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Design of radial turbomachinery for supercritical CO₂ systems using theoretical and numerical CFD methodologies

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Abstract

In high temperature waste heat to power conversion applications, bottoming thermodynamic cycles using carbon dioxide in supercritical phase (sCO₂) have recently become a promising developing technology that could outperform conventional Organic Rankine Cycle systems in terms of efficiency and compactness. Moreover, carbon dioxide is a fluid chemically stable, reliable, low-cost, non-toxic, non-flammable and readily available. Supercritical CO₂ power generation systems have been investigated by scientists and engineers mostly for large scale applications. However, when the electrical target output power is lower (50–100 kW), there are additional challenges on the turbomachinery design that need to be addressed. In the current research work, with reference to simple regenerative cycle architecture, the design of small scale sCO₂ radial compressor and turbine are firstly addressed through the similarity approach. Further to this study, numerical CFD simulations are performed to optimize the 3D design of the impellers and of the stators. In particular, steady state RANS simulations using the mixing plane approach are carried out taking into account real gas properties for CO₂.

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Nomenclature

β	Cycle pressure ratio [-]	<u>Subscripts</u>	
η	Efficiency [-]	cold	Cold source
c_p	Specific heat at constant p [$\text{J kg}^{-1} \text{K}^{-1}$]	comp	Compressor
h	Specific enthalpy [J kg^{-1}]	cy	Cycle
\dot{m}	Mass flow rate [kg s^{-1}]	el	Electrical
p	Pressure [Pa]	hot	Hot source
D	Diameter [m]	mech	Mechanical
H_{ad}	Isentropic enthalpy difference [J kg^{-1}]	s	Specific
N	Revolution speed [rad s^{-1}]	tot	Overall
Q	Flow rate [$\text{m}^3 \text{s}^{-1}$]	turb	Turbine
T	Temperature [K]	wf	Working fluid

1. Introduction

Conventional waste heat to power conversion systems are based on Organic Rankine Cycles (ORC) whose working fluids are not suitable for heat sources at high temperature ($>450^\circ\text{C}$). Furthermore, existing ORC systems have a relatively low efficiency at the lower power range increasing the need for alternative technologies that can operate both at higher temperatures and offer higher efficiency [1].

The supercritical CO_2 power cycle (sCO_2) operates in a similar manner to other Brayton cycles and uses Carbon Dioxide in supercritical phase as working fluid. Unlike other working fluids, near the critical point (31°C , 73.8 bar) CO_2 undergoes drastic density changes over small ranges of temperature and pressure and this allows a large amount of energy to be extracted at high temperature using relatively small size equipment, an order of magnitude smaller than steam or gas turbines. Additionally, CO_2 is low-priced, non-toxic, non-flammable and easy manageable [2]. The sCO_2 systems have been firstly conceived for nuclear or concentrated solar power generation applications [3,4]. However, the availability of high temperature waste streams in industrial environments and the limitations on the working fluids for ORC systems at the state of the art contributed to a wider awareness of the potential of sCO_2 systems.

If heat exchangers are crucial for the economic feasibility of a sCO_2 system [5], in the power range below 100 kWe turbomachinery design is undoubtedly the most crucial challenge from a technical perspective. In fact, the high power density leads to small dimensions and high revolution speeds that are challenging for high efficiency. Past research works employed scaling considerations based on the similarity approach proposed by Balje [6] as well as numerical CFD and FEA studies on radial compressors and turbines. In particular, the similarity studies concluded that for power outputs lower than 300 kWe, the turbomachinery technology that is advisable to employ is the single stage radial one with a specific speed in the range 0.4-0.7, such that efficiency is maximized [7,8]. As concerns the numerical studies, different CFD solvers were used. Nevertheless, a coupling with libraries of thermophysical properties to account for the real behavior of carbon dioxide was always performed [9-11].

This paper provides an overview of the design methodology employed in a small scale sCO_2 system for high temperature waste heat to power generation. Once the simple regenerated Brayton cycle was selected according to techno-economic considerations, a thermodynamic analysis coupled with real gas properties and Balje's correlations, provided the design specifics for the compressor-generator-turbine (CGT) unit of the sCO_2 system. In particular, size and speed were estimated and compared to constraints imposed by the bearing technology as well as by the manufacturability of the components. Finally the numerical CFD simulations were performed to optimize the 3D design of the impeller and the stator. In particular, steady state RANS simulations using the mixing plane approach were performed taking into account real gas properties for CO_2 .

2. Preliminary design

2.1. Thermodynamic modelling

The reference cycle architecture for the current study is the simple regenerated Brayton one using flue gas as hot source and water as cold one. This configuration is not as efficient as the recompression one [1,3] but definitely provides the most cost effective solution for the economic feasibility of the heat recovery approach especially at low power outputs (<100 kW_e). With reference to Figure 1, that shows the plant scheme and the entropy diagram of the sCO₂ system, assuming no pressure and heat losses at the interconnecting pipes, the working fluid is compressed (2-4), undergoes a heat gain (A-B) to be eventually expanded (5-6) and cooled back to the initial conditions (D-C). The regenerative heat transfer process occurs from the turbine outlet on the hot side (6-D) and from the compressor outlet with respect to the cold side (4-A) of the recuperator. The heat recovery process takes place in the heater (A-B) while the heat rejection occurs in the cooler (D-C). The modelling approach that has been pursued in the thermodynamic analysis of the sCO₂ system is based on steady state energy balances at the heat exchangers as well as on isentropic efficiency of compressor and turbine. Equations (1-7) are reported in Table 1. The software platform is Engineering Equation Solver (EES) [12] linked with the NIST REFPROP library [13] for the thermophysical properties of working fluids. The compressor and turbine efficiencies that have been assumed for the current analysis are reported in Table 2 together with additional input data.

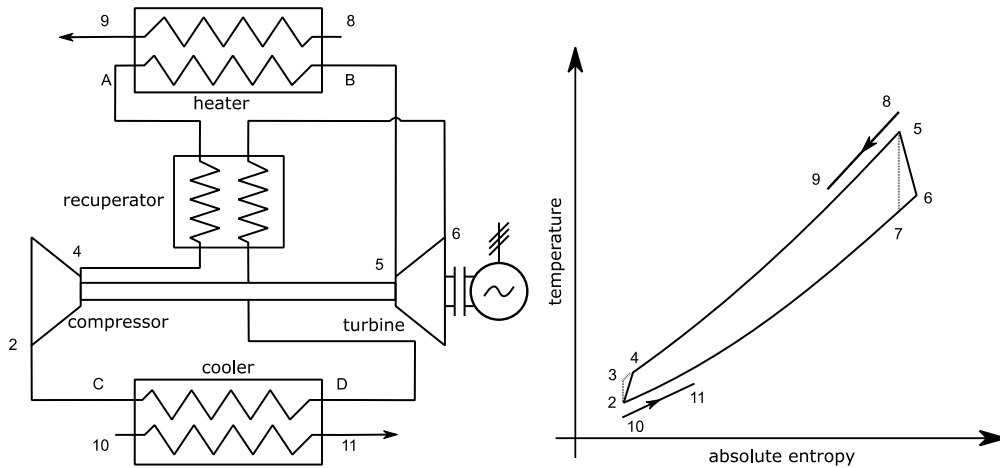


Fig. 1. Scheme and T-s diagram of the Simple regenerative Brayton cycle using supercritical CO₂ (sCO₂)

Table 1. Governing equations

Heater	$\dot{m}_{hot} c_{p,hot} (T_8 - T_9) = \dot{m}_{wf} (h_B - h_A)$	(1)
Recuperator	$h_A - h_4 = h_6 - h_D$	(2)
Cooler	$\dot{m}_{cold} c_{p,cold} (T_{11} - T_{10}) = \dot{m}_{wf} (h_D - h_C)$	(3)
Compressor	$\eta_{comp} = (h_3 - h_2) / (h_4 - h_2)$	(4)
Turbine	$\eta_{turb} = (h_5 - h_6) / (h_5 - h_7)$	(5)
Cycle efficiency	$\eta_{cy} = \frac{\dot{m}_{wf} ((h_5 - h_6) - (h_4 - h_2))}{\dot{m}_{hot} c_{p,hot} (T_8 - T_9)}$	(6)
Overall efficiency	$\eta_{tot} = \eta_{cy} \eta_{mech} \eta_{el}$	(7)

2.2. Turbomachinery design based on similarity considerations

The Balje's charts summarize total to static efficiencies of turbines and compressors with respect to non-dimensional parameters, namely specific speed and specific diameter [6]. Their expressions, proposed in Eqns. 8 and 9 respectively, allow to estimate reasonable values for revolution speed and wheel diameter since adiabatic head and flow rate are known from the cycle analysis.

$$N_s = N Q^{1/2} / H_{ad}^{3/4} \quad (8)$$

$$D_s = D H_{ad}^{1/4} / Q^{1/2} \quad (9)$$

For a given turbomachinery technology in Balje's charts, it is possible to draw a line that, for a given specific speed, provides a value of specific diameter that ensures the maximum efficiency. These lines, called Cordier's lines, were graphically retrieved from Balje's charts for the specific speed ranges strictly related to radial machines and taken into account in the sCO₂ model using Eqns. 10 and 11 for compressor and turbine respectively.

$$D_{S,comp} = 2.719 N_{S,comp}^{-1.092} \quad (10)$$

$$D_{S,turb} = 2.056 N_{S,turb}^{-0.812} \quad (11)$$

The turbine being the most influencing component for the actual energy recovery process, for a given value of its specific speed the model calculates the revolution speed of the turbine from Eqn. 8 and its diameter using Eqns. 11 and 9. Since the CGT configuration is considered a single shaft one, knowing the revolution speed from the turbine calculations allows to compute the compressor specific speed, specific diameter and impeller diameter using Eqns. 8, 10 and 9 respectively.

2.3. Parametric analysis

The effects of cycle pressure ratio and turbine inlet temperature are reported in Figure 2. Both sets of results were calculated neglecting thermal losses in pipes as well as pressure drops in heat exchangers and pipes. In Figure 2 the analysis was carried out with reference to a flue gas mass flow rate of 1 kg/s at 650 °C and assuming a constant temperature difference of 50 K between exhaust gas outlet and CO₂ inlet at the heater.

For a given cycle pressure ratio, a higher turbine inlet temperature leads to a lower amount of CO₂ mass flow rate in the supercritical loop. On the other hand, for a given turbine inlet temperature, a higher cycle pressure ratio leads to a lower turbine outlet temperature and, in turn, to a lower potential for regeneration. Therefore, at the sCO₂ heater, more thermal power is exchanged using a higher CO₂ mass flow rate. For a given cycle configuration, the net power output depends on the specific net work and the amount of working fluid mass flow rate. This fact explains the net electrical power trend that is shown in the top left chart of Figure 2: even though cycle pressure ratio and turbine inlet temperature both enhance the cycle efficiency and its net specific work, because of a lower amount of working fluid that is needed to balance the heat loads at the heater, the net power output decreases at high values of turbine inlet temperature. For instance, with a pressure ratio of 2 and a turbine inlet temperature equal to 400 °C, theoretical electrical power output would be over 87.4 kW with a 1st law efficiency of 24%. At 500 °C the cycle efficiency would rise to 28% but the net power output would drop to 75.7 kWe.

Mass flow rate resulting from the energy balance at the heater and cycle pressure ratio affect revolution speed and diameter of the turbomachinery according to Eqns. 8 and 9. In particular, for a given flow rate, the compressor and turbine will rotate faster and be smaller with increasing pressure ratio. On the other hand, for a given enthalpy rise/drop, smaller flow rates will reduce the size of the machine increasing its revolution speed. Furthermore, in small machines useful flow passages tend to have the same dimensions as leakage paths. Therefore, efficiency values largely accepted and achievable for MW-scale machines can be hardly assumed in kW-scale ones. In particular, for a given revolution

speed of the CGT, due to the high density of the CO₂, it is the compressor the most limiting machine in terms of size. Figure 2 provides some figures related to compressor wheel size and speed showing that cycle configurations with high efficiency demand small and fast machines whose specifics exceed the operational constraints mentioned above. Reasonable thresholds for cost effective turbomachinery are a revolution speed lower than 100,000 RPM and wheel diameter greater than 40 mm. Hence, the application of turbomachinery constraints on the thermodynamic design, limit the design configuration to a maximum cycle efficiency of 23% and a net output power range between 50 and 85 kW.

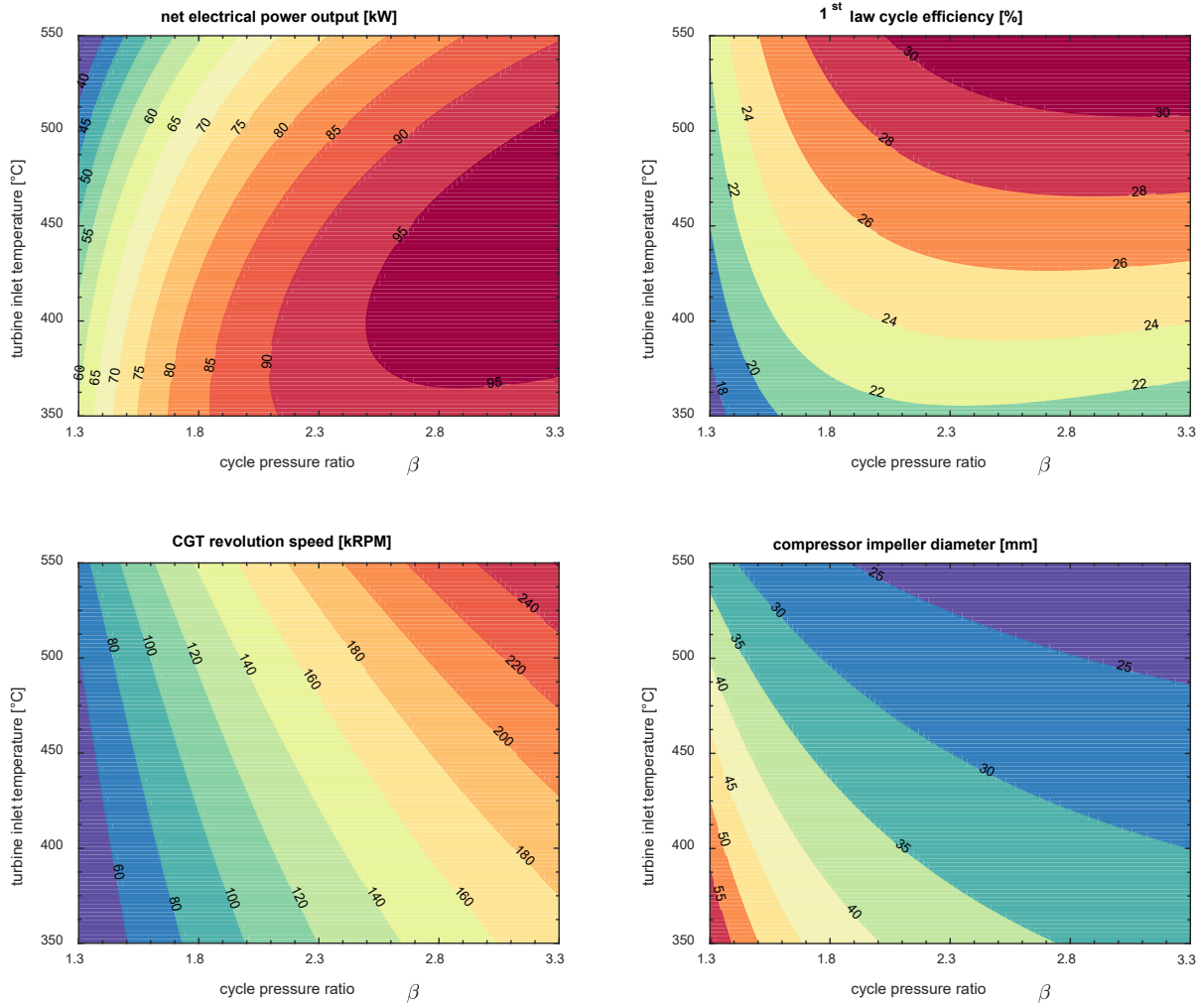


Figure 2 - Influence of sCO₂ cycle pressure ratio and turbine inlet temperature on: net electrical power output (a); cycle efficiency (b), revolution speed of the compressor-generator-turbine system (c); compressor impeller diameter (d)

3. CFD design

A 3D stationary Compressible flow will be considered; a classical coupled Navier-Stokes/Energy Solver is used to solve the general equations of the flow because it is more suited for near Mach velocity values, and the RANS K-Epsilon Model for the turbulence since it has an optimal calculation cost and is stable considering the meshing configuration. Since the fluid is in a supercritical CO₂ state the standard perfect gases equation of state is not

appropriate. The Peng-Robinson equation which has been shown to offer good accuracy near the critical point was employed.

3.1. Turbine

The simulation is split in two different domains; the first one is composed of the volute and diffuser which are designed to distribute the flow into the wheel. They have been optimized in a way that half of the expansion takes place in them. The second domain is composed of the wheel which is designed to convert the energy of the expansion into mechanical energy [14]. This domain is considered as a rotating reference and both centrifugal and Coriolis forces are included in the simulations. Since the velocity of the flow is subsonic at the interface between the two domains, a mixing plane interface is used. As the efficiency of a Turbine for compressible flow is dependent on the pressure ratio, the pressure is imposed at both the inlet and outlet of the domain.

As shown in Fig. 3, the simulation confirms that the chosen design of the Turbine allows for the expansion to happen half in the diffuser and half in the wheel, minimizing the pressure drop in the volute and allowing pressure to power conversion in the wheel.

The simulation shows efficiency of the turbine in the region of 70% at the nominal point.

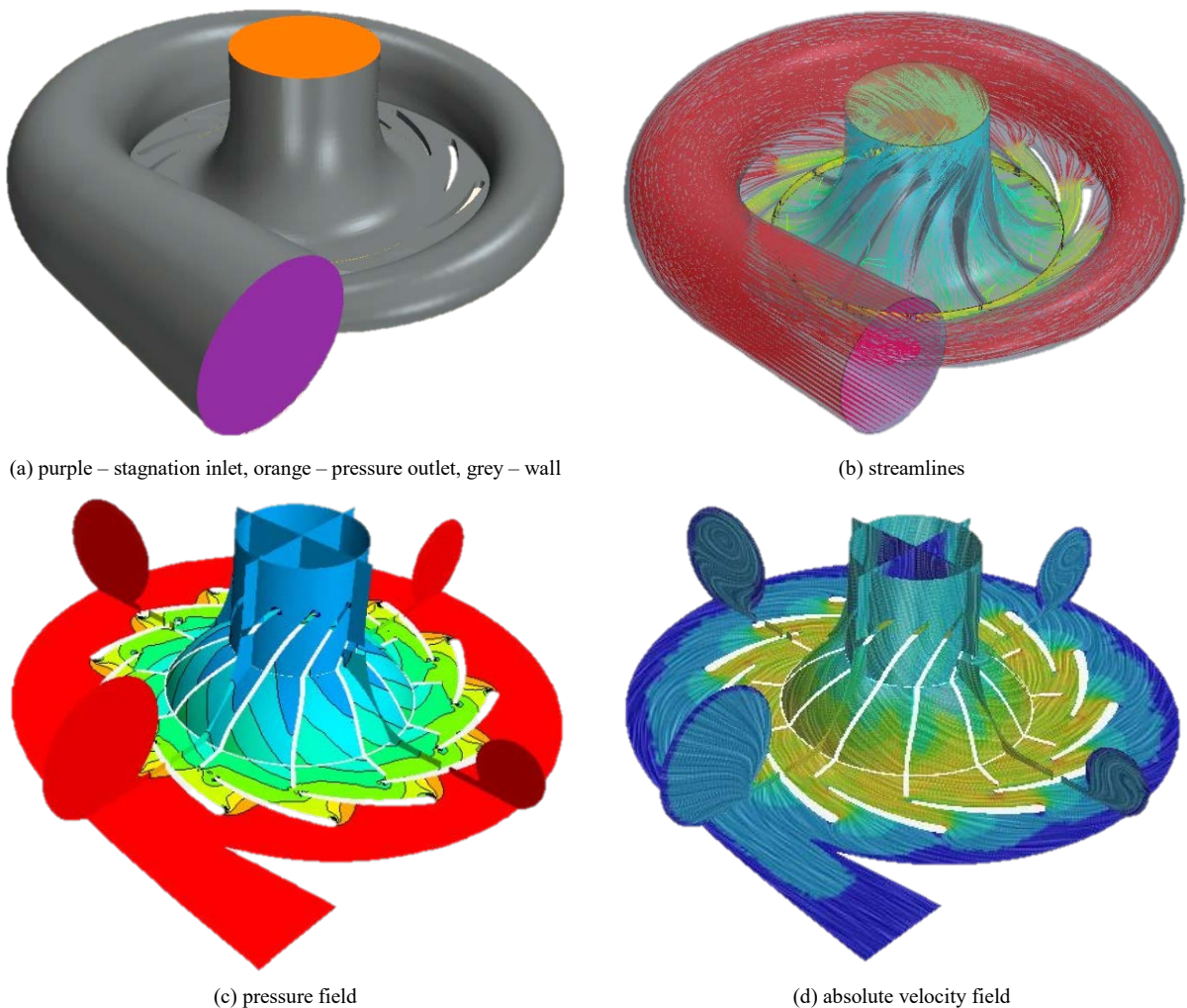


Fig. 3. Turbine CFD design: (a) boundary conditions, (b)-(d) results

3.2. Compressor

Since the outlet pressure in a compressor is higher than the inlet pressure, the pressure should not be imposed at both the outlet and the inlet like for the turbine. Therefore, for stability reasons the static pressure is imposed at the outlet, and the mass flow is imposed at the inlet. The pressure ratio is an output of the simulation not an input, allowing it to be established during the simulation and limiting reversed flows.

Similar to the turbine, this simulation is also split into two different domains, the first is composed of the wheel which has been designed to give the energy to the fluid and the second one which is composed of the diffuser and the volute, which are designed to limit flow rotation and increase the pressure [15].

As shown in Fig. 4, the simulation confirms that the chosen design for the compressor gives the required pressure ratio for the nominal rotational speed. For this design, the predicted compressor efficiency is 76%.

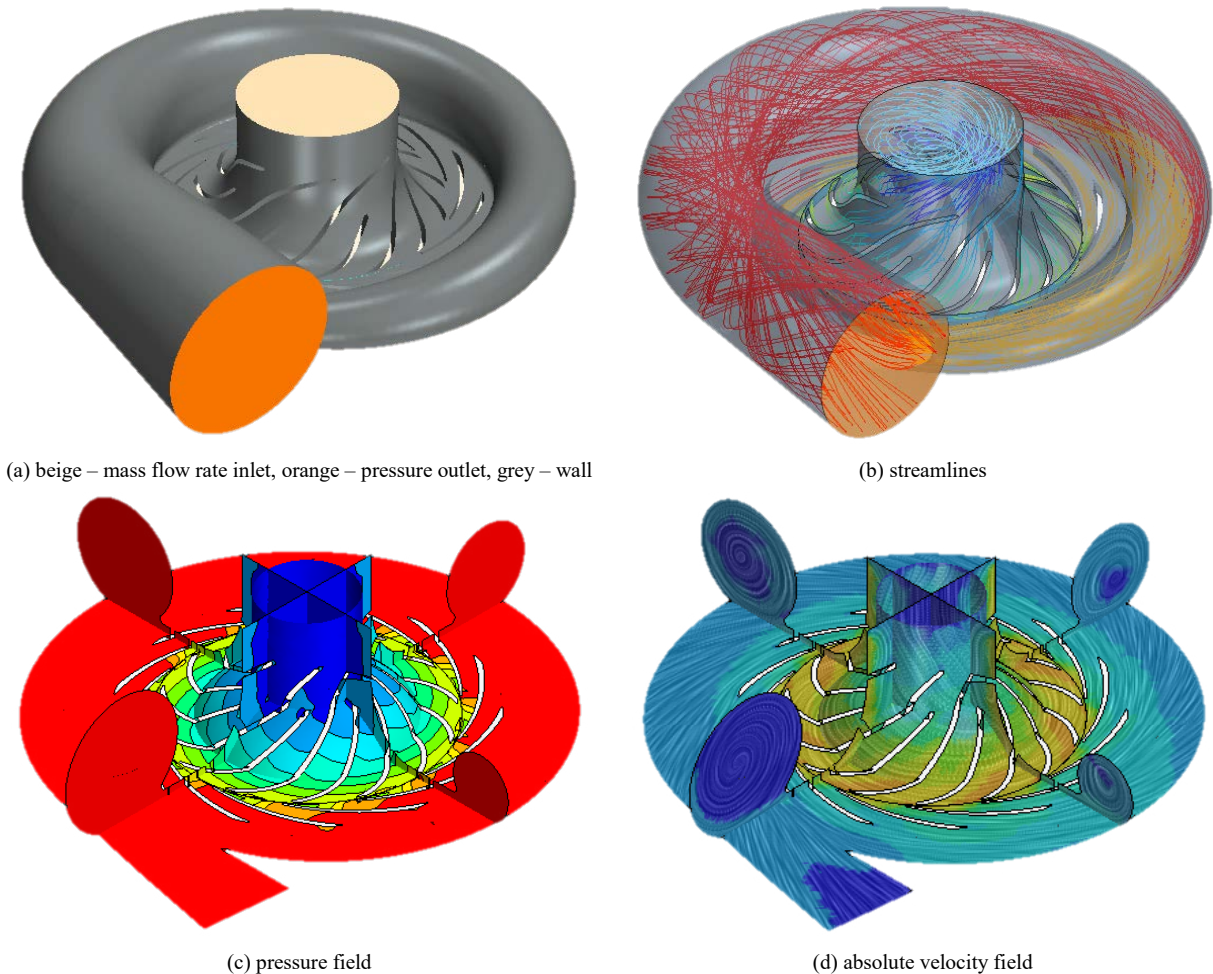


Fig. 4. Compressor CFD design: (a) boundary conditions, (b-d) results

4. Conclusions

The paper presented theoretical and CFD studies on the turbomachinery design for small scale supercritical CO₂ systems. With reference to a simple regenerative Brayton cycle layout, thermodynamic modelling and parametric

studies were carried out. The model takes into account real gas properties as well as Balje's correlations for an estimation of the rotational speed and size of the impellers which are constrained by operational and manufacturing limitations respectively. Once the 3D design of impellers and stator was complete for the compressor and turbine, RANS CFD simulations were performed to validate the design and estimate the efficiency. The turbine efficiency was found to be 70% and the compressor efficiency 76%.

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