COMPUTATIONAL FLUID DYNAMICS IN ROTARY POSITIVE DISPLACEMENT SCREW MACHINES

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Abstract
Positive displacement screw machines are classified as compressors, expanders, extruders, blowers, vacuum pumps, liquid and multiphase pumps. They are commonly used in industrial refrigeration, air conditioning, process gas compression and variety of liquid, multiphase and vacuum pumping applications. It is estimated that almost 20% of world energy consumption is used for various means of gas compression and pumping. Therefore, reliability and efficiency of such machines has large impact on economy and ecology important for every manufacturer of such machines.

Screw machines are normally designed with the aid of analytical tools, based often on one-dimensional flow models solved by numerical methods and validated by experiments. Continuing demands for improvements in accuracy when designing such machines for existing or new applications have generated a need to use advanced means of assessment of fluid flow and solid fluid interaction within these machines such as 3D Computational Fluid Dynamics and Computational Continuum Mechanics. The first use of CFD for analysis of screw machines was reported in late 1990’s. Since then, significant developments have been made to allow use of CFD in the design process of such machines. The most significant development which enabled such calculation methods was in representing the flow domains with the numerical grids capable of accurate and fast CFD calculation. This paper reviews the state of the art in application of CFD in modelling of positive displacement screw machines and outlines benefits which the use of such techniques may bring. The paper also identifies challenges and future development trends in application of CFD for rotary positive displacement screw machines.

Keywords
Computational Fluid Dynamics — Twin screw machines — Rotary positive displacement machines

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INTRODUCTION

Screw machines are rotary positive displacement devices capable of efficient operation with variety of fluids including gases, liquids and mixtures over a wide range of operating pressures and flow rates. Compared to other types of positive displacement machines, their design is simple, with rotors comprising the only moving parts. Thus, they can rotate at relatively high speeds and are therefore both reliable and compact. Usually these machines are formed of two rotors but they can also contain multiple rotors, one rotor driving two or more driven rotors.

Twin screw compressors are most common machines used for industrial compression of gases. These have been invented in 1878 by Heinrich Krigar in Germany but have not been in use until 1938 when Swedish company SRM licensed first screw compressor to Howden in Glasgow. Screw compressors can compress dry gasses in which case rotors are rotated through synchronising gears in order to maintain positive clearance between the rotors and to prevent their contact. More often twin screw compressors are operated with liquid injection to cool, seal and lubricate rotors which enables direct contact between the rotors and renders the need for expensive synchronising gears and internal seals. The most frequently used injection liquid in compressors is oil but it can be water or any other inert liquid. Consequently oil injected twin screw compressors comprise more that 95% of all screw compressors in use. Principle of operation and modelling of such compressors is extensively discussed in Stosic et al, 2005. Typical example of twin screw compressor is shown in Figure 1.

It is estimated that since the beginnings of industrial use of screw compressors, over 10 million of such compressors are produced worldwide. Japanese magazine for refrigeration compressors JARN reports that in 2013 some 137,000 refrigeration screw compressors are produced worldwide. Considering that a large proportion of screw compressors are smaller units used for air application and that the number of large gas screw compressors is significantly lower than refrigeration units, it is safe to say that over 500,000 of new screw compressors are put into operation every year. Although the authors could not identify a comprehensive source to estimate the size of the screw pump and vacuum pump market it is believed that the number of these machines will be several hundreds of thousands. With such large number of screw machines produced every year, the impact on environment and economy is significant and every effort should be made to make them operate more efficiently and reliably.

1. Nomenclature

- \( q_a \): flux source in general transport equation
- \( q_r \): volume source in general transport equation
- \( S \): cell surface
- \( v \): fluid velocity
- \( v_s \): surface velocity
- \( \Omega \): control volume
- \( n \): cell face normal vector
2. MODELLING SCREW MACHINES

2.1 Low order models

Early designs of screw compressors were based on the assumption of an ideal gas in a leak proof working chamber undergoing a compression process which could reasonably be approximated in terms of pressure-volume changes by the choice of a suitable value of the exponent "n" in the relationship \( pV^n = \text{Constant} \). The advent of digital computing made it possible to model the compression process more accurately and, with the passage of time, ever more detailed models of the internal flow processes have been developed, based on the assumption of one-dimensional non-steady bulk fluid flow and steady one dimensional leakage flow through the working chamber. Together with suitable flow coefficients through the passages, and an equation of state for the working fluid, it was thus possible to develop a set of non-linear differential equations which describe the instantaneous rates of heat and fluid flow and work across the boundaries of the compressor system. These equations can be solved numerically to estimate pressure-volume changes through the suction, compression and delivery stages and hence determine the net torque, power input and fluid flow, together with the isentropic and volumetric efficiencies in a compressor. In addition, the effects of oil injection on performance can be assessed by assuming that any oil passes through the machine as a uniformly distributed spray with an assumed mean droplet diameter. Such models have been refined by comparing performance predictions, derived from them, with experimentally derived data. A typical result of such modelling is the suite of computer programs described by Stosic et al, 2005. Similar work was also carried out by many other authors such as Fleming and Tang 1998 and Sauls, 1998. In recent years reports on development such models are still being made, for example Read et al, 2014 and Papes et al, 2015. Due to their speed and relatively accurate results, such mathematical models are often used in industry. However, these neglect some important flow effects that influence compressor performance, mainly in the suction and discharge ports.

2.2 3D Computational Fluid Dynamics

Screw compressor performance can be estimated more precisely by use of Three-dimensional Computational Fluid Dynamics (CFD) or Computational Continuum Mechanics (CCM). Computational fluid dynamics (CFD) covers a broad area, which attracted the interest of many investigators at the beginning of the computer era. It is based on the numerical simulation of the conservation laws of mass, momentum and energy, derived for a given quantity of matter or control mass. Finite volume method is most commonly used in CFD as described by Ferziger and Perić, 1995. The particular interest for the analysis of screw compressors is in the unsteady calculation with moving boundaries. As the rotors of a screw machine turn during operation of the compressor, the fluid volume in between them is deformed and the CFD grid which represents the fluid volume also needs to deform. Without capturing this deformation it is not possible to capture the real three dimensional fluid behaviour inside the working chamber. The challenge is in capturing the deformation of the main flow domain as well as in the leakage gaps which play essential role in the efficiency of screw machines. General grid generators are not capable of fulfilling this task and therefore efforts started almost two decades ago on grid generation for screw machines. The first report on the application of CFD in analysis of screw machines can be found in Stosić, Smith and Zagorac (1996). They presented a solution in both screw and scroll compressor geometry without full grid deformation but by the addition of a representative momentum source in the conservation equations. The results were encouraging for pressure distribution but did not provide full flow properties. A breakthrough was achieved in 1999 by Kovačević with the use of an analytical rack generation method, proposed by Stosić (1998), applied to generate an algebraic, adaptive, block structured, deforming grid calculation for twin screw rotors. Since then there have been several activities reported on the CFD analysis of twin screw compressors. The use of this method for screw compressor applications is justified by its ease of use and its speed. The analysis of the working chamber is transient in nature and requires a grid representing every time step rotor position and domain deformation. In this respect, algebraic methods can be used to recalculate the grid quickly. Kovačević, Stosić and Smith (1999 and 2000) successfully used an algebraic grid generation method together with boundary adaptation and transfinite interpolation which has been implemented in the program SCORG – (Screw Compressor Rotor Grid Generator). This has been written in FORTRAN with a C# front end application. In his thesis, Kovačević (2002) presented the grid generation aspects in detail. Kovačević et al. (2002a, 2002b, 2003, 2005 and 2006) has reported CFD simulations of twin screw machines to predict flow, heat transfer, fluid-structure interaction, etc. Kovačević et al. (2007) also published a textbook on the CFD analysis of screw compressors.

Figure 2. Typical representative of a numerical mesh for CFD calculation of screw compressors

Mujić et al. (2008) presented an optimisation of the discharge port area based on flow behaviour in the discharge chamber. They used CFD for relative comparison of port geometry modifications and their influence on predicted pressure pulsations has been used to judge sound spectrum and noise level from the compressor. These noise levels predicted by CFD solutions have been used for designing discharge ports with reduced noise levels. Mujić (2009) in his thesis presented a 3D CFD coupled model in which the boundary conditions for the discharge port were obtained as time varying data from 1D thermodynamic chamber models. Such an approach simplified the numerical analysis and also provided faster results from the CFD models. The procedure was implemented for Star CCM+ solver. It was found that the results predicted by the coupled model for sound pressure levels were closer to the full 3D CFD models and also in close agreement with the experimental measurements. Kethidi et al. (2011) conducted further studies on the influence of turbulence modelling on the CFD prediction of local velocity fields in twin screw compressors. Nouri et al. (2006) carried out cycle-resolved velocity measurements within a screw compressor using LDV and these data have been used by Kethidi et al. (2012) to compare with the results from 3D CFD models. Sauls and Branch (2013) used the results from CFD calculations to develop an improved one-dimensional thermodynamic model for refrigerant screw compressors, by extracting calibration coefficients that influence the pressure variation during the discharge process. Recently, Arjeneh et al. (2014) presented the analysis of flow through the suction port of a compressor with water injection. It was reported that it was difficult to stabilise a full 3D analysis with both deforming rotor domains and multiphase models. A simplified suction port model, with time varying boundary conditions, obtained from a full 3D single phase analysis was successful in predicting pressure variation in the suction port that agreed closely with experimental results. Also wetting of the port walls by the injected water was well predicted. Voordie, Vierendeels and Dick. (2004 and 2005) were the first to...
implement a grid conversion algorithm for unstructured to block structured mesh from the solution of the Laplace equation for twin screw compressors and pumps using differential methods. The use of differential methods requires the PDE to be solved for every rotor position and then the grid generation calculation of the solution has to be repeated from the equipotential and gradient lines. In his thesis, Voorde (2005) presented the principles of solving the initial Laplace equation and then using it to construct a block structured deforming mesh. Based on this grid generation, flow in a double tooth compressor and a twin screw compressor was analysed and the results were compared with experimental data over a range of discharge pressures and rotor speeds.

Papes, Degroote and Vierendeels (2013 and 2014) presented a 3D CFD analysis of an oil injected twin screw expander using the same differential grid generation approach. A real gas model for the working fluid R245fa was used and results for the different leakage flows were presented together with chamber pressure variation curves and performance analysis at different pressure ratios.

Recently CFX Berlin (2014) has introduced a software tool called TwinMesh to link with ANSYS CFX solver and this tool generates a grid for twin rotor machines on similar lines to that of the algebraic and differential approaches. Hesse et al. (2014) have presented the application of such a deforming grid for the analysis of an oil free twin screw compressor.

One of the major factors affecting the performance prediction of twin screw compressors by use of computational fluid dynamics (CFD) is the accuracy with which the leakage gaps are captured by the discretization methods. The accuracy of mapping leakage flows can be improved by increasing the number of grid points on the profile. However, this method faces limitations when it comes to the complex deforming domains of a twin screw compressor because the computational time increases tremendously. In order to address this problem, Rane et al (2012 to 2015) formulated an analytical grid distribution procedure that can independently refine the region of high importance for leakage flows in the interlobe space and produce single high quality mesh for screw rotor domains. By using this method the flow domains in the gaps are refined which improves accuracy of leakage flow predictions and the calculation of multiphase screw machines with the variety of solvers is made possible, which is the latest breakthrough in analysis these machines.

The boundary conditions used at the suction and discharge are specified pressure and temperature. In order to provide better location of the pressure specification, generally the ports are hypothetically extended and the boundary conditions are provided at the end that allow flow to oscillate into and out of the domain.

This paper reviews some important aspects of grid generation procedures developed by the research group at City University in last two decades which enabled accurate prediction of screw compressor performance by use of CFD. Additionally, several examples of use of CFD for analysis of different types of screw machines are presented to show opportunities for use of CFD in analysis and design of screw machines in industry and academia.

3. EARLY 3D CFD MODELLING AND VALIDATION

3.1 Computational fluid dynamics for screw machines

The working process of positive displacement screw machines is based on the principle of changing the size and position of a working domain volume which consequently changes the pressure within the working domain. Quantities such as mass, momentum, energy etc. are required for modelling of screw machines. Conservation of these quantities can be represented by a general transport equation for a control volume (1), (Ferziger and Peric, 1996)

\[ \frac{\partial}{\partial t} \int_{\Omega} \rho \phi d\Omega + \int_{S} \rho \phi \mathbf{v} \cdot n dS = \int_{S} \nabla \cdot (\rho \mathbf{v} \phi) n dS + \int_{S} q_{\phi, S} dS + \int_{\partial \Omega} q_{\phi, \partial \Omega} d\Omega \]  

Rotation of rotors deforms the working domain and the solution domain therefore changes with time due to movement of the boundaries. In the global coordinate system which is fixed, the only change in the conservation equation (1), caused by the movement of a boundary, is the appearance of the relative velocity \( (\mathbf{v} - \mathbf{v}_{\Omega}) \) in the convective term, where \( \mathbf{v}_{\Omega} \) is the velocity vector at the cell face. In such case, the general conservation equation can be written as (2),

\[ \frac{d}{dt} \int_{\Omega} \rho \phi d\Omega + \int_{S} \rho \phi (\mathbf{v} - \mathbf{v}_{\Omega}) \cdot n dS = \int_{S} \nabla \cdot (\rho \mathbf{v} \phi) n dS + \int_{S} q_{\phi, S} dS + \int_{\partial \Omega} q_{\phi, \partial \Omega} d\Omega \]  

The grid velocity \( \mathbf{v}_{\Omega} \) and the grid motion are independent of the fluid motion. However, when the cell faces move and if the grid velocities are calculated explicitly and, in turn, used to calculate the convective fluxes, the conservation of mass and other conserved quantities may not necessarily be preserved. To ensure full conservations of these equations, the space conservation law needs to be satisfied as given by (3),

\[ \frac{d}{dt} \int_{\Omega} d\Omega - \int_{S} \mathbf{v}_{\Omega} \cdot \mathbf{n} dS = 0 \]  

Space conservation can be regarded as mass conservation with zero fluid velocity. The unsteady terms in the governing equations involving integration over a control volume \( \Omega \), which is now changing with time, need to be treated in a way consistent with the space conservation equation with a deforming and/or moving grid. The governing equations required for the solution form a closely coupled, time dependent set of partial differential equations (PDE’s) and often employ a Finite Volume Method (FVM) to be solved. Resolving the mesh displacement is crucial for ensuring space conservation which requires the grid velocities and changes in CV volumes to be known at each new time step. Providing that the numerical mesh used for transient calculation of screw machine flow domains has structured topology with the constant number of computational cells for any rotor position, then the movement of vertices which define the mesh can be used for calculation of wall velocity \( \mathbf{v}_{\Omega} \) ensuring that the space conservation and the entire solution are fully conservative, Kovacevic et all, 2006.

However, if the numerical mesh does not keep the same topology throughout transient calculation, it is much more difficult to fulfill the conservation requirements. Demirdzic and Peric, 1998 showed that the error in mass conservation due to non-conformance of space conservation is proportional to the time step size for constant grid velocities and is not influenced by the grid refinement size. This has been investigated by Rane et al, 2012, to test if the user defined node displacement for structured mesh can be replaced by key-frame re-meshing which is the most commonly used method for deforming unstructured meshes. It was found that many limitations to key-frame re-meshing exist which make it unsuitable for analysis of screw machines. Namely, it requires time consuming pre-processing, has limited applicability to complex meshes and leads to inaccuracies in conservation of calculated variables.

3.2 Grid Generation

Grid generation approach may be numerical, analytical or variational, as outlined in Kovacevic et al, 2006. Numerical grid generation is based on solving an elliptic partial differential equation on the unstructured mesh in order to firstly obtain the division line between the rotor flow domains and later to distribute grid points within the domain, Vorbe et
The method can produce good quality meshes but requires significant time for grid generation and a finite element or finite volume solver to obtain the mesh. Applying the principles of analytical grid generation through transfinite interpolation with adaptive meshing, the authors have proposed general, fast and reliable algorithm for automatic mapping of arbitrary twin screw machine geometry, Kovacevic, 2002. On that basis, the authors have developed a program called SCORG (Screw COmpressor Rotor Geometry Grid generator), which enables automatic rotor profiling, grid generation and direct connection with a number of CFD solvers. Kovacevic et al, 2006.

3.3 CFD calculation and validation

The numerical mesh of the screw rotor flow domains generated by SCORG does not require use of a numerical solver for grid generation and is directly transferable to variety of Computational Fluid Dynamics or Computational Continuum Mechanics code. This ensures a fully conservative mesh for moving, stretching and sliding rotor domains and robust CFD calculation with all commercially available CFD solvers (Kovacevic, 2006). Apart of the rotor domains, the solver requires suction port and the discharge port. These stationary parts can be generated using SCORG or any commercial grid generator. Figure 2 shows the complete numerical grid of a twin screw machine ready for CFD calculation. The structured numerical mesh of rotors changes for every time step. Its movement is handled by relocation of vertices by importing the new coordinates before each time step. Their coordinates are calculated for all required rotor positions in advance. The structured meshes of two sliding rotor subdomains and stationary ports are in the solver connected by non-conformal interfaces. Typical results obtained for oil free screw compressor using commercial CFD solver Ansys CFX is shown in Figure 3. Full details of that study are presented in Rane et al, 2013 and 2015.

![Figure 3 Mass flow rate variations in the ports (left) and contours of pressure variation (right)](image)

The first experimental verification of the numerical results obtained using SCORG and commercial CFD solver Comet was reported in Kovacevic et al, 2002. This study was performed on the oil injected screw compressor with 'N' type rotors of a 5/6 lobe configuration and 128 mm male rotor outer diameter. The numerical mesh contained very moderate number of just over half of a million of cells of which around 200,000 were used to map the moving parts of the grid. The calculation was performed using segregated pressure based solver Comet of Adapco-CD with Euler-Lagrange treatment of multiphase flow calculating concentration of dispersed oil in air with average Souter diameter of oil droplets assumed at 20 micrometres. The turbulence model was K-omega. The converged solution obtained on an office PC was achieved with 120 time steps in approximately 30 hours of computing time. The results were compared with the measurements of the identical screw air compressor. Four piezo-resistive transducers were positioned in the housing to measure pressure fluctuations across the compressor.

![Figure 4 Oil injection and Comparison of measured and calculated pressures](image)

Obtained results were compared for various discharge pressures of 6, 7, 8 and 9 bar. Good agreement was obtained both for the integral parameters and the instantaneous pressure values, as shown in Figure 4. The mentioned report showed for the first time the distribution of oil in the working domain and discussed the effects of various factors and setup parameters on the calculation accuracy.
These included variations in mesh size, turbulence model, differencing scheme and many other factors. The results of the overall compressor were very close to measurements which indicated that the procedure for CFD calculation of screw compressors can be used in industry. However it was also shown that the use of different differencing schemes and turbulence methods significantly influence local velocity and pressure values in some regions of the machine such as discharge port and leakage gaps. Although these local values have a low impact on the overall performance, their influence on flow development had to be further investigated. Very few authors have analysed local effects in screw compressors. For example Vimmr, 2006, following on Kauder et al, 2000, analysed flow through a static mesh of the single leakage flow path at the tip of the male rotor to conclude that rotor relative velocity does not affect flow velocities significantly and that neither of the turbulence models they used significantly change the outcome of modelling. That was in agreement with the findings of Kovacevic et al, 2006, but also confirmed that the need for further validation of full 3D CFD results could not be obtained by simplified numerical or experimental analysis. Instead, a full understanding of the local velocities in the suction, compression and discharge chambers of the machine was needed to further validate the existing methods. Laser Doppler Velocimetry (LDV) was used for this further validation.

### 3.4 LDV flow measurements in a screw compressor

In order to measure flow velocities inside a screw compressor, the experiment was set up at City University where this technique was used to obtain measured values. The extensive study was performed in measuring velocities in the compression domain and in the discharge chamber of the test air screw compressor as discussed by Guerrato et al, 2007.

A transparent window for optical access into the rotor chamber of the test compressor was machined from acrylic to the exact internal profile of the rotor casing and was positioned at the pressure side of the compressor near the discharge port, as shown in Figure 5. After machining, the internal and external surfaces of the window were fully polished to allow optical access. Optical access to the discharge chamber was arranged through a transparent plate, 20 mm thick, installed on the upper part of the exhaust pipe. The optical compressor was then installed in a standard laboratory air compressor test rig, modified to accommodate the transmitting and collecting optics and their traverses. The laser Doppler Velocimeter operates in a dual-beam near backscatter mode. It comprised of a 700 mW argon-ion laser, a diffraction-grating unit, to divide the light beam into two and provide frequency shift, and collimating and focusing lenses to form the control volume. A Fibre optic cable was used to direct the laser beam from the laser to the transmitting optics, and a mirror was used to direct the beams from the transmitting optics into the compressor through one of the transparent windows. The collecting optics were positioned around 25% of the rotor chamber and 15% of the discharge chamber to the full backscatter position and comprised collimating and focusing lenses, a 100 µm pin hole and a photomultiplier equipped with an amplifier.

Coordinate systems shown in Figure 5 (a), (b) and (c) are applied to the rotors where cp and Rp are, respectively, the angular and radial position of the measured control volume and Hp is the distance from the discharge port centre. Taking the appropriate coordinate system, measurements were obtained at Rp = 48, 56, 63.2 mm, αp = 27º and Hp = 20 mm for male rotor, and at Rp = 42, 46, 50 mm, αp = 27º and Hp = 20 mm for female rotor.

The CFD calculation was performed using the numerical mesh generated from SCORG and the comparison with the measured data, obtained with the LDV technique. The rotor mesh consists of 935000 numerical cells. For the purpose of obtaining a grid independent solution, three different meshes were generated, the smallest consisting of 600000 numerical cells and the biggest with 2.7 million cells, which was the largest possible case that could be calculated by the single processor of the used desktop computer.

Figure 6 shows a comparison of the axial mean velocities in the compression chamber close to the discharge port. This figure shows very good agreement throughout Zone (1) and Zone (2), as defined in Figure 6. In Zone (3) both the measured and calculated velocities increase but the increase in velocities obtained from CFD is larger as a consequence of the inability of the used k-e model of turbulence to cope with the flow near walls in rather large numerical cells. Such a configuration of the numerical mesh is the result of the methodology used for generating and moving of the numerical mesh, as explained in more detail in Guerrato et al, 2007.
Conclusions derived from the measurements, are as follows: (1) Chamber-to-chamber velocity variations were up to 10% more pronounced near the leading edge of the rotor. (2) The mean axial flow within the working chamber decreases from the trailing to the leading edge with velocity values up to 1.75 times larger than the rotor surface velocity near the trailing edge region. (3) The effect of opening of the discharge port on velocities is significant near the leading edge of the rotors and causes a complex and unstable flow with very steep velocity gradients. The highest impact of the port opening on the flow is experienced near the tip of the rotor with values decreasing towards the rotor root.

The measurements confirm that turbulence plays a significant role in the flow between narrow leakage passages and the large main and discharge domains. It was assumed that the most probable reason for this slight disagreement in the CFD results with measurements is due to turbulence modelling. Therefore further research in the turbulence models for internal flow in the compressor ports is suggested. Favourably, the flow on both sides of that region appears not to be so turbulent. Due to that fact and because the internal energy in positive displacement machines is significantly larger than the kinetic energy, this does not greatly affect the overall estimation of performance. Despite this, further development and improvement of 3D CFD codes are needed.

4. APPLICATION OF EARLY 3D CFD MODELLING TO ANALYSIS OF SCREW MACHINES

4.1 Fluid-solid interaction

Interaction between compressor components and fluid flow within screw machines plays significant role on its performance and reliability. Kovacevic 2002, reported on investigation of this influence by use of Computational Continuum mechanics to determine fluid-solid interaction in screw compressors. In Computational Continuum Mechanics (Ferziger and Peric, 1995) the same generic transport equation (2) can be used to simultaneously define behaviour of various materials in the working domain including fluids and solids. If the variable \( \Phi \) in that equation is fluid velocity \( v_i \) and the material properties of such domain could be defined by Stoke’s law, this will form Newtonian fluid momentum equation. If on the other hand the variable \( \Phi \) assumes rate of change of the deformation of solid and the material properties cold be describe by Hooke’s law for thermo-elastic body then this equation represents solid momentum equation. Providing that both solid and fluid domains of a screw machine can be defined by a combined numerical mesh then Finite volume method could be applied simultaneously within the same solver to solve fluid flow and solid deformations. Kovacevic 2002, reported on the investigation of change in clearances for three common applications of screw compressors, namely an oil-injected air compressor of moderate pressure ratio, a dry air compressor, of low pressure ratio, and a high pressure oil flooded compressor. In all cases the rotors are of ‘N’ type with a 5/6 lobe configuration. The solver used for this investigation was Comet and the numerical mesh for the rotors and flow domains was generated by use of SCORG.

The rotor deformations in the ordinary oil injected screw compressor are shown in Figure 7 (left). The high pressure oil injected refrigeration \( \text{CO}_2 \) compressor with suction at 30 bar and \( 0^\circ \text{C} \) and discharge at 90 bar and \( 40^\circ \text{C} \) is shown in Figure 7 (right). The figure shows pressure distribution and deformation vectors and magnitude. In both cases the interlobe clearance gap is increased during the operation. For the medium pressure application these deformations are small, order of magnitude smaller than the clearance gap. In the high pressure application deformations are of the same order of magnitude as clearances. In order to make the results visible, the deformations are presented 20000 times enlarged. In the oil free air compressor, due to the lack of cooling, the air temperature rise is significant. For 3 bar discharge pressure the exit temperature has an average value of \( 18^\circ \text{C} \). The deformations of the rotor are presented in left Figure 8. The fluid temperature in the immediate vicinity of the solid boundary changes rapidly, as shown in
the right diagram of the same figure. However, the temperature of the rotor pair is lower due to the continuous averaging oscillations of pressure and temperature in the surrounding fluid. This is shown in the right diagram of Figure 8, where the temperature distribution is given in cross section for both the fluid flow and the rotor body. The deformation, presented in the figure, is increased 5000 times in order to make it visible. The rotor deformation has the same order of magnitude as the rotor clearance.

4.2 Coupled CFD and Chamber Model
It is possible to increase the speed of calculation of screw machines retaining accuracy of 3D models. Mujic et al, 2008 used the decomposition of the compressor geometry shown in Figure 9 to introduce the idea of coupled models. According to that, the components of the system of greater interest are modelled with full 3-D CFD model while the components of secondary concern are simulated with a thermodynamic model. This can combine the advantages of the fast computation of as chamber model as in Stosic et all, 2005 with the enhanced capabilities of the 3-D model, described in detail in Kovacevic et all, 2006.

Figure 9 3D domain of the screw compressor discharge chamber and full 3D model showing the interface

The inlet and outlet flows are the means by which a compressor chamber exchanges energy and mass with its surroundings. These occur through openings which generally change both in size and shape with time. More than one of them can be connected to the compression chamber at the same time. In the mathematical models mentioned earlier, these flows are introduced through the enthalpy and mass contributions to the fluid in the compression chamber. If all three chambers are simulated by a quasi one dimensional thermodynamic model, as discussed by Stosic et al, 2005, both the mass and energy flow estimates are based on the assumption of adiabatic flow through the suction and discharge cavities. However, if a one dimensional model of the compression chamber needs to be integrated with a three dimensional model of the suction and discharge chambers the exchange of mass and energy must be calculated by the summation of the boundary flows that occur in the three dimensional domains. Once the integrated flows are added to those of the one-dimensional model in the compression chamber, they can be used to calculate the thermodynamic properties in that chamber in the form of pressure, temperature and density. Mujic et al, 2008 and Mujic, 2009. The derived values of pressure and temperature in the compression chamber are used later as boundary conditions for the three dimensional models of the suction and discharge chambers. The example of the interface where these boundary conditions are applied is given in Figure 9.

4.3 Use of the CFD and coupled models for noise prediction
Identification of sources of noise in screw compressors and its attenuation becomes an important issue for the majority of applications. Pressure fluctuations in the discharge port affect not only aero acoustics in that domain but also a mechanically generated noise due to rotor rattling. It is believed that adequate porting can decrease the level of noise and increase the performance of the machine.

Mujic, 2009 presented comparison of results obtained by the chamber model, combined model and full 3D model to estimate pressure oscillations as a function of the shape of the port. The comparison of results obtained by modelling and measurements is shown in Figure 10.

Figure 10 Comparison of results provided by numerical models

The 3-D and coupled models offer better accuracy than the thermodynamic model, especially for higher harmonics of the gas pulsations. The discharge chamber geometry certainly does influence the gas pulsations and therefore the accuracy of the prediction is thereby improved in the case of the 3-D and coupled models. Additionally, since the thermodynamic model assumes uniform distribution of fluid properties across the control volume the value used for comparison of the results is that obtained at the centre of the discharge chamber. In the case of the 3-D model, the compared pressure values are those taken at the identical position
of the pressure probe in the real chamber. As both the 3-D and the coupled models include the momentum equation, they can account for pressure wave propagation through the discharge chamber. The pressure wave passes the measuring place and influences the value of the pressure at that place. Additionally, these two models provide information about other flow properties such as velocities within the chamber and can be useful in the analysis of fluid flow losses.

The accuracy and computational time for obtaining solution with each numerical model are shown in Figure 11. The chamber model requires modest computer resources and its computational time is much shorter than that required for 3-D computations. The accuracy of the 3-D and coupled models is better than that of the simple chamber model. The coupled model requires one order of magnitude lower computational time than the full 3-D model, for negligible loss in accuracy.

Mujic et al, 2010, used the coupled model to investigate the influence of the discharge port shape on the pressure pulsations in the discharge plenum (i.e. noise generation) and its effects on the performance. Figure 12 shows the modified discharge port of an oil injected screw compressor compared with the original port indicate with the drawn line and the effect on the pressure variations at the tip speed of 40 m/s and the discharge pressure of 8 bar. The reduction in pressure oscillations was about 10% which reduced noise up to 5 dB. At the same time, due to the reduction in the flow area of the discharge port, the specific power increased for just about 1%. The coupled model therefore allows fast and reliable optimisation of the compressor ports.

5. RECENT DEVELOPMENTS IN CFD MODELLING OF SCREW MACHINES

5.1 Single domain mesh with interlobe refinement for improved leakage flow capturing

One of the major factors affecting the performance prediction of twin screw compressors by use of computational fluid dynamics is the accuracy of representing the leakage by the discretization methods in grid generation Rane, et al, 2012. A method of improving the profile accuracy is by increasing the number of grid points on the profile. However, this method faces limitations when it comes to the complex deforming computational domain of the twin screw compressor because the grid quality deteriorates and computational time increases tremendously. In order to address this problem, an analytical grid distribution procedure has been developed (Rane et al, 2015) that can simultaneously refine the region of high importance i.e. the interlobe space and produce the conformal interface between the rotors.
By this means, the surface mesh on the casing is of the highest quality with regular quadrilateral cells. The surface mesh on the interlobe interface mostly follows axial grid lines with only small transverse movements in the vicinity of the top and bottom cusp’s which are cyclically repeating. The current implementation allows for a fully conformal interface with the equal index of the top and bottom CUSP points which ensures straight line in the axial direction. This also accurately captures blow-hole area. The features of the newly developed single domain mesh for two rotors are shown in Figure 13. The total grid size can be controlled by independent refining of the interlobe area between two cusp points and therefore reducing the overall mesh size but improving the quality of mesh in interlobe gap and blow-hole area.

### 5.2 Twin screw machines with variable rotor geometry

Gardner, 1969 patented screw compressor with variable pitch rotors. However such machines are rarely used as compressors due to the lack of efficient and economical manufacturing techniques. The variable pitch rotors are more common in vacuum technology but the rotor profiles are simple to produce. The conformal numerical mesh generated by SCORG, 2014 could be used for the CFD analysis of performance of compressors with variable geometry rotors. Rane et al, 2012 reported the analysis of variable rotor geometry using SCORG and Ansys – CFX solver.

Figure 14 shows the comparison of the sealing lines obtained for the uniform rotors and variable rotors. The sealing line on the uniform pitch rotors has the same length for each interlobe space along the rotor. The variable pitch rotors have the sealing line 20% longer at the suction and 20% shorter on the discharge end compared to the mid section which has the same sealing line length as the uniform pitch rotors. This indicates that variable pitch rotors have smaller leakage area towards discharge and higher volumetric efficiency compared to the constant pitch rotors. The performance of this oil free compressor of 128 mm 3/5 rotors was obtained using SST Turbulence model in Ansys CFX solver on the grid of nearly 2 million cells. Table 1

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**Table 1. Comparison of adiabatic and volumetric efficiencies of uniform and variable geometry rotor compressors**

<table>
<thead>
<tr>
<th></th>
<th>Volumetric Efficiency %</th>
<th>Adiabatic Efficiency %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>2.0 bar</td>
<td>3.0 bar</td>
</tr>
<tr>
<td>Uniform</td>
<td>$V_1$ 1.8</td>
<td>75.30</td>
</tr>
<tr>
<td>Uniform</td>
<td>$V_1$ 2.2</td>
<td>64.00</td>
</tr>
<tr>
<td>Variable Pitch</td>
<td>$V_1 &gt; 1.8$</td>
<td>66.20</td>
</tr>
<tr>
<td>Variable Profile</td>
<td>$V_1 &gt; 1.8$</td>
<td>62.80</td>
</tr>
</tbody>
</table>
shows a comparison of predicted volumetric and adiabatic efficiencies. The research confirmed that the variable geometry rotors have advantage in high pressure applications and that CFD can be effectively used to estimate performance and benefits of variable geometry screw machines.

5.3 Conical internally geared rotary compressor
The uniform pitch and variable section compressor with internally geared rotors is invented by start-up company Vertrotor, 2011. The 3/4 lobe compressor has cycloidal profiles as shown in Figure 15. In operation, the outer rotor is positioned on a central axis while the inner rotor rotates about an eccentric axis with varying centre distance from the suction to the discharge ends. Both axes are stationary in space. The numerical mesh is generated using SCORG, 2014. CFD analysis revealed interesting features of the machines such as flexibility for use with various pressure ratios and distribution of the pressure on one side of the machine as shown in Figure 15.

5.4 Multiphase CFD simulation of oil injected compressor
The cross section of the oil injected screw compressor with 4/5 configuration of “N” profile rotors, axis distance 93 mm and 108 mm male rotor diameter is shown in Figure 16. The oil injection is simulated by use of Ansys-CFX with full multiphase Euler-Euler scheme in the coupled pressure based solver. The turbulence model used is SST. The single domain numerical mesh for rotors was produced by SCORG while the stationary mesh of the ports was produced using ICEM. Figure 17 shows the comparison of measured and calculated data. On the left the integral volume flow rate was compared at two different speeds. The diagram on the right shows the comparison of internal pressures measured by use of 4 piezoelectric probes. The whole process of generating numerical mesh lasts for just few minutes. The calculation required 3 full cycles to stabilise which took around 4 days of calculation on the mesh ranging around 1 million cells. The results match very well and demonstrate that the single domain rotor grid is today the most suitable for multiphase flows in twin screw machines.

6. CONCLUSIONS
The last two decades saw growing interest for modelling and design of screw machines using 3D Computational Fluid Dynamics. Following early developments of the grid generation algorithms, extensive study was performed to validate accuracy of the 3D CFD results. Today CFD is still research tool used by academia and industry. To become widely used by industry the grid generation procedure and CFD simulation must become faster and more reliable. Coupled chamber and CFD models will find their use more often in industry. Further developments are also expected in grid generation especially addressing grid quality and leakage flows. Also more work is required in implementing real fluids and management of rotor clearances to better reflect reality.
7. ACKNOWLEDGEMENTS
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REFERENCES