2018

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Karvountzis-Kontakiotis, Apostolos; Singh, Gursharanjit; Kovacevic, Ahmed; and Rane, Sham Ramchandra, "CFD Modelling of a Twin Screw Expander Using a Single Domain Rotor Grid" (2018). *International Compressor Engineering Conference.* Paper 2525.
https://docs.lib.purdue.edu/icec/2525

CFD Modelling of a Twin Screw Expander Using a Single Domain Rotor Grid

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ABSTRACT

Grid generation for analysis of screw machines plays a significant role in the accuracy of Computational Fluid Dynamics predictions. Recently a new grid generation method, referred to as Casing-to-Rotor conformal mesh, was developed to generate fully conformal single domain mesh for the working domain between screw machine rotors and casing.

In this work, an analysis of the performance prediction of a twin screw air expander with this novel single domain mesh generated in SCORG© is compared with the results obtained with the mesh consisting of two domains and measured results obtained on the test rig. All grid generation techniques are available in SCORG© and their mathematical background is presented in this study. Stationary grids of the ports are generated using ANSYS commercial grid generator. The CFD calculations were performed in ANSYS CFX® solver. The simulations with the various grid techniques are compared with the experimental data from a twin screw expander obtained from a recent study. The results of this study show the impact of the grid generation on the prediction of the expander performance and confirm that the Casing-to-Rotor conformal mesh is recommended for use in modelling of screw expanders.

1. INTRODUCTION

Organic Rankine cycle (ORC) is widely recognized as a viable technology to convert low temperature heat into electricity (Smith, Stosic, and Kovacevic 2014). Compared to other emerging technologies, ORC systems have a number of advantages such as low maintenance, favourable operating pressures and autonomous operation (Besong 2015). Among the ORC components, selection of the appropriate expander and working fluid affects the overall cycle's efficiency, size and cost (Chen, Goswami, and Stefanakos 2010).

Expanders are classified into dynamic and positive displacement machines (Imran et al. 2016). Twin screw expanders belong to the latter group and compared to other expanders have the advantage of high isentropic efficiency (up to 70%), high pressure ratios (typically 2-10), simple structure, potential operation at relatively high rotational speeds and high power outputs as well as capability to handle multiphase fluids. Despite the number of publications on twin screw expanders, the experimental data are not readily available in open literature (Kovacevic and Rane 2013). Additionally, distribution and influences of oil and other liquids on the performance in multiphase screw machines are not fully understood. Therefore an advanced numerical grid generation is required (S Rane and Kovacevic 2017). It is expected that better understanding of the distribution of vapour, liquid as well as oil in multiphase expanders and their influence on leakage flows will lead to better designs and improvements in both efficiency and reliability of such machines.

Twin screw expanders can be numerically modelled either by chamber models (Read, Smith, and Stosic 2015) or with detailed CFD calculations (Papes, Degroote, and Vierendeels 2015). The so-called low dimensional thermodynamic models describe average fluid behaviour and give a limited information about the process inside the expander especially in case of multiphase flows. These barriers can be overcome using CFD analysis, which gives detailed information on flow phenomena that occur, such as compressible and unsteady flows, turbulence, multiphase flow and real gas fluids (S Rane and Kovacevic 2017).

In literature, there are two main grid generation techniques to mesh the rotor flow domain namely analytical and numerical. The first method is based on the pioneering work in the grid generation for screw machines by use of algebraic transfinite interpolation, which generates numerical meshes in flow sub-domains associated by each of the rotors. The subdomain meshes are then connected through sliding and stretching interfaces. This method described in detail elsewhere (Kovacevic, Stosic, and Smith 2000) is called Rotor-to-Casing (RC) method since the first boundary to be distributed is the rotor boundary and the mesh is rotating . The second algorithm so-called Casing-to-Rotor differs in that the first boundary to be distributed is the casing and the mesh generated by this means is stationary with the casing and stretches along the rotors. The first algorithm to produce such mesh was presented in (Vande Voorde, Vierendeels, and Dick 2004)). This algorithm is based on solution of elliptic differential equations to produce hexahedral meshes based on the initial tetrahedral mesh generated in the domain between the rotors and casing in the transverse coordinate plane. The main disadvantage of this method is the mesh generation speed and the limited ability to control the quality of the mesh in clearances. The third algorithm is based on combining advantages of the two previous methods, i.e. algebraic and differential grid method. The mesh for each domain is originally generated from the initial distribution on the casing using algebraic transfinite interpolation. Then the connecting boundary between two meshes is smoothed using differential grid smoothing. Following that, the algebraic method called background blocking is used to make conformal connectivity between the two subdomains and finally the differential smoothing is used to make the entire single domain grid smooth and orthogonal. This method is called in this study as the Casing-to-Rotor conformal grid (S Rane and Kovacevic 2017). Although these three options exist in literature, the use of the latest method has not been studied for investigation in twin screw expander operation.

The use of Rotor-to-Casing numerical mesh for the analysis of screw expanders was presented by (Kovacevic and Rane 2013). A set of different pressure ratios, with different operating speeds at fixed inlet gas temperature were studied with the variety of clearance settings to compare the CFD results performed using ANSYS CFX®. It was found that for the clearance distribution when the integral parameters such as flow and power matched well with the experiment, the internal pressure history had slight deviation from the measured values. It was concluded that the clearance distribution both in interlobe, radial and axial gaps has a strong influence on the performance of the expander but the sliding interface between the domains can (in the CFD solver used in the study) cause a non-physical dissipation which could contribute to differences between measured and calculated values in results.

The motivation of this study is to explore the effect of various grid configurations on the performance prediction of a twin screw expander. Experimental data from published literature were utilized to compare the differences of the three different meshes, namely Rotor-to Casing (RC), Casing-to-Rotor non conformal (CRNC) and Casing-to-Rotor conformal (CRC). The results of this study show the impact of the grid generation on the prediction of the internal pressure history as well as on the integral parameters, is the mass flowrate and the indicated power. The target of this study is to give insights from the air twin screw expanders simulation which can be transferred to a real gas screw expanders for a small scale ORC systems.

2. CFD ANALYSIS OF TWIN SCREW EXPANDER

A twin screw expander is a positive displacement machine that consists of a pair of coupled screw rotors inside the casing which form the working chambers. The ideal operating principals briefly consist of an isobaric filling up, following by an isentropic expansion and an isobaric discharge. Losses during the expansion process can affect the performance of the expander. Computational Fluid Dynamics (CFD) can describe in detail the performance of twin screw expanders and assist on a deeper analysis of complicated flow phenomena that occur, such as compressible and unsteady flows, turbulence, multiphase flow and real gas fluids. Grid generation is the first and most important process involved in computing numerical solutions to the equations that describe the twin screw expander operation. SCORG© has been utilised in this study as the CFD grid generation tool for the twin screw expander model and then the grid was imported in the CFD solver (ANSYS CFX®) for solution.

2.1 Grid Generation

The expander fluid domain consists of three (3) main regions namely the male and female rotor flow domain, the suction flow domain and the discharge flow domain. The rotors flow domain is the most challenging part of grid generation, as it includes moving meshing techniques to accurately predict the fluid flow. In this study the single domain technique is compared with the two other meshes consisting of two domains; all techniques are integrated in SCORG©.

The first grid method, which was pioneered by Kovacevic (Kovacevic 2002), is an algebraic grid generation that features boundary adaptation and transfinite interpolation. In this algebraic method (Kovacevic 2002), the rotor grid is generated in the O form which requires a flow domain between rotors and casing to be divided in two blocks that each belongs to one of the rotors (Sham Rane and Kovacevic 2017). Once O grid is constructed on the side of the male rotor and another on the female side. The division is achieved by use of rack and outer casing circles. Boundary nodes are first positioned on the rotor boundaries and rotate together with the rotor. Such a grid is being referred to as Rotor to Casing grid or "RC grid". In essence, each of the O grid block rotates and deforms. The two O grids used in this method slide relative to each other. The RC algebraic grid method is fast and robust but introduces two grid features which require further attention namely, a non-conformal interface between the O grids and degenerated hexahedral numerical cells in the CUSP. Both of these are problematic for some CFD solvers as these cannot handle them conservatively.

Table 1: Mesh Statistics of the three tested grids

Flow Domains	**Rotor-to-Casing (RC)**	**Casing-to-Rotor Conformal (CRC)**	**Casing-to-Rotor Non Conformal (CRNC)**
High Pressure Port			
Mesh Type	Tetrahedra	Tetrahedra	Tetrahedra
Elements (Thousands)	217	217	217
Nodes (Thousands)	42	42	42
Rotor (RC-CRNC-CRC)			
Mesh Type	Hexahedra	Hexahedra	Hexahedra
Elements (Thousands)	399	399	399
Nodes (Thousands)	472	472	467
Low Pressure Port			
Mesh Type	Tetrahedra	Tetrahedra	Tetrahedra
Elements (Thousands)	286	286	286
Nodes (Thousands)	53	53	53
Low Pressure Pipe			
Mesh Type	Hexahedra	Hexahedra	Hexahedra
Elements (Thousands)	50	50	50
Nodes (Thousands)	54	54	54
Total			
Elements (Thousands)	952	952	952
Nodes (Thousands)	621	621	616

Vande Voorde et al. (Vande Voorde et al. 2004) were the first to implement a differential grid generation algorithm for screw machines. They developed high–quality block structured grids starting from the solution of the Laplace equation obtained on an unstructured grid of the same geometry (Papes et al. 2015). The differential equation is a generic methodology that can be applied to a variety of twin rotor machines such as lobe pumps, tooth compressors, screw compressors etc. With the differential approach, the rotor domain is treated as a number of 2D cross sessions. This grid structure is referred in this study as Casing to Rotor conformal mesh or in short CRC grid type. Recently, Papes et al. (Papes et al. 2015) employed this method to provide insights of a twin screw expander performance for a small scale ORC system using the refrigerant R245fa.

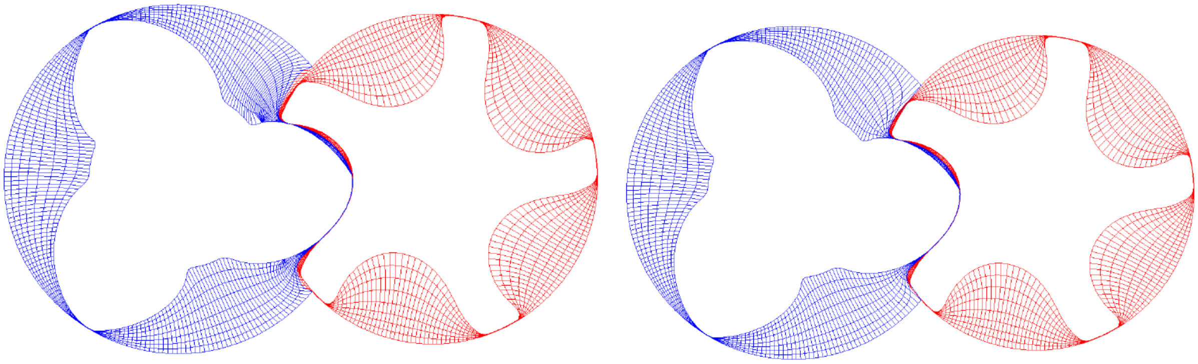

Figure 1: Numerical grids of expander rotors for the CR conformal (left) and the CR non-conformal (right).

More recently, Rane and Kovacevic (S Rane and Kovacevic 2017) presented a deforming numerical grid generation method for twin screw machines. The method utilizes algebraic transfinite interpolation to produce initial mesh upon which an elliptic partial differential equations (PDE) of the Poisson's form is solved numerically to produce smooth final computational mesh (S. Rane and Kovacevic 2017). The quality of the numerical cells has been validated and proved some significant improvements on two phase flows (Kovacevic and Rane 2017). The complete rotor grid for one of the cross sections for the CR conformal and the CR non-conformal are presented in Figure 1.

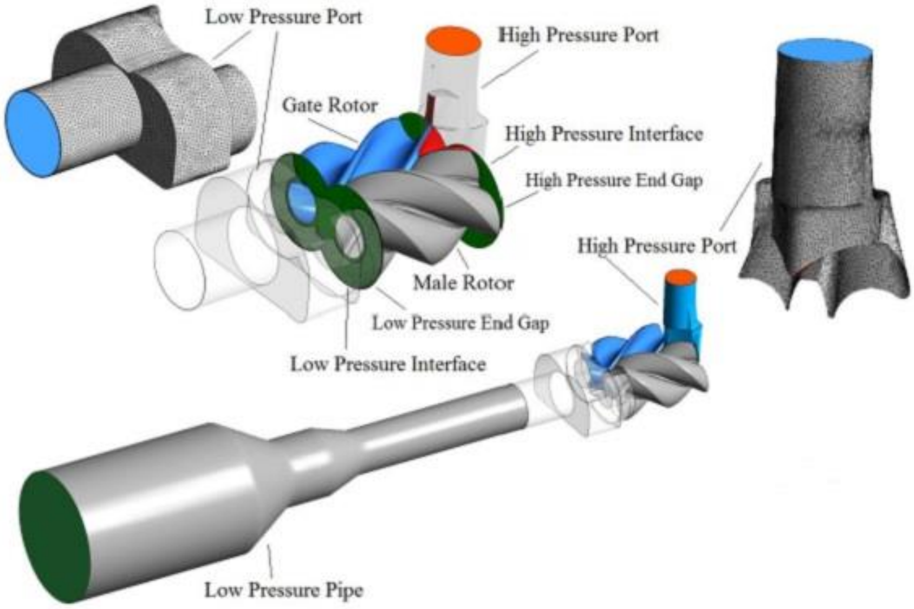

Figure 2: Flow domains of the twin screw expander (Kovacevic and Rane 2013).

In this study, the three grid generation methods are utilized to compare the effect of grid generation on the twin screw expander efficiency. Special focus is given in this study for the single domain rotor grid that is compared with the two domain rotor grids, all available in SCORG©. The CRC mesh generates a single domain rotor grid that conversely to the two domain grid, it presents the following advantages (S. Rane and Kovacevic 2017):

- The independent refinement of the numerical mesh in the interlobe leakage region provides a better accuracy in representation of rotor curvature in the gaps. In this respect, it was found that grid generation was more robust with a non-conformal interface between the rotor grid blocks.
- The single domain structured grid for the rotors eliminates the non-conformal interface between the two rotor domains, while still maintaining the fully hexahedral cell topology.
- The single domain grid can be handle from the majority of the commercial CFD solvers.

The grid of the rotors used in this study is comprised of 40x8x40 divisions in the circumferential, radial and axial direction per interlobe respectively in the male and female rotor areas as presented in a previous study (Kovacevic and Rane 2013). The mesh statistics for all grids used in the following presented transient simulations are briefly summarized in Table 1. The experimental and geometrical data of the selected expander in this study are introduced in session 3.

The mesh of the rotor has been generated using SCORG©. The mesh in the high and low pressure ports is tetrahedral and generated by ANSYS grid generator. The three (3) domains namely the high pressure parts, the rotor and the low pressure parts were assembled together in the ANSYS CFX® solver through non-conformal GGI interface. A schematic presentation of the twin screw expander flow domains is described in Figure 2. Further information of the model development can be found elsewhere (Kovacevic and Rane 2013).

2.2 Computational Set-Up

The numerical grids for rotors at each time step were computed using SCORG©, in advance of the CFD simulations. At each time step, the mesh for the appropriate position of the rotors is updated in the solver by use of an external subroutine. The ANSYS CFX® solver is set with a higher order advection scheme and the second order backward Euler temporal discretization. The convergence criteria for all equations were set to $1e^{-4}$ applying 10 coefficient loops for every time step. As simulation is transient, five (5) full cycles were simulated until a stable convergence limits are achieved and last cycle results were extracted as the final solution. The deviation for both mass flow rate and pressure ratio between 4th and 5th cycle were less than 1E-5.

The calculations assumed the Spalart-Allmaras turbulence model for all grid tested cases. An ‘opening’ boundary with a specified non-reflecting pressure head at the boundary location was defined. This type of boundary permits the flow to enter and leave the computational domain but affects the solution, depending on the location of the boundary relative to the source of the pulsations.

3. EXPERIMENTAL DATA

The experimental data of a small twin screw expander GL51.2 designed by TU Dortmund have been used in this study (Hütker and Brümmer 2013). This screw expander has a 3/5 lobe rotor combination and a relatively small internal volume $v_i = 1.47$. The outer diameters of the male and female rotors are 72mm and 67.5mm respectively, their centre distance is 51.2mm and the length of rotors is 101mm. The male rotor wrap angle is Φw = 200°. The available experimental data are only for dry air expansion and summarized in Table 2.

Table 2: Experimental data for expander GL51.2

Inlet Pressure [bar]	**2000 rpm**		**5000 rpm**		**10000 rpm**	
	Flow Rate [kg/s]	Power [W]	Flow Rate [kg/s]	Power [W]	Flow Rate [kg/s]	Power [W]
1.6	0.0292	511.9	0.0451	1318.8	0.0615	1748.1
2.0	0.0327	758.5	0.0511	1817.7	0.0786	3444.8
3.0	0.0409	1492.4	0.0737	3589.6	0.1179	7148.3

4. RESULTS AND DISCUSSION

4.1 Pressure Prediction

The experimental air data of the small twin screw expander GL51.2 have been utilized to validate the effect of grid generation on the performance of the expander. Figure 3 presents a full operating expansion cycle of the twin screw expander operating at 4000rpm and intake pressure 2 bar, while the working fluid is air. The three (3) previously presented grid generation methods are employed to simulate the performance of the expander. The working cycle initiates with the chamber filling that is achieved due to an increase in the volume formed between the rotors exposed to the high pressure port. Usually this part is characterised by pressure fluctuations due to the moving rotor and gas interaction as reported elsewhere (Kovacevic and Rane 2013), however those fluctuations are more obvious for the Casing-to-Rotor conformal mesh technique. Both Casing-to-Rotor conformal mesh and Casing-to-Rotor non-conformal mesh predict accurately the expansion process, while the difference on the re-filling phase is less compared to the Rotor-to-Casing mesh technique. The final phase of the discharge is well predicted from all grid generation methods.

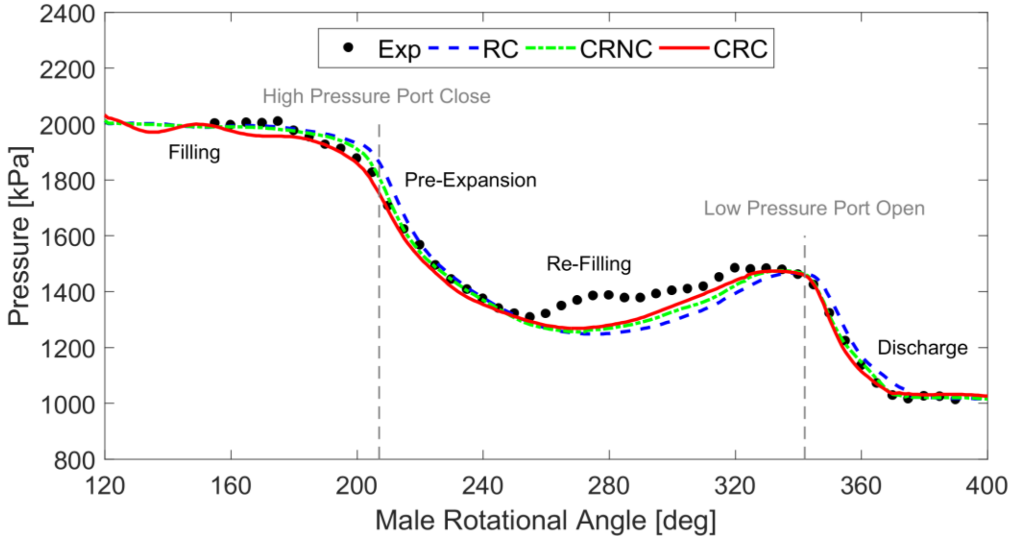

Figure 3: Diagram of indicated pressure of the twin screw expander at 4000rpm and 2 bar inlet pressure.

The difference with measured pressure of the three (3) examined methods is illustrated at Figure 4. The higher deviation is observed at the phase of re-filling and the main reason of that seems to be the effect of the clearance prediction on the performance of the expander. Minimum difference is observed at the regions of the two expansions, where Casing-to-Rotor non-conformal mesh seems to present the minimum deviation of the three mesh techniques. Overall, the average absolute difference of the predicted pressure trace is 1.78%, 1.96% and 2.56% for the Casing-to-Rotor non-conformal, Casing-to-Rotor conformal and Rotor-to-Casing mesh techniques respectively.

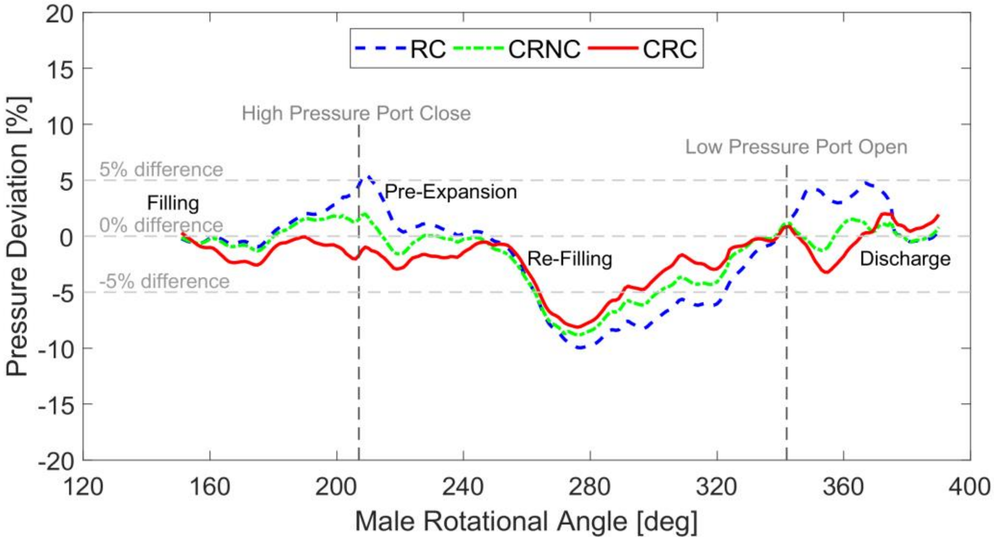

Figure 4: Diagram of pressure deviation of the twin screw expander at 4000rpm and 2 bar inlet pressure for the three different mesh techniques.

The three (3) employed grid generation methods were also tested against air experimental data at 10000rpm and 2 bar inlet pressure, as presented in Figure 5. Both the two domain meshes (Rotor-to Casing and the Casing-to-Rotor Non-Conformal) can better predict the expansion process in terms of pressure compared to the single domain mesh, however during the re-filling process the deviation from the experiment of the single domain mesh is less compared to the two domain techniques. The latter indicates that the influence of the clearance gaps is controlled better by the single domain method, while the interaction between the rotors can be better estimated by the two domains technique. It has to be noted that the clearance gaps have been investigated in this study and it was found that the

400µm gap presented the better matching with the experimental pressure trace, which is in agreement with a previous study (Kovacevic and Rane 2013).

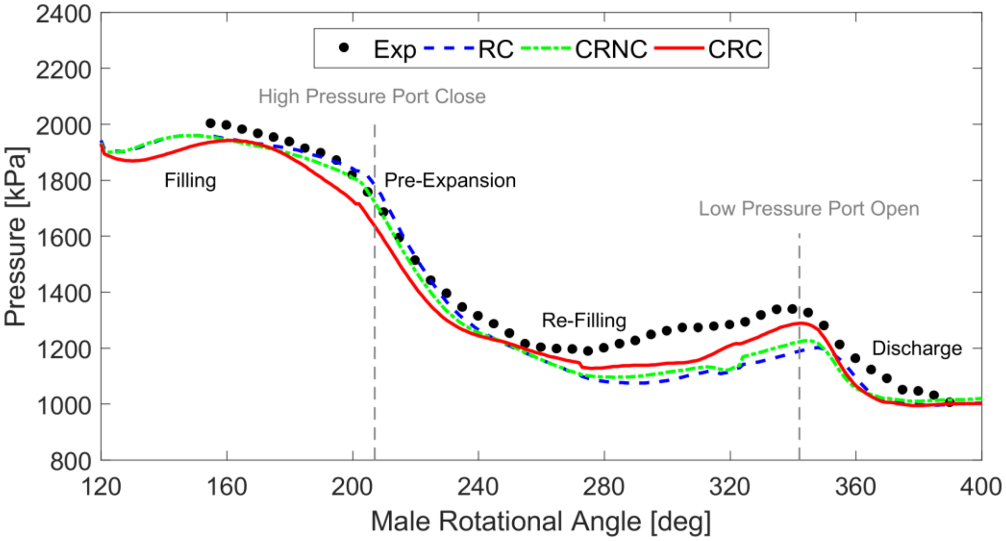

Figure 5: Diagram of indicated pressure of the twin screw expander at 10000rpm and 2 bar inlet pressure.

Figure 6 shows the deviation from the experiment of the three (3) investigated grid generation methods against experimental data. The Casing-to-Rotor non conformal grid generation method presents the minimum difference from the experiment at the expansion phase while the Casing-to-Rotor conformal grid generation method presents the minimum deviation from the experiment at the re-filling phase. Overall, the average absolute deviation from the experiment of the predicted pressure trace is 4.46%, 4.22% and 3.38% for the Casing-to-Rotor non-conformal, Casing-to-Rotor conformal and Rotor-to-Casing mesh techniques respectively. Compared to the 4000rpm operating conditions, the observed deviation from the experiment on the pressure traces is higher at 10000rpm, possibly due to the influence of the clearance gaps.

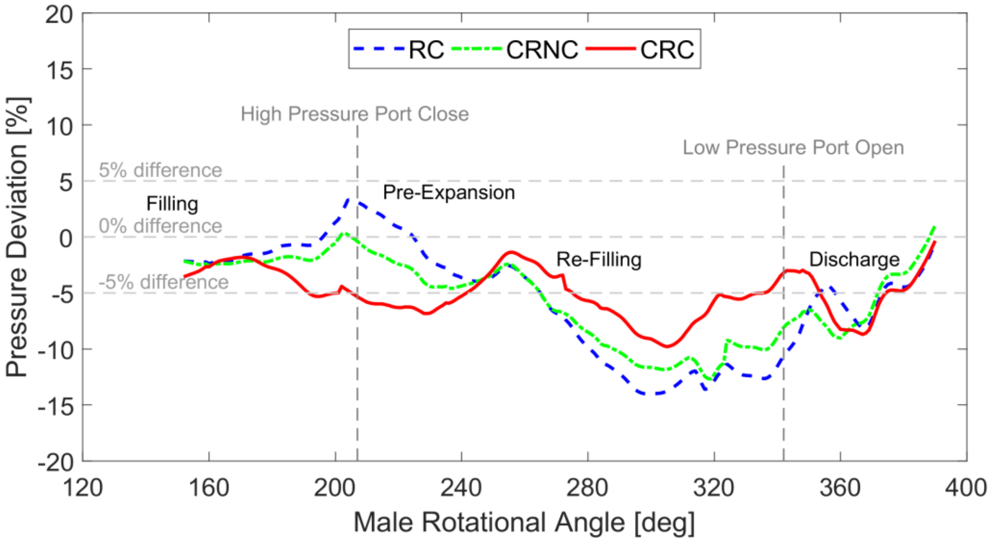

Figure 6: Diagram of pressure deviation of the twin screw expander at 10000rpm and 2 bar inlet pressure for the three different mesh techniques.

4.2 Prediction of Performance Characteristics

Apart from the prediction of the pressure trace, it is important to accurately predict the performance of the twin-screw expander in terms of mass flowrate and indicated power output. The predicted mass flowrates and indicated power outputs for the studied cases compared to measured values are illustrated in Figure 7. It is shown that the Casing-to-Rotor conformal mesh presents the lower deviation from the experiment values in the prediction of mass flowrate and indicated power which are 16.86% and 6.41% for the mass flow and 17.6% and 15.5% for the power output for 4000rpm and 10000rpm respectively. Both the two domain mesh techniques present deviations at the order of 30% for both mass flowrate and power output which is relatively high.

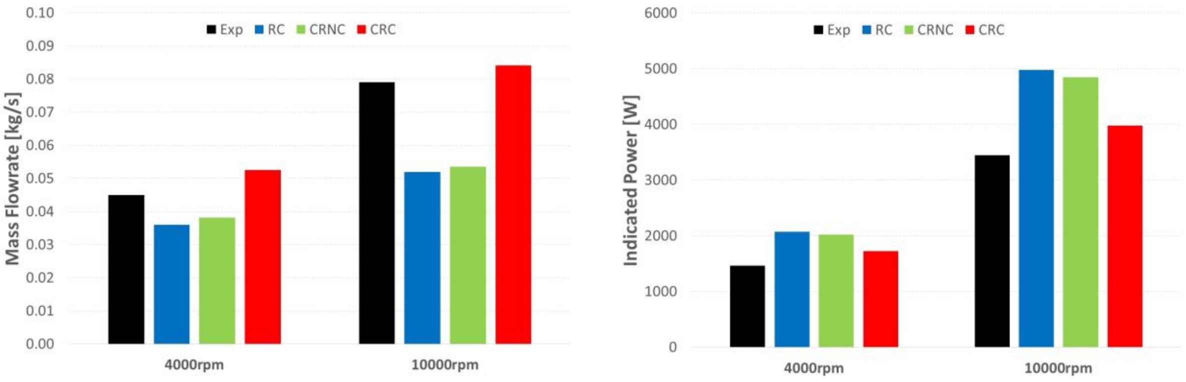

Figure 7: Effect of various grid generation methods on twin-screw expander performance prediction a) Left side: mass flowrate, b) Right side: indicated power.

6. CONCLUSIONS

Transient 3D CFD analysis of a twin screw expander has been successfully carried out using SCORG© grid generator and ANSYS CFX® solver. Three (3) different grid generation techniques were employed to predict and compared with experimental data found in literature. The comparison of the three (3) techniques showed the followings:

- The Casing-to-Rotor conformal (CRC) grids show minimum differences on the prediction of the pressure history within the twin-screw expander under all operating conditions.
- The single domain Casing-to-Rotor conformal (CRC) mesh presented the minimum difference compared to the other two grids on the prediction of the integral parameters i.e. mass flowrate and the indicated power output.
- At higher rotational speeds, it was found that the difference between the simulations and the experimental data was increased for both single domain and two domain grids. However, single domain grid gives better performance prediction results.
- The interlobe clearances in all three cases were identical. With the CRC mesh the influence of the sliding interface between the rotors is eliminated and it was found that the remaining difference between the experiment and predictions may cause the incorrect setting of clearances which were in the Rotor-to-Casing case set to be smaller in order to compensate for the diffusion caused by the sliding interface. This needs further investigation.

Casing-to-Rotor conformal mesh is suitable for use in air screw expander and is recommended for future use in modelling screw expanders for Organic Rankine Cycles.

NOMENCLATURE

CFD	Computational Fluid Dynamics	(–)
CRC	Casing-to-Rotor conformal mesh	(–)
CRNC	Casing-to-Rotor non-conformal mesh	(–)
GGI	Generalized Grid Interface	(–)
ORC	Organic Rankine Cycle	(–)
RC	Rotor-to-Casing conformal mesh	(–)

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ACKNOWLEDGEMENT

The authors would like to acknowledge the financial support of EPSRC to this project (EPRSRC Grant number EP/P009131/1).