

CFD simulation of a screw compressor including leakage flows and rotor heating

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Abstract. Computational Fluid Dynamics (CFD) simulations have promising potential to become an important part in the development process of positive displacement (PD) machines. CFD delivers deep insights into the flow and thermodynamic behaviour of PD machines. However, the numerical simulation of such machines is more complex compared to dynamic pumps like turbines or fans. The fluid transport in size-changing chambers with very small clearances between the rotors, and between rotors and casing, demands complex meshes that change with each time step. Additionally, the losses due to leakage flows and the heat transfer to the rotors need high-quality meshes so that automatic remeshing is almost impossible.

In this paper, setup steps and results for the simulation of a dry screw compressor are shown. The rotating parts are meshed with TwinMesh, a special hexahedral meshing program for gear pumps, gerotors, lobe pumps and screw compressors. In particular, these meshes include axial and radial clearances between housing and rotors, and beside the fluid volume the rotor solids are also meshed.

The CFD simulation accounts for gas flow with compressibility and turbulence effects, heat transfer between gas and rotors, and leakage flows through the clearances. We show time-resolved results for torques, forces, interlobe pressure, mass flow, and heat flow between gas and rotors, as well as time- and space-resolved results for pressure, velocity, temperature etc. for different discharge ports and working points of the screw compressor. These results are also used as thermal loads for deformation simulations of the rotors.

1. Introduction

Nowadays, screw machines are essential devices in many industrial plants and processes. As compressors they provide pressurized process gas or near-vacuum conditions, as expanders they produce energy from high-pressure air or water vapour. Dry screw machines only work with a gaseous fluid, e.g. air, and need tight gaps between rotating parts and the casing to prevent bypass flow; the rotors are typically synchronized by gears. For higher pressure ratios between pressure and suction side, oil or water are used as sealing and lubricating fluids.

From a fluid dynamics point of view, screw machines are quite complex. The geometry of the lobes and the casing is quite complex and due to rotation the shape of the fluid regions is deforming each time step. Compressibility and therefore acoustic aspects play an important role, and oil or water in-



jected machines require consideration of multi-phase effects. Though Computational Fluid Dynamics (CFD) is a broadly accepted tool, both in academia as well as in industry, to analyse fluid mechanics in complex systems in order to understand such systems, it is so far rarely used in industry for the examination and improvement of screw machines.

The numerical computation of screw machines requires accurate grid generation because the fluid flow is transient and depends on the rotor position. Furthermore, the grid needs a high resolution especially in the gaps and their vicinity. CFX Berlin has put its focus on the computation of positive displacement (PD) machines many years ago. Consequently, TwinMesh was developed by CFX Berlin with the aim to generate high quality grids in a short time. As a result, CFD can now be utilized on a day-to-day basis in industrial applications of PD machines.

The essential advantage of a numerical simulation is the visualization of the fluid flow inside the machine. Engineers commonly optimize PD machines based on experience, without knowing the detailed flow effects in particular. CFD results can give additional information and insights in local flow effects. This results in a better process understanding and thus, new ideas for product optimization.

In the following, the second chapter, a brief summary about available approaches to model PD machines will be given. In detail, three different methods will be presented and advantages and disadvantages will be discussed. The approaches realised within TwinMesh are shown in the third chapter. The fourth chapter shows workflow and setup for the simulation of a dry screw compressor. In the fifth chapter, simulation results are shown. Finally, a brief summary and outlook is given in the last chapter.

2. Methods for the Chamber Modelling

The fundamental challenge in PD machine modelling is the reproduction of the fluid domain depending on the rotor position. All physical processes involved depend on quite different length scales, starting at a few micro meters in the sealing gaps up to a couple of hundred millimetres in the working chamber. Thereby, local small scale effects can affect the macroscopic operating performance significantly. In such areas local discretisation in the fluid domain can be achieved utilising the following methods.

2.1. Immersed Solid Method

The immersed solid method is a comfortable method to investigate the rotor influence on the fluid flow inside a PD machine. Therefore, the fluid domain of the PD machine is meshed regardless the rotor geometry, i.e. the whole fluid domain is filled up with grid elements whereas the solid part of the rotor geometry is meshed independently. Commercial CFD codes, such as ANSYS CFX, then calculate the fluid flow inside the PD machine. During the simulation the region of overlap is determined each time step and momentum sources are applied to force the fluid there to follow the motion of the rotor. The advantage of this method is that the initial grids can be used for the whole simulation as remeshing or mesh deformation are avoided.

However, one of the main disadvantages is that this method only works for incompressible, single-phase flows and therefore, compressibility effects have to be neglected. Furthermore, the influence of the rotor surface on the flow is modelled insufficiently. For turbulent flows the results especially in the near wall region are rather loose. Very high numbers of elements are necessary to accurately resolve the near wall region. Since the gap position varies with time the grid also has to be refined circumferentially. CFX Berlin has investigated this method intensively in cooperation with the Technical University Berlin [1].

2.2. Remeshing

The remeshing method utilizes an algorithm that generates a new mesh during run-time depending on the rotor position and local mesh quality. At each time step the grid is deformed due to the new rotor positions, and a routine automatically decides whether this grid needs to be remeshed or not depending on the mesh quality. Thus, the user interaction is rather small. Compared to the immersed solid

method, the rotor surface is accounted for in a way that the near wall region can be treated more accurately by turbulence models. Also, multi-phase flows can be calculated.

However, the main disadvantage is that remeshing in small gaps is almost unavoidable for almost every angle increment. On the one hand, the time step size needs to be small in order to compute the mesh deformation accurately. On the other hand, every remeshing needs interpolated results from the previous time step, which can result in interpolation errors. Furthermore, the remeshing method must use an automatic grid generation program. Such programs usually use unstructured mesh elements that result in high elements numbers within the gaps or in poor mesh quality within the gaps.

2.3. Customised Grid Generation

In order to avoid the aforementioned disadvantages the grids must be customized by the engineer her/himself. Each new rotor position results in a change of the fluid domain and therefore, every position needs to be meshed individually. One popular software tool for this is ANSYS ICEM CFD Hexa which is capable of generating structured grids consisting only of hexahedral elements. Additionally, an O-grid type mesh can be utilized to mesh the rotor geometry, which is essential in accurately resolving flows in the gaps. If the topology, i.e. node number and element links, between the rotor positions remains the same, interpolation between the meshes is not necessary so that interpolation errors such as for the remeshing method are avoided.

The customized grid generation method is of high numerical quality and has been developed and utilized by CFX Berlin in cooperation with industrial partners [2, 3]. However, the time-consuming grid generation rules out that this method can be used efficiently for industrial purposes. Hence, TwinMesh has been developed by CFX Berlin to ensure high quality mesh generation at moderate operation times and user interaction.

3. Basics of TwinMesh

TwinMesh is a meshing software for PD machines with two axially parallel rotors, with complex rotor geometry, i.e. continuous (e.g. lobe pump) or discontinuous (e.g. screw compressor). Via IGES-format and alternatively point wise CSV-format, CAD-data of the rotor and casing can be imported that represents the fluid domain and is used for the structured grid generation. The topology usually contains two rotors, which are meshed using O-type grids and that are connected via an interface contour. Figure 1 shows the TwinMesh GUI in the case of a screw compressor.

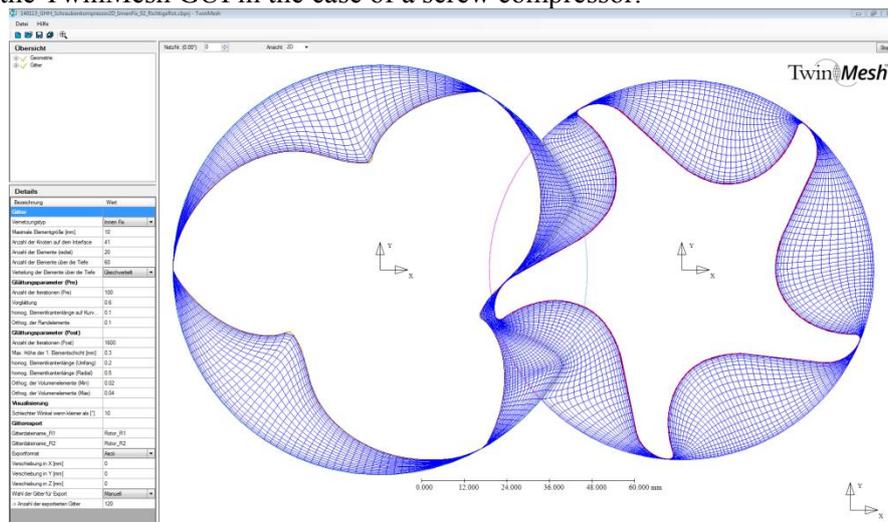


Figure 1: TwinMesh GUI for the mesh generation of a screw compressor.

After the import of the rotor and casing contours, TwinMesh generates 2D meshes for rotation angles of the rotors: For each 2D mesh, TwinMesh creates an interface line between both rotors and

initial O-type grids around each rotor. The initial meshes are smoothed with an explicit and iterative method with several target criteria: Equal node distance and normal mesh lines at boundaries, and small aspect ratios and equal face angles in the rotor region. There are several meshing strategies concerning where the boundary nodes are fixed: On the rotor surface (leading to sliding nodes on the casing and the interface), on the casing (leading to sliding nodes on the rotor surface, but allowing 1:1 interfaces between rotors and to the stator meshes), or a mixed type. The number of elements is directly dependent on the node distribution along the geometry contour and is defined by the user. Figure 2 shows the high quality of the mesh lines in the male and female chambers.

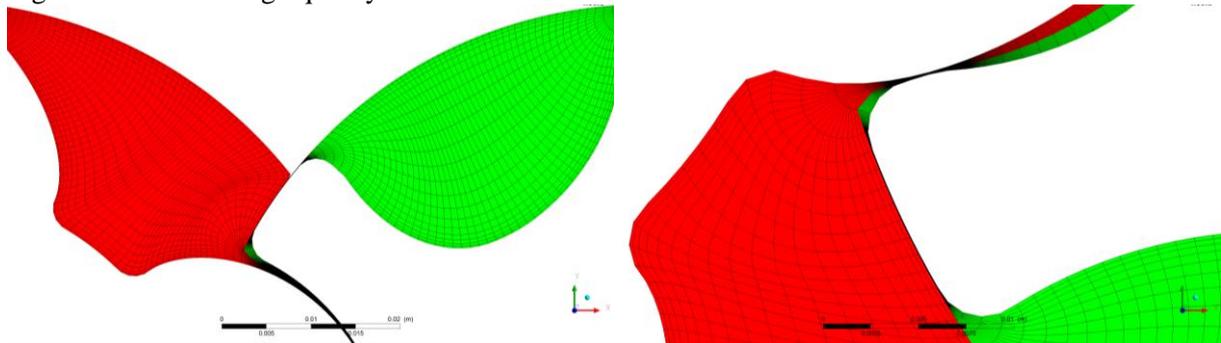


Figure 2: Mesh lines in a 2D cross section showing male (red) and female (green) chambers with 20 mesh lines in radial direction, refined boundary resolution, orthogonal mesh lines at boundaries and homogeneous resolution in gaps.

TwinMesh visualizes the mesh quality (minimum angle, determinant, aspect ratio, volume change) statistically for all meshes and as a coloured plot for a specified rotation angle. Once all 2D grids are generated, series of those grids are used to build appropriate 3D grids. Therefore, it is ensured before the simulation that all grids that will be used in the CFD solver have a high quality. In general, properties of a high quality mesh for PD machine simulations should fulfil certain criteria:

- Mesh should reflect the fluid domain as closely as possible.
- Interior angle $> 18^\circ$ and element size evenly distributed.
- Boundary layers should be adequately resolved with orthonormal elements.
- Small changes in node position between two subsequent angle increments.
- Number of meshes per revolution should be sufficient; preferably about 1° angle increments.

Mesh topology and node number remains the same for all 3D meshes so that the CFD solver needs no interpolation but directly uses the conservation laws for deforming meshes.

4. Workflow and Simulation Setup

ANSYS CFX was chosen as the solver as it provides a wide range of numerical models for the simulation of complex flows. For PD machine simulations the following models are of particular interest:

- Mesh deformation: mesh motion is included in the differential equations so that interpolation is not necessary; a FORTRAN routine is used that reads the TwinMesh data and calculates the mesh motion.
- Multi-phase models: cavitation in pumps, oil or water injection in compressors
- Complex fluid properties: Non-Newtonian or high-viscosity fluids in pumps, ideal or real gas models, dry and wet steam properties for compressors
- Heat transfer models: viscous heating, compressibility effects, heat transfer to/from solids
- Turbulence modelling: Reynolds-Averaged Navier-Stokes models and scale-resolving models

For the application of TwinMesh and ANSYS CFX on lobe pumps and gear pumps, see [4]. Geometry, setup and results for this screw compressor are based on a master thesis of one of the authors [5].

The simulation of a screw compressor starts with the geometric description of the rotating and stationary components of the machine, i.e. of both rotors, the casing and the fluid regions in between. In

this simulation the rotors are of SRM type A with 4 lobes for the male (300° wrap angle) and 6 lobes for the female rotor (200° wrap angle), see Figure 3. The rotors have a length of 168.3 mm, an axis distance of 80 mm and rotation speed of 12 333 rev/min of the male and 8222 rev/min of the female rotor. The gap between the rotors is $100\ \mu\text{m}$, between rotors and casing the gap is $50\ \mu\text{m}$.

Suction and discharge ports were added to the rotors, see Figure 4, with a suction port of 200 mm length and a final diameter of 50 mm and a discharge port of 300 mm length and a final diameter of 55 mm. Three different control edges at the discharge side were designed to get expected pressure ratios of 3, 4, and 4.6, respectively, see Figure 5.

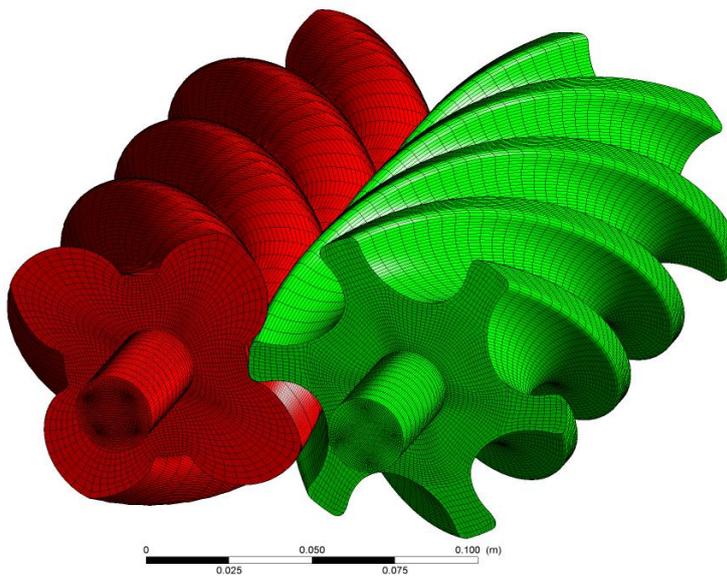


Figure 3: Geometry of male (left) and female (right) rotor with surface mesh.

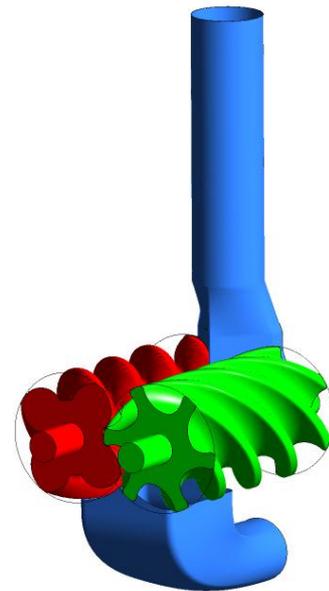


Figure 4: Geometry of suction (bottom) and discharge (top) port.

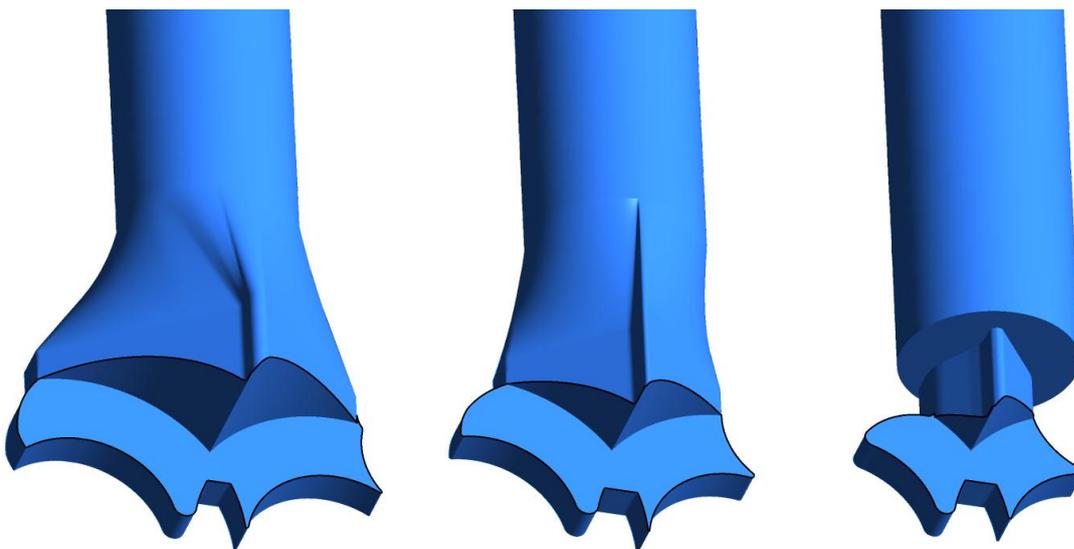


Figure 5: Three different control edges at the discharge side for expected pressure ratio 3 (left), 4 (middle) and 4.6 (right), i.e. for built-in volume ratios of 2.2, 2.7 and 3, respectively.

For the CFD simulation, the fluid region and, if a thermal simulation of the solids is desired, the solid regions have to be meshed. The resolution and the quality of the meshes have a great impact on both simulation time and result quality. With better and finer meshes, the results quality is improved, whereas coarse meshes may lead to a fast, but less meaningful simulation. For the fluid regions around the rotors, TwinMesh generates hexahedral meshes with fine resolution of gaps and smooth changes between small gaps (several microns) and larger chambers (several centimetres). In a grid sensitivity study [5], we found that a radial resolution of 20 elements, circumferential resolution of 300 to 400 elements, a spanwise resolution of 130 elements and a temporal resolution of 1° rotation angle ensure good results. With fewer elements in circumferential direction, the curvatures in the rotors cannot be resolved adequately; fewer elements in radial direction cause higher volume changes at interfaces leading to local errors.

The meshes for the stationary fluid regions, i.e. the supply pipes at suction and discharge sides, and the solid regions, are generated with common meshing tools as ANSYS ICEM CFD or ANSYS Meshing; here, structured hexahedral meshes are possible or unstructured hybrid meshes consisting of prisms for the adequate resolution of boundary layers and tetrahedrons for the inner parts. Hexahedrons have the advantages of a higher quality and less numerical effort. In contrast, the tetrahedrons and prisms are of more flexibility and less manual meshing effort.

In the setup shown in Figure 6, the meshes are combined and defined as fluid or solid regions:

- Meshes for rotating fluid regions around both rotors with axial and radial gaps from Twin-Mesh, rotated by reading mesh files via FORTRAN routine at run-time
- Mesh for stationary fluid region (pressure and suction side) from ANSYS Meshing
- Meshes for solid rotor regions from ANSYS Meshing, rotated by prescribed mesh deformation as rigid bodies

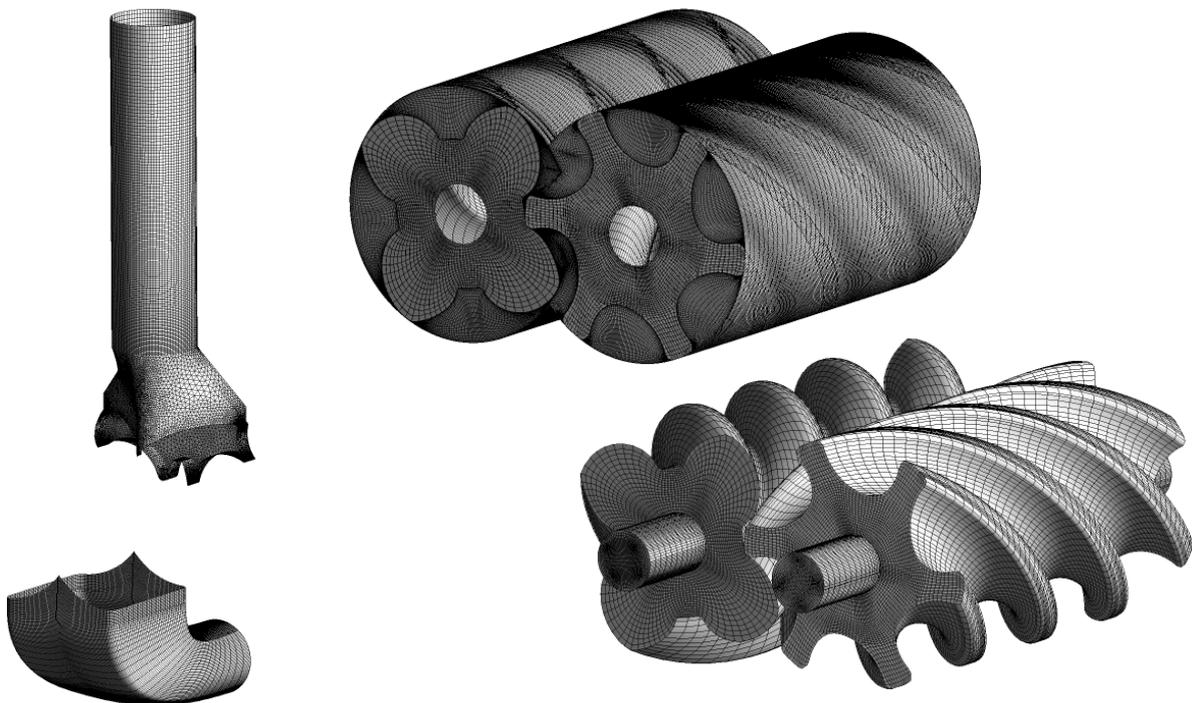


Figure 6: Stationary fluid domain (left) consisting of hexahedrons, tetrahedrons and prisms (approx. 1 mio nodes, 1.9 mio elements); both rotating fluid domains (top) consisting of hexahedrons (each approx. 550 000 nodes and elements); rotating solid domains (bottom) consisting of hexahedrons (each approx. 300 000 nodes and elements).

The different meshes are connected with interfaces so that flux of mass, momentum, turbulence and heat (for fluid-fluid interfaces) or heat (for fluid-solid interfaces) is conserved. Materials are assigned as air ideal gas for the fluid regions and steel as solid material. The user has to select appropriate physical and numerical models, e.g. whether viscous dissipation shall be taken into account or which turbulence model shall be used. Turbulence models are necessary to capture turbulent effects like increased friction and mixing without fully resolving turbulent structures spatially and temporally (direct numerical simulation). In these simulations, the shear-stress transport (SST) model is used, which is a Reynolds-Averaged Navier-Stokes (RANS) model so that turbulence is fully modelled. Hybrid models as Scale-Adaptive Simulation or Detached Eddy Simulation can resolve large turbulent structures while still modelling the smaller and near-wall scales. Furthermore, boundary conditions for all relevant numerical quantities are needed. For screw compressors, typically pressure and temperature at the inflow side (here 1 bar and 300 K) and pressure at the outflow side (here 3 bar) are prescribed; for the turbulent quantities, common conditions at the inlet are low or medium intensity.

In the simulation, time development is also discretized. With TwinMesh, rotor meshes for each time step have been generated and stored in this case for each 1° rotation angle of the male rotor. The time step size depends on this angle increment and the rotation speed and is $13.5 \mu\text{s}$ in this case. For each time step, the solver reads the corresponding rotor meshes and updates the connections between the parts and all quantities taking the mesh deformation and motion into account. Meshes were generated for a 90° rotation of the male rotor; then, simulation stops and a new simulation is initialized with the results of the previous one and run for the next 90 time steps, i.e. another 90° rotation. A typical initialization of the first simulation is zero velocity everywhere, and pressure and temperature at 1 bar and 300 K at the suction side and at 3 bar and 410 K (adiabatic compression) with linear interpolation at the rotors at the discharge side. Typically, several revolutions of the rotors are necessary to reach a periodic state.

The inlet and outlet boundaries are often positioned arbitrarily near the compressor to minimize computational effort. Prescribing the pressure at these artificial boundaries leads to numerical reflections of the pressure waves generated by the compressor, especially at the pressure side. The reflected waves and the outgoing waves superpose and form standing waves. So-called non-reflecting boundary conditions allow the waves to leave the computational domain. In ANSYS CFX, Navier-Stokes characteristic boundary conditions (NSCBC) can be used via Local One-Dimensional Inviscid (LODI) relations.

The result of the simulation includes temporally and spatially resolved fields of pressure, temperature, velocities, and turbulent quantities and derived quantities like density, shear strain rate, and eddy viscosity. Furthermore, integral quantities like moment on the rotors or force or heat flux on the walls are calculated within each time step. In order to consider heating of the solid rotors, they can be included in the simulation so that the heat flux from the compressed gas directly heats the solid material and vice versa. However, compared to the rotation of the rotors, a very slow process with several minutes in duration is needed to reach stationary temperature. Thus, several hundred thousand revolutions must be simulated. Alternatively, the simulation of the solid heating is decoupled from the fluid simulation by time-averaging the heat flows and imposing them on the solids for longer time scales of the order of minutes while using the solid temperatures in the fluid simulation as boundary conditions.

5. Simulation results

The aim of the screw compressor is to compress air from 1 bar to 3 bar; this can be illustrated by looking at the pressure in one chamber while the machine rotates, see Figure 7. In the beginning, the chamber is connected to the suction side at 1 bar and fills with air; after closing connection to the suction side, compression starts due to decreasing chamber volume until the control edge to the pressure side is reached so that the chamber is connected to the outlet. Depending on the geometry of the control edge (see Figure 5), it opens before the outlet pressure of 3 bar is reached (under-compression for the case with estimated pressure ratio 3 at approx. 2.7 bar) or at chamber pressures higher than the outlet pressure (over-compression for the cases with expected pressure ratio 4 and 4.6 at approx. 3.6

and 4.5 bar, respectively). In case of under-compression, gas initially flows from the outlet side into the chamber; in case of over-compression, gas immediately flows out of the chamber towards the outlet. Figure 8 shows pressure contours at a rotor angle of 26° (refers to $26^\circ + 2 \cdot 90^\circ = 206^\circ$ in Figure 7) for control edge designed for pressure ratio 4; for results with other pressure ratio, see [5]. The pressure peak has already left the compression chamber and moves (with speed of sound) towards the outlet. The strong pressure drop over the axial gap at the pressure side can be clearly seen here. Figure 9 shows pressure and temperature for this rotation angle in a cross section.

Figure 10 shows mass flow at inlet and outlet and torques on both rotors over the rotation angle. Mass flow at the inlet is almost constant at 0.133 kg/s, mass flow at the outlet fluctuates between 0.08 and 0.23 kg/s due to the periodic opening of the compression chamber at the control edge at 13° of the male rotor. Due to finite speed of sound, pressure and mass flow maximum reach the outlet later at approx. 70° of the male rotor. While the torque on the male rotor is quite high with an average of 18.2 Nm, torque on the female rotor is only 3.2 Nm in average. This leads to a power consumption of 23.3 kW on the male rotor and 2.8 kW on the female rotor; together 26.1 kW for the whole screw compressor.

Figure 11 shows leakage mass flows for the four male rotor gaps (sum of axial and radial part) and six female rotor gaps; gap mass flows up to 3% of total mass flow can be seen on male rotor and up to 2% on female rotor.

Figure 12 shows the temperature distribution on the rotor surface and thermal expansions of the rotor. The shaft ends are set to 70°C as a fixed boundary condition; the male rotor is heated up to 180°C and the female up to 160°C leading to a thermal expansion of over $300\ \mu\text{m}$ axially and $90\ \mu\text{m}$ (male) resp. $80\ \mu\text{m}$ (female) in radial direction. However, this expansion of the rotors (and the casing) is not taken into account in this CFD simulation. The high temperatures in the rotors are due to high heat input of approx. 560 W at high pressure side while approx. 380 W leave the solids at low pressure side and heat the gas, and 180 W are leaving the solid through the shafts; with shorter shafts, this cooling effect would be larger.



Figure 7: Chamber pressure over rotation angle of male rotor for all three control edges (see Figure 4); estimated pressure ratio 3 (blue line), 4 (orange line) and 4.6 (green line); vertical lines are for start of compression (red line, identical for all cases) and end of compression.

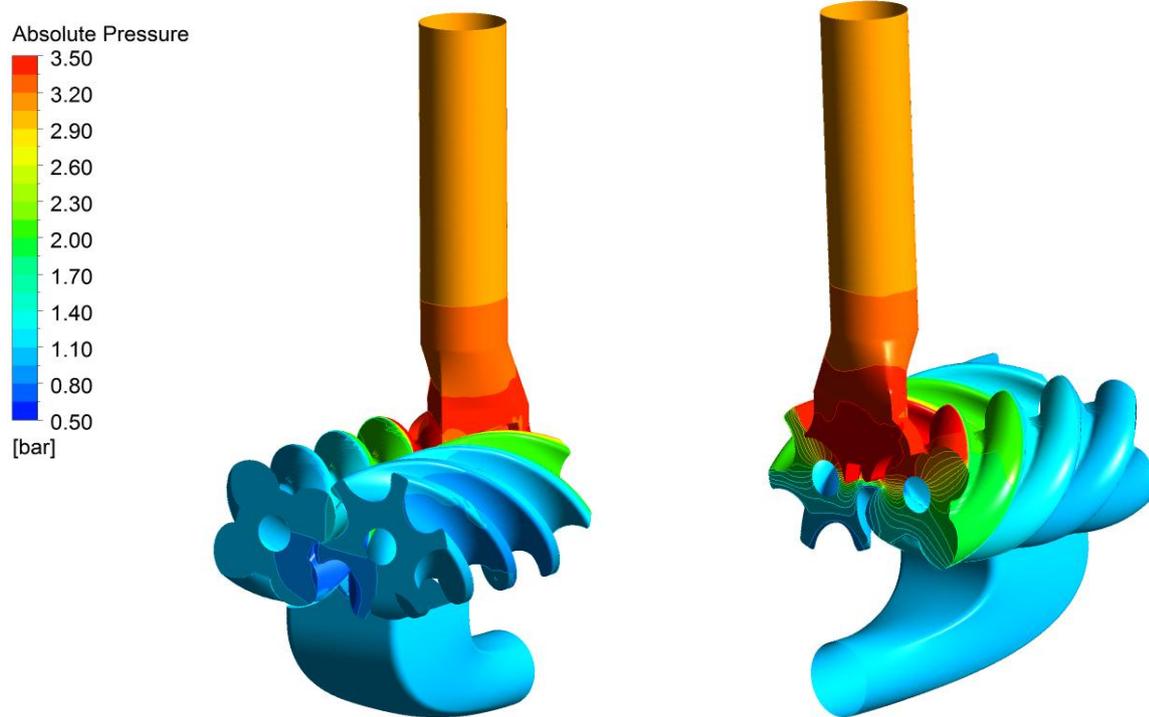


Figure 8: Pressure on casing wall and rotor surface at rotation angle 26°; control edge is reached at rotation angle 13°, control edge is for estimated pressure ratio 4.

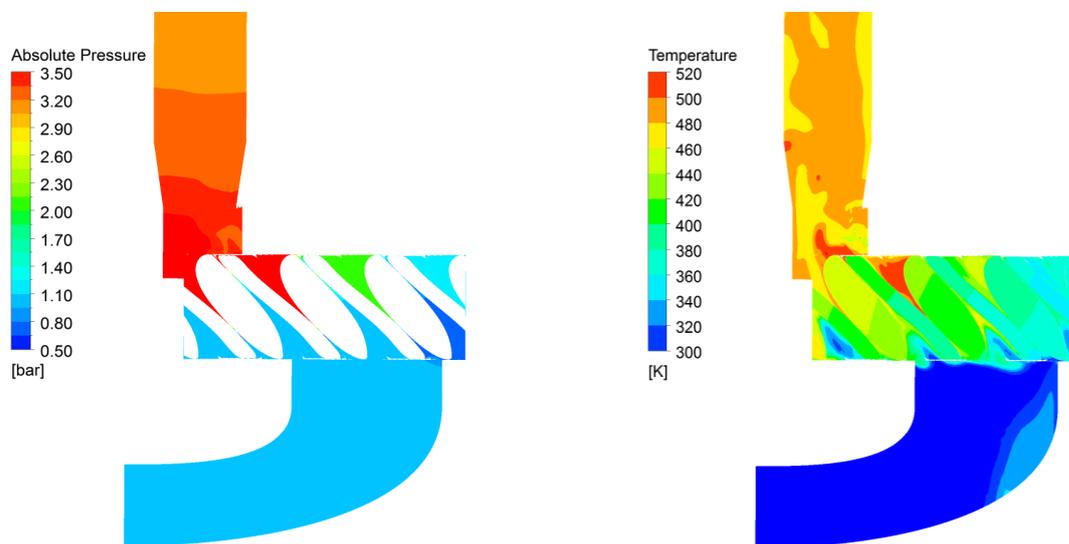


Figure 9: Pressure (left) and temperature (right) on mid cross section at rotation angle 26°.

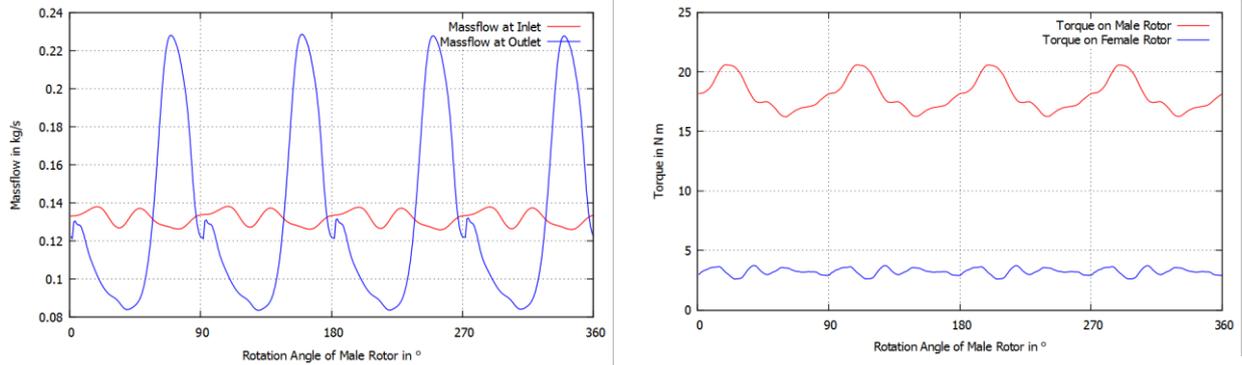


Figure 10: Mass flow (left) at inlet and outlet and torques (right) on male and female rotor over rotation angle of male rotor.

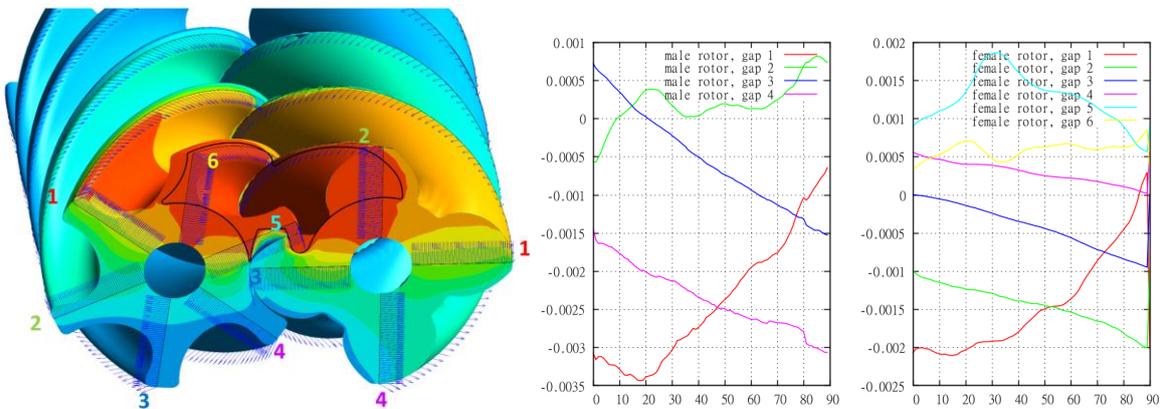
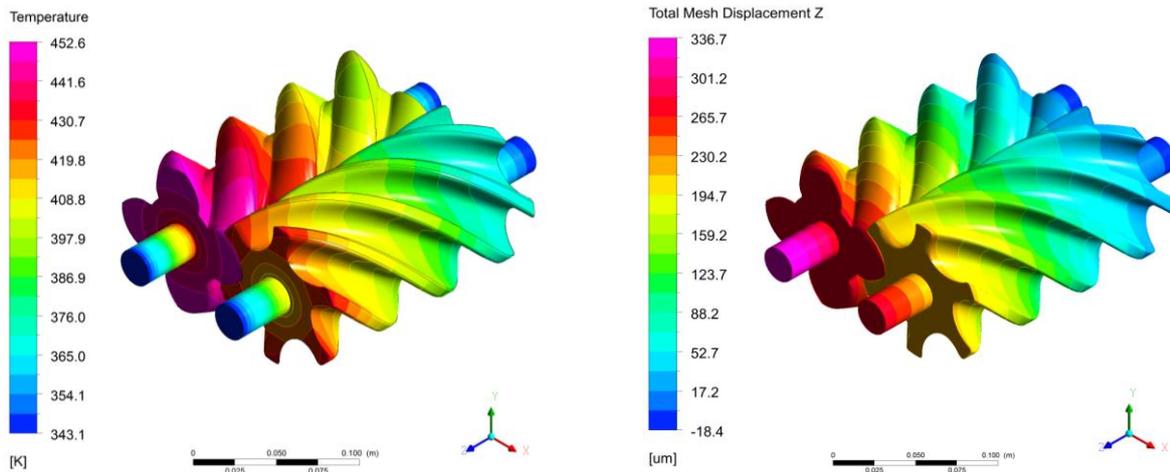


Figure 11: Position of axial and radial gap user surfaces at rotation angle 0° (left) with vectors showing rotation direction and pressure port as black line; mass flow through the gaps over rotation angle (right), positive means mass flow in rotation direction



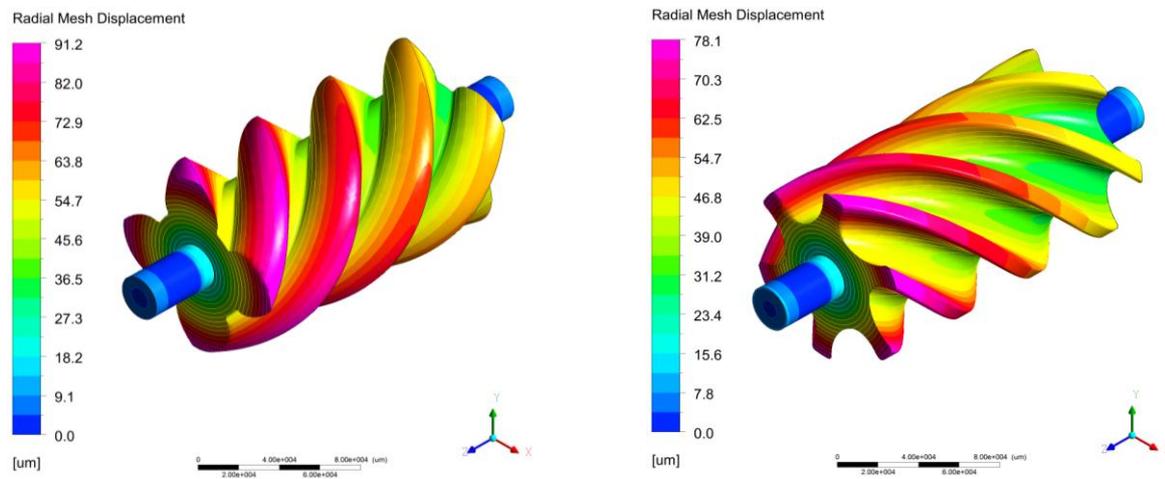


Figure 12: Results for the thermal expansion of the solid rotors; temperature on solid surface (top left) with shaft ends fixed to 70°C, axial expansion (top right) with right shaft end fixed, radial expansion of male (bottom left) and female (bottom right) rotor.

6. Summary and outlook

This paper shows simulation results for a dry screw compressor compressing air from 1 bar and 300 K to 3 bar and approx. 470 K. The simulations include axial and radial gaps and take the heating of the rotors into account. Meshes for the fluid regions around the rotors were generated with the special meshing program TwinMesh whereas those for stationary parts and the solid rotors were generated with ANSYS Meshing. TwinMesh creates hexahedral meshes for rotating PD machines with a high quality for each time step; these meshes are read by the CFD program during run-time. The transient simulations were performed with ANSYS CFX version 15.0.7 taking into account fluid flow, heat transfer including viscous dissipation and solids, and turbulence effects with the SST model.

We showed chamber pressure for three different control edges on the discharge side, one leading to under-compression, the other two leading to over-compression instead. For the case of moderate over-compression, pressure and temperature plots were shown for an arbitrary rotation angle. Here, the mass flow at the outlet showed a strong oscillation due to the periodic opening of the chambers. The main torque (on the male rotor) is approx. 18 Nm and the overall needed mechanical power is about 26 kW. Finally, thermal expansion results for both rotors in axial and radial direction were shown.

The usage of the thermal expansion results as a deformation of the rotors as well as the casing will be used in ongoing projects. Furthermore, additional work is needed to simulate oil or water injected screw compressors since multi-phase flows require very high mesh qualities for stable simulations.

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