopting a segmented strengthening strategy, the temperature difference between the inlet and outlet of the reforming chamber can be increased, which can effectively reduce the mole fraction of CO at the outlet. The application of sine fins significantly enhances heat transfer, improves methanol conversion rate, and CO mole fraction.

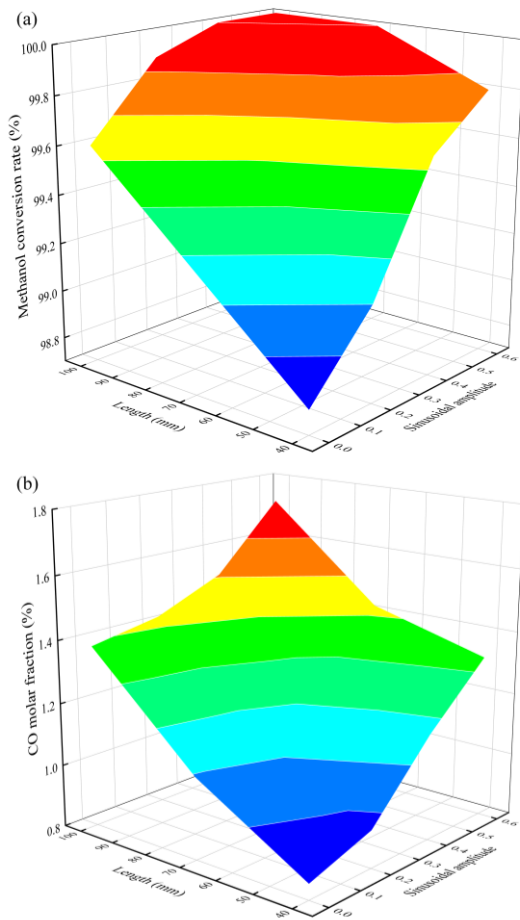


Fig.3 Effect of structure parameters on methanol conversion rate (a) and CO outlet molar fraction (b)

3.2 Optimization

Based on the influence of the length and the amplitude of the sine wave in the segmented reinforcement arrangement mentioned above, the genetic evolutionary algorithm NSGA-II was used to obtain the optimal structural parameters. Fig. 4 shows the Pareto front solution set obtained after optimization. In the Pareto front solution set, point B is considered the optimal solution as it is closest to the most ideal point A. The length and sine amplitude of the wavy fins represented by point B are 70 and 0.4, respectively. Under the optimal structural parameters, the methanol conversion rate and CO outlet mole fraction of the reformer can reach 99.6% and 1.3%, respectively. The MRFC system with segmented reformer can achieve an output power of 302 W at the methanol consumption of $212.5\text{g}\cdot\text{h}^{-1}$.

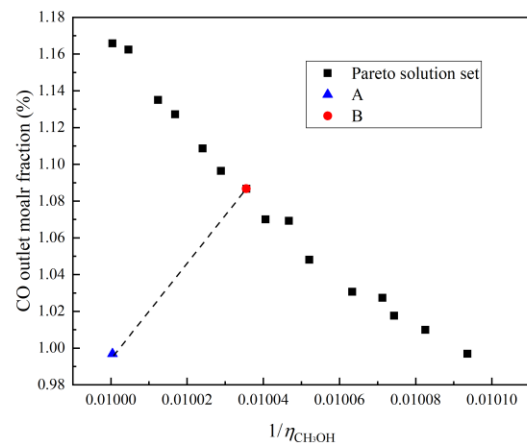


Fig.4 Pareto solution set

4. CONCLUSIONS

The reformer is a key component in MRFC for on-site H_2 production and operation of HT-PEMFC.

In this study, a segmented reformer was designed using heat transfer structure optimization to control the temperature segmentation of the reaction zone, achieving high conversion rate and low CO outlet molar fraction.

The multi-objective optimization of methanol conversion rate and CO output molar fraction was conducted to determine the optimal structures with the NSGA-II optimization algorithm.

For the output power, the MRFC with the segmented reformer can generate output power of 306 W, with a system efficiency of 49.3%, which provides reference significance for the commercialization of MRFC system.

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