Two Way Coupling of CFD Conjugate Heat Transfer Simulation with Solid Thermal Expansion in a Twin Screw Compressor

Hui Ding, Haiyang Gao, and Xiaonong Meng

Abstract Gas temperature changes due to compression can cause non-uniform thermal expansion in the compressor hardware, potentially impacting both its performance and lifespan. This paper proposes a fully-coupled simulation approach that incorporates gas compression, conjugate heat transfer (CHT), and solid thermal expansion. We will describe in detail the complete procedure for solving a two-way coupled computational fluid dynamics (CFD), conjugate heat transfer, and solid thermal expansion, including the technical challenges and proposed solutions. This approach has been applied to a twin screw compressor case. The simulation results indicate that the solid thermal expansion has significant impact on the performance of the compressor. This paper will also demonstrate that the approaches used are robust, fast, user friendly, making them readily applicable to industrial compressor systems.

Keywords Twin screw compressor · Conjugated heat transfer · Thermal expansion · FSI · CFD

1 Introduction

1.1 *Compressor Conjugate Heat Transfer and Thermal Expansion*

The temperature of a diatomic ideal gas can increase 32% when compressed to half in an adiabatic process. Gas temperature can raise further due to irreversible processes such as friction and mixing. These temperature changes can affect the solid components of the compressor and cause thermal expansion and stress, leading to excessive abrasion, changes in leakage gaps, and thermal-induced fatigue. Maintaining a small gap size in PD compressors is essential to separate gas pockets of high and low

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pressure, and altering these gaps can have a significant effect on the compressor's performance. Therefore, predicting and analyzing gap size changes due to thermal effects is crucial for compressor design and improvement.

However, most CFD studies of twin screw compressors only consider the fluid part of the compressor due to technical difficulties and simulation costs. Solid thermal effects are often ignored or completely decoupled from the CFD simulation. Generating a proper moving mesh for the moving/deforming rotor fluid volume is a challenge. Due to issue in handling small gaps, the high cost of remeshing, and the loss of accuracy during result interpolation, general purpose moving mesh solutions which generate a totally new mesh at each rotor position are rarely used for PD compressor. Hence, conventional techniques involving the deformation of an existing mesh are generally preferred. Because of really complex geometry, the moving mesh for twin screw is often generated using 3rd party special software for a set of predetermined rotor positions.

Besides complex geometry, another important issue is the cost of coupling slow heat propagation in solids with the very fast movement of the fluid machine. Ding et al. [1] have demonstrated that a simple direct coupling of conjugate heat transfer for twin screw is not practical. Coupling solid thermal expansion with geometry change in the rotor fluid volume requires deforming the fluid mesh based on local thermal expansion predictions. This is very difficult when using pre-created third-party rotor meshes.

Literature search shows that only a few studies have considered CHT with solids in their simulations. Rowinski et al. [2] simulated a twin screw expander coupled with solid fluid heat transfer using a "semi-transient" method. Ding et al. [1] used "Mixed Time Scale" method simulated CHT of a twin screw compressor. Thermal expansion of the rotors was also solved in this study, but not coupled with fluid volume geometry change. The current study is a continuation of the work done by Ding et al. [1] and involves coupling solid thermal expansion with fluid simulation to alter the fluid domain's geometry based on solid thermal expansion results. The following section will outline the simulation strategy, and the necessary capabilities utilized in the approach.

1.2 Proposed Simulation Approach with Required Capabilities/Tools

The proposed approach consists of 3 independent simulations: fluid simulation, solid heat transfer simulation, and solid thermal expansion simulation as shown in a flow chart displayed in Fig. 1. These simulations are run separately due to significant differences in their time scales. The approach involves two nested iteration loops: the CHT inner loop and the thermal expansion outer loop. The solid temperature field and thermal expansion are initialized before simulation iteration to provide boundary conditions and an initial mesh for fluid simulation. During Simulation 1,

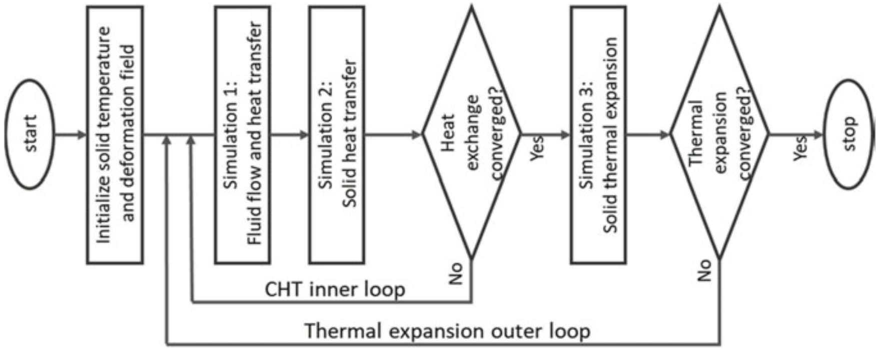

Fig. 1 Flow chart of proposed procedure

the fluid domain mesh is created and deformed based on available thermal expansion information, and transient simulation of fluid flow and heat transfer is solved for a repeating period. Heat exchange data between fluid and solid are collected during this simulation. Simulation 2 runs solid heat transfer simulation using the collected data as boundary conditions. If heat exchange balance is not achieved, the procedure returns to Simulation 1 with updated solid surface temperature. Otherwise, the conjugate heat transfer loop ends, and Simulation 3 solves solid thermal expansion based on the temperature field obtained in Simulation 2. Then, the convergence of thermal expansion is checked, and if not converged, the outer loop starts again. The collected thermal expansion data are used for mesh adjustment in fluid simulation.

To overcome the time scale issue, solid heat transfer simulation runs in steady state. This Mixed Time Scale Approach has been successfully used in many single phase and multiphase CHT simulations with high speed fluid machineries such as piston liquid cooling [3], e-motor liquid cooling [4], e-compressor CHT [5], and twin screw CHT [1]. The approach utilizes multiple innovative methods and tools, implemented in the commercial software Simerics-MP + .

Rotor Mesher: This study utilized the General Gear Template, originally designed for gear set meshes in gearboxes, to generate the twin screw rotor mesh. The template features: (a) modeling of spur/helical, internal/external gears, and more than two gears connected together, as shown in Fig. 2 for a helical planetary gear set mesh; (b) on-the-fly mesh generation in any specified rotation angle during simulation; (c) generation of a viscous layer mesh on gear surface which can benefit CHT simulation; (d) generation of a fluid rotor mesh representing a deformed rotor solid using localized geometry deformation information, which is critical for this study; (e) gear overlap protection by enforcing a minimum gap between solids. The General Gear Template has been previously tested in many gear cases [6] and a few twin screw cases [7].

CHT Data Exchanger: The exchange of heat transfer data between the fluid simulation and the solid heat transfer simulation is facilitated by a Data Exchanger Module, which is integrated into the same solver. This module automatically gathers the

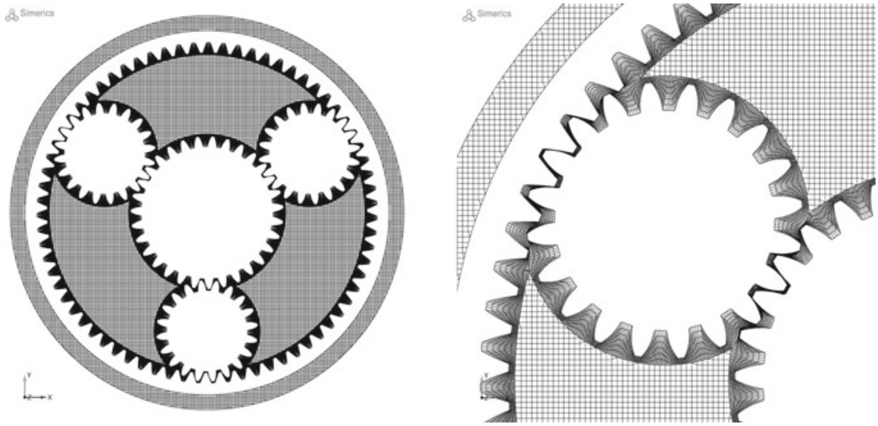

Fig. 2 Mesh of a helical planetary gear set

necessary heat exchange data, calculates appropriate time averages with the specified interval at the fluid–solid interface, and maps the data to the corresponding coupled solid or fluid simulation on different meshes. The Data Exchanger Module has been employed in various CHT coupling simulations mentioned earlier [3–5].

Solid Thermal Expansion Solver: This study uses a recently developed FEA capability to simulate the thermal stress and expansion of the solid. This FEA solver is based on classical finite element technology and offers all the advantages of a finite element solver, with the added flexibility to handle complex geometries. The solver works on general polyhedron meshes, which can be generated using Simerics-MP + proprietary binary tree meshing technique. It allows a mixture of hexahedron, tetrahedron, pyramid, prism, and polyhedron cell types, resulting in a hex-dominant mesh that offers superior speed, robustness, and accuracy. As the FEA solver can operate on the same binary tree mesh utilized in the current CFD solver for fluid flow and solid heat transfer simulations, coupling the simulations together becomes more convenient for the users.

1.3 Governing Equations and Physics Models

The CFD package, Simerics-MP + , used in this study solves conservation equations of mass, momentum, and energy of a compressible fluid using a finite volume approach. The standard two-equation $\kappa\varepsilon$ model with wall function is used to account for turbulence. Those equations combine with fluid properties to form a closed system. In the solver, each of the fluid properties can be a function of local pressure and temperature, and can be prescribed as an analytical formula or in a table format. Heat conduction in solids is also solved using a similar energy conservation equation. Please refer to Ding et al. [1] for more details.

Thermal Stress: The linear thermal stress problem can be solved by minimizing the potential energy of the system,

$$I(u) = \frac{1}{2}\int \nabla^s u : D(\nabla^s u - \varepsilon^0)d\Omega - \int u : bd\Omega - \int u : td\Gamma \tag{1}$$

$$u = N_a(\xi)u^a \tag{2}$$

$$\varepsilon^0 = \alpha(T - T_0) \tag{3}$$

In the above equations, u is the displacement, which can be approximated by shape functions and displacements at cell nodes, ε^0 is the thermal strain, it is caused by temperature change from stress-free temperature.

2 Twin Screw Compressor Test Case

The twin screw compressor studied in this research is an oil-free compressor with a 3/5 lobe arrangement [8]. It operates at male rotor speeds varying from 6000 to 14,000 rpm, with a male rotor diameter of 127.45 mm and a female rotor diameter of 120.02 mm. The center distance between the two rotors is 93.00 mm, and the rotors' length to diameter ratio is 1.6, with a male rotor wrap angle of 285.0 deg. Three independent models are created for three separate simulations: a fluid model, a solid heat transfer model, and a solid thermal expansion model. These models are coupled iteratively as described above to solve CHT and corresponding thermal expansion.

2.1 Fluid Model

The rotor section of the twin screw in the fluid model (Fig. 3) is meshed using Simerics-MP + General Gear Template. A 20-micron thick, two-layer boundary layer mesh is generated on the male and female rotor surfaces to capture CHT effects more accurately. The inlet and outlet ports of the fluid volumes are meshed using the Simerics binary tree unstructured mesher, and all fluid volumes are connected using the Mismatched Grid Interface (MGI). The fluid volume mesh comprises around 3.4 million cells, as shown in Fig. 4. A fixed total pressure and a fixed total temperature boundary conditions are set for the gas inlet, while the outlet is set to a fixed static pressure. The fluid–solid interface is set to a fixed temperature boundary condition with temperature values mapped from the solid model simulation results. Air is the simulated fluid, and the male rotor rotation speed is set at 8000 RPM. The fluid model takes approximately 2 h per male rotor revolution to run on an AMD workstation with 64 cores.

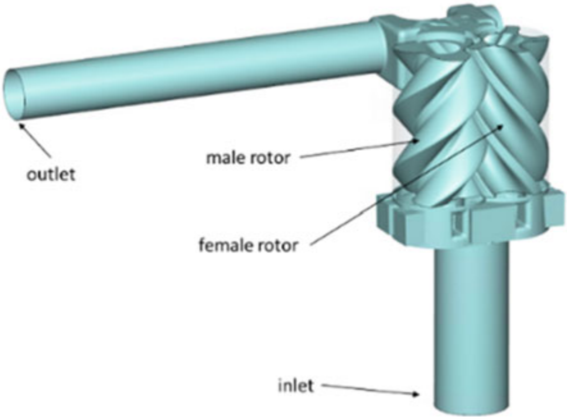

Fig. 3 fluid volumes

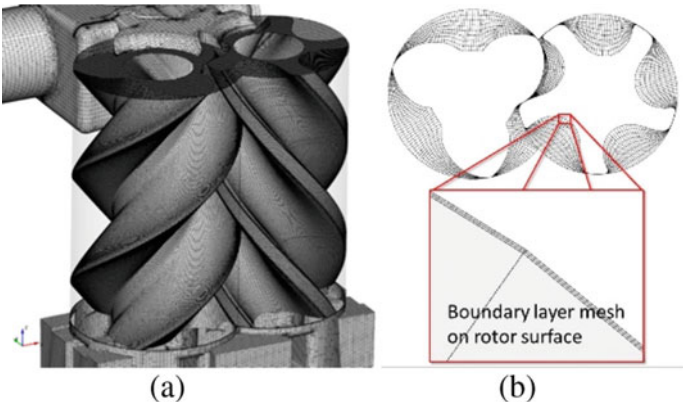

Fig. 4 Fluid mesh: **a** fluid volume mesh **b** cross-section of the rotor mesh

2.2 *Solid Heat Transfer Model*

The solid heat transfer model consists of three volumes: the case, the male rotor, and the female rotor, as illustrated in Fig. 5. All solid volumes are meshed using binary tree mesh with a total of about 0.4 million cells, as shown in Fig. 6. The solid–fluid interface is set as a fixed heat flux boundary with values mapped from the fluid model simulation results. The other boundaries of the solid rotor are assumed to be fully insulated. The outer surface of the case is set as a heat convection boundary. The solid model solves for steady-state heat conduction, and the simulation time for each run is less than one minute.

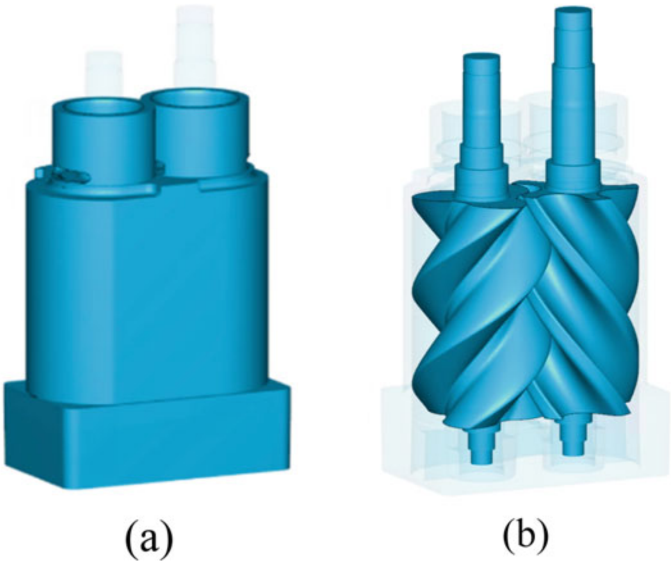

Fig. 5 Solid volumes: **a** case **b** rotors

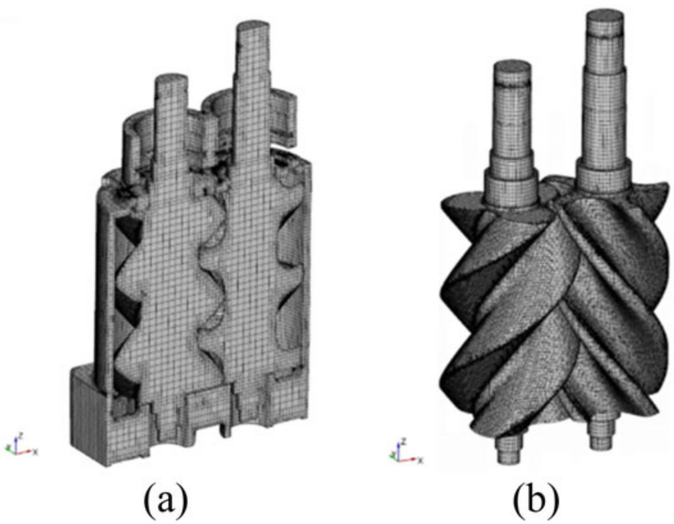

Fig. 6 Solid mesh: **a** case and rotor mesh in a cross section **b** rotor mesh

2.3 Solid Thermal Expansion Model

The solid thermal expansion model in this study only considers the male and female rotors due to insufficient information about the case solid components. The same rotor mesh used in the solid heat transfer model is also used in the thermal expansion study (Fig. 6b). In the simulation, the top and bottom surfaces of the rotor axials are fixed with zero displacement. The thermal expansion model reads the temperature field from the solid heat transfer simulation, runs a thermal expansion analysis, and save the displacement of the rotors in a data file. Later, the fluid model reads the displacement file to deform the fluid mesh for the next simulation iteration. The simulation time for each thermal expansion run is less than one minute.

3 Results and Discussion

In the simulation, the fluid inlet total pressure is 1 bar, outlet static pressure is 2 bar, and inlet total temperature is 300K. Both rotors are assigned proper rotational speed. Table 1 summarizes key simulation parameters. The solid case has a 10 W/m^2K heat convection on its outer surface with a 300 K environment temperature. Both fluid and solid are initially set to 300 K. A fixed number of iterations for the CHT inner loop is used. During the inner loop, the fluid model runs for one tooth rotation. The solid heat transfer model then runs a steady state simulation using the data from the fluid simulation. The CHT results from the solid simulation is used for the next fluid simulation. After 15 iterations or 5 revolutions of the male rotor rotation, the inner loop is considered complete. After that, the solid temperature field is passed to the thermal expansion model to calculate rotor expansion, which is used for the next iteration of the thermal expansion outer loop. In this study, the thermal expansion outer loop runs four iterations with total of 20 revolutions of male rotor rotation. The simulation is controlled by a Simerics-MP + batch file running in background without user interference.

Table 1 Simulation parameters

Parameters	Values
Gas	Air (using ideal gas law)
Gas inlet total pressure	1 bar absolute
Gas inlet total temperature	300 K
Outlet static pressure	2 bar absolute
Solid	Stainless steel
Solid density	7800 kg/m^3
Solid conductivity	30 W/mK
Solid heat capacity	450 J/KgK
Solid Young's Modulus	200 GPa
Solid Poisson Ratio	0.33
Solid thermal coefficient	1.2×10^{-5}/K
Compressor speed	8000 rpm (male rotor)

Figure 7 shows the instantaneous and cycle-averaged heat flux between fluid and solid rotors during the 20 male rotor revolutions to demonstrate procedure convergence history. The maximum instantaneous heat flux is about 500 watts. Once the solution has converged, the average heat flux becomes zero, which is correct because there is no heat source inside solid rotors, and other boundaries of rotors are assumed adiabatic.

The plot shows that the conjugate heat transfer converges quickly after the 1st outer loop iteration, and the 5-revolution inner loop iteration may not be needed for later outer loop iterations. The solid case carries about 90 watts of heat away from its outer surface by the environment.

Figure 8 displays pressure contour of rotors at 5 different crankshaft angles in the final iteration. Pressure inside each fluid pocket has similar values. The pressure value increases as a pocket moves from inlet to discharge due to volume reduction.

No abnormalities were found in the simulation results even with deformed rotor geometry, indicating proper handling of mesh deformation. The final averaged solid temperatures are 331.7 K, 355.7 K, and 352.4 K for the case, the male rotor, and the female rotor, respectively.

Figure 9a displays solid temperature distribution in a cutting plane, while Fig. 9b shows rotor surface temperature. The temperature inside rotors has a layered distribution from low to high when moving from inlet to discharge. As noted in [1], this pattern is different from the temperature distribution assuming adiabatic rotor surfaces.

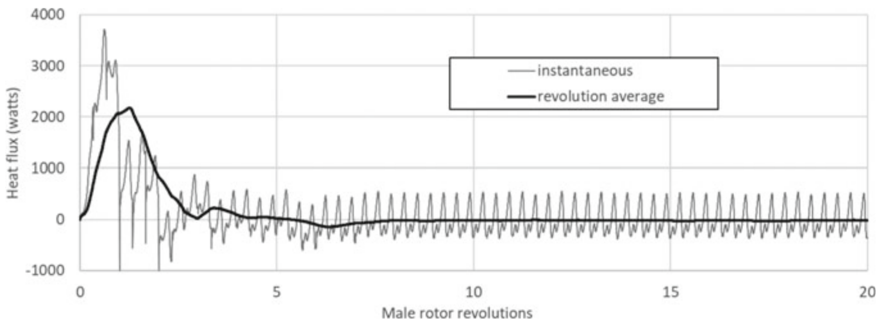

Fig. 7 Heat flux between fluid and solid rotors

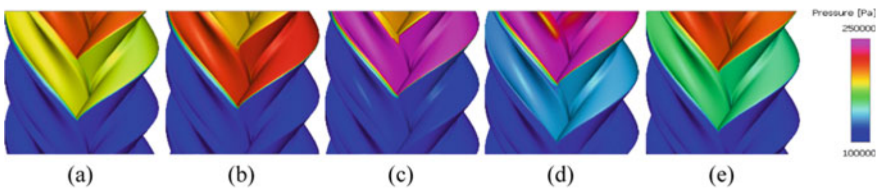

Fig. 8 Pressure contour at different male rotor crankshaft angles: **a** 24 degree **b** 48 degree **c** 72 degree **d** 96 degree **e** 120 degree

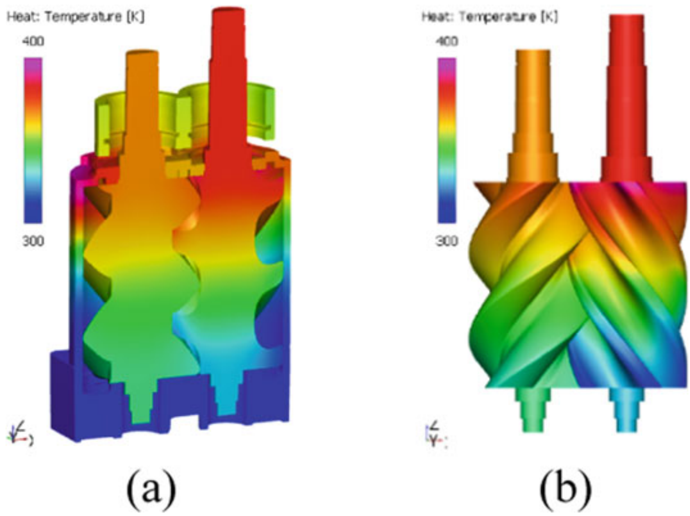

Fig. 9 Solid temperature **a** temperature in a cutting plane **b** rotor surface temperature

Figure 10 demonstrates the rotor thermal displacement in radial direction due to thermal expansion, increasing from center to out surface, with a maximum value of about 60 microns. Displacement also increases in the axial direction due to the temperature gradient. Figure 11 compares the rotor geometry before and after deformation, displaying a significant reduction in tip gap and a slight reduction in inter-lobe gap as a result of thermal expansion at one of the rotor positions. In the picture, grey area is the deformed fluid volume, and the red curves represent original geometry. Rotor thermal expansion significantly reduced tip gaps, assuming negligible case geometry thermal expansion.

Figure 12 shows the compressor mass flow rate plotted against the male rotor revolution. During the first outer loop iteration, when there were no shape changes caused by thermal expansion, the mass flow rate stabilized at approximately 11.7 kg/min. However, during the second iteration, when the rotor shape changed due to thermal expansion, the mass flow rate increased by more than 6% to 12.4 kg/min as a result of the reduction in gap size. The mass flow rate only underwent minor reduction during the third and fourth iteration. The reduction in mixing is attributable to less leakage, which results in lower gas temperature and, consequently, reduced thermal expansion. Eventually, the gap size slightly increased. The parameters listed in Table 2, which include mass flow rate, rotor average temperature, and rotor volume change due to thermal expansion, indicate that the coupling with thermal expansion has converged.

Table 3 compares gas mass flow rate and rotor power for the simulation results at the end of the first and the fourth outer iterations against experimental data [8]. The predicted flow rates have about 1 to 6% differences, and predicted powers have about 1 to 2% differences from the test data. The table shows that the prediction from

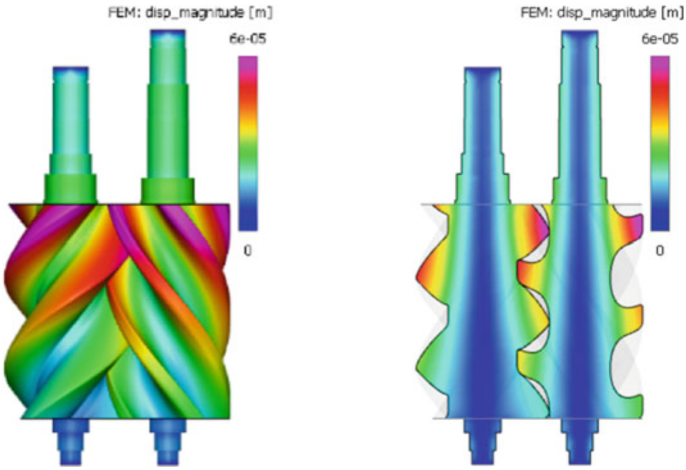

Fig. 10 Rotor displacement due to thermal expansion

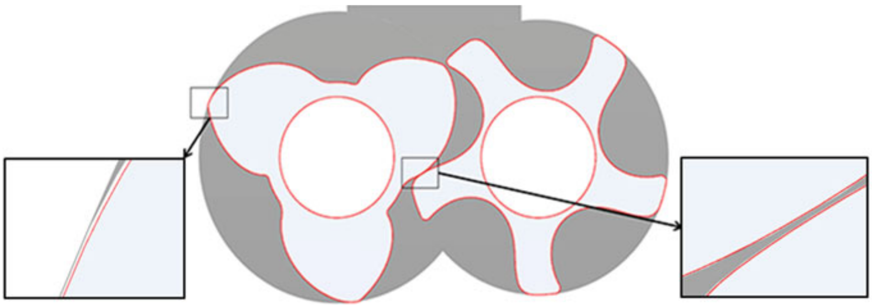

Fig. 11 Comparison of original and deformed gap size

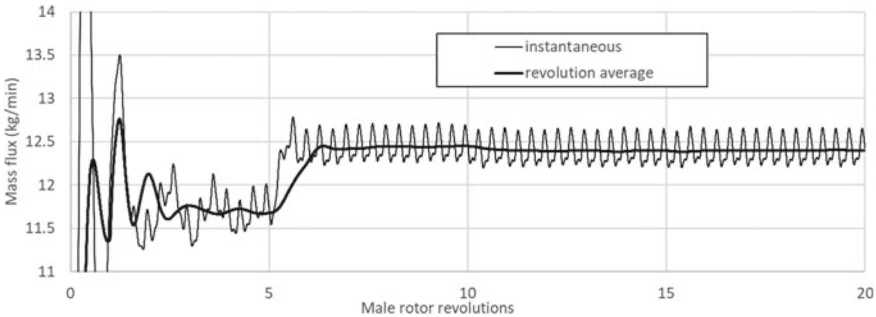

Fig. 12 Mass flow rate

Table 2 Thermal expansion loop iteration convergence

Iterations	1	2	3	4
Mass flow rate (kg/min)	11.70	12.43	12.39	12.40
Rotor average temperature (K)	357.80	354.14	354.05	353.89
Rotor volume change (mm^3)	0	6080	5690	5680

Table 3 Comparison of mass flow rate and rotor power

	1st iteration	4th iteration	Experiment
Mass flow rate (kg/min)	11.7	12.4	11.8
Rotor power (kw)	21.9	21.7	22.2

"original" rotor geometry matches the test data significantly better than the one from deformed geometry. The reason is that the deformed geometry could have double counted the thermal expansion effects since the "original" geometry had already been modified to consider potential shape changes due to thermal expansion, as mentioned by Kovacevic et al. [8].

4 Conclusion and Future Works

This study successfully attempted direct coupling of 3D CFD, CHT, and solid thermal expansion for twin screw compressors, with the aim of predicting thermal expansion effects on compressor performance. The method is divided into three coupled models: fluid flow and heat transfer, solid heat transfer, and solid thermal expansion. The solution procedure has a CHT coupling inner loop, nested in a thermal expansion coupling outer loop, and couplings are solved iteratively. Several new capabilities have been developed to fulfil the needs of this coupled procedure. With these added capabilities, setup and run such a simulation is very easy. The simulation results demonstrate stability and quick convergence of the proposed iterative procedure. The thermal expansion was found to cause a significant change in twin screw leakage gap size, which affected compressor performance, with a 6% increase in gas flow rate and 1% drop in power consumption for the simulated case. Added simulation time for solid heat transfer and thermal expansion was negligible compared to fluid simulation. Future work will include applying the procedure to twin screw compressor cases with more complete information to further evaluate the method's accuracy and improve simulation efficiency.

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