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Numerical Analysis of an Oil-free Twin Screw Compressor Using 3D CFD and 1D Multi-chamber Thermodynamic Model

Stuart Kennedy¹, Maria Wilson¹, Sham Rane²

¹Howden Compressors, Old Govan Road, Renfrew, PA4 8XJ, UK

² City, University of London, EC1V 0HB, UK

Email: stuart.kennedy@howden.com

Abstract. The application of three-dimensional computational fluid dynamics in twin-screw compressors provides an outstanding opportunity for developers to gain an understanding of the complex internal flow phenomena occurring within the machine. Equipped with this knowledge, design parameters, such as clearances and port geometry can be optimised, to enhance performance. However, as with all modelling, be it numerical or analytical, a high degree of certainty in the accuracy of the results is necessary.

This paper presents the results of a study of oil-free twin screw compressor in which the results of two modelling techniques are compared. The modelling techniques used are a one dimensional thermodynamic chamber model and a three dimensional computational fluid dynamic model. The paper presents an overview of an oil-free twin screw compressor machine, before describing important operating characteristics and the modelling techniques used. To validate, both models are compared against historical test data, this validation indicated the chamber model is more accurate. Following this, the focus will be on the comparison of key performance indicators, including, volume flow rate, volumetric efficiency, indicated power, and discharge temperature at varying duty points. The paper concludes that the difference between both models decreases as the compressor operating speed increases, although the level of variance is dependent on pressure ratio.

1. Introduction

The operating principle of the twin-screw compressor remains practically identical to that initially developed in the late 19th century. Development of the technology over the following 140 years has been steady, primarily coinciding with advancements in manufacturing techniques and computer processing capabilities. The latter has brought about an evolution of highly sophisticated mathematical modelling techniques, such as Finite Element Analysis (FEA), Computation Fluid Dynamics (CFD), and more specific to twin-screw compressors, the development rotor profile generation, grid generation and thermodynamic modelling software. With this, the modern-day screw compressor design engineer has a plethora of design tools at their finger-tips.

This paper presents the results of a study in which a selection of these tools are used to calculate performance characteristic of an oil-free screw compressor at specified speeds and pressure ratios.

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The tools used are; 3D CFD modelling and thermodynamic chamber modelling. A particular focus of the study will be on both the methodology undertaken and results obtained through CFD modelling, as this will be utilised extensively in future development work.

1.1 Oil-free Twin Screw Compressor - Overview

As the name suggests, in an oil-free twin screw compressor the working chamber is free from oil. This is opposed to the oil injected range of machines, where the oil is used to lubricate, control temperature and reduce internal leakages in the working chamber. Oil-free machines are typically used in industries where the working fluid must be free of any containments. Eliminating oil from the rotor chamber adds in own complexities and challenges, such as sealing arrangements, timing gears and increased operating temperatures. Additionally, as oil is absent from the working chamber, the induced efficiency losses that occur due to oil shear are avoided, meaning the oil-free screw compressor can operate at significantly higher tip speeds. With this, aspects such as gas velocities, vibration, and critical speeds must then be considered.

2. Modelling Methodologies

The performance characteristics of the machine can be calculated numerically, through CFD modelling or specially designed thermodynamic chamber modelling tools - such as that used in SCORGTM [1]. There are tremendous differences in the modelling methodologies. The greatest is the processing time and power required to obtain the results given the specified boundary conditions. Where the chamber model can output predictions in seconds, the CFD model would take days, ultimately due to quantity of calculations required. Additionally, to perform these calculations, a large amount of high specification processing power is required, whereas the chamber model can operate on a desktop machine. Further to this, the CFD model will provide an extensive range of results, including flow phenomena that can be numerically and visually interrogated; as opposed to the chamber model which outputs single calculated values relating to performance. This is not to say a particular model is superior, simply their use should be considered on a case to case basis.

2.1. Thermodynamic Chamber Model (SCORGTM)

One-dimensional mathematical modelling of screw machines has been used to great effect for many years. An accurate prediction of many aspects of machine performance can be obtained from the models which simultaneously solve thermodynamic processes, based on ideal or real gas laws, with the geometric parameters of the machine, including chamber volume, port areas and sealing line lengths. From the many modelling methodologies, that presented by Stosic et al [2] forms the foundation of the model used in this study. Described as multi-chamber thermodynamic model, the screw machine is divided into sub-domains representing each stage of the compression process. The challenge of computing time dependant flow variables within the control volumes is overcome by using a combination of differential equations to solve the rate of change of mass and internal energy, and algebraic equation to solve other internal flow behaviour such as velocity and leakages.

From a user perspective, the complexities involved in the computation of the aforementioned flow variables are hidden. As much as it is recommended to have a theoretical understanding of the model, developers have excelled in creating a tool that is as much user friendly as it is reliable. This study will utilise the thermodynamic model inherent to SCORGTM.

2.2. CFD Model

CFD modelling is rapidly being adopted in all areas of modern engineering practice to solve complex flow and heat transfers problems. An obvious application of this methodology is in twin screw compressors. However, the challenges involved in modelling and computing the complex physics and transient nature inherent to the machine have proven difficult to overcome. Nonetheless, through extensive and committed research, the development of design tools and users obtaining a greater understanding of the problems, it is now possible to undertake these simulations with a certain degree of confidence that a valid solution can be obtained. To obtain this, a host of 3D modelling and analytical tools are employed for pre-processing, solving and post-processing, these involve; 3D modelling, mesh creation, rotor grid generation and CFD software.

2.2.1. Rotor Grid Generation. The helically formed rotors - and the continuously varying volume that is formed between the male, female rotor rotors, and casing bore as they rotate - has offered the greatest challenge to developers for many years. Publications on techniques and methodologies are in abundance and presenting these is outside the remit of this study. However, techniques summarised in Kovacevic et al [3] provide an excellent overview of developments as well as describing the authors of the publication own methodology. This analytical grid generation procedure is presented in detail by Kovacevic [4] and expanded upon by work presented by Rane [1]. This methodology is at the core of



Figure 1: 3D Rotor Mesh

grid generation software $SCORG^{TM}$ - the tool used in this study.

Understanding the flow characteristics of the working fluid, or fluids, in the chamber is of great importance. Therefore, the grid used in the calculations must be of excellent quality to assure accuracy. The design tool, SCORG[™], provides the necessary means to achieve this. Dividing the male and female rotor into two sub-domains and then into a series of 2D domains, a numerical mesh for each rotor position is generated. This is then translated into a 3D mesh by positioning these in series, axially along the rotor length, an example of which, and those used in this study are shown in Figure 1. Furthermore, using a conformal boundary map at the sub-domain interfaces allows the male

and female rotors to be merged as one single domain.

These are 'N' profile rotors, which are generated using data points imported from rotor profile generation software SCORPATH^{TM,} as described by the authors [2]. This compatibility between software offers many benefits, of which the most important from a analysis perspective is the profiles used in the model are identical to those in the physical machine.

3. Case Study

The case study presents a comparison of calculated performance characteristics obtained from the described tools. The approach undertaken is to initially determine the variation between actual test data and each method, thus gaining an overall understanding of the level accuracy. Following this, the setup of both models will be described with particular attention taken to the CFD model set-up. Finally, each model will be used to predict performance at a range of operating conditions allowing the variance to be evaluated.

3.1. Machine Configuration

This case study involves a common machine configuration of 4 male and 6 female rotor lobes. Both rotors are of equal outer diameter at 255mm with an L/D ratio of 1.65, equating to a rotor length of 420.75mm. Typically, machines are defined by their built-in volume ratio (Vi), in this case this is 1.9. The specific duty of the physical compressor has not been defined. Therefore this study will focus on a range of speeds and pressure ratios of what are considered normal operating conditions. This will provide an extensive overview of the machine performance at various conditions.

3.2. Model Validation Study

An extensive study undertaken by Rane [1,6] presents a high level of accuracy between CFD modelling and test data is achievable when using a single domain rotor grid. To obtain additional confidence an attempt was made to validate this study's CFD set-up. In the absence of an identical prototype test

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machine, historical test results were examined to extract comparable performance data. The measured variables available are limited, therefore the volume flow rate is identified as the most suitable to validate the CFD model. Additionally, this data relates to machines operating with symmetric rotor profiles, therefore the rotor geometry/mesh in the CFD model is modified accordingly to reflect the compressor configuration.

In addition to validating the CFD model, the opportunity is taken to compare the volume flow rates predicted by the chamber model, thus gaining an overall evaluation of the accuracy of each method. The machine was tested at a constant speed of 7385 rpm at 0.988barA suction pressure with pressure ratios of 1.52 and 1.93. The measured and calculated volume flow rates are shown in Figure 2a, with the associated error in Figure 2b.



Given the results, it can be established that in both models there is an under prediction of volume flow rate. The chamber model calculates approximately 4%-5% less flow. The CFD results indicate an under-prediction of the volume flow by approximately 8%. It can be identified that in both cases, the results have the correct trend, with decreasing flow rates at increasing discharge pressures, this reflects what is theoretically expected.

From the several factors that may be accountable for the degree of error identified in the CFD model, the most likely reasons are: rotor mesh quality, the machines physical geometry and its alteration as it responds to heat transfer. Firstly, to ensure numerical accuracy, as well as capturing flow characteristics more precisely, the rotor mesh must be generated to an acceptable level of quality and quantity. Therefore, a full sensitivity study examining the change in calculated results with consecutive cases of grid refinement will be undertaken in future work.

Secondly, the rotor thermal expansion that will occur during operation and the consequential modification to internal clearances introduces additional factors of uncertainty (also applicable to chamber model). The complex interaction between the working fluid and the rotor is currently not captured in the model, which adds a degree of inconsistency in the validation study. Options available to resolve this are to include fluid-solid interaction in the model, or one could calculate theoretical thermal expansion of the rotors and model the revised clearances, the latter will be the focus of a future study.

3.3. Aspects of the CFD Model

By taking advantage of the functionality of a range of tools as shown in Table 1, the CFD model is created. As listed, the calculations are completed by the ANSYS CFX solver [7], chosen due to its compatibility with SCORGTM, and it's known reliability and robustness and in computing highly deforming mesh type models. As with all computational analysis, it is critical the mesh quality is of a high standard and undertaking a full mesh dependency study is prudent. However, due to the time restrictions, this has been omitted from the current study. The authors are reliant on effectiveness of the tools used and previous experience to create a high quality mesh.

Stage	Part	Software	
		Autodesk Inventor	
	3D Geometry	ANSYS Design Modeller	
D		ANSYS SpaceClaim	
Pre-processing		ANSYS Meshing	
	Meshing	ANSYS ICEM	
		SCORG	
	Set-up	ANSYS CFX	
Solver		ANSYS CFX	
Post-processing		ANSYS CFX	
		Microsoft EXCEL	

Table 1: I	Design Tools
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3.3.1 Rotor Mesh As discussed in Section 2.2.1, SCORGTM is used to generate the 3D rotor fluid domain. The tool allows the user to define certain mesh parameters to calculate a suitable mesh. Key parameters used to generate the mesh are defined in Table 2 as represented in Figure 3.

Parameter	Description	Input
Α	Circumferential Divisions	40
В	Radial Divisions	7
С	Angular Divisions	40
D	Interlobe Divisions	60
Е	Type of Distribution	Casing to Rotor - Conformal

Table 2: 2D Grid Set-up



Figure 3: 2D Grid Parameters

A review of the mesh quality determines the adequacy of the above mesh, the statistics of the 2D and 3D rotors summarised at Table 2. These indicate a good overall quality rotor mesh, with <1% of the cells in the 3D mesh not meeting the recommended orthogonality and expansion factor quality criteria. Additionally this illustrates the 2D mesh quality depreciates during transformation to a 3D mesh - ultimately it is this 3D mesh quality calculated by the CFD solver that is important.

	Orthogonality		Expansion Factor		Aspect Ratio				
	Good	Acceptable	Poor	Good	Acceptable	Poor	Good	Acceptable	Poor
2D	99%		<1%	96%		4%	98%		2%
3D	72%	27%	1%	99%	1%	<1%	100%		

Table 3	Rotor	Mesh	Quality
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3.3.2 Stationary Domains Mesh Figure 4a illustrates the 3D model used in the simulation. Due to the complex geometry, it was decided to deconstruct the stationary domains into simpler geometry, or sub-domains, to allow, when possible, an effective hexahedral cell structure to be created, as shown in Figure 4b. This does however mean additional interfaces must be added at each sub-domain - meaning improved processing speed may come at a cost of numerical accuracy. However, the overall global mesh quality calculated indicates the risk of numerical error is minimised.





3.3.3 CFD Boundary Conditions To provide a extensive list of results, performance is interrogated at a total of 9 duty points. This is achieved by applying discharge pressures of 2.0, 2.5 and 3.0 barA, to represent under, optimum and over compression, respectively, and varying speed of 4000, 5500 and 7000rpm at each of these pressure points - as summarise in Table 4

Speed (RPM)	Working Fluid	Suction Pressure (bar A)	E Press)ischarg sures (b	ge ar A)	Suction Temperature (K)
4000						
5500	Air	1.0	2.0	2.5	3.0	293.0
7000						

Run	PDischarge	Speed
1	2.0	4000
2	2.0	5500
3	2.0	7000
4	2.5	7000
5	2.5	5500
6	2.5	4000
7	3.0	4000
8	3.0	5500
9	3.0	7000

Table 4: Case Set-up

Due to the varying speed and discharge pressures, the order in which the calculations are undertaken must be carefully considered to minimise numerical instability. It is predicted that the change in discharge pressure will effect solver stability more than a change of speed, therefore it is decided to calculate a specified discharge pressure and increase/decrease the speed, then change the discharge pressure and repeat. It is key to obtain a balance between numerical accuracy, stability and time taken to solve. Based on experience gained from previous studies, it is decided that each set-up will be calculated for 6 male rotor rotations (960 time steps) to gain stability, then 1 further rotation in which the results are recorded - the run sequence is shown in Table 5.

 Table 5: Simulation Workflow

3.3.4 Solver Parameters The calculations are performed by an Intel Xeon X5650 processor, with 48 GB of available RAM. The solver, running parallel with 8 available 2.66GHz cores, used a High Resolution Advection Scheme and Second Order Backward Euler Transient scheme with a SST - k Omega turbulence model. For convergence, the maximum number of co-efficient loops is set to 10 iterations per time step, with convergence criteria of $1e^{-04}$. For stability, it is necessary to apply underrelaxation factors to solve momentum and continuity equations.

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3.4 Thermodynamic Model

As discussed in Section 2.1, the thermodynamic chamber model used is that inbuilt in SCORGTM. Additionally, as the same software is used to create the rotor mesh, the process of obtaining thermodynamic results is extremely efficient, as the rotor geometry and internal clearances used in the calculations are already defined. As this is a study into oil-free machines, the thermodynamic model set-up is somewhat simplified. Furthermore, as the CFD does not calculate power losses due to bearings and seals, another element of the set-up is removed. This means only a few variables are defined for each calculation, those being rotor speed, operating pressures and the working fluid properties. The boundary conditions listed in Table 4 are used to calculate the results for 9 of the cases; typical results presented by the thermodynamic model are; Volume Flow, Mass Flow, Indicated Power, Volumetric Efficiencies, Specific Power and Gas Discharge Temperatures.

4.0 Results

The results present the performance calculations, applying the boundary conditions listed above, from both models. From here a clear comparison can be drawn, the variance calculated and conclusions drawn.

4.1 Mass Flow Imbalance - CFD model

To ascertain a degree of certainty of numerical accuracy in the CFD model prior to comparing with the chamber model, the mass flow imbalance between the suction and discharge boundaries is calculated. The error percentage between these is listed below in Table 6. As shown the error is <2% in all cases, showing good balance between what is entering and leaving the domain, thus it can be concluded that the quality of the mesh has resulted in high numerical accuracy.

	Pressure Ratio			
Speed	2:1	2.5:1	3:1	
4000	0.1%	0.3%	0.01%	
5500	0.3%	-1.2%	0.7%	
7000	1.2%	-0.6%	2.0%	

 Table 6: Mass Flow Imbalance

4.2 Volume Flow Rate and Volumetric Efficiency

The achievable volume flow rate of a machine is a key component in the selection process. Therefore, it is extremely advantageous to have the capabilities to accurately predict this, given a specified rotor profile, built-in volume ratio, and at a range of pressure ratios and speeds. Firstly, focussing on the calculated volume flow rates, Figure 5a shows the change in volume flow rate with speed for each pressure ratio. As shown, the overall trend of the volume flow rates in each model are a well matched. However, when comparing the variance between CFD results and the chamber model, as shown in Figure 5b, there is a recognisable difference in prediction of flow rate, which is particularly evident at lower speeds. For example, at 4000 rpm, it can be observed that the variance increases from 8.6% at P.R. 2:1 to 15.8% at P.R. 3:1. Interestingly, in all cases as the speed increases, this variance between models decreases. Also worth highlighting is from 5000 rpm to 7000 rpm, the variance at each pressure ratio is relatively stable. This shows clearly CFD model will predict flow rate more accurately at higher speeds.

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Figure 5a: Volume Flow Rate

Figure 5b: Volume Flow Rate Model Variance

The volumetric efficiency is a key performance indicator of the screw machine, defined as the ratio actual volume flow rate to the theoretical capacity. With reference to Figure 6, there is a clear trend in the behaviour of each model. Both the chamber and CFD models predict the volumetric efficiency to increase as the speed increases - this behaviour reflects what is theoretically expected. At all pressure ratios, the variance between models decreases as the speed increases which reflects the overall behaviour of the volume flow rate results. Thus, it is established that at low pressure ratios and high rotational speeds, both models are closely matched.



4.3 Indicated Power and Adiabatic Efficiency

Indicated power is defined as the rate of work transferred from the screws to compress the gas, commonly calculated directly from the pressure-volume curve, or using angular velocity and torque. In this study, power consumed by bearings and seals is neglected, as these losses cannot be calculated by means of CFD.

With reference to Figure 7a, as expected, the indicated power increases with speed and pressure ratio. At all pressure ratios, it can be identified that the variation between the predicted indicated power increases as speed increases. The CFD model predicts greater indicated power than the chamber model in all cases; ranging from 4-6kW at 4000 rpm to approximately 19kW at 7000 rpm.

An additional performance characteristic of interest is specific power. The specific power describes the power consumed to deliver a cubic metre per minute of working fluid (air). Therefore, a low specific power is a useful indicator of efficient machine performance. Figure 7b illustrates the trends of both models. It can be identified that the difference in models is less than 0.5 kW/m³/min in all cases.

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4.4 Gas Discharge Temperature

As discussed in Section 1.1, gas temperature is a critical operating parameter, therefore having the ability to predict this is extremely valuable. The omission of oil in the rotor chamber will naturally result in high gas temperatures, that will over time transfer heat to the compressor components. In this study the fluid domain walls, such as those of the rotor bore and the discharge casing, are adiabatic. Therefore, conjugate heat transfer between the fluid and structure is not computed. Although this fluid-structure interaction would be most desirable, it does not devalue knowing only the gas temperature. As this can be used in theoretical calculations for heat transfer, and subsequent structural analysis for deformation.

Additionally, the isentropic relationship between pressure and temperature ultimately means the greater the pressure ratio, the greater the gas discharge temperature. Historically, this has imposed operating limitations to oil-free twin screw compressors.

The results in Figure 8a present the average gas temperatures (over speed range) for each pressure ratio. As shown in both models, the trend reflects that expected, however there is a noticeable variation. The CFD model predicts a higher gas temperature compared to the thermodynamic chamber model - this deviation ranges from 15-30 Deg. C or 15-17% as shown in Figure 8b



5.0 Conclusion

This paper presents the comparison of performance characteristics predicted by numerical CFD and thermodynamic modelling techniques typically used to evaluate twin-screw compressors. Through the validation study undertaken, it is recognized the thermodynamic chamber model prediction is closer to actual machine performance than the calculations of the CFD model. It is with this it is assumed the chamber model is the bench mark in which the CFD is compared to at various duty points. Given the results, the following can be concluded:

• Volume Flow Rate - the CFD model under predicts volume flow rate at lower speeds. As operating speed increases, there is a noticeable improvement in closeness between both models.

Furthermore, it is identified the variance increases as operating pressure ratio increases. Thus, it can be concluded in this case, CFD provides more accurate results at higher operating speed and lower pressure ratios.

- Power As the operating speed increases, the difference in calculated indicated power increases. With the CFD model predicting higher indicated power in all cases. As the specific power is a function of volume flow rate, this is impacted by the increased accuracy at higher speeds as described above.
- Discharge Temperature the CFD model over predicts gas temperature at discharge, in all cases. The variance in results also increases as the pressure ratio increases.

It can be established from the results presented that the thermodynamic chamber model calculates consistent results, with identifiable trends in flow rate, power and temperature. In contrast, the CFD model is sensitive to operating conditions, both the operating speed and pressure. As a consequence, the variation between models is inconsistent. Both the magnitude and inconsistency of the variance between the models highlights the importance of undertaking a grid sensitivity study, with the aim of reducing the variance.

Overall, the study undertaken is successful in calculating performance characteristics using numerical and thermodynamic modelling techniques. It is also worth highlighting the comprehensive results obtained from the CFD simulation provides the opportunity to visually and numerically examine internal flow phenomena. Therefore, making it an extremely advantageous tool in the optimisation and development of twin screw machines.

Having now created a functional CFD model provides the opportunity to undertake further work which will involve a grid sensitivity study, additional validation and investigating the impact modifying internal clearances due to thermal expansion has on performance.

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