

THERMAL MANAGEMENT OF METHANOL STEAM REFORMING REACTOR BY BACK PROPAGATION NEURAL NETWORK AND PARTICLE SWARM OPTIMIZATION ALGORITHM

Zhenzong He^{1,2,3}, Shijie Sun¹, Xinyu Jiang¹, Junkui Mao^{1,3}, Fengli Liang^{1,3}, Yao Fu⁴*

1. College of Energy and Power Engineering, Nanjing University of Aeronautics and Astronautics, Nanjing 210016, China
2. Low-carbon Aerospace Power Engineering Research Center of Ministry of Education, Nanjing 210016, China
3. Collaborative Innovation Center for Advanced Aero-Engine, Beijing 100191, China
4. Aviation Key Laboratory of Science and Technology on Aero Electromechanical System Integration, Nanjing, China

* Corresponding author, E-mail: hezhenzong@nuaa.edu.cn

Methanol steam reforming (MSR) reactor is a device that converts the methanol into hydrogen. Since the MSR is an endothermic reaction, the methanol conversion is usually affected by the heating conditions. So, to improve the methanol conversion, the heating condition should be managed. This study aims to present a framework and methodology for studying the thermal management of a determined MSR reactor by controlling the heating conditions. Firstly, the characteristics of a three-dimensional MSR reactor are carried out, and the effects of the inlet condition parameters e.g. heating parameters and fuel supply parameters, on the methanol conversion are investigated. Then, the performance prediction of the MSR reactor is studied using several common intelligence algorithms and the corresponding surrogate models are obtained. The back propagation neural network (BPNN) surrogate model shows the best prediction accuracy than stepwise linear (SL), radial basis function neural network (RBFNN), linear support vector machines (L-SVM), and random forest algorithms (RFA). Finally, the thermal management of the MSR reactor is carried out by combining the surrogate model and particle swarm optimization (PSO) algorithm to obtain better performance. The results show that hydrogen production of the MSR reactor can be generally guaranteed by the characteristic curves of the heating parameters and fuel supply parameters, and the methanol conversion can be maintained steadily above 93% within the whole period of the hydrogen production requirements.

Key words: Methanol steam reforming; Thermal management; Surrogate model; Hydrogen production

1. Introduction

Hydrogen is considered the best alternative to traditional aviation fuels (such as domestic RP-3 aviation kerosene) because of its high calorific value, zero emission and no pollution. Its application in aerospace and other fields has received wide attention from domestic and foreign research institutes and aero-engine manufacturers [1]. Despite many advantages as a clean energy source, hydrogen has challenges in storage and transportation. Storage and transportation technology is a key factor that enables hydrogen efficient development and utilization. It is also one of the bottlenecks that currently limit the large-scale use of hydrogen [2, 3]. Therefore, more and more scholars focus on separating and extracting hydrogen from its carriers using physical and chemical methods to meet the demand for hydrogen in modern society.

As a basic chemical fuel, methanol has many advantages, such as low cost, easy storage, low toxicity, high hydrogen-to-carbon ratio and sulfur-free [4]. Therefore, it stands out among many hydrogen production materials. With the appearance of high-efficiency and low-cost catalysts, hydrogen production by MSR has also attracted widespread attention in the industry due to the high hydrogen production, mild reaction, and low reaction temperature (523 K~573 K) [5, 6]. Li et al. [7] studied the catalytic methanol reforming hydrogen production technology and pointed out that among all hydrogen carriers, methanol shows great potential in hydrogen production due to its sustainability and transportation convenience. The reforming reactor is a key component for converting methanol to hydrogen, and its design is crucial to improve the efficiency of methanol steam reforming to hydrogen. To effectively improve methanol conversion and hydrogen production in reactors and reduce the energy consumption of the device, the reactor usually has a high specific surface area and high heat transfer efficiency so that it fully utilizes the heat provided by the external heat source to achieve efficient methanol reforming [8, 9]. Perng et al. [10] investigated the effects of parameters such as internal heater temperature, porosity, and porous sheath thickness of a cylindrical reformer on methanol conversion, hydrogen, carbon monoxide, and carbon dioxide production, as well as temperature and velocity fields under the same inlet conditions. The results showed that the methanol conversion and the hydrogen production rose with the increasing heater temperature, porosity, and porous sheath thickness.

Since the MSR is an endothermic reaction, the methanol conversion is usually affected by the heating conditions, which mean the heating conditions should be optimized to improve the methanol conversion. Therefore, the optimization problem should consider the production of hydrogen to meet the needs of other devices such as fuel cells while maximizing the conversion of methanol. Recently, the neural network has played an important role in performance prediction due to its ability to integrate multiple sources of information, process heterogeneous data, and capture changing dynamics. Moreover, the neural network also has strong feature extraction and abstraction capabilities. To optimize the MSR performance of a cylindrical reactor, Zheng et al. [11] used back propagation neural network (BPNN) to establish mathematical prediction models of the reaction performance of different reactors, optimized the computational model using genetic algorithm (GA) to obtain the optimal reaction parameters. The reliability of the optimal reaction parameters of the cylindrical hydrogen production reactor is verified through experiments. Pajak et al. [12] studied the optimal design of catalyst distribution in a small-scale methane/steam reforming reactor and used genetic algorithm (GA) for optimization to find the optimal value of methane conversion and the minimum value of the difference between the highest and lowest temperature in the reactor. Na et al. [13] took the catalyst

loading distribution inside the microchannel reactor as the variable. An optimization method combining CFD and genetic algorithm (GA) is used to optimize the temperature rise in the microchannel.

To find the best combination of the parameter to maximize the H₂ yield, Chen et al. [14] used neural networks to perform the predictions of CH₃OH conversion and H₂ yield in terms of the operating parameters of the methanol steam reforming reactor. Qi et al. [15] used the backpropagation (BP) neural network algorithm to develop the mapping relation model between the membrane reactor's prime operational parameters and fuel cell output performance for future integration system design and control application. Vo et al. [16] used artificial neural network to develop an optimization method for the adsorption-enhanced MSR process. Taking H₂ purity and CO₂ capture rate as constraints, the optimization was carried out to minimize the cost of hydrogen production.

The structure of the present work can be found in Figure 1. This study investigates the characteristics of the three-dimensional CFD MSR reactor proposed in the previous paper [17], and uses several common intelligent algorithms, namely back propagation neural network (BPNN), stepwise linear (SL), radial basis function neural network (RBFNN), linear support vector machine (L-SVM) and random forest algorithm (RFA) to predict the performance of the MSR reactor and obtain the corresponding alternative model. In addition, the BPNN proxy model was used to study the performance prediction of the three-dimensional CFD MSR reactor, and the PSO algorithm was used to optimize the reforming reactor. Finally, based on the determined hydrogen output demand curve, the optimal change laws of the heating condition parameters and fuel supply parameters was obtained to ensure a satisfactory methanol conversion rate.

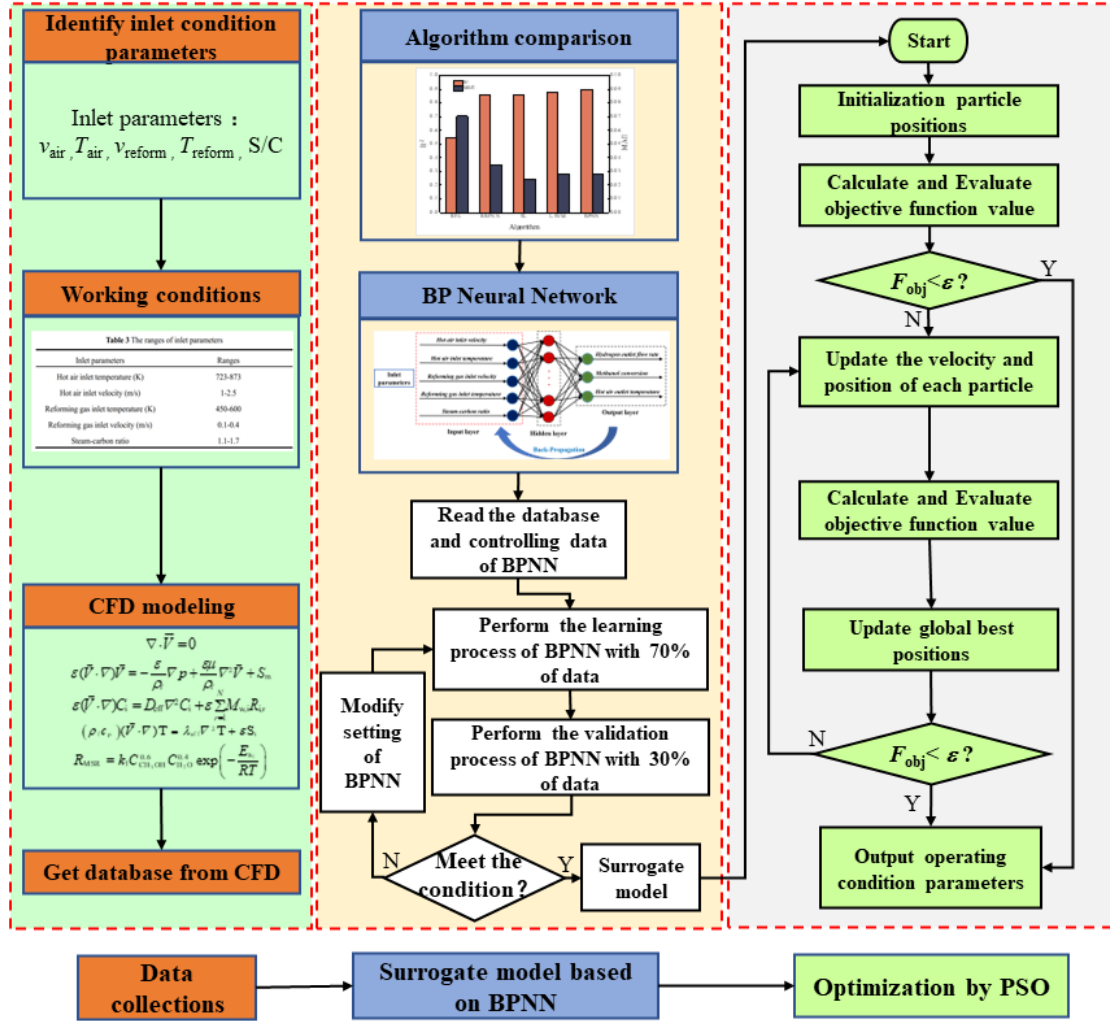


Fig. 1 The structure of the present work

2. Numerical methods

2.1. Model description

In our previous work [17], the cylindrical reforming reactor was designed with wave ribs to improve the reforming characteristics and increase the efficiency of the methanol reforming while minimizing the energy consumption of the device. The schematic diagram of the overall structure and cross-sectional dimensions of the reforming reactor are shown in Figure 2. The heat for the reforming reaction may be supplied by the waste heat from a heat engine device, e.g. the engine exhaust gas. The methanol and steam are introduced into the reactor in a certain mixing ratio. The geometrical parameters of the reactor are shown in Table 1.

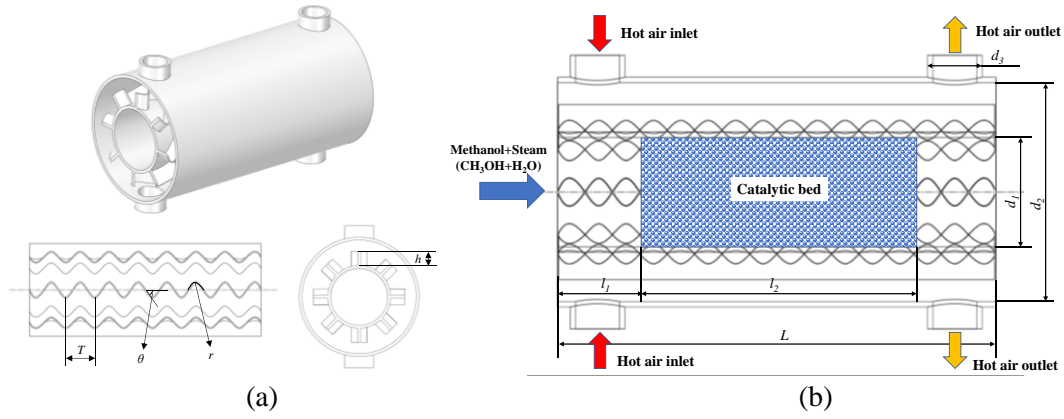


Fig. 2 Structural diagram of reforming reactor: (a) Three-dimensional structure; (b) Model dimension.

Table. 1 Geometrical parameters of the reforming reactor

Parameters	Value
Reforming reactor length, L (mm)	160
Ingress segment length, l_1 (mm)	30
Catalytic bed length, l_2 (mm)	100
Reforming gas channel diameter, d_1 (mm)	40
Hot air channel diameter, d_2 (mm)	80
Hot air inlet and outlet diameter, d_3 (mm)	20
Wall thickness (mm)	2
Rib height h (mm)	10.46
Angle of rib θ ($^\circ$)	53.49
Radius r (mm)	9.98
Cycle T (mm)	49.8

To simplify the model and calculations, the following assumptions are made [9]:

- (1) All gases are assumed to be ideal and incompressible, and the effect of changes on gas density is neglected.
- (2) The external surface of the reactor is considered adiabatic.
- (3) The effect of gravity is neglected.
- (4) The porous catalyst layer is considered isotropic and homogeneous with uniform morphological properties. Also, the chemical reactions take place only in the catalyst.

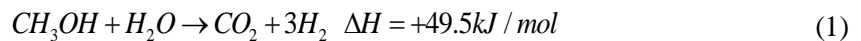
2.2. Mathematical model of reforming reactor

The reforming reactor model comprises five control equations, i.e., continuity, momentum, component mass fraction, energy, and chemical reaction equations. Using the homogeneous model, the control equations of model are as follows.

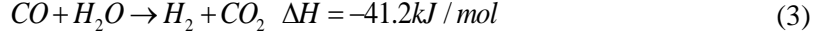
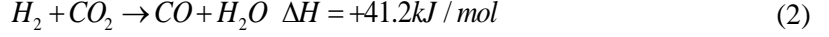
2.2.1. Chemical reaction equation

Purnama et al. [18] pointed out that the MSR reaction was faster than the reverse water gas shift reaction (rWGS). Therefore, the chemical reaction equations can be derived as:

- 1) Methanol steam reforming reaction



- 2) Water gas shift reaction



The rate of the above chemical reaction is calculated by the Arrhenius model, which is expressed as,

$$R_{MSR} = k_1 C_{CH_3OH}^{0.6} C_{H_2O}^{0.4} \exp\left(-\frac{E_{a1}}{RT}\right) \quad (4)$$

$$R_{WGS} = k_2 C_{CO_2} C_{H_2} \exp\left(-\frac{E_{a2}}{RT}\right) - k_{-2} C_{CO} C_{H_2O} \exp\left(-\frac{E_{a2}}{RT}\right) \quad (5)$$

where k is the reaction pre-exponential factor, E_a is the activation energy corresponding to the reaction. The relevant parameters are shown in Table 2.

Table. 2 Material properties and relevant parameters

Parameters	Value
Catalytic bed density ρ (kg/m ³)	1480
Catalyst thermal conductivity λ_s (W/(m·K))	1
Catalytic bed porosity ε_0	0.5
Mass diffusion coefficient D_k (m ² /s)	6.8×10^{-5}
Gas constant R_g (J/(mol·K))	8.314
Pre-exponential factor of steam reforming reaction k_1 (s ⁻¹)	8×10^8
Pre-exponential factor of water gas shift reaction k_2 (m ³ /(mol·s))	4×10^8
Pre-exponential factor of reverse water gas shift reaction k_{-2} (m ³ /(mol·s))	4×10^8
Activation energy of steam reforming reaction E_{a1} (J/mol)	7×10^4
Activation energy of water gas shift reaction E_{a2} (J/mol)	1×10^5
Activation energy of reverse water gas shift reaction E_{a-2} (J/mol)	1×10^5

During the reaction, the methanol conversion can be obtained from Equation (6),

$$X_{CH_3OH} = \frac{C_{CH_3OH,in} - C_{CH_3OH,out}}{C_{CH_3OH,in}} \times 100\% \quad (6)$$

where $C_{CH_3OH,in}$ denotes the mass fraction of inlet methanol, $C_{CH_3OH,out}$ denotes the mass fraction of outlet methanol.

2.2.2. Continuity equation

$$\nabla \cdot \vec{V} = 0 \quad (7)$$

where \vec{V} is the velocity.

2.2.3. Momentum equation

$$\varepsilon_0 (\vec{V} \cdot \nabla) \vec{V} = -\frac{\varepsilon_0}{\rho_f} \nabla p + \frac{\varepsilon_0 \mu}{\rho_f} \nabla^2 \vec{V} + S_m \quad (8)$$

where S_m is the source term of momentum generated by the porous catalyst, which can be calculated from Equation (9).

$$S_m = -\frac{\mu}{\rho_f K} \vec{V} - \frac{\beta \vec{V}}{2} |\vec{V}| \quad (9)$$

where ε_0 is the catalyst porosity, which is taken as 0.5 in this paper by reference [9] in order to enable the reaction to occur stably, ρ_f is the density of fluid, K is the permeability, β is the inertia loss coefficient in every direction in the porous material of the conversion catalyst, μ is the dynamic viscosity of mixture.

2.2.4. Component mass fraction equation

$$\varepsilon_0(\vec{V} \cdot \nabla)C_i = D_{\text{eff}}\nabla^2C_i + \varepsilon_0 \sum_{r=1}^N M_{w,i}R_{i,r} \quad (10)$$

where C_i denotes the mass fraction of every substance (CH_3OH , H_2O , H_2 , CO_2 and CO), and the last term is the source term for chemical reaction induction in the catalyst. D_{eff} is the effective mass diffusion coefficient based on the Stefan-Maxwell equation [19]. To describe the effect of porosity ε_0 and curvature τ on porous catalysts, the effective mass diffusion coefficient is expressed as:

$$D_{\text{eff}} = \frac{\varepsilon_0}{\tau} D_k \quad (11)$$

where D_k is the mass diffusion coefficient of gas mixture; ε_0 is the porosity and τ is the curvature.

2.2.5. Energy equation

$$(\rho_f c_p)(\vec{V} \cdot \nabla)T = \lambda_{\text{eff}}\nabla^2T + \varepsilon_0 S_i \quad (12)$$

where ρ_f is the density of fluid, c_p is the specific heat capacity at constant pressure. T is the temperature, λ_{eff} is the effective thermal conductivity. Usually, to calculate the effect of porous medium in the energy equation, it can be expressed as:

$$\lambda_{\text{eff}} = \varepsilon_0 \lambda_f + (1 - \varepsilon_0) \lambda_s \quad (13)$$

where λ_f and λ_s are the fluid thermal conductivity parameter and solid thermal conductivity parameter in porous media, respectively.

$$S_i = -\sum_{i=1}^N \left(\frac{h_i^0}{M_{w,i}} + \int_{T_{\text{ref}}}^T C_{p,i} dT \right) (R_{i,r}) \quad (14)$$

where source term S_i is zero in the reactor except for the catalyst region.

2.3. Boundary conditions

The boundary conditions are listed in Table 3. Velocity-inlet and pressure-outlet boundary condition was used along with coupled wall condition for heat exchange between heating and reacting channel. Also, the operating pressure is kept at 0.1 MPa.

Table 3 The boundary conditions

Parameters	Ranges
Hot air inlet temperature (K)	800-880
Hot air inlet flow velocity (m/s)	1.0-3.0
Reforming gas inlet temperature (K)	523-573
Reforming gas inlet flow velocity (m/s)	0.1-0.5
Steam-carbon ratio	1.1-1.9
The operating pressure (MPa)	0.1

2.4. Grid independence analysis and numerical model validation

The details of the grid independence analysis and numerical model validation are available in our previous work [17] and are not repeated here.

3. Results and discussion

3.1. Effect of condition parameters on the characteristics of the MSR reactor

In a reforming reactor, the methanol conversion is influenced by the parameters such as the temperature of hot air and reforming gas, the flow velocities of hot air and reforming gas, and the steam-carbon ratio. The effects of the inlet condition parameters on the methanol conversion are shown in Figure 3.

Figure 3(a) shows the effects of hot air inlet flow velocity and temperature on methanol conversion. Studies have found that under constant temperature, increasing the hot air velocity leads to higher methanol conversion rate. The likely explanation is that the increase of the reforming reactor's internal flow Reynolds number, which is affected by increasing hot air inlet velocity, leads to an increase in the heat transfer coefficient. Thus, the convective heat transfer of the catalytic tube wall is enhanced, allowing more heat to be used for the methanol reforming inside the reactor, which results in more methanol participating in the reaction and higher methanol conversion obtained. In addition, the influence of increasing hot air inlet flow velocity on methanol conversion is more obvious when hot air temperature is high. For example, when $T_{\text{air}}=800$ K, the hot air velocity increasing from 1.0 m/s to 3.0 m/s leads to the methanol conversion increasing from 83.2% to 92.3%. Meanwhile, when $T_{\text{air}}=880$ K, the methanol conversion changes from 87.1% to 96.9% with the same hot air flow velocity range.

When the inlet flow velocity of hot air remains constant, the methanol conversion also increases with an increase of the hot air temperature. Taking $v_{\text{air}}=1.0$ m/s as an example, when the hot air temperature increases from 800 K to 880 K, the methanol conversion increases from 83.2% to 87.1%. Assuming that the chemical reaction temperature in the reactor remains invariable, an increase in the hot air temperature leads to a greater temperature difference for convective heat transfer within the reactor. According to Newton's cooling formula, a larger temperature difference benefits more heat to be transferred to the catalytic bed, promoting the methanol reforming reaction. However, considering that there is an optimal reaction temperature range (523 K-573 K) for methanol reforming and the heat resistance of reactor materials is limited, the hot air temperature should not be too high. Furthermore, it can be found that if the temperature and velocity of hot air increase in the same proportion, increasing the temperature of the hot air has a more significant effect on improving the methanol conversion inside the reactor. This indicates that for the present reactor, increasing the flow velocity of hot air to increase the Reynolds number, improves the heat transfer efficiency and enhances the methanol conversion is not as effective as increasing the hot air temperature.

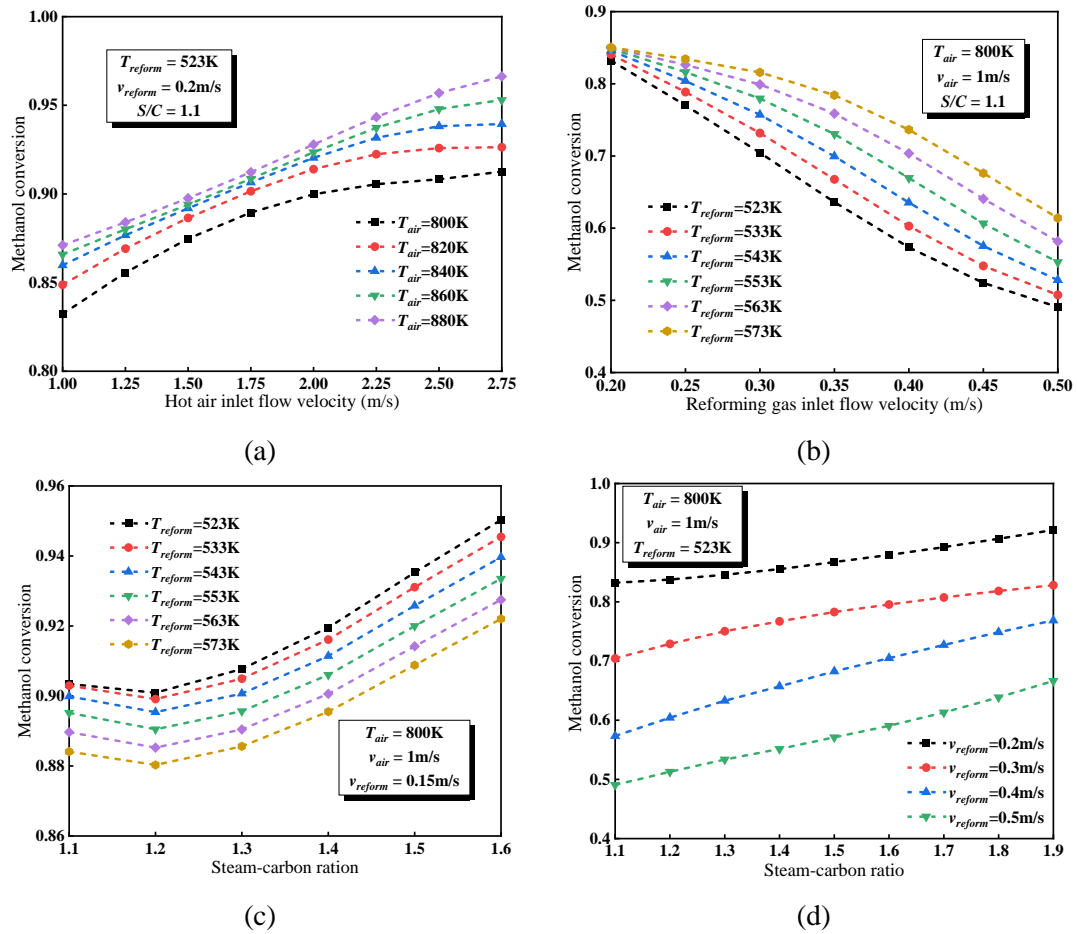


Fig. 3 Effects of condition parameters on methanol conversion: (a) hot air inlet flow velocity and temperature; (b) reforming gas inlet flow velocity and temperature; (c) reforming gas inlet flow velocity and steam-carbon ratio; (d) reforming air temperature and steam-carbon ratio.

Figure 3(b) shows the impact of reforming gas inlet flow velocity and temperature on methanol conversion. Increasing reforming gas inlet velocity results in a significant decrease in the methanol conversion when the reforming gas temperature is constant. For instance, taking $T_{\text{reform}}=523$ K as an example, when the reforming gas velocity increases from 0.1 m/s to 0.5 m/s, the methanol conversion decreases from 99.4% to 49.1%. This is because increasing reaction gas velocity reduces the residence time of reactants inside the reforming reactor, preventing reactant from fully contacting with the catalyst. As a result, the methanol gas flows out of the reactor without participating in the reaction, leading to a lower methanol conversion and methanol waste. The outlet contains a high methanol gas concentration, further lowering the reactor's conversion. When the velocity of reforming gas is unchanged, an increase in the temperature of the reforming gas leads to a gradual increase in the methanol conversion. Taking $v_{\text{reform}}=0.3$ m/s as an example, when the temperature of the reforming gas increases from 523 K to 573 K, the methanol conversion increases from 70.4% to 81.6%. The reason for this is that within the optimal temperature range (523 K-573 K) for MSR, as the temperature of the reactant gas entering the reactor increases, the temperature of reactor also increases, which affects catalyst activity and leads to an acceleration of the reaction rate for hydrogen production. Therefore, the methanol conversion is negatively correlated with the inlet flow velocity of the reforming gas and positively correlated with the inlet temperature of the reforming gas.

Figure 3(c) shows the effect of the steam-carbon ratio and reforming gas inlet flow velocity on methanol conversion. When reforming gas inlet flow velocity is constant, the methanol conversion

positively correlates with the steam-carbon ratio. For example, at $v_{\text{reform}}=0.1$ m/s, when the steam-carbon ratio increases from 1.1 to 1.9, the methanol conversion increases from 90.3% to 99.2%. This is because the MSR reaction is reversible, as shown in Eq. (1), and an increase in the steam-carbon ratio (an increase in water content) favors the forward reaction, promoting methanol conversion. Therefore, increasing the steam-carbon ratio favors improving the methanol conversion.

Figure 3(d) shows the effect of the steam-carbon ratio and reforming gas temperature on methanol conversion. A similar conclusion can be obtained, i.e., increasing the steam-carbon ratio and reforming gas temperature helps accelerate the reforming reaction and improve methanol conversion.

3.2. Performance prediction of MSR reactor using different intelligence algorithms

The traditional CFD method has the advantages of high accuracy and operability, but it is complex and time-consuming. Intelligence algorithms can establish a mapping relationship between input and output parameters, so obtaining calculation results faster [20]. Five commonly used intelligence algorithms are applied to study the prediction performance of MSR reactor, and the regression models are compared. The number of data points is 100, 70% of which is used for training, 15% of which is used for validation and 15% of which is used for test. The hyperparameters of the three methods are shown in the Table below.

Table. 4 The hyperparameters of three methods

Methods	Hyperparameters
L-SVM	The penalty factor $c=4.0$, radial basis function parameter $g=8.0$
RFA	The number of trees =100, minimum number of leaves=5
RBFNN	The expansion speed of the radial basis function $r_{\text{bf_spread}}=100$

The coefficient of determination R^2 and mean absolute error (MAE) are used to evaluate the fitness of algorithms. The R^2 and MAE are calculated as follows:

$$R^2 = 1 - \frac{SS_{\text{res}}}{SS_{\text{tot}}} = 1 - \frac{\sum (y_i - y_i^*)^2}{\sum (y_i - \bar{y})^2} \quad (15)$$

$$MAE = \frac{1}{m} \sum_{i=1}^m |y_i - y_i^*| \quad (16)$$

where SS_{res} represents the sum of residuals of squares, SS_{tot} represents the sum of total squares, y_i represents the actual value, and y_i^* represents the output value of the artificial neural network, \bar{y} represents the average of the actual value.

The value of the coefficient of determination R^2 is between 0-1. The closer the value of R^2 is to 1, and the smaller the value of MAE, the better the fitting performance of the model. The coefficient of determination R^2 and MAE of the five intelligence algorithms are shown in Figure 4. As can be seen, the R^2 of SL, L-SVM and BPNN are greater than 0.8, especially the BPNN ($R^2=0.97$). Moreover, the MAE of the BPNN is 0.0347, which is the lowest. As a whole, the BPNN shows better regression performance. Therefore, the BPNN is used to predict the reforming reactor performance.

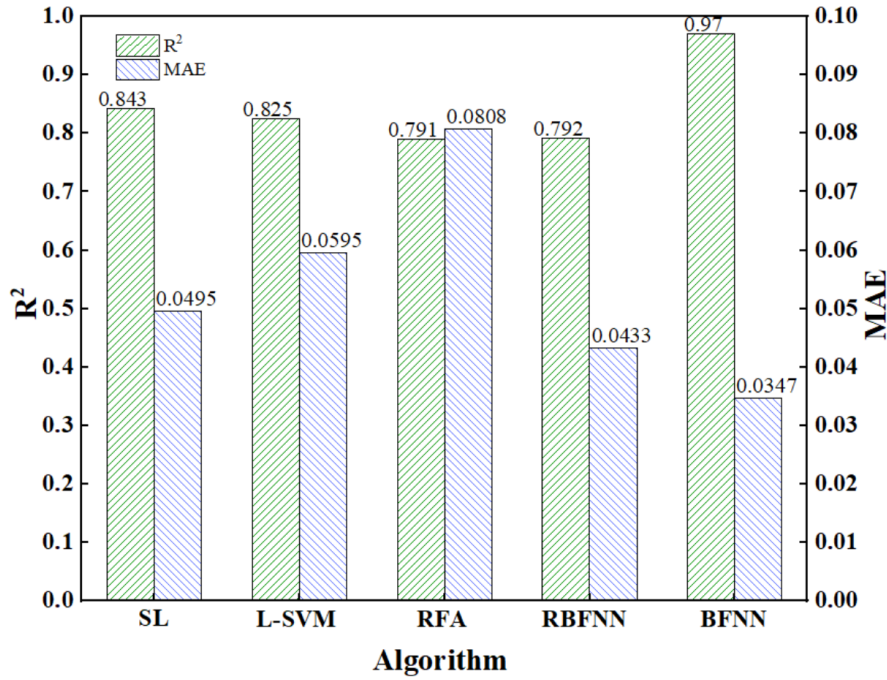


Fig. 4 The MAE and R² of the prediction results of different intelligence algorithms

3.3. Research on thermal management of the MSR reactor

The thermal management of the reforming reactor is to control the decision variables in a given model under certain constraints to obtain optimal solutions for the given the objective functions. Therefore, the most important process for the optimization model of the MSR reactor can be divided into three steps: selecting decision variables, determining objective optimization functions, and establishing corresponding constraints.

1) Selecting decision variables

The decision variables are usually selected according to the degree of the influence of parameters on the reforming reactor. For the MSR reactor, the inlet condition parameters, which affect the methanol conversion of the reforming reactor are selected as the decision variables, i.e. the temperature (T_{air}) and flow velocity (v_{air}) of hot air, the temperature (T_{reform}) and flow velocity (v_{reform}) of reforming gas, and the steam-to-carbon ratio (S/C).

2) Determining objective optimization functions

This work focuses on the main objective of meeting the load demand of fuel cell during one operating cycle, by adjusting the reactor's hydrogen production output and maintaining high methanol conversion. Therefore, the objective optimization function of MSR reactor can be expressed as:

$$F_{\text{obj}}(v_{\text{air}}, v_{\text{reform}}) = \min \left\{ r_1 \left\| m_{\text{H}_2}^* - m_{\text{H}_2, \text{net}} \right\|_2^2 + r_2 \left\| 1 - \frac{1}{\eta} \right\|_2^2 \right\} \quad (17)$$

where $m_{\text{H}_2}^*$ represents the hydrogen production demand, $m_{\text{H}_2, \text{net}}$ is the output hydrogen production of reactor, η is the methanol conversion, r_1 and r_2 are the weight coefficients. The first term on the right side of equation aims to adjust the device's output hydrogen production to meet the load demand, while the second term aims to maximize the methanol conversion of MSR reactor.

3) Establishing corresponding constraints

To operate within a certain range and conditions for the reactor, many limiting factors constitute the constraints of the optimization model. The hot air in this paper is assumed to come from the exhaust gas, and the temperature of supplied hot air is usually constant. Moreover, various reports mention that the optimal temperature for MSR on the copper-based catalyst is 523 K, and the inlet steam-carbon ratio is set to 1.3 [9]. To optimize the properties of the reactor, the inlet condition parameters mentioned above remain constant as much as possible. Therefore other specific constraints are:

$$\begin{cases} v_{\text{air}} > 0 \\ v_{\text{reform}} > 0 \end{cases} \quad (18)$$

Figure 5 shows the hydrogen consumption characteristics over one cycle. The horizontal axis represents dimensionless time, indicating the temporal sequence within a working cycle. It does not express specific time units and is used to study the temporal variation trend of periodic phenomena. The surrogate model of the MSR reactor obtained by the BPNN is used as the direct problem model, and the PSO algorithm studied in the present work is selected as the inverse problem model to study the optimization of the reforming reactor. The detail of the PSO algorithm is available in reference [21], and the difference is that the particle dimension is set as 2 for there are two operating condition parameters (v_{reform} and v_{air}) to study.

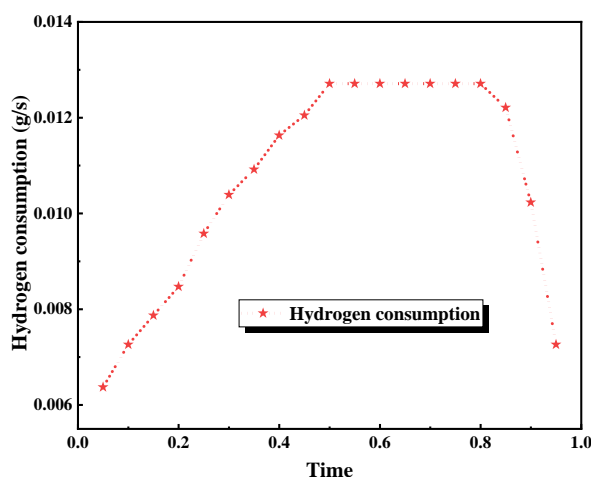


Fig. 5 Hydrogen consumption over time

Figure 6 shows a satisfactory agreement between the predicted hydrogen production and the actual hydrogen consumption demand. Figure 7 shows the methanol conversion of the MSR reactor over time, and the methanol conversion can be kept stable at over 93%, indicating that the reactor has maintained excellent reforming performance. Figure 8 shows the prediction of condition parameters (v_{reform} and v_{air}) varying over time. It can be seen that the flow velocity of hot air and reforming gas gradually increase or decrease as the hydrogen production demand rises or declines within the cycle. The heat supply also tends to be stable during the steady demand for hydrogen production. All these studies indicate that the methodology consisted of the BPNN surrogate model and the PSO algorithm can be used to study the thermal management of the reforming reactor to improve the properties of the reforming reactor. The characteristic curves of the condition parameters within the whole cycle can be obtained to guarantee hydrogen production demand and excellent methanol conversion.

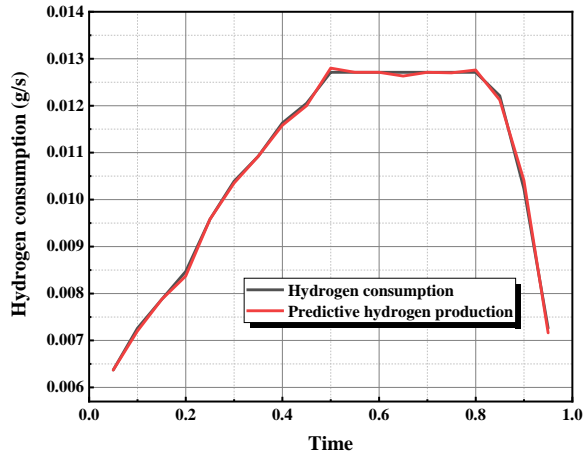


Fig. 6 The prediction of output hydrogen production

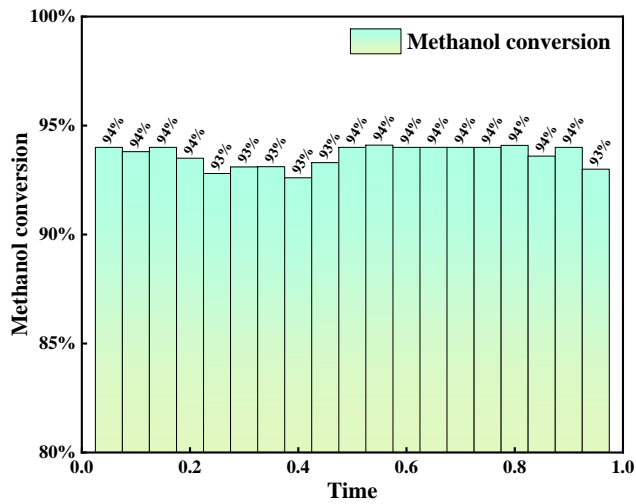


Fig. 7 The methanol conversion of methanol steam reforming reactor over time

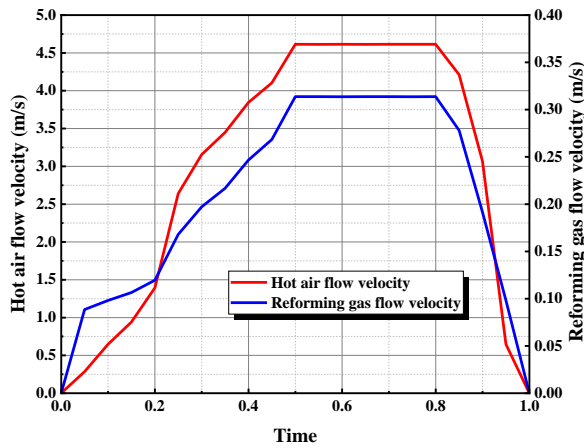


Fig. 8 The flow velocity of hot air and reforming gas optimized over time

4. Conclusions

The present work firstly carried out the CFD analysis for the MSR reactor, and then the surrogate model of the reforming reactor is studied by different intelligence algorithms, and the coefficient of determination R^2 and mean absolute error (MAE) are used to evaluate the fitness of different

intelligence algorithms. Finally, the thermal management of the MSR reactor is studied by the PSO algorithm. The research conclusions are as follows:

(1) Increasing both the temperature and flow velocity of the hot air can improve the methanol conversion effectively. However, different conclusions will be obtained by increasing the temperature and flow velocity of the reforming gas. The methanol conversion can be improved by increasing the temperature or decreasing the flow velocity of the reforming gas. Moreover, larger steam-carbon ratio is more conducive to the MSR reaction, which can also improve the methanol conversion.

(2) The R^2 of the SL, L-SVM and BPNN are greater than 0.8, especially the BPNN ($R^2=0.97$). Moreover, the MAE of the BPNN is 0.0347, which is the lowest value. The results show that the BPNN surrogate model is better than the algorithms mentioned above.

(3) With the help of the thermal management of the MSR reactor by the BPNN surrogate model and the PSO algorithm, hydrogen production can be generally guaranteed by the characteristic change curves of the inlet condition parameters of the reforming reactor. Moreover, excellent methanol conversion ($\geq 93\%$) can be maintained steadily within the cycle.

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