

MULTIPHYSICS NUMERICAL INVESTIGATIONS OF HOT COMPONENTS IN A sCO_2 POWER PLANT TURBINE

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Abstract. To achieve a higher energy conversion efficiency, the use of supercritical CO_2 (sCO_2) in closed-loop Brayton and Rankine cycles has become relevant in the last decades due to an increased interest in its properties. sCO_2 allows a more efficient heat transfer, chemical stability, non-flammability, and greater system efficiency. The necessity of a sealing system, which creates a barrier between the high-pressure fluid in the turbine and compressor and low-pressure regions, became essential for high-efficiency preservation and plant emissions reduction. In this regard, Dry Gas Seals (DGS) become one of the substantial components for sCO_2 turbomachinery design due to lower leakage and higher efficiency than a traditional labyrinth radial seal. The high fluid pressure and density, connected to a small size sealing clearance and a high rotational speed, results in a significant friction heat, which characterizes the domain temperature distribution. The necessity for a thermal analysis of the domain becomes compelling to respect the maximum temperatures allowed in the turbomachine. When drawing up a thermal analysis, the high computational costs of a 3D simulation of the fluid domain (CFD) could be unfavourable due to the different orders of magnitude of secondary flows cavity sizes and DGS seals gaps, and the necessity to run a high number of simulations to define a geometrical sensitivity and optimization of crucial zones. A segregated conjugate heat transfer (CHT) iterative procedure has been implemented, relating a commercial 1D fluid modeller (Altair Flow Simulator) and a commercial finite element solver (Ansys Mechanical). To assess the procedure developed, 3D CFD simulations and CHT analysis of specific critical areas of the domain have been carried out. The segregated approach, implemented within the European project CO2OLHEAT, showed results in line with 3D CFD and CHT analysis, reducing computational time and cost.

1 INTRODUCTION

In recent years, the use of supercritical carbon dioxide (sCO_2) as a working fluid for closed-loop Brayton and Rankine cycles become relevant in the industrial field due to its particular thermodynamic properties. The sCO_2 is a carbon dioxide state which occurs above its critical point (7.4 MPa and 31 °C). Here, CO_2 shows unique characteristics which make it useful for a variety of applications such as Waste Heat Recovery, Power Generation, industrial processes and extraction of natural resources (solar and fossil). In the supercritical region, the CO_2 properties are halfway between a gas and a liquid [1]: the density is similar to that of a fluid, while the dynamic viscosity is on gas levels. The high fluid density is convenient for carrying out processes that require high mass transfer rates and allows lower component dimensions [2]: the smaller the components, the lower the noise and vibrations are. Moreover, the sCO_2 allows an efficient heat transfer, chemical stability and non-flammability, making it safer than other traditional working fluids and thus reducing the plant footprint and greenhouse gas emissions [3]. Finally, the power cycle reaches high thermal efficiency levels (nearly 50%). Due to the characteristics expressed is simple to understand how the interest in this topic is increasing both from an industrial and academic point of view.

Despite the defined advantages, the sCO_2 power cycles show significant technical challenges. The smaller size of the turbo machinery implies a higher rotational speed causing a series of new challenges to the design and operation for sCO_2 [4]. To diminish the efficiency loss, safety hazards and environmental concerns, another aspect to consider is the sCO_2 leakages control.

One of the main types of mechanical seals is exemplified by the labyrinth seal, used to prevent leakage between two surfaces, such as a rotating shaft and its housing. It consists of a series of interlocking grooves on one surface and a set of mating fins on the other surface, which create a tortuous path for the fluid to follow. Despite being the typical seal technology applied in traditional steam turbines [5], for sCO_2 power cycles, they suffer from high leakage due to the high operating pressure, resulting in significant efficiency loss. In light of this, dry gas seals (DGS) emerge as a core technology for sCO_2 closed-loop cycles.

The DGS is a dynamic seal consisting of a rotating and static ring including which a few micron gap is originated and maintained from a resulting balance between a hydrodynamic and elastic force, thus reducing the leakages. As shown by Bidkar et al. [6] the use of existing sealing technology (i.e. labyrinth seals), instead of DGSs, on a $450MW_e$ sCO_2 turbine can result in a loss of 0.55% to 0.65% points in the thermodynamic cycle efficiency. Moreover, the smaller the cycle efficiency, the higher the CO_2 leakage is.

The high temperatures, pressure and velocities could influence the DGS characteristics. As shown by Brown [7], the working temperatures depend on the seal material: using elastomers, the temperatures range from 4°C to 233°C while by using non-elastomers extend from -157°C to 650°C. At the same time, as suggested by Steinmann et al. [8], venting sCO_2 into the atmosphere can lead the CO_2 to become solid (dry ice formation) due to lamination (Joule-Thomson effect). In [8] a test campaign to test DGSs for a sCO_2 Re-compression Closed Brayton Cycle (RBCB) pilot plant at different boundary conditions was conducted. It was observed that low leakages reduce the risk of ice formation on the primary vent side, improving seal reliability and how, in general, the seal gas inlet temperature and pressure should be selected carefully to avoid this phenomenon. Based on the above, the development and evolution of sCO_2 power cycles must go hand in hand with the DGS thermal behaviour analysis.

Many works, with the aim of a better understanding of DGS thermal management, are found in literature both from a numerical and experimental point of view. Shahin et al. [9] defined a 3D computational study for spiral DGS evaluating the laminar and turbulent flow with RNG $k-\epsilon$ and LES for equivalent geometrical and operating conditions, finding that the laminar flow simulations agree with the experimental data more than the turbulent flow, which overestimates the pressure distribution inside the seal. When the Reynolds number is less than a critical Reynolds number, the fluid flow could be considered laminar [10].

Concerning the numerical modelling, Pengyun et al. [11] studied the real gas effect on the DGSs performance. The real gas equation of state is applied to better characterize the fluid behaviour around the critical point. It was found that the real gas behaviour affects the leakage of the DGS but not the opening force.

To better represent the heat transfer between the fluid and the solid objects, especially in cases where there is a significant thermal interaction, the Conjugate Heat Transfer (CHT) analysis is often employed. Since simultaneously the CHT solves the fluid flow and heat transfer equations, the computational cost increases and could be prohibitive when considering the difference in characteristic length in the DGS domain. Hong et al. [12] performed a comprehensive CHT analysis through a multi-physics approach to reduce the computational cost of the analysis: three computational models were solved step-by-step, to overcome the computational cost problem. It was observed that by reducing the film gap the friction heat generated increases. Therefore, Zakaria [13] further investigates the DGS thermal behaviour in sCO_2 with CHT simulations, validating the results through experimental data with air.

In this regard, the present work aims at implementing a segregated CHT model, developed among our research group, the University of Florence "Heat Transfer and Combustion" group, and firstly presented in the paper by Rafanelli et al. [14], within the European Project CO2OLHEAT (Supercritical CO_2 power cycles demonstration in Operation environment Locally valorising industrial waste HEAT), conceived to recover waste heat from an existing cement plant. A general description of the plant cycle and components and project state-of-the-art could be found in the work of Toni et al. [15].

Being the CO2OLHEAT project at its early stages, no experimental data are available for the model assessment: 3D Computational Fluid Dynamics (CFD) simulations and CHT analysis of specific critical areas were performed, introducing a higher precision level from a numerical point of view. Despite this, the numerical model was experimentally confirmed in [14] on a similar DGS test bench, described in [8].

2 NUMERICAL MODEL

To reduce the computational cost of a fully coupled CHT, where the fluid and solid domains are solved simultaneously, the development of a segregated approach represents a compelling alternative. In literature, many works with the aim of presenting a decoupled CHT approach are present, exploring various domains. Weilun et al. [16] established a model to evaluate the internal cooling performance of a composite cooling structure. Andrei et al. [17] presented a decoupled procedure aimed at predicting cooling performances and metal temperature of gas turbine blades and nozzles. Similar targets are shown in [18]. Hereafter, the segregated CHT approach, and the fluid and solid domains are illustrated.

2.1 Segregated CHT approach algorithm

The numerical approach, extensively presented in [14], uses the fluid network solver Altair Flow Simulator and the language ANSYS Mechanical APDL to perform a Finite Element Analysis (FEA). The solution transfer between the two solvers is achieved through a Matlab code, which sets the convective heat transfer and the convective power as Boundary Conditions (BCs) respectively for the 2D thermal model and the 0D fluid network. A schematic representation of the procedure is shown in Figure 1.

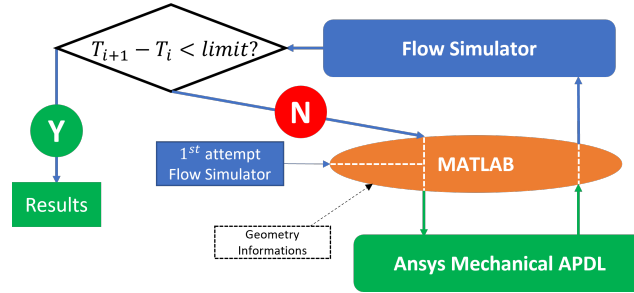


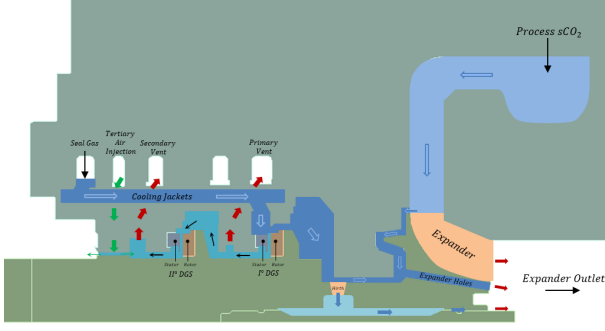
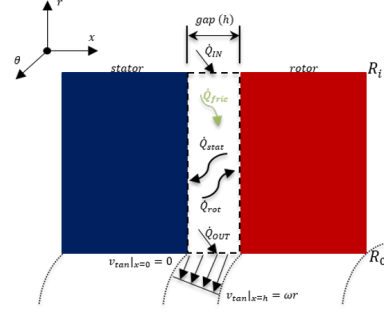
Figure 1: Coupling Algorithm

Altair Flow Simulator computes the fluid temperatures which are set, together with the calculated HTC, as BCs for the FEA. Then, the mechanical model outputs are imposed as BCs for the fluid network. This iterative loop is repeated until convergence is reached i.e. the temperature variations between two consecutive steps is below 0.5%. The lower the leakage flow, the larger the temperature fluctuations are: for this reason, a temperature under-relaxation factor was introduced to reach convergence even for strongly critical conditions.

2.2 Fluid Network

The commercial fluid solver Altair Flow Simulator has been used to discretize the fluid domain through a 1D model in which 0D fluid chambers are connected through fluid elements. The conservation equations for mass, momentum, angular momentum and energy are solved iteratively until convergence is reached. The CO2OLHEAT power unit consists in an integrated gearbox expander compressor where the impellers are assembled in an overhung configuration, which requires a sealing system to avoid sCO_2 leakages. The discretized fluid domain, shown in Fig. 2, is representative of the region behind the expander impeller.

Specifically, part of the process sCO_2 leaks behind the impeller and is mixed with a seal gas injected through 12-tubes (Cooling Jackets) circumferentially arranged, manufactured within the fixed power plant housing, with a mass-flow rate of 0.25 kg/s at 100°C and 195 bara. The mix of the hot process gases and a large part of the seal gas mass flow is reinjected at the expander outlet through 12 holes (Expander Holes), also circumferentially arranged, and manufactured within the rotating impeller. On the other side, part of the seal gas mass flow goes through an hirth-coupling, used to precisely align and transmit torque between the impeller and the rotating domain: the mass flow is then reinjected at the expander outlet. Furthermore, the remaining seal gas mass flow flows through the tandem DGS configuration: the mass flow is split between a stream which goes through the primary vent and one through the secondary vent (after the second DGS). To further avoid the sCO_2 leakages in the surroundings, an air


Figure 2: Test bench fluid network scheme

Figure 3: DGS gap flow field

tertiary seal injection is defined: part of the air mass flow is released in the ambient while the remaining mixes with the sCO_2 and goes through the secondary vent. Due to the temperature limit of the seal, the estimation of the friction heat is fundamental in the preliminary thermal-management design phase of the power plant. Flow Simulator is able to internally calculate the friction heat with validated stator-rotor cavities correlations [19][20], which however are not valid for the DGS gap, characterized by a low-passage area and a very stretched aspect-ratio section. For this reason, the friction heat generated is externally computed by the Matlab script with the expression experimentally validated found in literature [13][21].

Referring to Figure 3, under the hypothesis of linear velocity in the axial and radial directions, the fluid velocity can be expressed as follows:

$$v(x, r) = \frac{\omega r x}{h} \quad (1)$$

where h is the gap size, r and x are the radial and axial directions and ω is the rotational speed along the x direction. This equation is based on the Laminar Couette flow hypothesis for the DGS gap, confirmed in [22][23]. Shear stresses at wall can be defined as:

$$\tau = \mu \frac{\partial v}{\partial x} = \frac{\mu \omega r}{h} \quad (2)$$

where μ is the dynamic viscosity. Considering the friction torque M as the integral of shear stresses at the wall multiplied by the radius, the heat power generated through the seal can be calculated as:

$$\dot{Q}_{fric} = \omega M = \omega \int_0^{2\pi} \int_{R_0}^{R_i} \frac{\mu \omega r^2}{h} r dr d\theta = \frac{2\pi \mu \omega^2}{h} \frac{R_i^4 - R_0^4}{4} \quad (3)$$

where R_0 and R_i are respectively the inner and outer DGS radii. The low-passage area, together with the high rotational velocity brings to high HTCs in the DGS gap. This aspect, combined with a low mass-flow rate makes the fluid almost isothermal through the gap since most of the generated heat is transferred to the solid. Zakariya et al. [13] showed how the fluid held only 5% of friction heat across the gap.

Furthermore, real gas Joule-Thomson (J-T) leakage cooling shall be considered for a proper fluid temperature calculation. This was externally evaluated by computing the Joule-Thomson coefficient μ_{JT} using the COOLPROP library to calculate the fluid thermodynamic properties. In the test bench analyzed the fluid temperature difference across the seal is almost zero

(isothermal transformation) since the J-T cooling is balanced by the friction effect: this is in line with the results found by Zakariya et al. [13].

This approach was only applied in the DGS gap where the standard correlations for the evaluation of the friction heat and HTC are not valid and the real gas J-T effects can't be neglected. In all other regions, the friction heat is internally computed by the fluid solver, and the HTCs are externally estimated by the MATLAB script through the Dittus-Boelter correlation [24]. Specifically, statoric and rotoric HTCs are evaluated starting from the swirl number S definition which correlates the fluid tangential velocity with the rotating velocity, allowing to compute the Reynolds number from a stationary and rotating point of view. Setting the Prandtl number equal for the statoric and rotoric interface, the HTCs are computed by the MATLAB script and set as boundary conditions, together with the bulk temperatures obtained from the fluid solver, on the mechanical model.

2.3 CFD Analysis

CFD simulations were carried out to numerically validate the use of the Dittus-Boelter correlation for the Heat Transfer coefficients (HTCs). This was performed through a double-run technique with adiabatic and fixed temperature simulations. To reduce the computational cost the domain analyzed is limited to the high-pressure region shown in Figure 4, thus not considering the DGS gaps. The CFD simulations were run through the commercial Navier-Stokes solver ANSYS CFX [25]. Turbulence was modelled with the two-equation SST $k-\omega$ model [26] with automatic wall treatment. The computational grid was created to reach a near-unit value of the y^+ . Moreover, a high-resolution scheme was implemented to compute the advection fluxes of continuity, momentum and total energy equations, with a second-order accuracy as a result. Lastly, the Augier Redlich-Kwong Equation of State (EoS) available in ANSYS CFX was used to take into account the real gas effects for the sCO_2 .

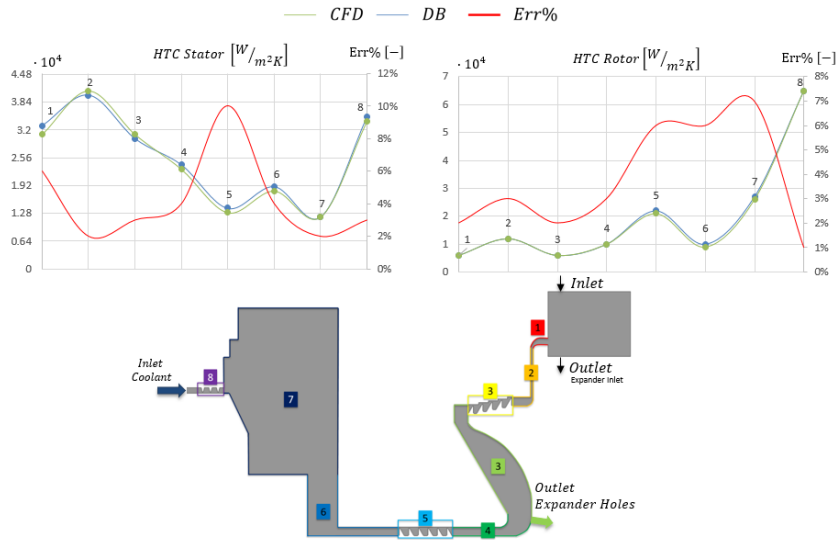


Figure 4: CFD Domain and Statoric and Rotoric HTC distributions

From the results shown in Figure 4, the Dittus-Boelter correlation can correctly catch the

HTC distributions both for the static and rotating wall, introducing a maximum percentage error of about 10% between the two approaches. The maximum error is found specifically in regions where the geometry is far from the typical cylindrical duct on which the correlation is based (i.e. labyrinth seals). The comparison shows how the fluid network accuracy is acceptable with a slight overestimation in the HTCs values: the error introduced by the correlation is negligible in a preliminary thermal-management design phase.

2.4 Mechanical Model

The solid geometry implied in the segregated procedure is presented in Figure 5 by differentiating between the statoric (light grey) and rotoric (dark grey) domains. A steady-state thermal finite element analysis was set in ANSYS Mechanical using the ANSYS Parametric Design Language (APDL). Worth mentioning is the presence of a thermal barrier used to shield the region of interest from the high-temperature working fluid. A sensitivity analysis for the thermal barrier, in terms of material and thickness, was tackled in [15], using the segregated CHT procedure.

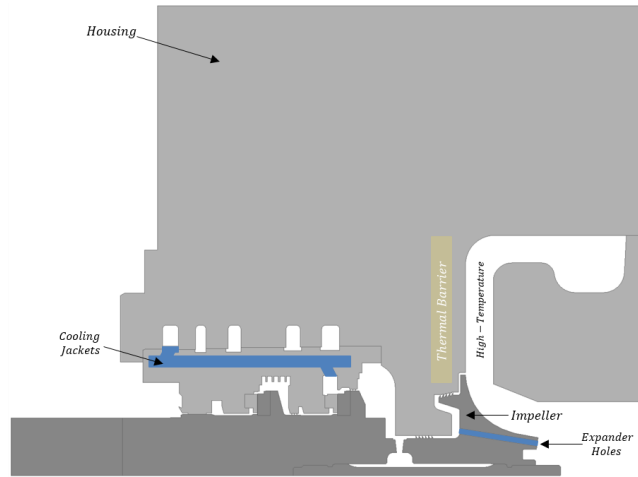


Figure 5: Solid domain: stator (dark grey) and rotor (light grey)

One important aspect to address in the solid domain modelling is the Inlet and Outlet tubes' effect on the overall temperature distribution. Since the solid domain was modelled as 2D axisymmetric, a specific modelling approach for 3D circumferentially arranged tubes was developed. The Cooling-Jackets tubes, aimed at providing the seal gas needed to avoid sCO_2 leakages, were discretized as 2D surfaces (equal to their section) where the thermal conductivity and the heat transfer coefficients were re-calculated in proportion with volume and wet area, respectively. The volume proportion for the thermal conductivity was performed considering the volume of the 12 tubes (V_{fluid}) against the volume of the solid of revolution (V_{tot}) obtained by revolving the 2D tube section around the rotational axis (as expressed in 4).

$$k_{eq} = \frac{V_{fluid}k_{fluid} + V_{solid}k_{solid}}{V_{tot}} \quad \text{with} \quad V_{solid} = V_{tot} - V_{fluid} \quad (4)$$

On the other side, the wet area proportion was defined by considering the real tubes' wet area (A_{wet}) against the solid of revolution surface area (A_{tot}). The equivalent HTC, HTC_{eq} , is computed as follows:

$$HTC_{eq} = \frac{A_{tot}}{A_{wet}} HTC_{wet} \quad (5)$$

The same approach was also applied to the Expander Holes. As shown in the results section 3, the developed approach introduces a negligible solid temperature overestimation compared to the CHT analysis, which setup will be tackled in the next section.

2.5 Conjugate Heat Transfer (CHT) Analysis

The segregated CHT procedure (SP) was assessed and verified through a complete 3D Conjugate Heat Transfer (CHT) analysis, where a fully coupled CFD solution of the fluid and the solid domain is defined. Despite the high computational costs, CHTs are widely used in the academic and industrial fields to evaluate, in the preliminary design phase, thermal distributions in high-temperature components.

Analyzing the SP preliminary results, the fluid appears to be almost isothermal in the area next to the sealing system due to a balance between the friction heat and the J-T cooling. Based on this and to avoid prohibitive computational costs due to differences in characteristic lengths in the DGS domain, the direct coupling between the solid and fluid domain was only limited to the high-pressure part of the fluid domain, thus neglecting the DGS gaps and the region after it. Similar conclusions were also defined for the hirth region.

Likewise, the CHT simulation has been carried out in ANSYS CFX, considering a 30° sector due to the tubes' periodicity.

Regarding the solid model, the thermal boundary conditions applied for all the areas where no direct coupling between the two domains is expressed, come from the SP solution. Depending on the region, heat fluxes or bulk temperatures and HTCs were applied as boundary conditions. For all the other areas, the boundary conditions are program controlled: the solver can correctly transfer the solution mutually between the two domains.

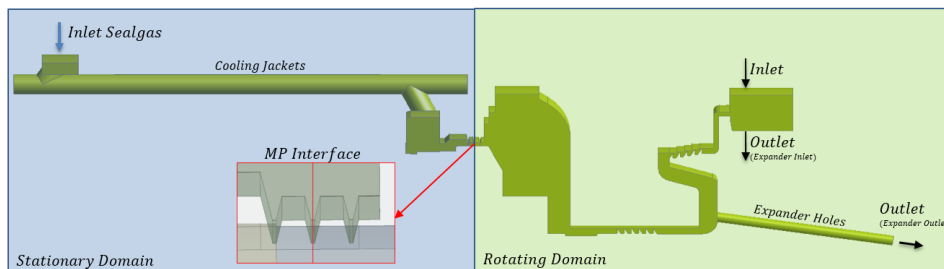


Figure 6: CHT Rotating and Stationary Domain

Concerning the fluid model, further modelling was needed to take into account the rotating expander impeller. The expander holes co-rotate with the impeller while the cooling jackets are integral to the fixed power unit housing. Hence, the fluid domain was divided between a stationary and rotating domain (Figure 6) relating the two through a Mixing Plane (MP) Interface. The idea behind the MP concept is that each fluid zone is solved as a steady-state problem and the solution transferred between the two interface sides is a circumferential average of the flow data on both sides. The profile averaging methods applied at the interface were the

area and mass-averaging ones. Specifically, to overcome solution stability problems, the solution was initiated with area averaging and then switched to mass-averaging, which provides a better representation of the total quantities than the area-averaging method. The first may not be representative of the momentum and energy of the flow [25]

3 RESULTS

In this section, the SP outcomes will be compared to the CHT ones in terms of thermodynamical properties and flow field. In general, the SP is able to correctly predict the results presented by a higher-order CFD analysis, thus reducing the computational time and costs required. The fluid domain temperatures and pressure distributions for both approaches are presented in Figure 7, together with contour plots for the aforementioned variables, outputs of the CHT analysis.

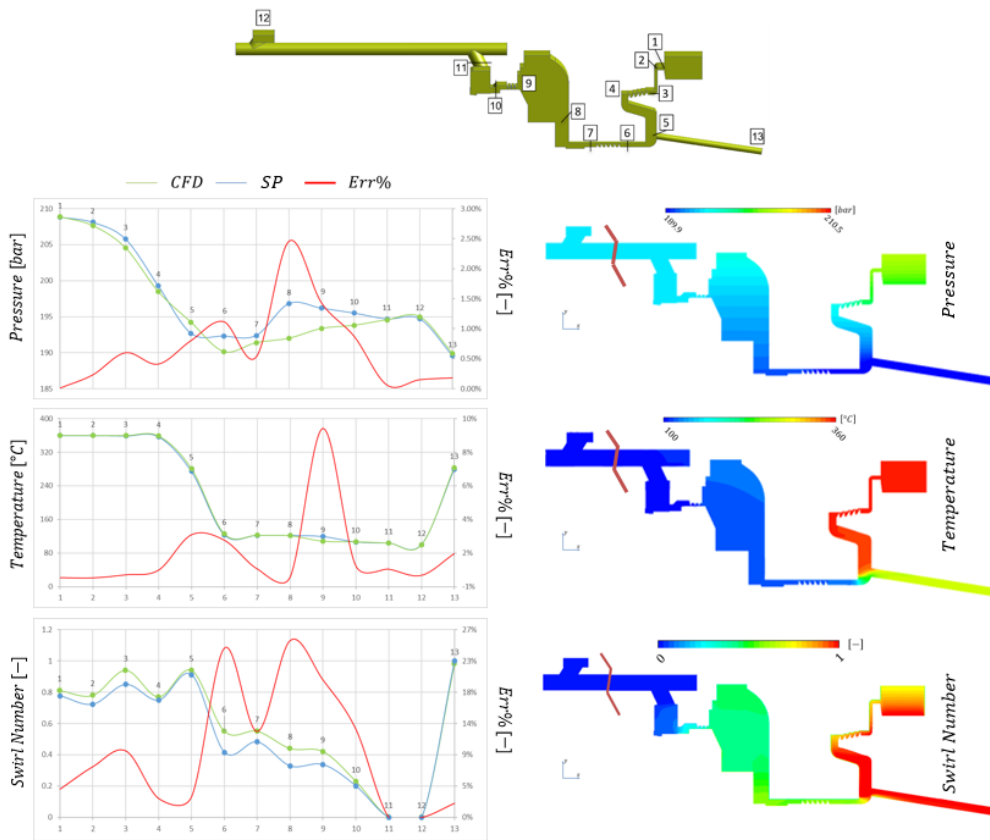


Figure 7: Comparison between CHT and SP in terms of Temperatures, Pressures, and Swirl Number Distributions

The SP accurately catches the pressure and temperatures distributions shown by the CHT: a percentage error of about 2.5 % for pressure and about 10% for temperatures is introduced by the SP in specific regions where the three-dimensionality of the flow field becomes significant, such as the plenum region around 8-9. The overestimations shown by the SP define a "conservative approach" that is convenient in the preliminary phase of the thermal management design of the power plant analyzed.

Furthermore, the SP exhibits a slight underestimation of the swirl number, always as illustrated in Figure 7. Specifically, this is connected to the inherent uncertainty of the approach where a 2D model aims at replicating a turbulent 3D flow field: the turbulence connected to the 3D recirculation regions is underestimated by the SP, which isn't able to describe the tangential flow field correctly. Despite the underlined deviation, the SP accurately detects the swirl number trend.

As defined, the quantification of thermal distributions is fundamental in the preliminary power plant design phase to preserve material integrity, thus avoiding phenomena such as thermal decomposition and fatigue, which can occur in elastomeric secondary sealing elements. So, the solid temperature distribution evaluation is cardinal for the subsequent design phases.

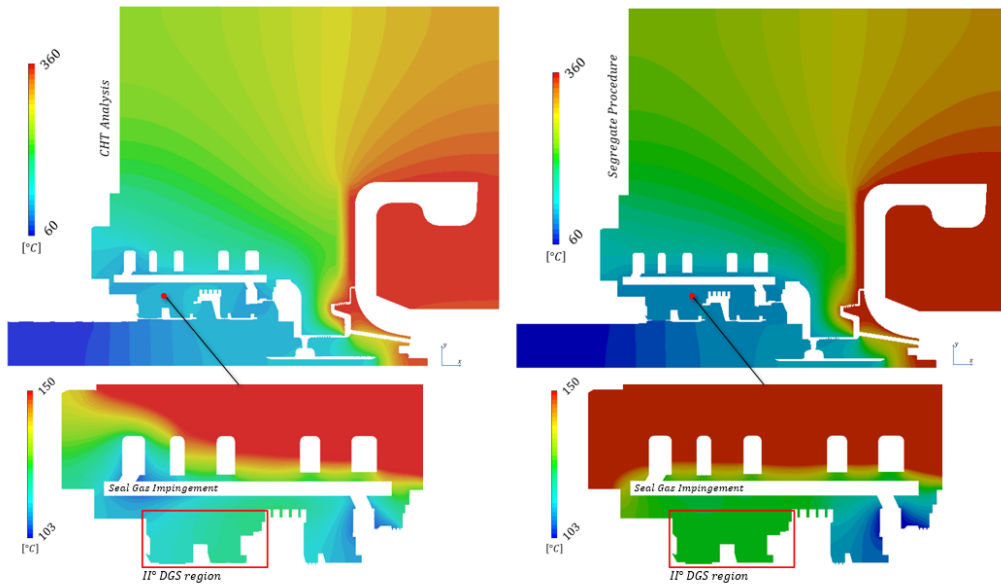


Figure 8: CHT and SP Midplane Solid Temperature Distributions

Figure 8 shows an excellent agreement between SP and CHT temperature contours on the midplane: the SP correctly detects the Min and Max temperatures reached in the domain, giving equivalent results. However, in the II° DGS region, a slight temperature overestimation ($\approx 4^\circ\text{C}$) results from the SP. The approach under discussion, as explained before, underestimates the 3D behaviour of the flow field: for example, the cooling determined by the seal gas impingement on the Cooling Jackets' walls is not perceived by the approach. Moreover, the Inlet and Outlet tubes model described in section 2.4 minimally affects the temperature distribution in that region. Despite the simplifications introduced, the SP correctly catches the temperature range obtained by the CHT. Both cases show maximum temperatures lower than the maximum temperature allowed, defined by the material employed for the different power plant components.

4 CONCLUSIONS

To achieve a higher energy conversion efficiency, the use of supercritical CO_2 (sCO_2) in closed-loop Brayton and Rankine cycles have become relevant in the last decades due to an

increased interest in its particular thermodynamic properties that led to an increase in cycle efficiency and a decrease in turbomachinery dimensions. To reduce the hazard of a sCO_2 leakage in the power plant surroundings, which could affect the newly increased efficiency and the plant emissions, the mechanical and thermal management design of a sealing system becomes essential. DGSs are key components from this point of view. The present work aimed to verify and validate a segregated CHT approach with a 3D CHT analysis, limited to a specific part of the domain analyzed, the CO2OLHEAT power unit. The SP has been discussed first in the work of Rafanelli et al. [14], while the power unit is described in detail in the work of Toni et al. [15]. At first, a validation through 3D CFD simulations of the Dittus-Boelter correlation used for the HTC's quantifications was performed. The results show a good agreement between the CFD and the correlation employed, introducing an overestimation of about 10%, which is negligible in the preliminary thermal-management design phase. Secondly, the complete CHT analysis has been carried out by limiting the direct coupling between the fluid and solid domain to the high-pressure region. The SP accurately caught the fluid pressure and temperature distributions showed by the CHT with a temperature and pressure overestimation, respectively of about 9% (≈ 10 °C) and 2.5% (≈ 5 bar). Moreover, the SP can precisely describe the swirl number trend indicated by the conjugate analysis, despite a slight underestimation. Regarding the solid temperatures, the SP correctly detects the Min and Max temperatures reached in the domain with a negligible overestimation of ≈ 4 °C in the II° DGS region. Future developments of this work could be represented by:

- The comparison with experimental data, when available.
- The CHT analysis of the entire domain, considering also the low-pressure region and so, the low-passage area gap of the DGSs.
- The development of a new 2D pseudo-solid model for the discretization of 3D fluid structures, such as the Cooling Jackets and the Expander Holes.

To conclude, the low computational cost of the SP makes it compatible with the industrial design time requirements compared to the CHT analysis. Specifically, the computational cost of the CHT, in terms of CPU*Time, is almost 100k times higher than that required by the SP.

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