Challenges in 3D CFD Modelling of Rotary Positive Displacement Machines

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Abstract. The use of Computational Fluid Dynamics (CFD) and Computational Continuum Mechanics (CCM) for analysis of rotary positive displacement machines is exponentially increasing which was mostly allowed by the development of methods for generating numerical grids of complex domains within the machines. However there are several challenges with the commercial CFD/CCM codes which are preventing generic use of CFD. These are conservativeness of spatial discretisation caused by the inappropriate grid generation, numerical instabilities and dissipations caused by misalignments and application of inappropriate discretisation of equations and the speed and accuracy of multiphase models used in CFD of positive displacement machines.

In this paper the authors will review methods used for modelling of rotary positive displacement machines and challenges which developers and users of these methods face. The paper will also offer some solutions and directions for resolving these issues.

Keywords: Rotary Positive Displacement Machines, CFD, Conservativeness, Numerical dissipation, Convergence, grid generation

1. Introduction

Twin screw compressors are a type of rotary positive displacement machines mostly used in industrial applications such as oil and gas, refrigeration and air compression. They represent approximately 80% of the millions of industrial positive displacement compressors produced globally each year. More than 87% of screw compressors are oil injected, remaining being oil free. Other rotary positive displacement machines are mostly used in commercial and domestic applications, primarily air-conditioning and refrigeration. About 200 millions of rolling piston (or better known as rotary) compressors are annually produced for domestic refrigeration and air-conditioning, about 15 million of scroll compressors and much smaller number of rotary vane are used in refrigeration and variety of other applications. When rotating in the opposite direction, these will be able to reduce pressure of the working fluid and extract power. Recently rotary positive displacement machines are applied in power recovery systems such as Organic Rankine Cycles. In such cases these will operate with phase changing organic fluids and oil injection. Rotating positive displacement machines are also used for pumping liquids and mixtures of liquids, gasses and solids as well in vacuum applications. Liquid pumps may be subject to cavitation. Reliability and efficiency of such machines operating with multiphase fluids is of utmost importance for economy and ecology.

The control of the clearance gaps is the most important issue for efficiency and reliability of rotary positive displacement machines. The effective depth of the main working chamber in a rotary positive displacement machines can be up to four orders of magnitude larger than the clearance gap. Thermal and force deformations of a machine elements could easily be of the size of the clearance gap and increase or reduce it so that it can either ruin the performance or cause catastrophic failure of the machine. This phenomena is still not fully understood and the most promising method of understanding and preventing this is use of Computational Continuum Mechanics (CCM) and Computational Fluid Dynamics (CFD).

The use of CFD and CCM for analysis of rotary positive displacement machines is exponentially increasing which was mostly allowed by the development of methods for generating numerical grids of complex domains within the machines. However there are several challenges with the commercial CFD/CCM codes which are preventing generic use of CFD. These are conservativeness of spatial discretisation caused by the inappropriate grid generation, numerical instabilities and dissipations caused by misalignments and application of inappropriate discretisation of equations and the speed and accuracy of multiphase models used in CFD of positive displacement machines.

2. Generation of Structured mesh required for conservative multiphase flow calculations

Computational Fluid Dynamics (CFD) can provide a useful means of modelling distribution of oil in a compressor and study the physical phenomenon in detail. A prerequisite for 3D modelling of multiphase screw machines is the ability to generate a good structured numerical mesh which could efficiently and accurately utilise capabilities of general CFD solvers. The pioneering work on development of a numerical grid for analysis of screw machines was by Kovačević [5], [6]. To allow generation of the structured mesh, the flow domain around two rotating rotors of a screw machine is divided into two subdomains by the rack plane each belonging to one of the rotors. Then the nodes are distributed in the transverse cross sections on the domain boundaries formed by the casing and rack on the outside and the rotor surface on the inside of the rotor flow domain. A 2D numerical mesh is made in each transverse cross section along the rotor length by use of an algebraic grid generation method with boundary adaptation and transfinite interpolation. These 2D meshes are then connected along the axis of the rotor so that these form structured 3D numerical mesh. The deformation of the mesh is obtained by movement of nodes between time steps. This method is the only method devised so far to ensure fully structured moving mesh and therefore fully conservative solution of transport equations. For the reference in this text, this method will be called Transverse Structured Body Fitted mesh (TSBF). An example of mesh generated in this way is shown in Figure 1.

Figure 1 Configuration of a structured numerical mesh for the flow domain of the male rotor

This method allows generation of two types of meshes, i) the mesh that rotates with the rotor or ii) the mesh which is stationary on the casing but deforming on the rotor surface. Both have been implemented in the program SCORG [4], generic grid generator for screw machines. The first method is caller Rotor-To-Casing generation method in which numerical mesh rotates with the rotation of the rotors. It allows excellent representation of the rotor geometry and refinement of the mesh in clearances but requires special attention in CFD solver to handling of the interface between the two rotor meshes. Kovačević et al. (2007) have reported on CFD simulations of twin screw machines to predict flow, heat transfer, fluid-structure interaction, etc using the Rotor-To-Casing mesh. In the same work, a test case study of an oil injected compressor using source terms in transport equations with a segregated pressure based solver was reported. Vande Voorde et al. [17] used an algorithm for generating block structured mesh from the solution of the Laplace equation for twin screw compressors and pumps using differential methods. Reports on analysis of dry air screw compressors and twin screw expanders with real gas models are available in literature using these techniques (Papes et al., [10]). Recently, Arjeneh et al. [1] have presented the analysis of flow through the suction port of a screw compressor with water injection. It was reported that it was difficult to stabilize the solver in a full 3D analysis with both deforming rotor domains and multiphase models. Although several attempts have been made in the recent past to extend the CFD technology to oil injected compressors, it has proven to be difficult to achieve the desired grid structure and the modelling conditions that can provide stability to the numerical solvers.

Rane [9] in his thesis proposed a new analytical approach for grid generation that can independently refine the interlobe region of the screw rotors. This method is called Casing-To-Rotor indicating that the numerical mesh is attached to the casing and it slides on the rotor face. It was demonstrated that such a grid refinement improves the prediction of the mass flow rates. The same algorithm has been extended to produce a rotor grid that eliminates the interface between two rotors, called conformal interface, and thereby to provide a desirable grid for modelling of oil injected or multiphase machines. This recent developments has been reported by Rane and Kovacevic in [12], [13] and [8]. Use of this grid generation method enables much more conservative solution in variety of different CFD solvers as reported in [7]. However, there is a possibility to improve the quality of such mesh and further improve the speed and accuracy of a CFD solution by implementing elliptic numerical smoothing and orthogonalisation of the mesh generated by use of analytical grid generation. The casing-to-rotor mesh is generally more suitable for calculation of oil injection in screw machines since it avoids existence of sliding interfaces with complex geometrical shape.

The numerical mesh for screw machines produced by dividing the mesh in separate rotor subdomains and producing the 2D mesh in transverse cross sections before joining it in the 3D mesh results in a structured fully conservative mesh necessary for accurate modelling of screw machines.

3. Main numerical issues when modelling Screw Machines

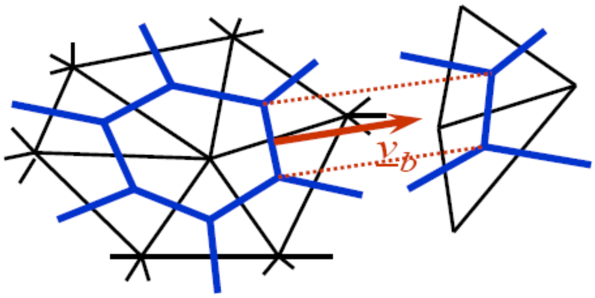
Screw compressors fall in category of rotating positive displacement machines (PDM). Pressure is increased in PDM on the account of volume reduction of the trapped gas and that is why these machines are also called 'volumetric'. CFD is originally developed for modelling of open flows in which the change of pressure in the domain is caused by the change in velocity which is consequence of changes in geometry of the flow domain. However, in PDM, velocity changes are much smaller and pressure increase depends on the change of volume. For analysis of such machines and to ensure full conservativeness of the solution, it is essential that the space conservation is preserved. The TSBF grid generation method presented in this paper produces such meshes and is the only known fully conservative method known so far. It has been used also by other researchers and practitioners, for example by Viereendels group from University of Gent [10], [17] and CFX Berlin [15]. Both have applied same principle of producing 2D numerical meshes in transverse plane and joining them in a 3D mesh. The only difference is that they produced internal grid points using differential method. Some alternative grid generation techniques have also been tested but have not been so successful. One of these is described by Rowinski in [14] which uses cut-Cartesian numerical mesh that changes the number of points for each time step. Another one is use of overset meshes [11]. Both of these methods are not conservative and require modelling of leakage flows which reduces their accuracy and application.

In this paper four aspects that affect accuracy and applicability of results produced by CFD codes are presented.

3.1. Issue 1: Conservativeness

The principle of continuity applied to solving fluid flow problems in CFD states that for the accurate solution it is necessary that the flow domain, space and time discretisation as well as discretisation of equations are conservative, i.e. the sum of all inputs and outputs to the domain as well as to each numerical cell has to be equal to 0. For positive displacement machines it means that the overall machine space, as well as each numerical cell need to be conserved in time so that the solution is conservative. As shown in Figure 2 by Vierendeels, each conservation equation for mass, momentum and energy contains variable v_b which represents velocity of the cell boundary in each time step during transient calculation. In order to allow conservative solution of these equations it is necessary to calculate this velocity accurately in each step which can be done by the Space conservation law shown in the same figure. This is easy to calculate explicitly providing the numerical cells are existing in time and only change their position and shape for each time step which is caused by movement of boundaries. If this condition is satisfied, the numerical mesh will be conservative and it will allow conservative solution, which is the case with TSBF (Transverse Structured Body Fitted) meshes.

$\underline{v}_b$ is the velocity of the control volume edge



$$\frac{\partial}{\partial t}\int_V \rho\, dV + \int_S \rho\,(\vec{v}-\vec{v}_b).\vec{n}\, dS = 0$$

$$\frac{\partial}{\partial t}\int_V \rho\vec{v}dV + \int_S \rho\vec{v}(\vec{v}-\vec{v}_b).\vec{n}dS = \int_V \rho\vec{f}dV + \int_S \vec{T}dS$$

$$\frac{\partial}{\partial t}\int_V \rho E dV + \int_S \rho E(\vec{v}-\vec{v}_b).\vec{n}dS = \int_V \rho\vec{f}.\vec{v}dV + \int_S \vec{n}.\vec{\sigma}.\vec{v}dS - \int_S \vec{q}.\vec{n}dS$$

$$\xrightarrow{\rho, p, E = cst,\ \vec{v}=0} \boxed{\frac{\partial}{\partial t}\int_V dV = \int_S \vec{v}_b.\vec{n}\, dS}$$

Space conservation law

Figure 2 Requirement for conservation of space and equations used for solving problems with moving and deforming meshes
(adopted from J. Vierendeels, Ghent University, Introduction to CFD in PD machines, Short Course, London, Sept 2015)

However, cut-Cartesian or overset meshes cannot ensure that this condition is satisfied directly since for each new time step the mesh is generated without preserving the structure of the mesh. Even if the wall velocity can be calculated for newly generated cells, it cannot be guaranteed that this will be conservative. Therefore, these meshes are by nature non conservative which leads to solutions that do not converge as expected. The example of the solution produced with the non-conservative grid generation method for piston compressor is presented by Sham et al in [11].

3.2. Issue 2: Speed and accuracy of a numerical solver

Solution of equations shown in Figure 2 depend on the discretisation method. Most commonly used solvers are so called pressure based solvers. Since pressure is not a field it does not have conservation equation. Instead, pressure is obtained by balancing momentum and continuity equations through pressure correction equation. This solution can be performed using segregated and coupled pressure based solvers.

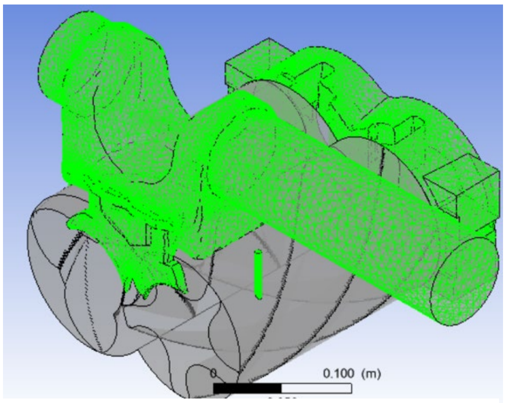


Figure 3 Numerical mesh of an oil-injected screw compresseor

In order to compare the solution accuracy and speed of several solvers an experiment was conducted to obtain performance predictions of the oil free screw compressor on the numerical mesh shown in Figure 3. The compressor in question has "N" rotor profile, 3/5 configuration of rotors, main rotor diameter of 128 mm and L/D ration of 1.6

Figure 4 shows the difference in the process of solving transport equations by use of segregated and coupled solvers by most common commercial CFD solvers.

In segregated solvers each equation of mass, energy, momentum etc is solved separately in so called internal iteration loops until the desired convergence criteria is obtained. Following that the pressure correction is obtained and the equations are balanced in the external iteration loops until both momentum and continuity equations result in velocities within the tolerance range. Such system requires lower memory than coupled solution but can become quite unstable when pressure correction is applied sometimes leading to temperatures, pressures and densities beyond the expected range.

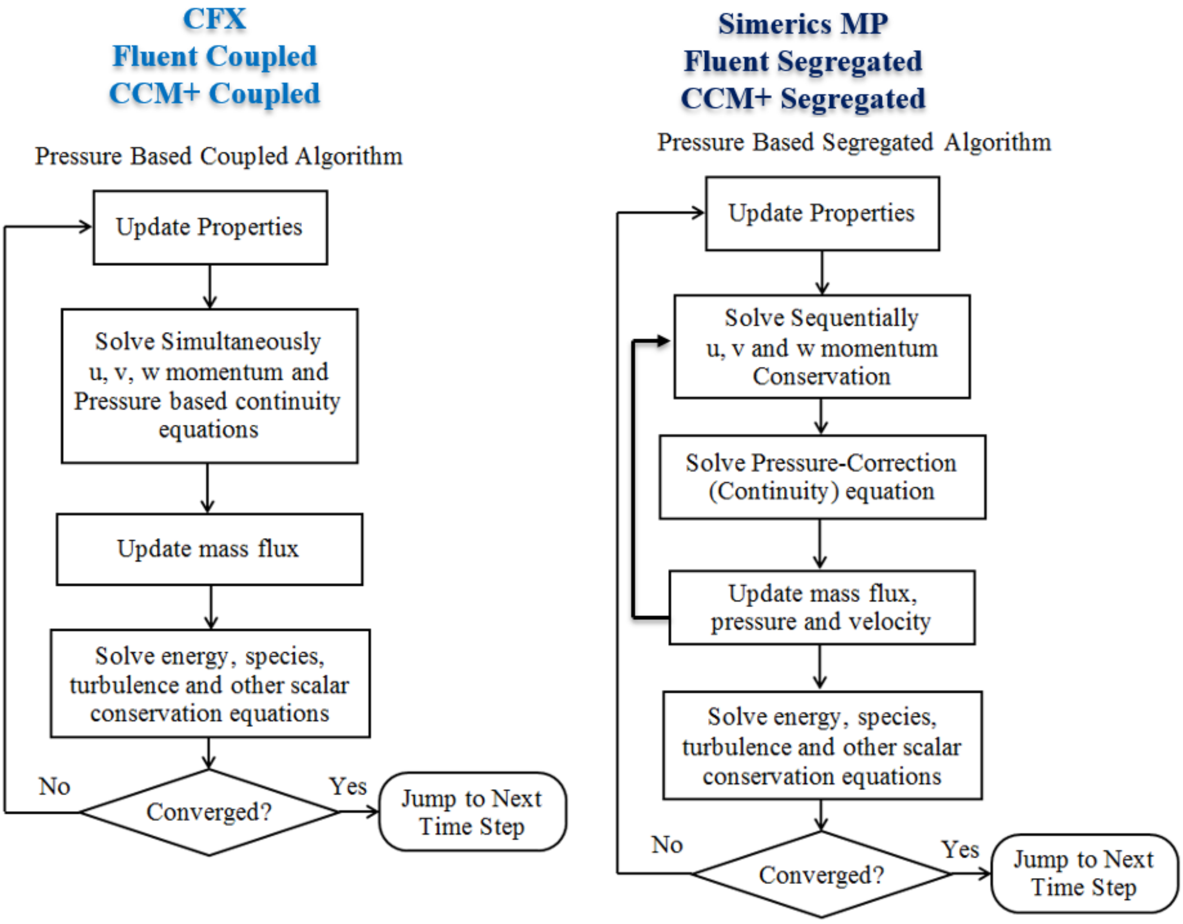
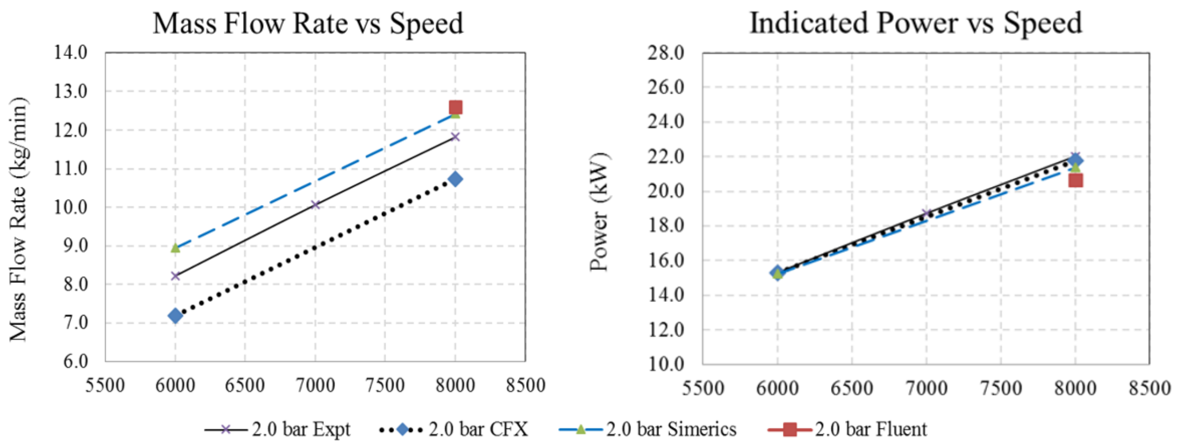


Figure 4 Schematic view of processes in segregated and coupled solvers

Coupled solvers solve the entire system simultaneously and generally achieve better stability of the solution but require much longer time to obtain converged solution.

Three solvers are used in this experiment, namely, CFX coupled solver, Fluent segregates solver and Simerics MP also segregated solver. In all cases the numerical mesh contained 582,000 numerical cells in the rotating parts of the compressor. Figure 5 shows the comparison of mass flow and power calculations and the speed of all three tested solvers. It is shown that the selection of discretisation scheme can results in speed and accuracy differ for an order of magnitude from each other.



Solver	Total number of time steps	Calculation time per time step / total	Coefficient Loops	Error in cycle averaged mass flow
CFX	1000	7.30 mins / total = 5 days	6	1.01
FLUENT	1000	2.40 mins / total= 1.7 days	10	0.99
SIMERICS MP	1000	1.5 min / total = 1 day	10	1

Figure 5 Comparison of integral results and speeds of some popular CFD solvers

3.3. Issue 3: Alignment of grid to leakage flow direction

As mentioned before, a TSBF numerical mesh could be generated as casing-to-rotor or rotor-to-casing as shown in Figure 6. It is clear from these figures that in both cases velocity vectors are aligned with the radial direction of cells which are generated between the casing and the rotors but they are not aligned with the orientation of cells in circumferential direction. The reason is that the numerical mesh is always generated in transverse cross sections.

Such an orientation of cells and direction of flow can cause diffusion in the solution. Let us consider a 2D convection-diffusion equation (1).

$$\frac{\partial \phi}{\partial t} + \vec{v}.\nabla \phi = \upsilon \nabla^2 \phi \qquad (\upsilon = \mu / \rho) \tag{1}$$

If this equation is discretised in the Cartesian coordinate system with no slip conditions, central differencing scheme, the equation will result in:

$$\frac{\partial \phi}{\partial t} + u\frac{\phi_{i,j} - \phi_{i-1,j}}{\Delta x} + v\frac{\phi_{i,j} - \phi_{i,j-1}}{\Delta y} = (\upsilon + u\Delta x)\frac{\phi_{i-1,j} - 2\phi_{i,j} + \phi_{i+i,j}}{\Delta x^2} + (\upsilon + v\Delta y)\frac{\phi_{i,j-1} - 2\phi_{i,j} + \phi_{i,j+i}}{\Delta y^2} + H.O.T. \tag{2}$$

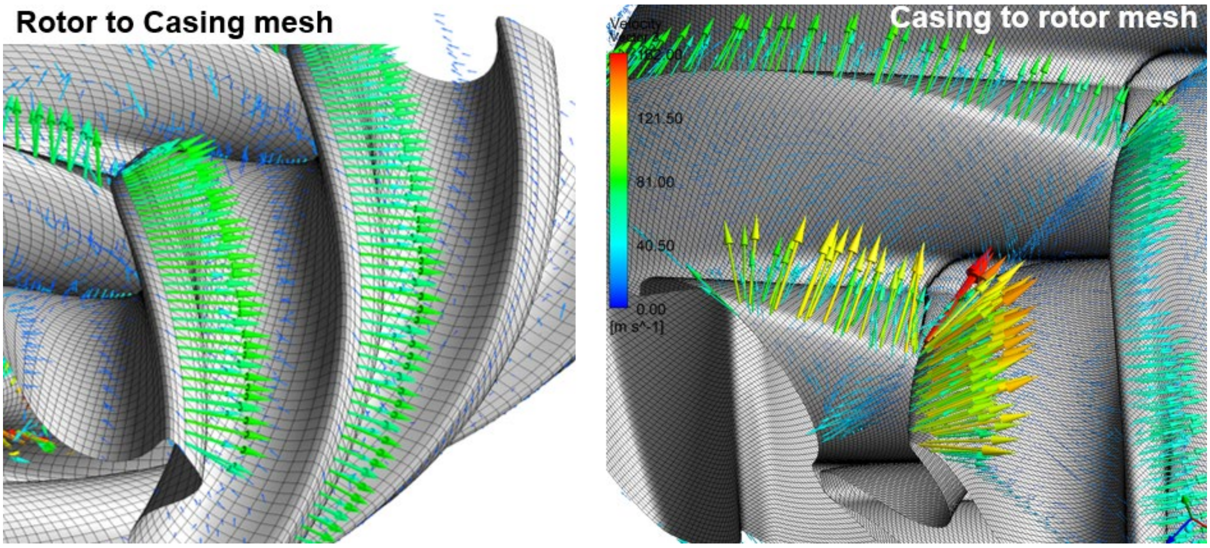


Figure 6 Velocity vectors in leakage paths of TSBF meshes

Considering boundary conditions with velocities of 1 m/s and 2 m/s respectively on boundaries. Assuming the no-slip conditions, if the numerical mesh is aligned to the flow direction, there will be no mixing between the two streams i.e. no artificial diffusion on the right hand side of Equation (2). This situation is shown in Figure 7 Left.

However, if the numerical grid is not aligned to the flow direction, there will always be numerical diffusion irrespective of the mesh quality or the order of discretisation as shown in Figure 7 Right. Similar situation will happen in unstructured meshes.

The preferred numerical mesh to resolve this issue would be Normal rack structured body fitted mesh which will have 2D cross sections positioned along the helix of the rotor. Such mesh is being developed at City, University of London as shown in [9].

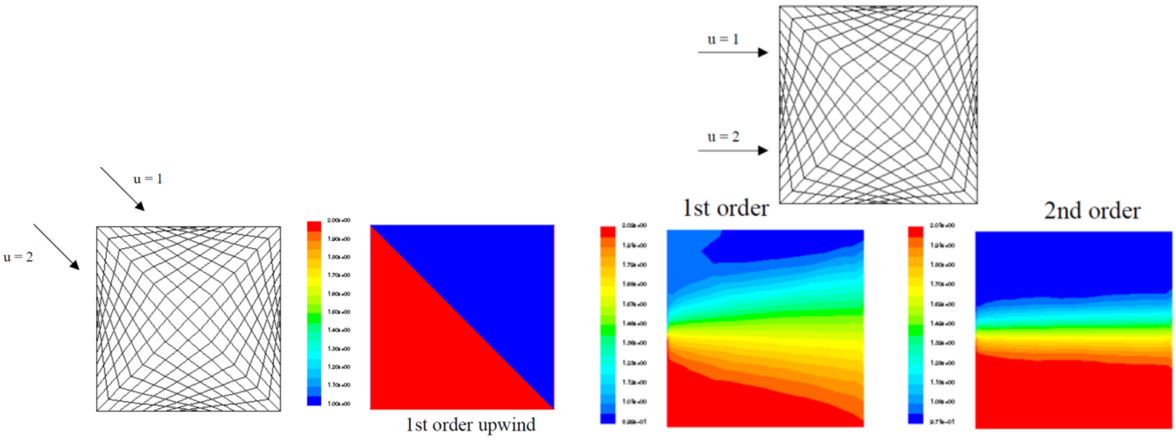


Figure 7 Demonstration of artificial numerical diffusion caused by misalignment of the numerical grid to the flow direction
(Left – grid is aligned to the flow direction; Right – flow is not aligned to the flow direction) from J. Vierendeels, Ghent University, Introduction to CFD in PD machines, 3rd Short Course, London, Sep 2017

3.4. Issue 4: Selection of multiphase solver for oil injected screw machines

The complexity of the flow inside a screw compressors makes modelling challenging since variety of flow regimes can occur within the relatively small working domain. The oil injected in the compressor breaks in droplets of a certain size but once it hits the rotor surface a part of it will form a film which sticks to the walls. The film grows and spreads until the injection nozzle is cut-off from the compression chamber by the rotors trailing lobes. Further rotation causes flooding of the chamber whose volume is continuously reducing. In order to capture such complex mechanism, a multiphase model used in CFD is required to account for large changes in oil volume fraction and distribution. Crowe et al. [3] have presented review of multiphase flow regimes as a function of the disperse phase concentration.

The three main methods used for multiphase modelling in CFD are capable to represent some of the multiphase flow regimes.

The first method is called Euler-Lagrange. It can be applied if the concentration of the dispersed phase is low and the individual droplets exist in the flow with a negligible momentum. In that case the compressed gas can be treated as the continuous phase while the oil droplets are treated as particles in the Lagrangian frame which have just one way coupling. This means, the oil will move with the flow and only heat transfer between phases will occur. Such a computational model has five transport equations for the gas phase and one momentum (motion kinematics) equation for the liquid phase that needs to be conserved separately.

The second approach called Eulerian – Eulerian inhomogeneous method is used for conditions which occur in heavily oil flooded operation. In addition to the oil droplets, the oil film on the rotors and housing will occur resulting in oil being dragged along with the compressed gas. Under such conditions, both oil and gas are treated as continuous phases which exchange both energy and momentum. Such a computational model requires significant computational resources and requires solving five transport equations for each phase including momentum, energy and volume fraction. The pressure field solution obtained from the common continuity equation is shared by the two phases. The relative slip and shear between the gas and oil is calculated as the difference between the individual velocities obtained by separate momentum equations. In describing multiphase flow the concept of phase volume fractions is utilized. The phase volume fraction represents the space occupied by each phase in a computational cell in which each phase must satisfy conservation of mass, momentum and energy individually. This is regarded to be the most accurate treatment for any multiphase flow regime and is most likely required for oil injected screw compressors.

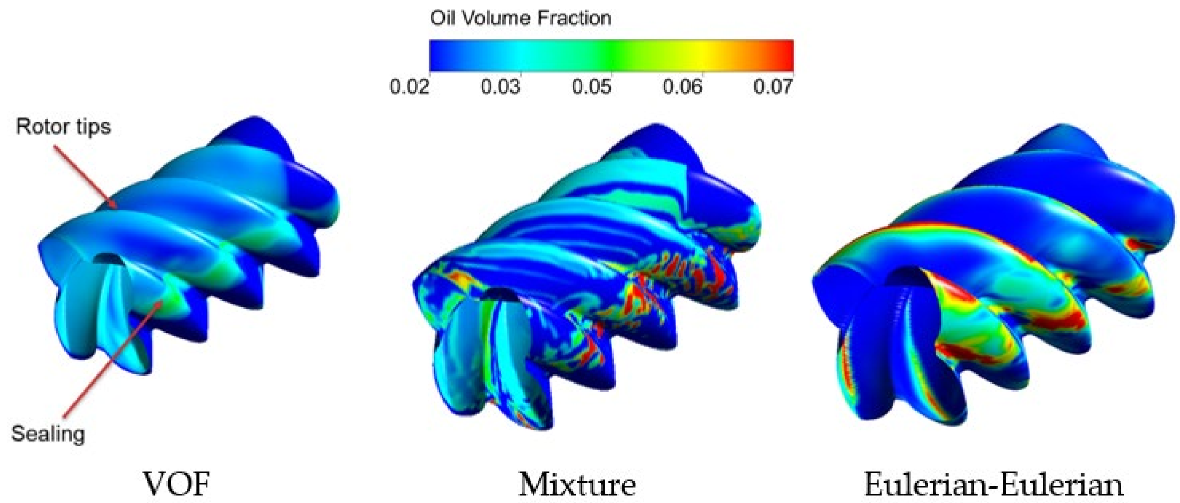


Figure 8 Comparison of three mixture models for oil injected screw compressors

The third model is a simplification of the Eulerian – Eulerian approach. It can be applied to flows which have negligible slip between two phases, for example a multiphase flow with fluids of similar physical properties. In this Euler – Euler homogeneous multiphase treatment both phases share a common pressure solution and velocity field. Such model requires five equations for the continuous phase and an additional concentration equation for distributed phases. More on this could be found in [6]. There are several sub variants of this method which could be used in modelling of screw machines in different applications providing the interaction of phases can be modelled appropriately.

In the recent publication by Basha et.al, [2] three multiphase models have been considered and compared as shown in Figure 8

It was concluded in the study that both mixture and VOF models are capable of predicting overall performance of the flow and power close to measured values. The mixture model predicts flow with 0.9% and power with 4.5% error compared with measured values. The VOF model predicts flow with 3.5% and power with 5.7% error compared with measured values.

Pseudo single-phase models are computationally economical, and on average a 22% improvement in time was observed with pseudo-single fluid models compared to the Eulerian–Eulerian.

The study shows a good comparison of oil distribution within the compression chamber, which differs between mixture and VOF models. With the VOF model, smooth distribution of oil volume fraction was observed due to the air and oil phases being treated as non-interpenetrating. With the mixture model, the distribution of oil phase was different since the phases are penetrating and the slip between phases is included. However, the Eulerian–Eulerian model which was originally solved in CFX still shows distribution closer to expected reality.

4. Conclusions

Modelling positive displacement machines using CFD is complex task which requires careful consideration of several modelling aspects.

Firstly, the conservativeness of the solution depends on the numerical grid used. The 3D mesh obtained by successive generation of 2D structured numerical meshes in transverse planes ensures full conservativeness and if generated from casing-to-rotor it is the most suitable for accurate prediction of oil injected flows.

Secondly, selection of a differencing scheme significantly affects the speed and accuracy of solution. Segregate solvers are able to produce good results much faster than coupled solvers but are still unstable in some cases.

Thirdly, structured mesh allows the alignment of numerical grid to the leakage flows which plays significant role in future modelling to reduce leakages in screw machines. Generation of the mesh from normal planes is expected to further improve the accuracy of flow calculation in clearances.

Finally, Euler-Euler nonhomogeneous model is the most accurate for calculating oil-injected screw compressors but it still requires significant time for obtaining solutions.

Future work of authors will be dedicated to developing new methods to address issues listed above.

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