Bi-Directional System Coupling for Conjugate Heat Transfer and Variable Leakage Gap CFD Analysis of Twin-Screw Compressors

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Abstract. Oil-free twin-screw compressors are essential in various industrial applications where clean compressed gas is required. Due to the absence of the cooling oil in these machines, thermal deformations are large. Hence, design clearances are generally set at a relatively large value of more than 150 μm. Leakage through these clearances are the primary source of flow loss. It is essential to predict the change of the gap size in operation accurately so that the design clearances can be minimised, allowing reliable operation and maximising compressor efficiency. To achieve this, CFD and Structural solvers were combined. The CFD model uses a single domain deforming grid of the twin-screw rotors generated in SCORG grid generator, together with ANSYS CFX flow solver. The thermal model of the rotors and housings uses ANSYS Structural solver. Two modelling systems were coupled bi-directionally to obtain variation in the radial leakage gap size for calculation of performance in the CFD model. The predicted compressor performance thus obtained was compared with measurements of flow, internal pressure-rise, power, specific power, volumetric and adiabatic efficiency. For the test case, three variations of radial gap size were evaluated, two of them with the uniform gap size of 10 μm and 160 μm and the third one with a variable gap size as predicted by the bi-directionally coupled model. The coupled model predicted this gap size to vary from 24 to 117 μm, thus predicting an improved flow and volumetric efficiency by 8.2%, lower indicated power by 2.5% and a higher adiabatic efficiency by 5.5%, in comparison to the design gap size of 160 μm. These predicted gap sizes could be used to improve the design clearances of the compressor by reducing them from 160 to 120 μm which would result in a better performance during operation.

1. Introduction
Oil-free twin-screw air compressors are essential in various industrial applications where clean compressed gas is required. As a result of the absence of oil within the working chamber, during compression, the internal temperature of the gas may rise up to 130°C. This causes large thermal deformation of the rotors and casing. Accordingly, the design clearances are generally set at a value of about 150 μm, which is much larger than in oil flooded machines. Leakage through clearances being the primary source of loss, it is essential to predict the resulting gap size variation accurately to enable safe design clearances to be set at a minimum reliable value and thereby improve the compressor efficiency. Kovačević et al. [1, 2] presented various techniques for CFD modelling of twin-screw machines and in the chapter on fluid-solid interaction, the analysis of rotor deformation is discussed for several cases such as a 127 mm oil injected air compressor operating from 1.0 to 7.0 bar, dry air operation from 1.0 to 3.0 bar, and a high-pressure CO₂ refrigeration compressor with suction conditions of 30.0 bar at 0°C and a discharge pressure of 90.0 bar at 40 °C. Deformation levels in the range of 70 to 100 μm were reported in these studies. The Comet solver for computational continuum mechanics was employed for
both fluid and structural calculations. In their three-part literature from 2006, Sauls et al. [3, 4 5] proposed a procedure whereby an initial thermodynamic chamber model computational result is used to define boundary conditions for intermediate thermal analysis of refrigeration compressor components, followed by calculation of deformation and clearance variation along the rotor-to-rotor mesh line and in the rotor-to-housing gaps. A similar approach that couples the chamber model KaSim to the ANSYS solver was described by Nikolov et al. [6] to estimate the influence of rotor and casing thermal deformation on the performance of a screw expander in an ORC system, based on the iterative coupling of a thermodynamic chamber model and 3D FEM thermal analysis. More recently, Ding et al. [7] used an approach similar to [1, 2] to solve Conjugate Heat Transfer (CHT) and deformation of solid parts of a dry air compressor. The Simerics-MP+ solver was used in conjunction with the SCORG grid generator. Buckney [8] applied a procedure to calculate CHT and clearance variation in SCORG chamber models which was extended to 3D FEM analysis by Husak et al. [9].

### Table 1. Specification of the dry air twin-screw compressor

| Rotor profile | N Type | Rotor Data |
|---------------|--------|------------|
| Axis distance | 93.00 mm | Main Rotor Gate Rotor |
| Rotor length  | 203.913 mm | Lobes 3 5 |
| Built-in volume index | 1.8 | Outer diameter 127.324 mm 120.262 mm |
| Interlobe gap | 160 microns | Wrap angle 285.00° 171.00° |
| Axial gap     | 160 microns | Radial gap 160 microns 160 microns |

A bi-directional system coupling approach that utilizes CFD and Structural solvers in co-simulation is presented here. The CFD model uses a single domain deforming grid of the twin-screw rotors generated in SCORG and ANSYS CFX flow solver. The thermal model of the rotors and housing uses the ANSYS Structural solver. System coupling by means of CHT analysis is used to map the fluid-solid boundaries where the local heat transfer coefficient, wall adjacent fluid temperature and heat flux are exchanged in a co-simulation loop. Additionally, a considerable saving in computational time has been achieved by attributing a large time-scale factor to solid heat conduction. The compressor specification is listed in Table 1 and a photograph of the N-profile [10] rotor pair is shown in Figure 1, taken from the suction side axial end. Estimates of the housing temperature distribution, exit air temperature, compressor performance and internal pressure distribution were compared with measured values for validation of the model. The bi-directional system coupling approach used, improved the reliability of the performance results obtained from the computational models.

### 2. Methodology of the bi-directional system coupling

As shown in Figure 2, the bi-directional system is comprised of five analytical models, which are coupled and managed via the ANSYS Workbench platform. Each model is identified by an alphabetical letter and its elements are numbered as cells. For example, C5 describes the setup cell of the structural analysis model. The compressor design data, the rotor CAD model and the grids required for the CFD model are generated externally by SCORG. The system coupling procedure is an iterative process that starts with an initial CFD solution to get an estimate of the temperature field. In the current work, the initial CFD solution was obtained with an assumed radial leakage gap of 10 μm. This is derived from a combined flow and CHT analysis with uniform leakage gap sizes. However, the component E estimates the leakage gap size, based on the deformation data received from component C during the simulation process. ANSYS CFX solver with a Finite Volume Method (FVM) is used for both models. Once the initial flow field and temperature distribution are known, the housing and rotor surface temperature data are transferred as boundary conditions to the component B which defines the thermal analysis model. The thermal analysis model uses a Finite Element Method (FEM) to solve temperature distribution in the metal components and the results are transferred as body loads to the transient structural analysis model in the component C. Components C and E are connected via the system coupling component D. In the current work, the housing deformation has been accounted for only in components C and E. For
simplification, the rotor deformation is not considered. Accordingly, in order to account for rotor deformation, the leakage gap size is set at a lower value of 30 μm in the model and is updated by the housing deformation data as the simulation progresses.

Figure 2. Components of the bi-directional system coupling analysis.

3. Numerical modelling of the system components
   CFD modelling of a twin-screw compressor is challenging due to the complex deformation of the working chamber. To achieve a reliable numerical model, the in-house grid generator SCORG is used as shown in Figure 2. Details of the methodology used for CFD analysis in this paper can be found in examples of the use of the SCORG grid generator in references [11 - 18].

3.1. Screw compressor CFD model with CHT
   The CFD model of the twin-screw compressor is detailed in Figure 3. The whole compressor block is split into several domains as shown in Figure 3a.

Figure 3. CFD model of the twin-screw compressor with CHT, a) domains and boundaries, b) 3D rotor grid and discharge port, c) 2D rotor grid at one position.
Namely, these are the suction port, the rotor fluid domain, the discharge port, the main rotor solid domain, the gate rotor solid domain and the housing solid domain. High-pressure axial end leakage has not been included in the present study. In Figure 3b, the housing and the radial and axial discharge port areas are highlighted. In Figure 3c a cross-section of the rotor grid generated by SCORG is shown at one rotor position. The rotor domain is a fully hexahedral cell structure with both rotors contained in a single grid [12, 13]. All other domains are generated using a tetrahedral cell structure. The domains are connected in the CFD solver through non-conformal interfaces. The compressed gas is air as an ideal gas, with a molar mass of 28.96 kg/kmol, a specific heat capacity at constant pressure of 1.0044e03 J/kg K, a dynamic viscosity of 1.831e-05 kg/m s and a thermal conductivity of 2.61e-02 W/m K. Both the rotor and housing components, are assumed to be made of structural steel with a density of 7850 kg/m³, a coefficient of thermal expansion of 1.2e-05 units/°C, a tensile yield strength 250 MPa, Young’s modulus 200 GPa, Poisson’s ratio 0.3 and thermal conductivity 60.5 W/m K.

| Table 2. Specification of the numerical setup in the ANSYS CFX solver. |
|---------------------------------|---------------------------------|-----------------|-----------------|
| Mesh deformation                | User defined nodal displacement | Advection scheme | High Resolution |
| Mesh in ports                   | Tetrahedral (ANSYS Mesh)        | Inner loop coefficients | Up to 10 iterations per time step |
| Outlet boundary condition       | Opening (Static pressure 2.0 bar, backflow acts as total pressure and temperature) | Transient scheme | Second order Backward Euler Δt = 5.55556e-05 sec CHT solid time scale τ = 10^6 |
| Inlet boundary condition        | Opening (Total pressure 1.0 bar and temperature 25°C) | Convergence criteria | r.m.s residual level 1e-05 |
| Turbulence model                | SST – k Omega (Standard Wall Functions) | Relaxation parameters | Solver relaxation fluids 0.1 Solver relaxation scalar 0.2 |

In Table 2, the main numerical setup parameters of the CFD solver have been specified. It is noted that in the transient scheme and solver time-step definition, a large scaling factor of 10^8 has been applied to accelerate the conjugate heat transfer analysis. By this setting, the flow solver progresses in time with a time-step size of 5.55556e-05 sec while the heat transfer in the solid parts of the model progresses with an average diffusion timescale close to 600 sec.

| Table 3. CFD model grid size and quality metrics. |
|---------------------------------|-----------------|-----------------|-----------------|-----------------|
| Mesh deformation                | User defined nodal displacement | Advection scheme | High Resolution |
| Mesh in ports                   | Tetrahedral (ANSYS Mesh)        | Inner loop coefficients | Up to 10 iterations per time step |
| Outlet boundary condition       | Opening (Static pressure 2.0 bar, backflow acts as total pressure and temperature) | Transient scheme | Second order Backward Euler Δt = 5.55556e-05 sec CHT solid time scale τ = 10^6 |
| Inlet boundary condition        | Opening (Total pressure 1.0 bar and temperature 25°C) | Convergence criteria | r.m.s residual level 1e-05 |
| Turbulence model                | SST – k Omega (Standard Wall Functions) | Relaxation parameters | Solver relaxation fluids 0.1 Solver relaxation scalar 0.2 |

Grid size and quality factors in various domains have been reported in Table 3. The average quality of cells in the rotor domain is critical for the stability of the solver. The rotor domain grid with a very high expansion factor and high aspect ratio of cells could be processed using a double precision calculation.

3.2. Housing thermal model
From the CHT calculations of the initial CFD model, with a radial gap size of 10 μm, the data of the time averaged housing bore surface temperature is transferred to system B to serve as a thermal load for the deformation calculation. The housing thermal model calculates heat conduction in the metal and provides volumetric temperature data for the housing deformation model of system C. The bore temperatures imported from the CFD solution and the housing thermal model setup are shown in Figure 4a, while the calculated housing temperature and transferred to system C is illustrated in Figure 4b.
Figure 4. Thermal and structural model of the compressor housing, a) Bore temperature from CFD, b) housing temperature, c) supports and system coupling boundaries.

3.3. Coupled CFD and housing deformation model
System C presented in Figure 4c is a transient structural model of the housing which is coupled with the CFD system E through the system coupling D. In the structural model both local surface forces acting on the bore are received from the CFD system and the volumetric temperature is received from system B. Thus, the deformation of the housing is calculated under both the net force and the thermal load. The force load is dependent on the position of the rotors and gets updated every coupling iteration. The instantaneous deformation of the housing bore is transferred to the CFD system E as an incremental boundary displacement, and this changes the radial leakage gap size with time and space. Other supports defined in the structural model are also represented in Figure 4c.

Figure 5. Data exchange routine of the bi-directional system coupling.

3.4. Routine for Data exchange
Figure 5 illustrates the setup used for bi-directional data transfer during calculations. Two data transfer units are defined, one for the force due to compression pressure rise from CFD model to the structural model and another for deformation due to thermal and force load from the structural to the CFD model. The flow solver leads the loop, and the time step size is defined in order to set the main rotor speed at 6000 rpm for the set rotor grid advancement per step. In order to reduce computational cost only one coupling iteration is defined per time step with r.m.s convergence level of 0.01.

4. Results and discussion
The above methodology has been applied to solve flow, CHT and housing deformation in a dry air compressor at 6000 rpm speed operating at 1.0 bar suction pressure, 24°C suction temperature and 2.0
bar discharge pressure. Measurement results at this operating condition were recorded at the City, University of London test facility and are available as compressor performance data and compression chamber pressure cycle data [12, 13]. These data have been used for comparison with three numerical cases; Case 1 is with the uniform radial leakage gap size of 10 μm, used as an initial CHT solution, Case 2 is with the design specified uniform radial leakage gap size of 160 μm and Case 3 is with the variable radial leakage gap obtained using the bi-directional system coupling with the housing deformation and an initial gap size of 30μm.

4.1. Conjugate heat transfer analysis
When the solid components of the screw compressor unit are included in the CFD model, heat flux conservation is achieved between the fluid and solid parts and the assumption of adiabatic walls at the housing and the rotor surfaces could be eliminated. This helps to achieve more accurate heat transfer results that consequently impact the compression process. The temperature distribution on rotors, in the compression chamber and in the discharge port is presented in Figure 6. The results are compared between the three cases. With a 10 μm radial leakage gap, the peak temperature reaches to 133.7°C. With a 160 μm radial leakage gap, the leakage is substantially increased and hence the peak air temperature reaches 156.9°C. While, with the variable radial leakage gap the peak air temperature is around 151.4°C.

![Figure 6](image1.png)

**Figure 6.** Instantaneous air temperature distribution, a) radial gap 10 μm, b) radial gap 160 μm, c) variable radial gap.

On the rotor and housing components, a larger time scale factor was applied to achieve close to steady operating temperature results. A time averaged temperature distribution is presented in the rotor and housing section in Figure 7 after 20 compression cycles. The differences in air temperature observed in Figure 6 influence the CHT results of the metal temperature here. With a 10 μm radial leakage gap, peak time averaged temperature in the solid reaches 98°C. With a 160 μm radial leakage gap, the time averaged temperature in the solid increase to 129°C. While, with the variable radial leakage gap the time averaged temperature in the solid is around 120°C.

![Figure 7](image2.png)

**Figure 7.** Time averaged rotor and housing temperature distribution, a) radial gap 10 μm, b) radial gap 160 μm, c) variable radial gap.

4.2. Variation of radial leakage gaps
Due to the thermal non-uniformity on the housing and the rotors, and high metal temperature, the housing deforms. This deformation causes the clearance between the rotor outer diameters and the housing bore diameter to vary significantly from their design values. Results of the calculated variation
in the radial leakage gap size after 20 compression cycles are presented in Figure 8. It can be observed that the gap size distribution is highly non-uniform, and ranges from 24 to 117 μm over both the main and gate rotor bores. It should be noted that the rotor deformation has not been accounted in the current study and hence an initial gap size of 30 μm was specified in the radial leakage clearance. The obtained non-uniform gap size distribution is an impression of the housing deformation on this initial uniform 30 μm clearance.

**Figure 8.** Non-uniform variation of the radial leakage gap size, as captured in the CFD model.

A detailed evaluation of the radial gap size variation in presented in Figure 9. Figure 9a is for a set of axial locations on the main rotor bore, while Figure 9b is for the same axial locations on the gate rotor bore. These axial locations have been defined in Figure 8. It can be observed that at 25 mm from the discharge end, the housing deflection is the highest and here the leakage gap varies from 55 to 115 μm, from the low-pressure CUSP (intersection of the bore diameter) to the high-pressure CUSP, respectively on both housing bores. CUSP locations have been indicated in Figure 8. The gap variation at the suction end is small due to the relatively low temperature and a fixed support boundary applied on the intake flange. At 1 mm from the discharge end, the gap variation is lower than at 25 mm due to higher housing stiffness provided by the end wall. At axial locations, between 25 and 150 mm, the gap variation shows a gradual change with lower gaps at the low-pressure CUSP as compared to the high-pressure CUSP for

**Figure 9.** Variation of the radial leakage gap size along the housing bore axis, a) main rotor bore, b) gate rotor bore.
both housing bores. This nature of leakage gap size distribution results in lower volumetric efficiency and higher specific power of the compressor. The data could be used to redesign the housing with cooling jackets and stiffness elements.

4.3. Pressure distribution

The pressure-angle diagram of the compression cycle is compared between the three cases in Figure 10a, and the instantaneous distribution of pressure on the rotors is presented in Figure 10b. The pressure-angle diagram is compared with measurements at the same operating condition.

![Pressure Angle Diagram](image1)

**Figure 10.** Compression cycle pressure distribution, a) pressure-angle diagram, b) instantaneous pressure in the rotors and suction port.

With a radial gap size of 10 μm, the initial pressure rise is more gradual and lower than the measured value. After about 150° main rotor angle, the pressure rises more steeply, and the peak pressure exceeds that of the measured value, to reach about 2.71 bar. This is followed by pressure pulsations of a higher magnitude in the remaining cycle. In the case of a radial gap size of 160 μm, the initial pressure rise exceeds that of the measured value, up to a rotor angle of 175°, but the peak pressure, at about 2.2 bar, is lower than the measured value. The variable leakage gap size also estimates a similar initial pressure rise, higher than the measured value and the peak pressure is about 2.3 bar.

4.4. Housing deformation and stress distribution

The distribution of deformation magnitude on the housing is presented in Figure 11a. It can be observed that the highest deflection is about 115 μm which correlates in magnitude as well as location to the radial leakage gap variation presented in Figure 8 and Figure 9. These results confirm validity of the bi-directional coupling setup and accuracy of the coupling solver.

![Deformation and Stress](image2)

**Figure 11.** Housing structural analysis results, a) deformation, b) Von Mises equivalent stress.

The distribution of the Von Mises equivalent stress in the housing material is presented in Figure 11b. For the specified thermal and force load and the locations of the supports such as fixed axis distance, axial end face planar displacement and fixed mounting on the suction flange, produce locally high stress in the discharge end of the housing. The maximum stress magnitude is about 150 MPa which is within the material tensile strength of 350 MPa.
4.5. Compressor performance

A comparison of the compressor performance parameters is presented in Table 4. The measured performance data at 6000 rpm was available at 2.0 bar discharge pressure [12, 13]. With a fixed radial gap clearance of 10 μm the flow was 17% higher than that measured. With a larger radial gap of 160 μm, the flow was reduced considerably and was 18% lower than the measured value. With a variable radial gap that ranged from 30 to 120 μm, the flow was reduced and about 11% lower than that measured.

| No | Case                  | Flow m³/min | Torque kW | Indicated Power kW | Specific Power kW/m³/min | Discharge Temperature °C | Volumetric Efficiency % | Adiabatic Efficiency % |
|----|-----------------------|-------------|-----------|--------------------|--------------------------|--------------------------|-------------------------|-------------------------|
| 1  | Measured              | 7.036       | 25.397    | 15.15              | 2.153                    | 129.4                    | 68.98                   | 67.59                   |
| 2  | Radial Gap 10 μm      | 8.244       | 24.355    | 15.30              | 1.856                    | 114.1                    | 80.83                   | 78.39                   |
| 3  | Radial Gap 160 μm     | 5.751       | 23.849    | 14.98              | 2.606                    | 135.1                    | 56.38                   | 55.84                   |
| 4  | Variable Radial Gap   | 6.223       | 24.454    | 15.36              | 2.469                    | 132.5                    | 61.01                   | 58.94                   |

The torque obtained from the CFD model relates to the indicated power only. However, the measured torque includes the mechanical losses. Hence a mechanical efficiency of 95% has been assumed here in order to compare the calculated results with the measured values. At 10 μm gap, (Figure 10a), the internal pressure rise is higher, hence the torque and indicated power is 1% higher than that measured. With 160 μm clearance, the indicated power is 1% lower than the measured and with a variable gap, the indicated power is 1.4% lower than that measured. These results can be correlated with the nature of the pressure distribution represented in Figure 10a. The discharge air temperature is 12% lower with 10 μm gap, 4.4% higher with 160 μm gap and 2.4% higher with the variable gap model. Based on the flow results, the volumetric efficiency is 11.85 units higher with 10 μm, 12.6 units lower with 160 μm and 8 units lower with the variable gap model in comparison to the measured values. Based on the indicated power, the adiabatic efficiency is 10.8 units higher with a 10 μm gap, 12 units lower with a 160 μm gap and 8.6 units lower with the variable gap model. Between the three models, the difference in specific power is of the same order as that of the flow, as the indicated power is very close in all three of them.

5. Conclusions

High temperature of the gas during compression, and the thermal deformation resulting from it, limits the maximum pressure that can be achieved in a dry air twin-screw compressor. Due to these factors, the leakage gap sizes tend to be over specified in the design, leading to lower volumetric efficiency and higher specific power. In order to improve the accuracy of computational models used, a bi-directional system coupling approach that solves CFD and structural models in co-simulation has been presented here. The following conclusions can be drawn from the study:

- Adding compressor metal components in the CFD model eliminates the requirement to specify a boundary condition at the fluid-solid interfaces for the conjugate heat transfer analysis.
- Bi-directional system coupling can be used to predict a variable radial leakage gap size, thereby improving the accuracy of performance prediction. For the test case the gap size was found to vary from 24 to 117 μm.
- A comparison between 10 μm, 160 μm and a variable radial leakage gap calculation indicated that time averaged peak temperature in the solid reaches 98°C, 129°C and 120°C respectively.
- The coupled model predicted an improved flow and volumetric efficiency by 8.2%, lower indicated power by 2.5% and a higher adiabatic efficiency by 5.5%, in comparison to the design gap size of 160 μm.
- The presented solution was a conceptual test, as rotor deformation was not included, and housing deformation was used to vary an initial 30 μm radial leakage gap. The system needs to be developed further to account for rotor deformation.
- Interlobe and high-pressure axial end leakage gaps are also required to be incorporated, to further improve the numerical model.
Such an improved CHT analysis with bi-directional system coupling can be used to accurately estimate the thermal deformation and leakage gap changes in the compressor during operation and improve the reliability of the performance results obtained from the computational models.

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