

Optimised design of fuel cell hydrogen recirculation system based on ejector[#]

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ABSTRACT

With the advantages of simple structure, easy maintenance and low cost, the ejector is an ideal cycling device for proton exchange membrane fuel cells, but it is difficult to have a good performance at low power. Aiming at the problem that it is difficult to adapt the ejector to the circulation demand under full working conditions, this paper summarizes the general design flow of the fixed structure ejector by comparing the three design methods of one-dimensional computation, CFD simulation and algorithmic optimization, and describes the advantages and disadvantages of the various schemes by comparing the single ejector, a new structure of the ejector, a two-stage ejector in parallel, and a combination of the ejector and the hydrogen circulating pump for the hydrogen circulation. The advantages and disadvantages of each scheme are described, with a view to contributing to the research on the design of ejectors and hydrogen circulation schemes.

Keywords: ejector, PEMFC, hydrogen recirculation

NONMENCLATURE

Abbreviations

PEMFC	Proton Exchange Membrane Fuel Cell
CFD	Computational Fluid Dynamics
NXP	Nozzle exit position
MIGA	Multi-island Genetic Algorithm
EBF	Ellipsoidal Basis Function
NLPQL	Non-linear Programming by Quadratic Lagrangian
ILPM	Integrated Lumped Parameter Model

Symbols

λ	Flow ratio
λ_{H_2}	Hydrogen flow ratio
m_p	Primary flow rate
m_s	Secondary flow rate
y_{H_2O}	Vapour mass fraction
M	Mach number

A	Cross-sectional area of pipe
f	Coefficient of pipe friction
x	Axial distance of pipeline
D	Pipe Diameter
X	flow resistance
k	Specific heat ratio
p	Static pressure
m	Mass flow
dm	Mass flow rate of injected and evaporated gases
y	Quantities related to fluid velocity
T_0	Stagnation temperature
F_A	Influence coefficients corresponding to area change
F_f	Influence coefficients corresponding to friction
F_{T_0}	Influence coefficients corresponding to stagnation temperature change
F_m	Influence coefficients corresponding to flow rate change
T	Temperature
c_p	Constant-pressure specific heat capacity
k_p	Isentropic index (physics)
v	Specific volume
V	Velocity
g	Accelerations
lower labels $i, o, x, 1, 2, 3$	State i, state o, section x, section 1, section 2 and section 3
upper labels ' and "	Primary and secondary flow

1. INTRODUCTION

PEMFC as a key carrier of hydrogen energy utilisation, is one of the most probable energy devices to replace the internal combustion engine in the future^{[1][2]}. In order to ensure that the electrochemical reaction of the PEMFC proceeds normally, usually incorporate a

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hydrogen recycling device to recycle hydrogen from the anode outlet to the inlet, which improves the hydrogen utilisation rate and enhances the safety of the system. In addition, hydrogen recirculation can help maintain the water content inside the PEMFC^[3].

Two commonly used hydrogen recirculation devices are ejectors and hydrogen recirculation pumps. Hydrogen circulation pumps are capable of adjusting the rotational speed to meet the circulation needs under various operating conditions, but they incur additional power consumption and higher costs. In contrast, the ejector is simple, easy to maintain, and less costly, and is considered an ideal hydrogen circulation device in the PEMFC. However, the application of the ejector is limited by the fact that it can only perform good hydrogen recycling capability when the output power of the electrostack is higher than 50% of the maximum power^[4].

This paper focuses on the problem of narrow working range of PEMFC ejector, analyses and summarizes the relevant research results at home and abroad, and points out the development direction of the design of PEMFC ejector and hydrogen circulation scheme.

2. EJECTOR DESIGN METHODS

The existing ejectors are divided into two forms: fixed structure and new structure. The traditional ejector is a fixed structure, as shown in Fig. 1(a). The existing design methods are mainly for the traditional fixed-structure ejectors, which are highly influenced by the structural parameters, and the performance of the ejector at each size is limited to only a specific operating interval^[5].

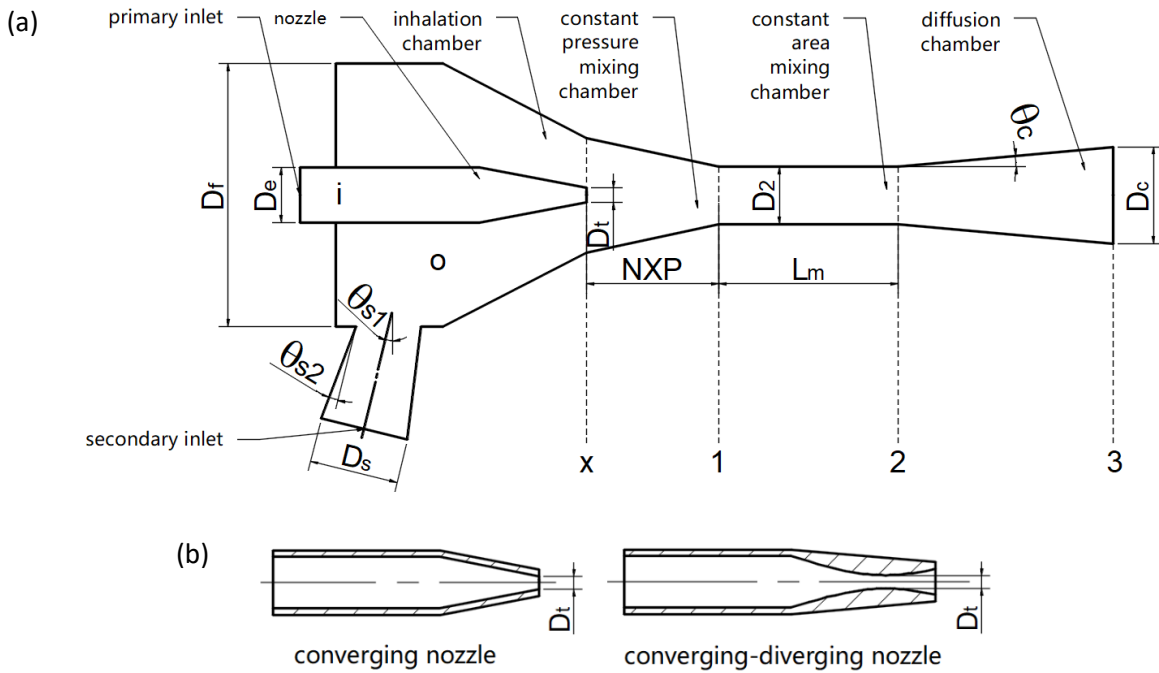


Fig. 1 Schematic diagram of ejector structure (a) ejector (b) nozzle

Existing design methods generally choose the flow ratio or hydrogen flow ratio as the evaluation index of the PEMFC system ejector performance. The formulas are respectively:

$$\lambda = \frac{m_s}{m_p} \quad [1]$$

$$\lambda_{H_2} = \frac{m_s(1 - y_{H_2O})}{m_p} \quad [2]$$

2.1 One-dimensional calculations

One-dimensional calculations of ejectors are performed based on the one-dimensional gas dynamics of compressible gases. Initial one-dimensional gas

dynamics studies focused on solving the fluid characteristics within a section of pipe. Sczeniowski^[6] investigated the frictionless heat-generated flow characteristics of a fluid in a constant-area pipe. Chambre and Lin^[7] presented equations for the combined effects of area changes, heating, combustion, and molecular weight and specific heat changes in a pipe. Shapiro^[8] for the first time took the case of having gas injected into the main flow into account and proposed a one-dimensional computational equation for the gas flow in the steady state, as shown in Eq. [3].

$$dM^2 = F_A \frac{dA}{A} + F_{T_0} \frac{dT_0}{T_0} + F_f \left(4f \frac{dx}{D} + \frac{dX}{0.5kpAM^2} - 2y \frac{dm}{m} \right) + F_m \frac{dm}{m} \quad [3]$$

$$V_2 = \frac{\omega v_2}{A} \quad [5]$$

$$\frac{m'}{g} V_1' + \frac{m''}{g} V_1'' + p_1 A = \frac{m}{g} V_2 + p_2 A \quad [6]$$

where,

$$\begin{cases} F_A = -\frac{2M^2 \left(1 + \frac{k-1}{2} M^2\right)}{1 - M^2} \\ F_f = \frac{kM^4 \left(1 + \frac{k-1}{2} M^2\right)}{1 - M^2} \\ F_{T_0} = \frac{F_m}{2} = \frac{M^2(1 + kM^2) \left(1 + \frac{k-1}{2} M^2\right)}{1 - M^2} \end{cases}$$

Edelman^[9] firstly selected the value of specific heat ratio in Eq. [3], and then calculated the values of influence coefficients corresponding to different Mach numbers, and obtained the numerical solution table of influence coefficients in Eq. [3]. Shapiro and Edelman's research constitutes a modern one-dimensional design of the ejector. The theoretical basis for the modern one-dimensional design of ejectors is formed by Shapiro and Edelman.

Initially, the theory on one-dimensional calculations of ejectors focused on analytical methods for the characterisation of the fluid inside the mixing chamber, while methods for the design of the ejector were lacking. Flügel^[10] firstly proposed an analysis method applicable to the combined case of constant pressure and constant area mixing and compared the results of the analyses with the experimental data of the ejector, showing a good agreement, and he concluded that mixing in a tube of constant area of the tube is better for total mixing. In addition, Keenan and Neumann^[11] also performed calculations for a combination of constant pressure and constant area mixing and came to the same conclusion. Based on this, they also proposed a one-dimensional analysis method for a simple ejector without diffusion chamber and showed good agreement by experimental comparisons: as shown in Fig. 1(a), the flow rates of the primary and secondary streams at cross-section 1 are calculated according to the principle of reversible adiabatic expansion, and assuming that the pressure p_1 at 1 is known given that the pressure p_2 is known at 2, and all of the Eqs. [6] can be obtained from Eqs. [4] and [5] by means of Eqs. values of the quantities, if the equation [6] is not satisfied, the assumed value p_1 is adjusted for calculation until the equation is valid. In 1950, Keenan and Neumann^[12] were the first to propose a method for the design of an ejector with a diffuser.

$$c_p T_i = \frac{k_p}{k_p - 1} p_2 v_2 + \left(\frac{m}{A}\right)^2 \frac{v_2^2}{2g} \quad [4]$$

Huang^[13] classified the operating modes of the ejector into critical, subcritical and counterflow modes according to the backpressure, and they added the analysis of the obstruction to Keenan's theory, and proposed a new method for the design of the ejector. Sokolov^[14] classified the ejectors according to the nature of the primary and secondary flow, and gave the corresponding one-dimensional analysis method for each type of jet, and based on the experiments summarised the calculation formula and empirical coefficients, and put forward the theory of one-dimensional design of the jet that can be applied in engineering.

Researchers have developed a one-dimensional computational model of the ejector for the PEMFC system to address these special needs. Based on the design theory of Huang, Karnik^[15] established a control-oriented one-dimensional model of the PEMFC ejector by assuming that the primary stream and the circulating gas are pure hydrogen; Kim^[16] carried out the design of an ejector with a humidified hydrogen stream according to the humidification requirements of the PEMFC. Based on the Sokolov design theory, Xu^[17] carried out the design of an ejector for an 80kW high-pressure PEMFC system and verified its performance through experiments, and the results showed good consistency. Zhu^[18] considered that there is less water vapour condensation in the shrinking nozzle ejector compared to the shrinking and expanding nozzles, and therefore established an analytical model for the PEMFC shrinking nozzle ejector. The analytical model of the PEMFC shrinking nozzle ejector was developed. Their model can only analyse the flow rate based on the dimensions, while Fan^[19] deduced the required flow rate for operation based on the PEMFC operating conditions, and then calculated the structural dimensions of the constriction-type nozzle ejector based on the analytical model proposed by Zhu. The design outputs two dimensions of the nozzle outlet diameter, D_t , and the mixing chamber diameter, D_2 . However, Liu^[20] considered that the assumption of equal pressure between the inhalation chamber and the inlet of secondary flow in Fan's model was not consistent with the actual situation, so he modified the pressure of the inhalation chamber in the model and carried out the model validation, and the results showed that the simulation data of the corrected model matched the

experimental data more closely and the optimisation of the model was achieved.

The one-dimensional calculation method is already a mature ejector design method, and the one-dimensional design flow of the existing PEMFC ejector is shown in Fig. 2.

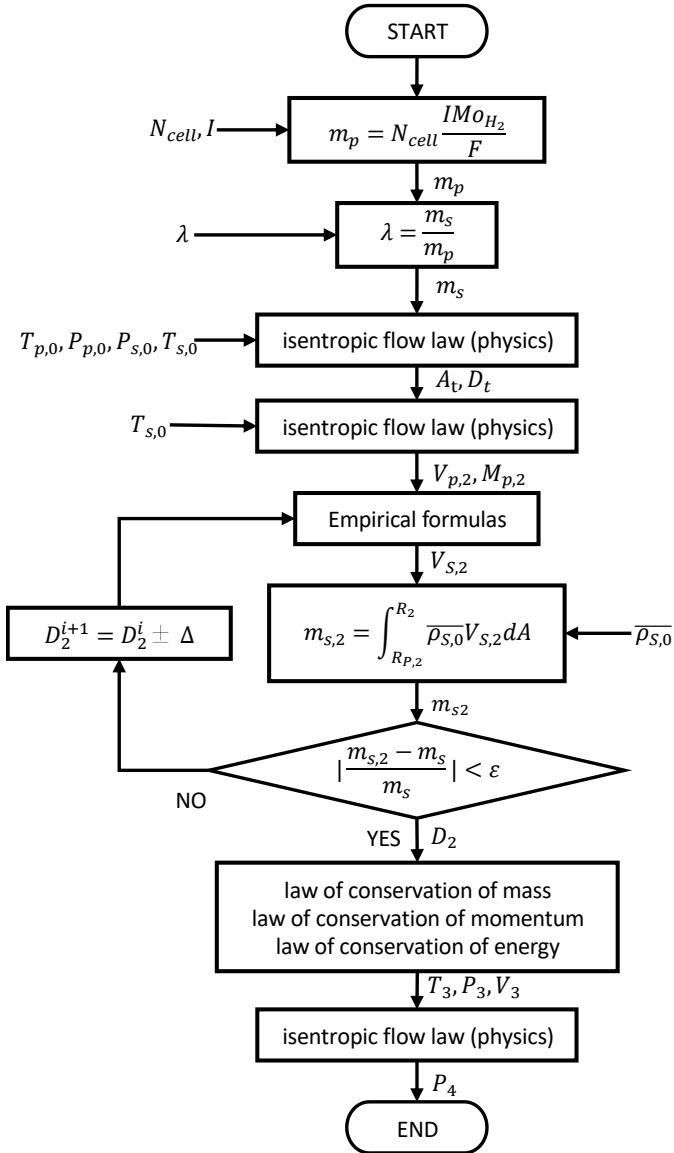


Fig. 2 Block diagram of the one-dimensional computational flow of the ejector

The one-dimensional calculation method can calculate the two key dimensions of nozzle outlet diameter and mixing chamber diameter according to specific design parameters, while the secondary inflow port diameter, diffusion section angle, and individual axial dimensions cannot be obtained as accurate values, and are mostly obtained based on empirical formulas. This method is a faster solution process, but the structural parameters of the ejector involved are not comprehensive, and is currently used to give an initial range of parameters, and other methods such as CFD

simulation are used for the subsequent optimisation process.

2.2 CFD simulation

The method of designing the ejector through fluid simulation is to change the influencing parameters one by one by controlling variables for simulation comparison and analysis, and select the parameter values corresponding to the best performance. The specific process is as shown in Fig. 3.

The methods of designing the ejector through CFD simulation are divided into two-dimensional and three-dimensional. However, the two-dimensional model performs the simulation with poor accuracy^[21]. Since the three-dimensional CFD simulation of the ejector design takes into account the non-uniformity of the radial flow field distribution, the design optimisation of the ejector is now mostly carried out by three-dimensional simulation.

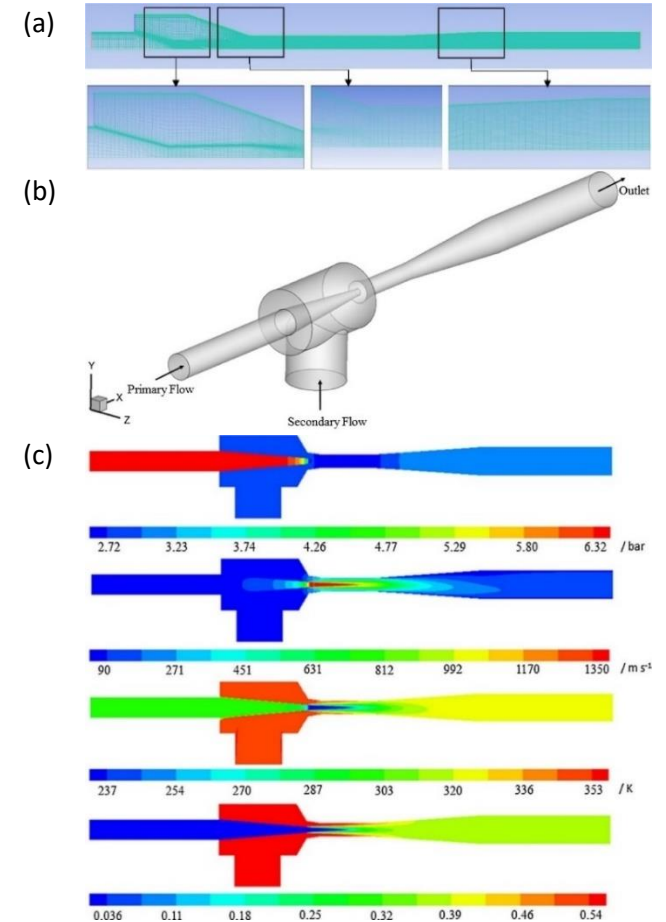


Fig. 3 CFD simulation of (a) 2D axisymmetric mesh^[22](b) 3D mode^[21](c) cloud map of pressure, velocity, temperature, and vapour distribution^[21]

The ejector design based on 3D CFD simulation is carried out by changing a single dimension in the model, simulating it under the same meshing and the same

boundary conditions, comparing the effect of the dimension on the ejection ratio, and selecting the dimension corresponding to the maximum ejection ratio as the design output. The nozzle outlet diameter D_t and the mixing chamber diameter D_2 are the key factors affecting the ejector performance. While most of the studies obtained these two parameters directly by one-dimensional calculation.

In addition to the critical dimensions, a number of scholars have investigated the influence laws of structural parameters such as NXP , secondary flow structure, mixing chamber length L_m , and diffusion chamber angle θ_c on the ejector performance by CFD simulation. Zhang^[23] and Hosseinzadeh^[24] investigated the influence law of the NXP on the ratio, and found that the extreme difference of the ratio was less than 0.5 when other structural parameters were unchanged. The studies of Yin^[21], Zhang^[25] and Zhou^[26] showed that the ratio increased with the increase of the diameter of the secondary inflow port D_s , and the extreme difference is less than 0.4, while parameters such as the position of the secondary inflow tube, the skew angle $\theta_{s,1}$ and the convergence angle $\theta_{s,2}$ do not have much influence on the ejector performance, and the corresponding extreme deviations of the ratios are less than 0.1. Dong^[27] investigated the influence of the length of the mixing chamber, L_m , on the ejector performance by three-dimensional CFD simulations, and the results showed that the ratio increases firstly and then decreases with increasing of L_m , and the optimal range of the mixing chamber length exists. optimal mixing chamber length range, and the extreme difference of the ratio is less than 0.3. Zhang^[25] and Li^[28] investigated the effect of the diffusion chamber angle θ_c on the ratio, and found that there existed an optimal diffusion chamber angle at both high and low operating conditions, and the extreme difference of the ratio was about 0.2, but the effect of θ_c on the ratio was greater at low power. Their study showed that the nozzle outlet position, secondary inflow port diameter, and mixing chamber length have less effect on the ejector performance than the nozzle outlet diameter and mixing chamber diameter.

In conclusion, the structural parameters that have the greatest influence on the ejector performance are the nozzle outlet diameter and the mixing chamber diameter, and the nozzle outlet position, the secondary inflow port diameter, and the mixing chamber length also have a certain influence on the ejector performance, while other parameter variations have almost no influence on the ratio. The CFD simulation-based ejector design method can clearly show the flow state at each

point in the ejector, and the non-critical parameters can also be studied, but the disadvantage is that the geometric model needs to be constantly adjusted and the mesh delineation and boundary conditions setup need to be repeated, the computational process is relatively cumbersome, and the lack of experimental validation may result in a larger deviation from the actual one.

2.3 Algorithmic optimisation

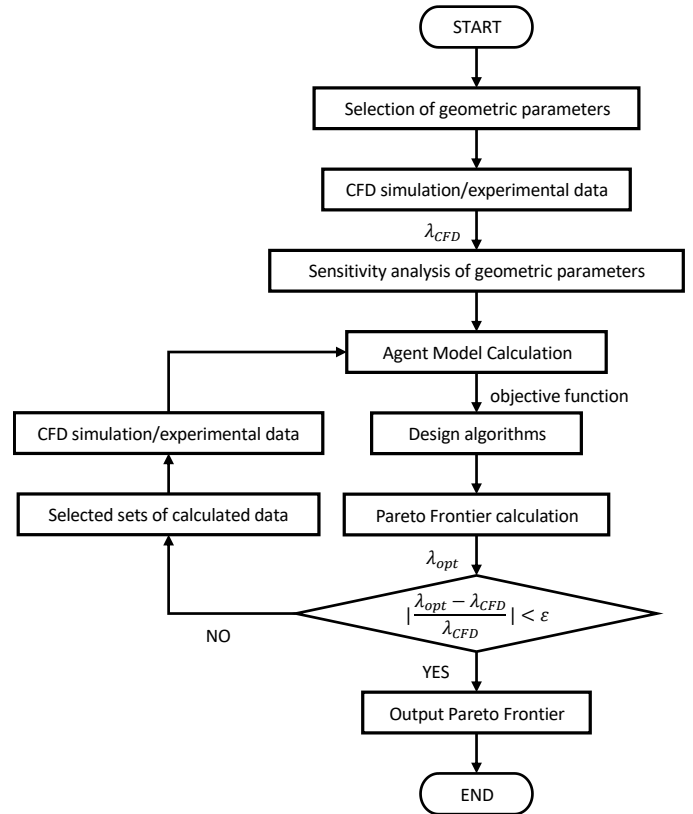


Fig. 4 Flowchart of ejector algorithm optimisation

Algorithmic optimisation is a design method that uses simulation or experimental data as inputs to efficiently find the optimal combination of structural parameters of the ejector through an algorithm. Maghsoodi^[29] used four structural parameters, namely, nozzle outlet position, mixing chamber length, diffusion chamber length and diffusion chamber angle, and the priming ratio as inputs and outputs, respectively, of an artificial neural network based on simulation data obtained by CFD using 167 set of data to establish the relationship between the inputs and outputs. Then the relationship between the inputs and outputs obtained from the artificial neural network is used as the objective function of the genetic algorithm for optimisation, and the priming ratio is improved by 0.3% compared to the pre-optimisation period. Wu and Yao^[30] used the CFD simulation results as a control group for algorithm

optimization, and solved the Pareto front for six parameters such as D_t , D_2 , NXP , L_m , etc. by using the Kriging agent model and the MIGA, and the ejection ratio was improved by 8.8% compared to the pre-optimization. 8.8%. After that, they^[31] believed that the EBF neural network model can better approximate the complex nonlinear relationship between the structural parameters and the lead-in ratio, so they proposed another EBF neural network model and NLPQL algorithm to optimise the structural parameters of the ejector, and the optimised firing ratio was improved by 3.9%.

The algorithmic optimisation process of the ejector is shown in Fig. 4.

Algorithmic optimisation takes into account the coupling between parameters, which can greatly improve the efficiency of optimisation, but the algorithm is difficult to design and often requires simulation or experimental data as input, which prolongs the design cycle of the ejector.

3. EJECTOR-BASED HYDROGEN RECIRCULATION SYSTEM

3.1 Fixed structure ejector

The structure of the hydrogen circulation system based on fixed structure ejector is shown in Fig. 5.

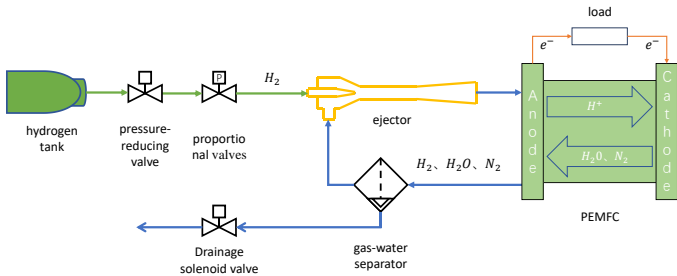


Fig. 5 Hydrogen recirculation system structure with single ejector

When the ejector is used in the PEMFC system, in addition to the optimization of the structure of the ejector itself, many scholars have researched the matching problem between the ejector and the PEMFC system. Bao^[32] established a dynamic model of the PEMFC system including the ejector, and investigated the effect of current on the operating parameters of the battery through simulation, and the results showed that when the current was instantly reduced, the injection ratio suddenly dropped to 0 and then The results show that when the current is instantaneously decreased, the ratio plummets to 0 and then rises rapidly, and the air metering ratio, cathode inlet pressure, and the pressure difference between the two poles are unable to follow the instantaneous decrease of current. Based on this,

they^[33] designed a two-freedom linear state feedback controller based on Kalman estimator and an adaptive model prediction controller with an online neural network identifier for the poor transient response of the model, which improved the transient response performance and anti-interference capability of the model. Besagni^[34] presented an ILPM- CFD model, which takes into account the efficiency of each component of the ejector under different operating conditions, and can more accurately predict the performance of the ejector under different power. Dadvar^[35] investigated the correlation between the design parameters of the electrostack and the design parameters of the ejector by analysing the effects of the cell activation area, the number of single cells, the diameter of the nozzle, and the diameter of the mixing chamber on the output efficiency of the fuel cell and the efficiency increment when it is maximal. corresponding current density value, based on which two dimensionless parameters, the size ratio $G^* = N_{cell} \cdot A_{cell}/A_t$ and the diameter ratio $\beta_D = D_2/D_t$, were proposed, in which G^* establishes a link between the stack design and the ejector design. Ma^[36] investigated the matching design problem between the ejector and the PEMFC system, quantified the ejector in the overall operating range of practical boundary conditions, and established the design of the PEMFC system including the circulation ratio $(m_p + m_s)/m_p$, the hydrogen circulation ratio $[m_p + m_s(1 - y_{H_2O})]/m_p$, the minimum current $I_{min,1.5}$ for a certain hydrogen circulation ratio (the minimum current for hydrogen circulation ratios greater than 1.5), and the relative hydrogen circulation ratio γ (the ratio of the hydrogen circulation in the case of the secondary flow wetting ratio to the hydrogen circulation ratio when the secondary stream is dry) of a comprehensive ejector performance evaluation system, suggesting that both the hydrogen circulation ratio for low primary stream flow and the sensitivity to relative humidity variations should be considered when designing the ejector.

3.2 New structure ejector

The new structure of the ejector widens the operating range to some extent compared to the fixed structure ejector, but its reliability and durability need to be further verified.

Most researchers use the programme of changing the nozzle outlet area to make the ejector adjustable, there are two main ways: (1) adding a needle valve. On this basis, Brunner^[37], Jenssen^[38], and others investigated the characteristics of an inclined-straight spiked conical needle valve adjustable ejector, as shown

in Fig. 7(a), and through the equation $A_n = (\pi/4)\{D_t^2 - [D_s + 2X_n \tan(\alpha_s)]^2\}$ calculated the needle valve position under different working conditions. (2) Change the number of nozzles. Du^[39] proposed a co-axial dual-nozzle ejector structure, as shown in Fig. 7(b). Song^[40] proposed a co-focal twin-nozzle structure, as shown in Fig. 7(c). Xue^[41] proposed a confocal four-nozzle ejector structure, and its performance was evaluated by simulation, which shows that the best performance is achieved when two non-adjacent nozzles are working at the same time, and it extends the lower power limit of the ejector operation to 20 kW.

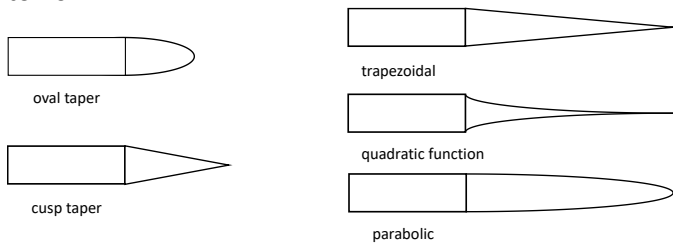


Fig. 6 Needle Valve Linear

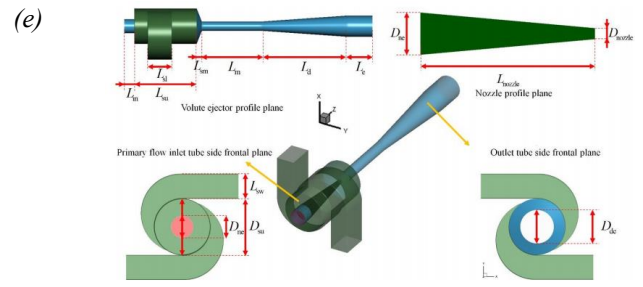
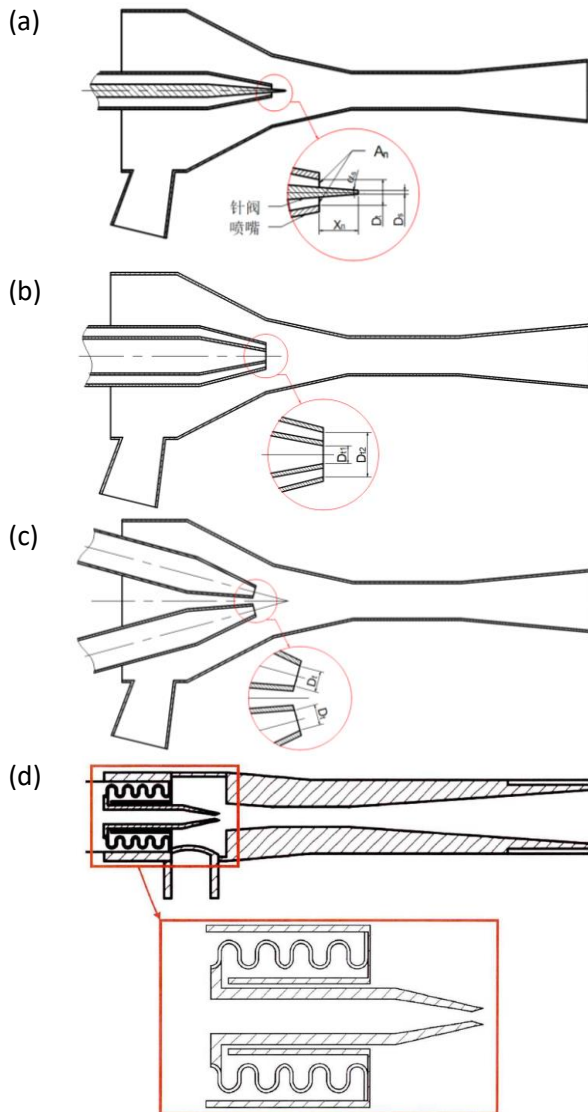


Fig. 7 New structure ejector (a) Needle valve adjustable ejector (b) Co-axial dual nozzle ejector (c) Co-focal dual nozzle ejector (d) Nozzle position adjustable ejector[42] (e) Worm shell ejector[20]

In addition, some scholars have also broadened the range of ejector use by changing other structural parameters. Zhang^[42] designed an ejector based on a bellows to achieve automatic adjustment of the nozzle outlet position, as shown in Fig. 7(d). Liu^[20] thought that the new nozzle structure may increase the occurrence of water vapour condensation phenomenon, which is not applicable to the PEMFC hydrogen cycle, so he designed a snail shell ejector, as shown in Fig. 7(e).

3.3 Two-stage ejectors in parallel

Using two fixed structure ejectors connected in parallel as shown in Fig. 8. This scheme is used to widen the operating range of the ejector by controlling the opening and closing of the solenoid valves so that the ejector operates in different operating intervals. two-stage ejector cycling scheme has been investigated by Kim^[43] and James^[44]. Kim designed two identical ejectors based on 60% of the half power of the PEMFC, and proposed a control strategy to make the ejector I work individually for less than 23kW, and to make the two ejectors work individually for more than 23kW. Above 23kW makes both ejectors work simultaneously, which is achieved by controlling the solenoid valve of the branch where ejector II is located; while James use a hydrogen diverter valve to divide the primary flow into two streams with different flow rates and control the secondary flow rates of the two ejectors through two solenoid valves to make the two ejectors work individually at high and low power, respectively; however, they did not give a quantitative design scheme.

Parallel ejector programme effectively widens the working range of a single ejector, and lower cost, simple control, easy to operate and maintain, but this programme in a very small power is still unable to meet the needs of the cycle, and need to be designed according to the power of a number of ejectors, to a certain extent, increase the workload.

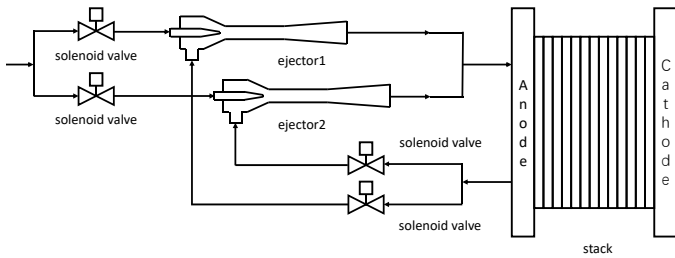


Fig. 8 Schematic diagram of two-stage ejector in parallel

3.4 Combination of ejectors and hydrogen circulation pumps

The combination of an ejector and a hydrogen circulation pump as a hydrogen circulation device for the PEMFC system can ensure its circulation needs at a low power, and it can play a better performance for the scenarios with frequent load changes. When the fuel cell is in the low power zone, the ejector performance is not good, then the hydrogen circulation pump is activated to circulate hydrogen, when in the high power zone, the ejector alone can meet the demand. This solution not only avoids the problem of poor performance of the ejector in the low power zone, but also reduces the power consumed by the hydrogen circulation pump.

The circulation scheme using a combination of ejectors and hydrogen circulation pumps can be arranged in both parallel and series, as shown in Figure 9.

There are fewer studies for the series mode, and most of them focus on the parallel mode. In 2005, Argonne Laboratories^[45] proposed a parallel connection between an ejector and a hydrogen circulation pump, with check valves on both circulating gas branches to prevent backflow, but the check valves have a high flow resistance, which may weaken the performance of the circulating subsystem. He^[46] proposed a scheme without check valves, which improves the problem, by adding an additional supply line with a flow control valve to deliver the gas directly to the anode inlet at low loads, and the opening and closing of the flow control valve corresponded to the change of load conditions.

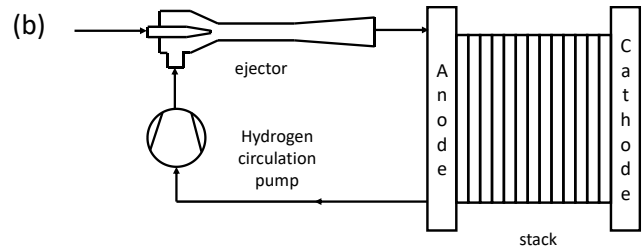
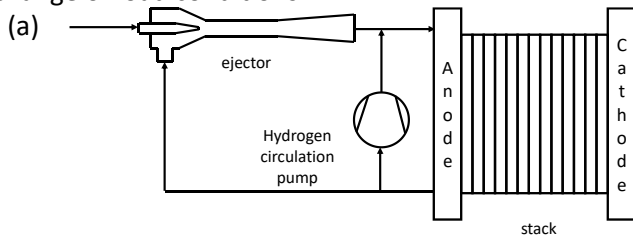


Fig. 9 Schematic diagram of the use of a ejector in combination with a hydrogen circulation pump (a) parallel scheme (b) series scheme

4. CONCLUSIONS

Aiming at the problem of poor performance of the ejector under low power, this paper analyses and summarizes the performance improvement method of the hydrogen cycle of the proton exchange membrane fuel cell. Firstly, the design methods of the ejector are summarised, which mainly include one-dimensional calculation, CFD simulation and algorithmic optimisation, and these three methods are usually not carried out individually. The actual design process generally starts with the one-dimensional model calculation to give a preliminary size range, and then CFD simulation and algorithmic search for the optimal combination of structural parameters. Considering the advantages of simple structure, reliable operation and lower cost of the ejector, the principles and current research status of several ejector-based hydrogen circulation schemes are compared. In the fixed structure ejector scheme, the matching problem between the ejector and the PEMFC system is investigated to improve its performance at low power; the new structure of the ejector can widen the range of use, but reduces the reliability; the parallel connection of two-stage ejectors can be used to make the two ejectors work at different power by controlling the solenoid valves, but it still can not satisfy the demand of smaller power circulation; the combination of the ejector and the circulating pump can well cover the circulating demand of all working conditions, which is suitable for the application scenario of frequent load change, but requires complex control strategy. In conclusion, the optimisation of structural parameters and the use of multi-stage circulation devices can effectively broaden the scope of use of the ejector.

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