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Three-dimensional CFD Modelling of a Roots Blower for Hydrogen Recirculation in Fuel Cell System

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ABSTRACT

Fuel cell system has gained extensive attention due to increasing tendency of environmental protection, and Roots blower has great potential as the recirculation pump in its hydrogen recirculation system while there are rare of research about this ancillary component. In this paper, a three-dimensional, transient model of a three-lobe Root pump was established and solved and the internal flow characteristic was investigated. The results show that pressure ratio can influence the mass flow rate and torque significantly and high pressure ratio will lead to mass flow reflux. The most dramatic variation of pressure occurs in the moment that the displacement chamber connects with the exhaust region. The vortex will arise from both the inlet and outlet pocket. Different methods are needed to reduce the vortexes since their position are quite different in the inlet and outlet pocket.

Keywords：FCV, Hydrogen recirculation pump, Roots blower, CFD transient modeling, leakage flow

1. INTRODUCTION

Fuel cell vehicles (FCV) are considered as the best candidates for internal electric engine in the future because of its high power density, low emission, low operation temperature and short start-up time. In a PEM fuel cell system, the hydrogen fuel must be supplied with more than it is required for a given load. The best way to use those excess gas at the exit of fuel cell stack is to recirculate it back to stack's inlet. Some researches about hydrogen recirculation system (HRS) and the associated control systems have been carried out in recent years[1-3]. Different recirculation types, including recirculation pump, ejector, combination of pump and ejector or pumpless system have been researched to achieve high efficiency. However, the published literatures are mainly focused on the comprehensive system of HRS or the influence of it to the overall performance of FCV, and there are rare of research about the ancillary components for proper fuel cell system operation.

Roots blower has great potential in this application as the recirculation pump due to its advantages such as low cost and high reliability, and it has been widely researched as a kind of general machinery. Most prior research focused on geometric design or different shapes of rotors. Mimmi and Pennacchi[4,5] examined dynamic pressure loads acting on the helical and spur shaped rotors, indicating that increasing the reservoir and using helical shaped rotors can improve dynamic loads regularity and decrease system vibrations. Hwang and C.F. Hsieh[6,7] proposed new rotor profiles using the trochoidal curve or cycloid curve with variable trochoid ratio to improve sealing performance between the rotor tip and the chamber and achieve high volumetric efficiency. Tong and Yang et al.[8-10] presented a complete synthesis procedure to design rotor profile for high-sealing roots pumps by deriving a novel deviation function with given flow rate functions.

With the rapid development of CFD simulation in both software and hardware, numerical simulation has become one of the three main methods to deal with complex problems in fluid mechanics. Houzeaux and Codina[11] developed a finite element method to simulate the flow in rotary displacement pumps, a method that able to solve leakage problems in the gap and gear intersection while the transient Navier-Stokes equations must be solved in a series of configurations. Huang and Liu[12] used RNG k-ε turbulent model, second-order upwind difference scheme to simulate an involute-type three-lobe positive discharge blower, and the results were compares those from semi-empirical formulas. Strasser[13] applied a simulation of a large-scale metering gear pump through a moving-deforming grid method, and Second-order upwinding and bounded central differencing schemes were used to reduce numerical diffusion. Shu-Kai Sun[14] established two simulated 3D cases to analyze flow characters in working chambers and inlet/outlet pockets of a Roots pump by using a dynamic mesh method, and the results were validated by tests. Heish[15] compared the difference between cylindrical and screw type Roots pumps in terms of their outlet flow rates and pressure pulsation.

Although much research has been conducted about the Roots mechanical, its applications are limited as the vacuum pump, blower or compressor, and the working medium are focused on air or liquids as water in the published literature. While hydrogen recirculation pump has a significant difference with traditional Roots mechanical in operation condition and characteristics of the working medium. So it is an important issue to realize the fluid flow in the hydrogen Roots pump. The mathematical model and fluid analysis are presented and discussed in the following sections.

2. NUMERICAL SIMULATIONS

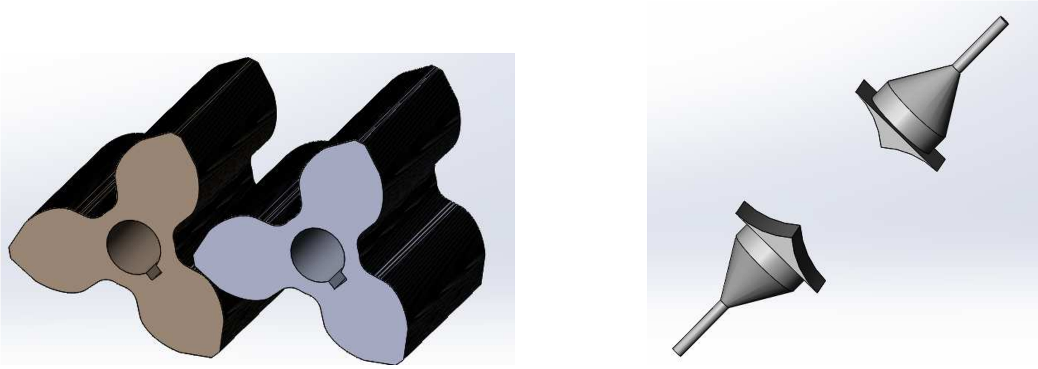
2.1 The Geometry of Roots Pumps

The roots pump in this project had two three-lobe rotors, as seen in Fig.1a. The rotors have a diameter of 37.5mm and a length of 50mm. Theoretical suction volume of it was 0.72~1.67 m3/min with rotational speed 3000~7000 r/min. The gaps between the rotors and the casing were 50μm and between two rotors 100μm. The fluid domain included the deforming part which was the cavity between rotors and pump's cylinder and the stationary part which included the suction and discharge ports as well as the solid regions as shown in Fig.1b.

2.2 Grid Generation

The deform-and-remesh or dynamic method is one of the common methods in modeling the flow filed in a positive displacement machine but often causes bad quality even illegal grids due to the significant change in shape of fluid domains. The overlapping grids or overset method is a comfortable approach to investigate the rotor influence inside a PD machine, but it often lakes of conservation because the interpolation between meshes and a very high number of elements is necessary to resolve the gaps accurately.

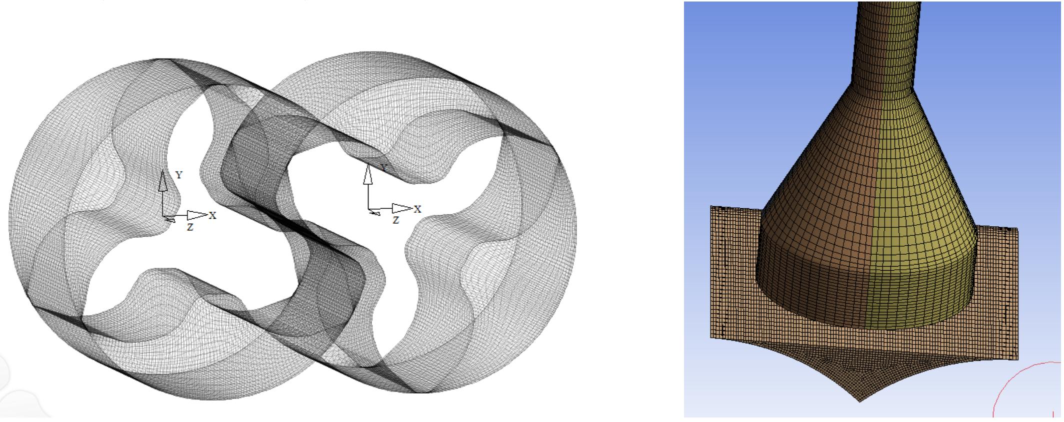
Customized grid generation can avoid disadvantages of above two methods. Kovaccevic et al. pioneered in grid generation for screw rotors with algebraic method through the computer code called SCORG(Screw Compressor Rotor Grid Generation), and Twinmesh is another meshing software to generate high quality grids for the moving parts of PD machines.



a) Geometry of rotors b) Geometry of suction and discharge ports

Figure1： Geometry of rotors and stationary ports

In this project, Twinmesh was used to pre-generate the hexahedral structured meshes of the deforming fluid domain as shown in Fig.2a. The fluid domain between the rotors and the casing was divided into two parts, and was connected via an interface contour. Meshes for each new rotor position needed to be generated individually and all of them had same mesh topology and node number. Fig.3 showed the meshes in a 2D cross section in detail and we can see that there was high resolution of gaps (dozens of micrometers) and smooth changes between small gaps and larger chambers (several centimeters).



a) Grids of deforming domain b) Grids of stationary domain

Figure 2：Meshes of simulation

All other meshes, i.e. the supply pipes at suction and discharge sides, and the solid regions were generated with ANSYS Meshing (Fig.2b) and the whole stationary fluid regions consisted of 149,294 elements. In sum the total global fluid domain consisted of 641,750 elements adding 229,500 elements of each part of deforming domain.

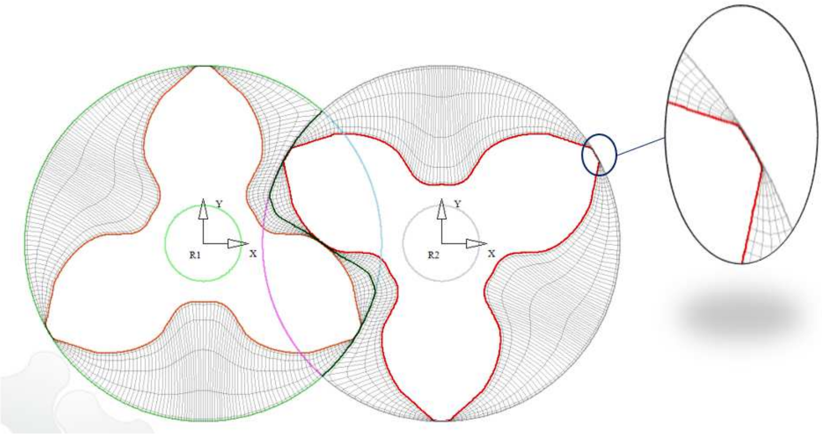


Figure 3：Details of structured grids of deforming domain

2.3 Simulation Setup

The meshes for different parts were connected with Generalized Grid Interface and the model of Roots pump was carried out based on ANSYS CFX platform. The fluid was hydrogen, with its density changed as an ideal gas. In these simulations, the Shear Stress Transport (SST) model was used, which can resolve large turbulent structure while still modeling the smaller and near-wall scales. Transient term discrete method of the governing equations was the implicit time step -- a second order backward Euler (2nd order accurate).

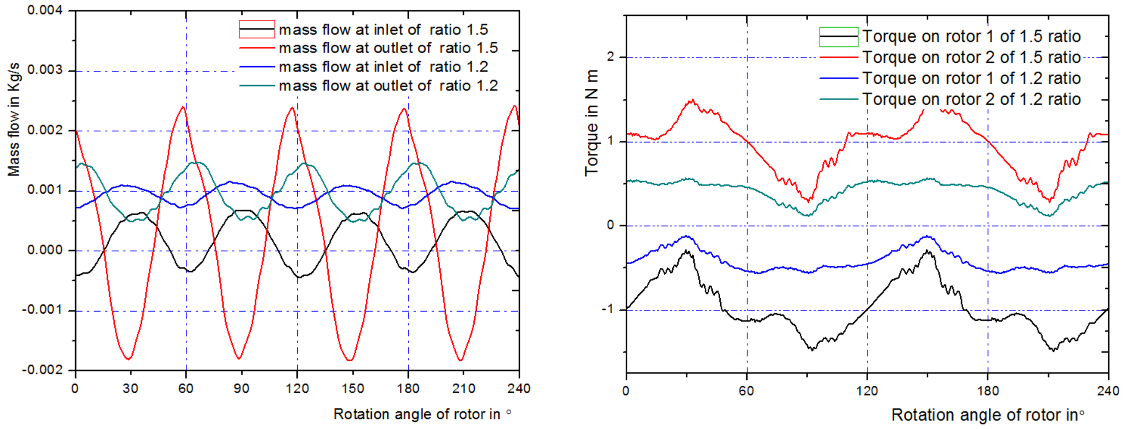
The working process was similar to an adiabatic process due to high rotation speed and the wall condition was assumed to be adiabatic. Both total pressure and temperature were given at inlet and outlet boundary. The inlet pressure was 1.0bar and temperature 293.15 K, and the outlet pressure changed in pressure ratio of 1.2 to 1.5.

With TwinMesh, the meshes were generated and stored in this case for every 1 rotation angle, and the time step size was decided by both rotation angle size and rotation speed. The simulation was considered as steady when the difference of average mass flow between the inlet and outlet boundary was lower than 1%.

3. RESULTS AND DISCUSSION

3.1 Mass Flow and Torques

The variation of mass flow at inlet and outlet and torque on both rotors over rotation angle under different pressure ratio is shown in Fig.4. It can be seen that the mass flow rate at both inlet and outlet shows regular periodic variation, while the fluctuation at outlet is more violent than it at inlet. High pressure ratio amplifies the fluctuation and when the pressure ratio is 1.5, a mass flow reflux can be observed at inlet and outlet. In a rotor rotation cycle, the flow rate shows six fluctuations because of the interaction of two rotors, and the frequency of this variation is twice the number of rotor's lobes. In the variation of torque, because of same profile design two rotors bear same torque value and change cycle of 120° which is two times of mass flow change, the only difference is a phase difference of 60°. High pressure ration also means large fluctuation range in the variation of torque.

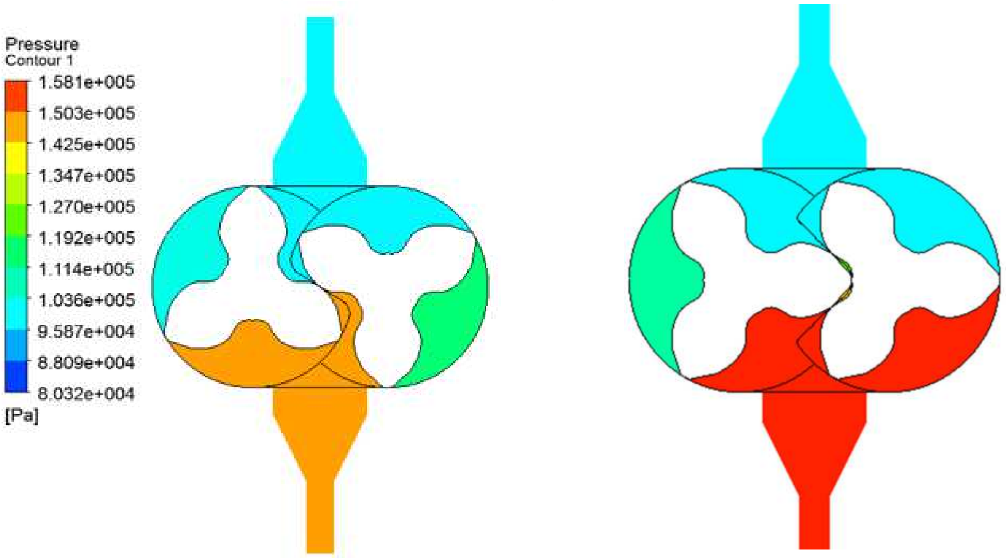


a) Mass flow variation with rotation angle b) Torque variation with rotation angle

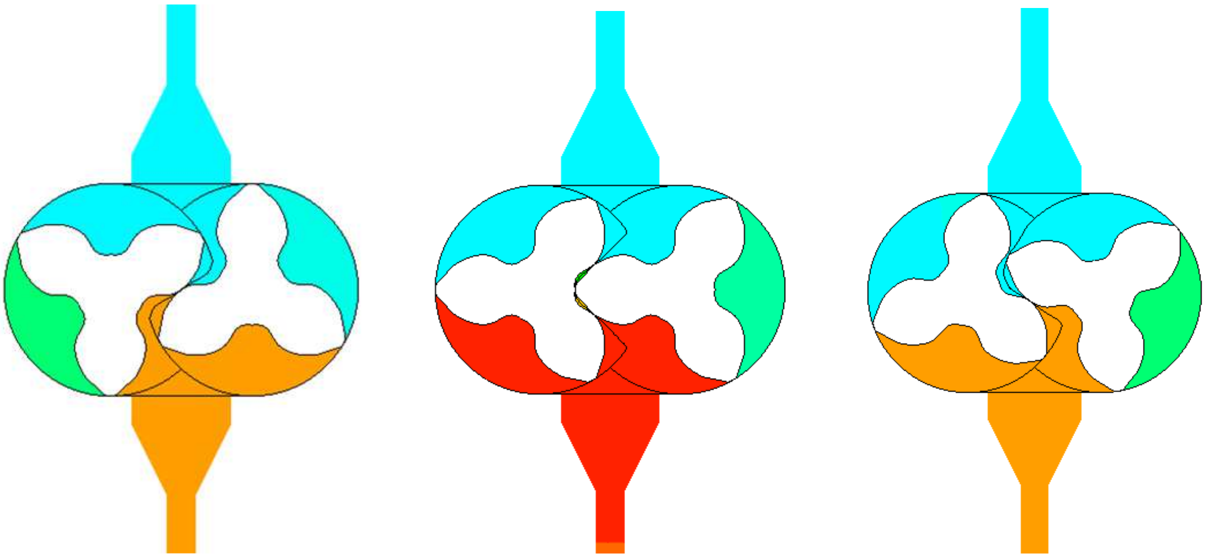
Figure 4: Mass flow and torque under different pressure ratio

3.2 Pressure Field

Pressure fluctuation of the internal flow is known to play a crucial role in understanding and predicting the unsteady flow and noise generation mechanisms. Fig.5 describes the pressure distribution of a stable cycle case in which the suction pressure is 1.0bar and discharge pressure 1.5bar, rotating speed is 6000r/min, and the clearance 0.05mm.



a) θ=0°/120°/240° b) θ=30°/150°/270°



c) θ=60°/180°/300° d) θ=90°/210°/330° e) θ=110°/230°/350°

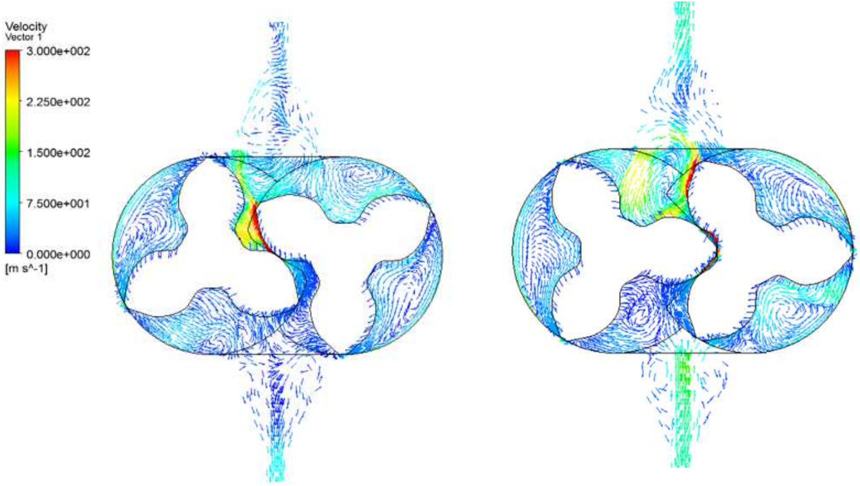
Figure 5: Pressure fields on middle face with rotation angle

From a to e the rotating angle of the rotor is 0°~110°, and that of another two rotors 120°~230° and 240°~350° respectively. A complete cycle is represented in the diagram as the suction process of a-e-a, displacement process a-c, and the last compressing and discharge process c-e-a-c. This set of images clearly shows that the pressure remains relatively stable and has small fluctuation in the intake region, increases slowly in in the displacement chamber and has an undulant fluctuation around a higher value in the exhaust region. The variation range of the pressure is 82.5kPa to 174.1kPa, and the most dramatic variation occurs in the moment that the displacement chamber connects with the exhaust region.

3.3 Velocity Field

Fig.6 shows the variation of velocity in Roots pump, and the legend is fixed in the range of 0 to 200m/s in order to show the whole velocity field better. Fig.6 a) has the same rotation angle with Fig.5 a), and so are Fig.6 b-e).

The fluid flows into the suction region and moves along the surface of rotors. A vortex arises in the radial direction with the rotation angle of 30°. The vortex moves with the rotor as the rotor rotates and then disappeared after the rotating angle of 90°. This is because that the connection channel between the working chamber and intake region becomes narrow at this time and the flow tends to be slow. When the angle is 120°, the working chamber is closed and then maintained with rotor's rotating until the angle reaches 180°.



a) θ=0°/120°/240° b) θ=30°/150°/270°

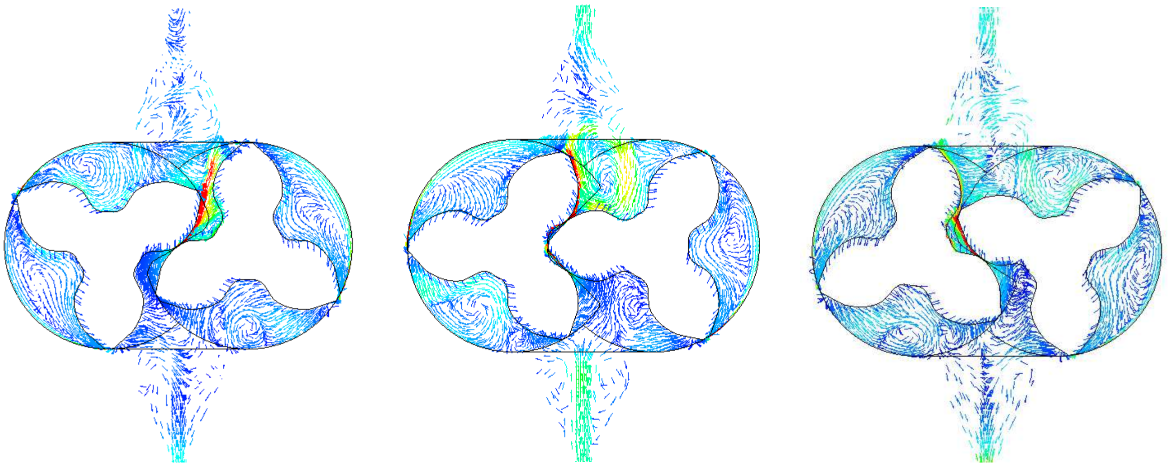
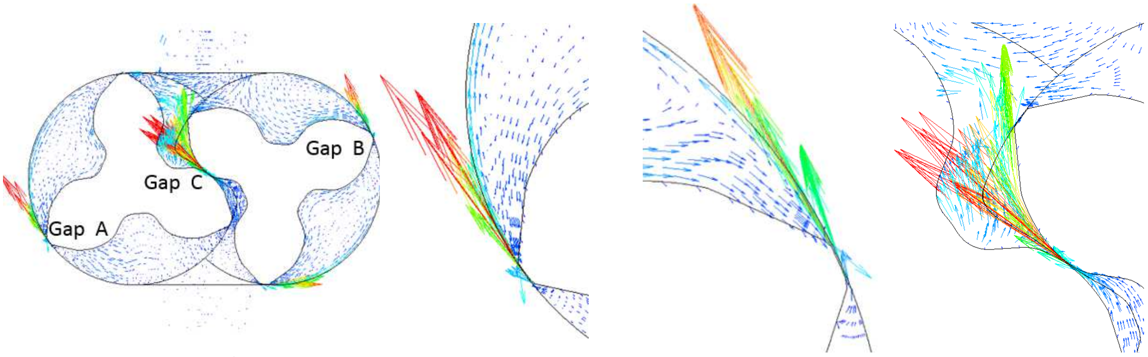

c) θ=60°/180°/300° d) θ=90°/210°/330° e) θ=110°/230°/350°

Figure 6: Velocity fields on middle face with rotation angle

After 180°, the closed chamber connects with the exhaust region. The high-pressure fluid flows into the working chamber and collides with the normal flow. So a vortex distributed alternately in two rotors' chambers is formed. After the pressure in the chamber is high enough, the fluid begins flow into exhaust pocket with rotor's rotating and causes the pressure in exhaust pocket rises again. Then another flow-back will be taken place. This kind of fluid back-flow in exhaust pocket repeats itself and causes intensified discharge pressure pulsation.

It can be seen that the rotation angle has great effects on the distribution of inlet and outlet velocity. The fluctuation of outlet velocity is much higher than that of inlet velocity. The vortex exists at both the inlet and outlet pockets, and it is the main cause of discharge pressure pulsation and the aerodynamical noise made by the pump. The vortex in the inlet pocket is close to the rotors while in the outlet pocket is near the cylinder wall. This indicates different methods are needed to reduce the vortexes and noises.



a) Distribution of velocity b) Velocity in gap A c) Velocity in gap B d) Velocity in gap C

Figure 7: Distribution of velocity vector at rotating angle 10°

Fig.7 shows the distribution of velocity vectors in middle face at the rotating angle of 10°. At this moment, we can see that compared with other regions, the velocity in gap A(0.05mm), gap B(0.05mm) and gap C(0.1mm) are much larger. The velocity in gap A is larger than that in gap B because there is a greater pressure difference between the two sides of the chamber. Moreover, the flow direction in three gaps is all in the opposite direction of the main flow. It can be seen that the high pressure at exhaust pocket has a strong influence on the whole velocity distribution and the high-speed back flow will lead to significant energy dissipation.

4. CONCLUSIONS

A numerical simulation of the three-dimensional unsteady flow in a Roots pump for hydrogen recirculation used in fuel cell system was presented in this paper. Twinmesh was used to generate structured meshes of the deforming fluid domain in cylinder which has a high resolution of gaps and smooth changes between small gaps and larger chambers. The governing equations were solved with second order backward Euler scheme using Shear Stress Transport turbulent model. The following conclusions can be drawn from the results of investigation:

- The mass flow variation at the outlet is more violent than in the inlet. High pressure ratio amplifies the fluctuation and will lead to mass flow reflux. The frequency of mass flow variation is twice the number of rotor's lobes in a rotor rotation cycle. Two rotors bear same torque value and its change cycle is two times of mass flow change.
- Pressure remains relatively stable and has small fluctuation in the intake region, increases slowly in in the displacement chamber and has an undulant fluctuation around a higher value in the exhaust region. The most dramatic variation occurs in the moment that the displacement chamber connects with the exhaust region.
- The velocity field of the Roots pump is influenced by the pressure field. The gaps between rotors and casing, as well as between two rotors, are filled with the back-flow gas with high velocity. This will lead to significant energy dissipation. The vortex will arise from both the inlet and outlet pocket. It is close to the rotors in the inlet pocket, while near the cylinder wall in the outlet pockets. This indicates different methods are needed to reduce the vortexes and noises.

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