Numerical investigations of the flow distributions with a transient three-dimensional multi-component ejector model

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Abstract. Ejector is a promising hydrogen recirculation for proton exchange membrane fuel cell (PEMFC) systems since it does not require parasitic power consumption. However, the complicated transport mechanisms inside the ejector remain unclear. In this study, the heat and mass transport processes are investigated by a transient three-dimensional multi-component model. The distribution of velocity, temperature, and pressure are presented. To avoid water vapor condensation, the maximum primary flow pressure should be limited to prevent the formation of a low temperature region at the nozzle throat. Compared with the converging-diverging nozzle, the convergent nozzle is recommended since it increases the condensation of water vapor. To predict the lowest temperature, the relationship between the relative pressure and the temperature is further obtained by curve fitting methods.

1. Introduction

Ejector is a promising device for the hydrogen recirculation in proton exchange membrane fuel cell (PEMFC) systems. Meanwhile, it also recycles the heat and moisture, enhancing energy utilization and anode humidification. However, several technical challenges remain to be solved, such as narrow working ranges, inaccurate flow control, and complicated transport mechanisms.

In the past decades, both numerical and experimental researches have been conducted. Experiments were mainly focused on the effects of fluid component, operating conditions, and structural designs. Li et al.[1] established an ejector test facility to study the effects of water vapor on the hydrogen recycle entrainment ratio. Arun et al.[2] used the schlieren flow visualization method to investigate the velocity distributions. It was found that shock waves were generated and influenced by velocity differences between the primary flow and the secondary flow. As regards modeling studies, Mazzelli et al.[3] comprehensively compared the two-dimensional (2D) model with a three-dimensional (3D) model. It was concluded that the 3D model generated more accurate results such as mass flow rate and entrainment ratio. Yin et al.[4] optimized the ejector geometric parameters to improve the entrainment ratio with a 3D steady-state model. To investigate the transient processes, Ankit et al.[5] proposed the inertial effect, which was found to be negatively correlated with the primary flow pressure. Lijo et al.[6] investigated the transient phenomena within a vacuum ejector. Ferrari et al.[7] developed a 3D ejector model for the SOFC recirculation. The model was validated against their experimental data. Despite aforementioned researches, the distribution of parameters (velocity, temperature, and pressure) inside the ejector are still not fully revealed. Water vapor condensation inside ejectors can cause severe damages to the performance and reliability. However, the studies to prevent vapor condensation are hard to find in literature. Investigating the transport processes inside ejectors not only helps improving performances but also gives advice on the prevention of water vapor condensation.

In the study, a transient 3D multi-component ejector model is developed since there are multiple
components in the fuel cell anode exhaust. The distribution of velocity, temperature, and pressure along the primary flow direction are presented. The differences between two turbulence models are studied. For guiding the choice of the working conditions, the relationship between primary flow pressure and the lowest temperature in ejector is investigated.

2. Mathematical method

2.1 Geometric parameters

As shown in Figure 1, the high-pressure hydrogen enters the ejector through the primary flow tube. The velocity of the primary flow increases dramatically. Meanwhile, the pressure declines rapidly due to the convergent nozzle. The vacuum region is formed at the nozzle throat. Therefore, the secondary flow can be drawn into the ejector by the pressure difference between secondary flow and the vacuum region. Subsequently, the primary flow and the secondary flow are fully mixed in the mixing tube. At the diffuser section, mixed gases restore the pressure and temperature to meet the fuel cell anode inlet requirements. In this study, geometric parameters are set the same as Dadvar et al. [8] and the operation conditions are adopted from reference [4].

Figure 1. Structural parameters of the ejector.

2.2 Governing equations

Continuity equation:

\[
\frac{d\rho}{dr} + \nabla \cdot \left( \rho \vec{U} \right) = 0
\]  
(1)

Where \( \rho \) is density (kg m\(^{-3}\)), \( t \) is time (s) and \( \vec{U} \) is body velocity (m s\(^{-1}\)).

Momentum equation:

\[
\frac{d\rho\vec{U}}{dr} + \nabla \cdot \left( \rho \vec{U} \vec{U} \right) + \nabla p = 0
\]  
(2)

Where \( p \) is pressure (Pa).

Energy equation:

\[
\frac{d\rho E}{dr} + \nabla \cdot \left( \rho \vec{U} E \right) + \nabla \cdot \left( \rho p \vec{U} \right) = 0
\]  
(3)

Where \( E \) is total energy (J kg\(^{-1}\)).

Species transport equation:

\[
\frac{d}{dr} \left( \rho Y_i \right) + \nabla \cdot \left( \rho \vec{U} Y_i \right) = -\nabla \cdot \vec{J}_i
\]  
(4)

\[
\vec{J}_i = -\rho D_{diff, i} \nabla Y_i
\]  
(5)
Where \( Y_i \) is mass fraction of \( i \) species (hydrogen, water vapor, nitrogen), \( J_i \) is the diffusion flux \( (\text{kg m}^{-2}\text{s}^{-1}) \) of \( i \) species, \( D_{\text{diff},i} \) is the diffusion coefficient of \( i \) species.

In this study, the ejector is mainly designed for fuel cell systems. The operating conditions are listed in Table 1. The ejector is initially filled with pure hydrogen. The initial temperature is the same as ambient temperature. The RNG \( k-\varepsilon \) turbulence model is adopted for all cases.

| Parameters                          | Values |
|-------------------------------------|--------|
| Primary flow temperature \( T_p \) (k) | 293    |
| Secondary flow temperature \( T_s \) (k) | 353    |
| Primary flow pressure \( P_p \) (kPa) | 450/325|
| Secondary flow pressure \( P_s \) (kPa) | 300    |
| Secondary flow water vapor mass fraction | 0.55   |
| Secondary flow nitrogen mass fraction | 0.05   |
| Secondary flow hydrogen mass fraction | 0.4    |

2.3 Numerical procedures

The simulations are conducted based on the open-source software OpenFOAM, and the rhoCentralFoam solver is adopted for calculation. However, the rhoCentralFoam solver in OpenFOAM cannot solve the flow problems with multiple components [9]. Therefore, the species transport equations are added to the solver owing to the existence of various gas species (including hydrogen, nitrogen, and water vapor) in the fuel cell system. The variable time step is used to accelerate the convergence speed and improve the calculation stability. Since the solver is a transient one, the steady-state solution does not exist. Therefore, when the relative error of mass rate between time points is less than 0.03, a relatively stable state is considered to be reached. All simulations are conducted based on the Tianhe-HPC1 system at the National Supercomputer Center in China.

3. Results and discussions

The numerical results are validated with experimental data [10] in two different turbulent models, which are \( k-\varepsilon \) RNG and \( k-\omega \) SST, respectively. Figure 2 illustrates the comparison of mass flow rates with different turbulence models. It is seen that the two different turbulence models can predict the
flow rate of the primary flow well. When it comes to the secondary flow, both models overestimate the mass flow rate. The $k$-$\omega$ SST model predicts more accurately when the pressure is lower (125kPa), and the error increases significantly when the pressure is higher (175kPa). In general, the fluctuation of $k$-$\varepsilon$ RNG is smaller than $k$-$\omega$ SST. Therefore, the $k$-$\varepsilon$ RNG turbulence model is finally selected.

Figure 3 shows the distribution of velocity, pressure, and temperature along the primary flow direction. The differences between two different primary flow pressures (325kPa, 450kPa) are presented. The abscissa represents the relative position in the z-direction, 0 represents the inlet of primary flow, and 1 represents the outlet. The result shows that the velocity gradually increases in the nozzle (0.05-0.3) and the pressure gradually decreases in the nozzle. In addition, the maximum value of velocity and the minimum value of pressure occur at 0.3, where is the nozzle throat position. Note that the maximum velocity of 450kPa is much larger than 325kPa (Figure 3 (a) shown) and the vacuum region pressure of 450kPa is lower than 325kPa (Figure 3 (b) shown).

The Figure 3(c) shows the temperature variation inside the ejector. It is found that the minimum of temperature occurs at the nozzle throat. Higher primary flow pressure results in lower temperature at the nozzle throat. The lowest temperature is about 268K with the primary flow pressure being 450kPa. Compared to the inlet region of primary flow, the temperature drops by nearly 25K. However, the secondary flow from fuel cell anode exhaust contains water vapor, which will condense due to the low temperature at the nozzle throat position. If the primary flow pressure is 325kPa, the lowest temperature drops a little (only 3-4K). Therefore, the inlet primary flow pressure of ejectors for fuel cell systems must be limited to prevent water vapor condensation. Since the converging-diverging nozzle results in lower temperature than the converging nozzle [11], the converging-diverging nozzle is not suitable for PEMFC systems.

For working fluids including water vapor, predicting the lowest temperature helps prevent water vapor condensation, which improves the ejector stability. As shown in Figure 4, the relationship between the relative pressure of the primary flow and the lowest temperature inside the ejector is investigated. A linear fitting equation is proposed for predicting the lowest temperature inside the ejector. The details of linear fit equation are shown in Table 2. It can be seen that there is a linear negative correlation between the relative pressure of the primary flow and the lowest temperature. The lowest temperature of the ejector inside can be predicted by this equation which can guide the choice of the primary inlet pressure.
Table 2. The parameters of the linear fit equation.

| Description       | Types and value         |
|-------------------|-------------------------|
| Equation          | $y = a + b \times x$    |
| Plot              | Temperature             |
| Weight            | No Weighting            |
| Intercept         | $342.17277 \pm 1.80675$ |
| Slope             | $-0.16631 \pm 0.00463$  |
| Residual Sum of Squares | 0.9397                |
| Pearson's r       | -0.99845                |
| R-Square(COD)     | 0.9969                  |
| Adj.R-Square      | 0.99613                 |

Figure 4. Linear fit of relative pressure to temperature.

4. Conclusions
In this study, a transient three-dimensional multi-component ejector model is established for investigating the heat and mass transport processes inside the ejector. The $k$-$\omega$ SST model better predicts the ejector performance than $k$-$\varepsilon$ RNG if the primary flow pressure is lower than 125kPa. Conversely, the predictive ability of $k$-$\omega$ SST is better than $k$-$\varepsilon$ RNG at high pressure. The distribution of velocity, pressure, and temperature along the primary flow direction are presented. The results indicate that the most dramatic change occurs in the nozzle throat. The velocity rises significantly while the pressure and temperature drops. The maximum value of the primary flow pressure of ejector systems for fuel cell systems should be limited to prevent water vapor condensation caused by low temperature region. The diverging nozzle is more suitable than the converging-diverging nozzle. A linear fitting equation of primary flow relative pressure to lowest temperature is proposed to prevent condensation inside the ejector.

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References
[1] F. Li, J. Du, L. Zhang, J. Li, G. Li, G. Zhu, M. Ouyang, J. Chai, H. Li, (2017), Experimental determination of the water vapor effect on subsonic ejector for proton exchange membrane fuel cell (PEMFC), International Journal of Hydrogen Energy 42(50) 29966-29970.
[2] K.M. Arun, S. Tiwari, A. Mani, (2019), Experimental studies on a rectangular ejector with air, International Journal of Thermal Sciences 140 43-49.
[3] F. Mazzelli, A.B. Little, S. Garimella, Y. Bartosiewicz, (2015), Computational and experimental analysis of supersonic air ejector: Turbulence modeling and assessment of 3D effects, International Journal of Heat and Fluid Flow 56 305-316.
[4] Y. Yin, M. Fan, K. Jiao, Q. Du, Y. Qin, (2016), Numerical investigation of an ejector for anode recirculation in proton exchange membrane fuel cell system, Energy conversion and management 126 1106-1117.
[5] A. Mittal, G. Rajesh, V. Lijo, H.D. Kim, (2014), Starting Transients in Vacuum Ejector-Diffuser System, Journal of Propulsion and Power 30(5) 1213-1223.
[6] V. Lijo, H.D. Kim, G. Rajesh, T. Setoguchi, (2010), Numerical simulation of transient flows in a vacuum ejector-diffuser system, Proceedings of the Institution of Mechanical Engineers, Part G: Journal of Aerospace Engineering 224(7) 777-786.
[7] M. Ferrari, M. Pascenti, A. Massardo, (2018), Validated ejector model for hybrid system applications, Energy 162 1106-1114.

[8] M. Dadvar, E. Afshari, (2014), Analysis of design parameters in anodic recirculation system based on ejector technology for PEM fuel cells: A new approach in designing, international journal of hydrogen energy 39(23) 12061-12073.

[9] C.J. Greenshields, H.G. Weller, L. Gasparini, J.M. Reese, (2010), Implementation of semi-discrete, non-staggered central schemes in a colocated, polyhedral, finite volume framework, for high-speed viscous flows, International journal for numerical methods in fluids 63(1) 1-21.

[10] K. Nikiforow, P. Koski, H. Karimäki, J. Ihonen, V. Alopaeus, (2016), Designing a hydrogen gas ejector for 5 kW stationary PEMFC system–CFD-modeling and experimental validation, International Journal of Hydrogen Energy 41(33) 14952-14970.

[11] NAKAGAWA Masafumi, M.S. BERANA, KISHINE Akinori, (2009), Supersonic two-phase flow of CO2 through converging–diverging nozzles for the ejector refrigeration cycle, International Journal of Refrigeration 32(6) 1195-1202.