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AI-BASED OPTIMIZATION OF PROTON EXCHANGE MEMBRANE FUEL CELL CENTRIFUGAL COMPRESSOR VIA THREE-DIMENSIONAL COMPUTATIONAL FLUID DYNAMICS MODEL AND DATA-DRIVEN SURROGATE MODEL

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ABSTRACT

Air compressor is an important sub-component in fuel cell systems. Previous experimental and numerical studies still cannot provide an effective method for the quick and deep modification for fuel cell centrifugal compressor structure. To improve the compressor pressure ratio and efficiency, this paper develops a novel artificial intelligence (AI) framework for fuel cell centrifugal compressors by integrating three-dimensional (3D) computational fluid dynamics (CFD) models, machine learning and genetic algorithm. Based on the simulated results, the surrogate model is developed, which is subsequently coupled with NSGA-Ⅲ algorithm to find the Pareto-optimal front. A set of optimized parameters are obtained. Based on the CFD model, the performance of the optimized compressor is comprehensively compared with the original compressor design. It is found that the flow uniformity inside compressor is greatly enhanced, leading to a better performance.

Keywords: centrifugal compressor, AI, data-driven surrogate model, SVM, NSGA-Ⅲ.

1. INTRODUCTION

Proton exchange membrane fuel cell converts chemical energy into electricity, has been widely used in a variety of applications [1]. As an important sub-component, centrifugal compressor is considered as one of the most promising air compressor fuel cell system [2]. Centrifugal compressors for fuel cell have specific characteristics that are not different from previous compressors [3]. Therefore, it is necessary to redesign and optimize the fuel cell compressor.

A lot of researches have been carried out on the centrifugal compressor for PEMFC systems. Qi et al. [4] used commercial software CFTurbo to design low flow rate and low specific speed centrifugal compressors. However, the designed compressor relied on commercial software database and could not meet the requirements of high pressure ratio and high efficiency. Zhang et al. [5] optimized aerodynamic performances with impeller parameters based on the genetic algorithm and data mining method. But the optimization method has a long iteration cycle. The method of combining machine learning and genetic algorithm for multi-objective optimization has been used in other turbomachinery researches [6, 7]. However, few researches of multi-objective optimization framework for fuel cell centrifugal compressor were found in literature.

In this study, a three-dimensional (3D) centrifugal compressor model is developed in ANSYS. Based on the simulation results, an AI framework is presented, which combines support vector machine (SVM) with NSGA-Ⅲ algorithm. The framework is used to optimize the designed centrifugal compressor. The 3D model is further adopted to verify the effectiveness of optimized parameters, and the mechanisms that result in performance improvement have been explained.

2. AI FRAMEWORK

2.1 Design target

To meet the requirement of a 130 kW fuel cell stack, a single-stage centrifugal compressor is designed. The air mass flow is calculated based on the Faraday law [8].

$$m_{air} = \frac{N_{stack} I A_{cell} \xi M_{air}}{4F \times 0.21 \times 1000} \tag{1}$$

In this paper, the minimum current density for stack is set as 0.1 A cm^{-2}, and the stoichiometry ξ is set as 1.4. The maximum current density is set as 2.2 A cm^{-2}, and the stoichiometry ξ is set as 2.3. Correspondingly, the target mass flow rate of centrifugal compressor ranges from 6.24 g s^{-1} to 226 g s^{-1}. According to the flow range, a centrifugal compressor with a rated power point of 160 g s^{-1} 10000 rpm is designed, as shown in Fig 1.

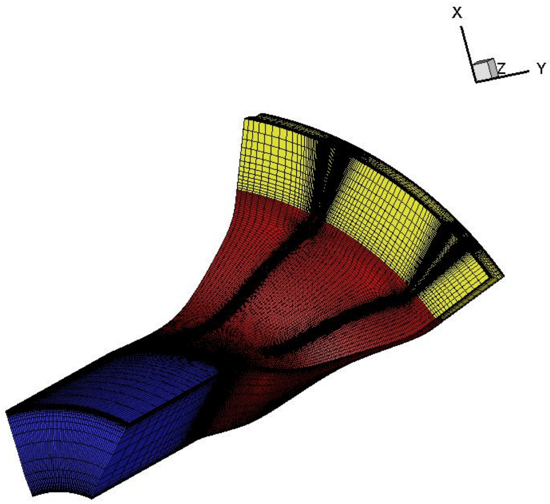


Fig 1 Computational domain

2.2 Governing equations

In this study, air is assumed to be compressible ideal gas, and effects of gravity are neglected. The governing equations include continuity equation, momentum equation, and energy equation.

$$\frac{\partial \rho}{\partial t}+\nabla\cdot(\rho U)=0 \tag{2}$$

$$\frac{\partial \rho U}{\partial t}+\nabla\cdot(\rho UU)=\nabla\cdot p+\nabla\cdot\tau \tag{3}$$

$$\frac{\partial \rho h}{\partial t}+\nabla\cdot(\rho Uh)+\frac{\partial \rho K}{\partial t}+\nabla\cdot(\rho UK)-\nabla\cdot(\alpha_{\mathrm{eff}}\nabla h)=\frac{\partial p}{\partial t} \tag{4}$$

2.3 Boundary conditions

CFX 2019 R1 is adopted for numerical calculation. The inlet boundary is set away from impeller inlet 40 mm for calculation accuracy. Total pressure and mass flow rate are adopted for inlet and outlet boundary, respectively. The wall is set to be adiabatic. The shear stress transport (SST) turbulence model is adopted. The convergence criterion is set as 10^{-6}. The dimensionless wall distance between the wall and the first node (y+) is about 5~10 in the all components. Hexahedral meshes are used. The flow inside tip-clearance between stationary shroud and rotary impeller is computed as a part of the entire flow domain. The frozen rotor method is used for the data exchange between stationary region and rotary region. Automatic wall function is selected to achieve the accuracy for low Reynolds number form and the wall function formulation. Considering the large amount of data used in machine learning, the single passage steady state calculation is used to generate the database.

2.4 Grid independence study

The grid number in the computational domain ranges from 0.4 million to 1.4 million. It is found that the increase of grid number from 1.15 million to 1.4 million brings negligible difference. Therefore, the grid number of 1.15 million is adopted.

2.5 SVM and NSGA-III

Support vector machine (SVM) is widely used in machine learning. SVM is adopted in this paper. The database is randomly divided into training set and test set, and the test set does not participate in training during the whole process. The ε – SVR is more suitable for regression problems. In order to calculate the nonlinear function, radial basis function kernel is chosen. The five-fold cross-validation is conducted to search the optimal values of *c* and *g*. The relationship can be mathematically expressed as:

$$\pi=S(R_{1h},R_{1s},R_2,\beta_1,\beta_2,b) \tag{5}$$

$$\eta=S(R_{1h},R_{1s},R_2,\beta_1,\beta_2,b) \tag{6}$$

For fuel cell vehicles, the operating conditions are changing during the road conditions. In this paper, three operating cases are considered, and the details are given in Table 1.

Table 1 Case details.

Case	Rotating speed	Mass flow rate ratio
Case 1	100000 rpm	100%
Case 2	120000 rpm	150%
Case 3	60000 rpm	70%

In multi-objective optimization problem, it is difficult to obtain an optimal value that satisfies each objective function. If one objective function is improved, at least the other objective function will be weakened. This is called the Pareto optimal solution.

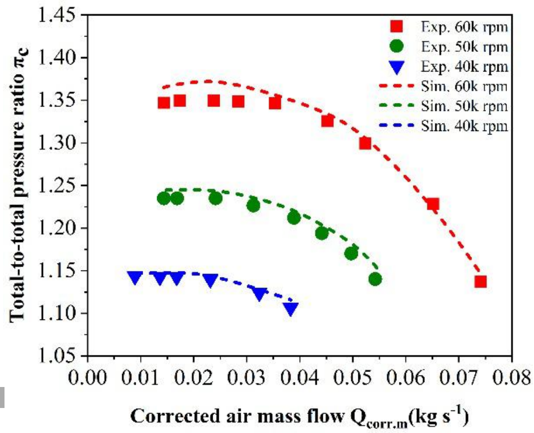
The genetic algorithm (GA) is an algorithm that simulates the natural selection and genetic mechanism of Darwinian biological evolution. The NSGA-III proposed by Deb et al. [9] is a non-dominated sorting multi-objective optimization genetic algorithm. Considering different requirements for pressure ratio and efficiency in vehicle road conditions, different weights in object function have been set. The pressure ratio weight under accelerated conditions is larger, and the efficiency weight under common conditions is larger. The proportion of the pressure ratio in case 1, case 2 and case 3 is set as 0.3, 0.5, 0.2, respectively. The proportion of the efficiency in case 1, case 2 and case 3 is set as 0.3, 0.2, 0.5, respectively.

In total, there are 200 populations. The crossover rate and the mutation rate are 0.95 and 0.1, respectively. The maximum iterations are 1000. The Pareto-optimal front not change after 300 iterations. The fitness values are the total-total pressure ratio and total-total isentropic efficiency.

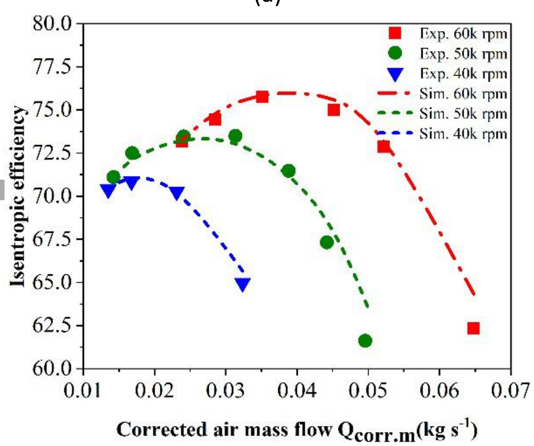
3. RESULTS AND DISCUSSION

3.1 Model validation

To verify the 3D CFD model, comparison between experimental data and simulation data is shown in Fig 2.



(a)



(b)

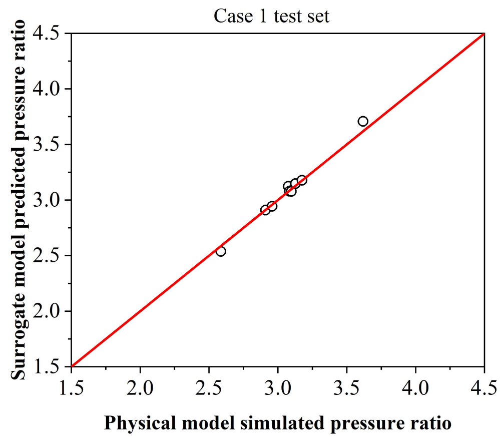
Fig 2 Comparison between simulation results and experimental data [2]. (a) Total-to-total pressure ratio. (b) Total-to-total isentropic efficiency.

The maximum relative error of total pressure ratio and isentropic efficiency are less than 2% and 5%, respectively. Simulation data and experimental data are well matched.

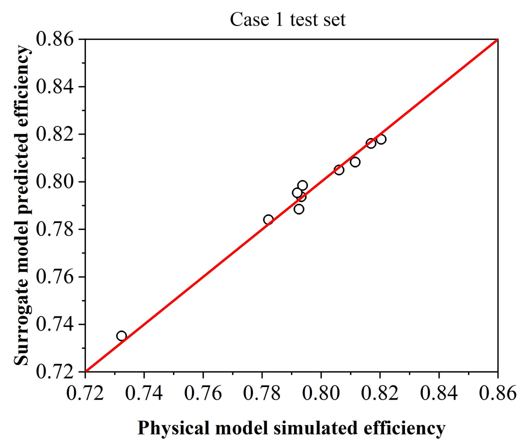
3.2 Prediction performances

To evaluate the accuracy of surrogate model, root mean squared error (RMSE), square correlation coefficient (R-square), mean percentage error are adopted.

Fig 3 shows the predicted performance in the dataset of case 1. The surrogate model performance of case 2 and case 3 are similar to case 1. The other two cases also reached a high prediction level. RMSE, R-square and mean percentage error in the test set are showed in Table 2.



(a)



(b)

Fig 3 Predicted performance. (a) Pressure ratio in the test set at case 1. (b) Isentropic efficiency in the test set at case 1.

Table 2 Prediction accuracy.

Test set in Case 1	RMSE	R-square	Mean percentage error, %
Pressure ratio	0.0371	0.9766	2.6143
Isentropic efficiency	0.0028	0.9856	0.0025

3.3 Comparison of original model and optimized model

Fig 4 shows the entropy at 50% span in case 1. It is found that the flow of the optimized impeller is more uniform and the entropy increase is smaller. The separation flow at impeller leading edge decreases indicating the impeller blade angle is more reasonable. The flow separation in optimized model is reduced and the energy loss is smaller. From the perspective of impeller height, both 20% span and 80% span achieve a more uniform flow field of the optimized model, too.

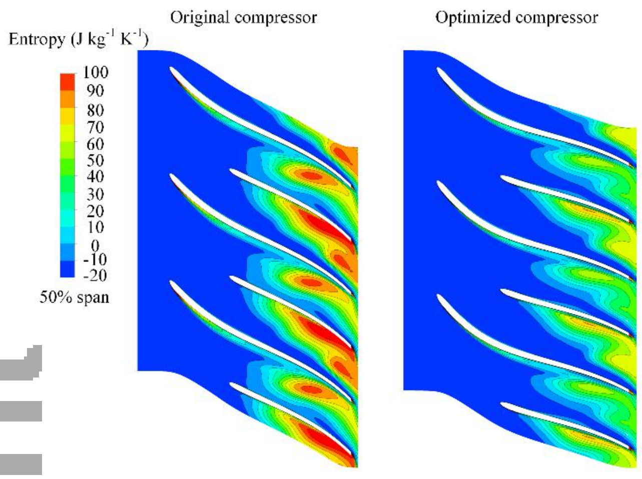


Fig 4 Comparison of Entropy between original compressor and optimized compressor.

After CFD calculation, the performance of the optimized model is significantly better than the original model. At case 1, the pressure ratio is increased by 0.71%, the isentropic efficiency is increased by 4.19%. At case 2, the pressure ratio is increased by 12.47%, the isentropic efficiency is increased by 6.86%. At case 3, the pressure ratio is increased by 0.62%, the isentropic efficiency is increased by 1.60%.

4. CONCLUSIONS

A comprehensive three-dimensional (3D) centrifugal compressor model for fuel cell systems is developed. A novel AI framework combining SVM and NSGA-III algorithm is developed to achieve multi-variable global optimization for improving centrifugal compressor pressure ratio and efficiency. The advantages of proposed AI framework are summarized as follows:

(1) Both the CFD model and the SVM model have shown a reliable predicted result for the performance of compressor.
(2) From the perspective of entropy variation, it is seen that the flow field is greatly modified.
(3) At large mass flow rate operating point, the pressure ratio and efficiency of the optimized compressor are greatly increased.

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