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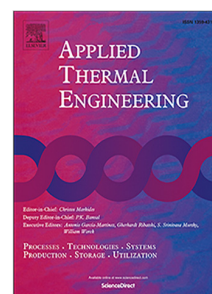
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Salma I. Salah, Francesco Crespi, Martin T. White, Antonio Muñoz, Andrea Paggini, Marco Ruggiero, David Sánchez, Abdulnaser I. Sayma



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Axial turbine flow path design for concentrated solar power plants operating with CO₂ blends

Salma I. Salah^{a,*}, Francesco Crespi^b, Martin T. White^{a,c}, Antonio Muñoz^b, Andrea Paggini^d, Marco Ruggiero^d, David Sánchez^b, Abdunaser I. Sayma^a

^aThermo-Fluids Research Centre, Department of Engineering, City, University of London, Northampton Square, London, EC1V 0HB, United Kingdom

^bDepartment of Energy Engineering, University of Seville, Camino de los descubrimientos s/n, 41092 Seville, Spain

^cThermo-Fluid Mechanics Research Centre, School of Engineering and Informatics, University of Sussex, Brighton, BN1 9RH

^dBaker Hughes, Turbomachinery & Process Solutions, Baker Hughes, Via Felice Matteucci, Firenze, 50127, Italy

Abstract

The utilisation of certain blends based on supercritical CO₂ (sCO₂), namely CO₂/TiCl₄, CO₂/C₆F₆ and CO₂/SO₂, have been found to be promising for enhancing the performance of power cycles for Concentrated Solar Power (CSP) applications; allowing for up to a 6% enhancement in cycle efficiency with respect to a simple recuperated CO₂ cycle, depending upon the nature of the used blend and the cycle configuration of choice. This paper presents an investigation of the impact of adopting these sCO₂-based blends on the flow path design for a multi-stage axial turbine whilst accounting for aerodynamic, mechanical and rotordynamic considerations. This includes assessing the sensitivity of the turbine design to selected working fluid and imposed optimal cycle conditions. Ultimately, this study aims to provide the first indication that a high-efficiency turbine can be achieved for a large-scale axial turbine operating with these non-conventional working fluids and producing power in excess of 120 MW. To achieve this aim, mean-line aerodynamic design is integrated with mechanical and rotordynamic constraints, specified based on industrial experience, to ensure technically feasible solutions with maximum aerodynamic efficiency. Different turbine flow path designs have been produced for three sCO₂ blends under different cycle boundary conditions. Specifically, flow paths have been obtained for optimal cycle configurations at five different molar fractions and two different turbine inlet pressure and temperature levels of 250 & 350 bar and 550 & 700°C respectively. A total-to-total turbine efficiency in excess of 92% was achieved, which is considered promising for the future of CO₂ plants. The highest efficiencies are achieved for designs with a large number of stages, corresponding to reduced hub diameters due to the need for a fixed synchronous rotational speed. The large number of stages is contrary to existing sCO₂ turbine designs, but it is found that an increase from 4 to 14 stages can increase the efficiency by around 5%. Ultimately, based on the preliminary cost analysis results, the designs with a large number of stages showed to be financially feasible compared to the designs with a small number of stages.

Keywords: Axial turbine, CO₂ cycles, mean-line design, CO₂-blends, flow path design.

*Corresponding author

Email addresses: salma.salah.2@city.ac.uk (Salma I. Salah), crespi@us.es (Francesco Crespi), Martin.White@sussex.ac.uk

Highlights

- Axial turbine designs are obtained for CO₂ blends at optimal cycle conditions.
- Recuperated, precompression, and recompression cycle configurations are optimised.
- Turbine designs are achieved using a validated mean-line aerodynamic design model.
- The aerodynamic model is integrated with mechanical and rotordynamic constraints.
- Cycle and turbine efficiencies greater than 50% and 92% were achieved respectively.

1. Introduction

The performance of Concentrated Solar Power (CSP) plants is significantly affected by the thermal efficiency of the power block; where a maximum cycle efficiency of 42% can be obtained by conventional subcritical steam Rankine cycles operating at a maximum steam temperature of 540°C [1]. Further efficiency enhancement in conventional steam cycles, by up to 4.5%, can be achieved by operating at supercritical conditions. Unfortunately, this would result in an increase in the power block capital cost [1] and in slower plant dynamics (less flexibility) during startup and shutdown. Supercritical CO₂ (sCO₂) cycles have been proposed due to their potential to outperform traditional steam cycles for CSP applications if maximum cycle temperatures exceed approximately 550°C [2–5]. This could bring about large reductions in the Levelised Cost of Energy (LCoE) and increase the competitiveness of CSP plants in comparison with conventional power generation systems.

The efficiency enhancement enabled by supercritical CO₂ cycles is primarily a result of reducing compression work through increasing the working fluid density throughout the compression process, alongside the subsequent positive impact on the potential for internal heat recovery. This can be enabled by either condensing the working fluid, or by performing the compression process close to the critical point of CO₂. Nonetheless, achieving this is not feasible for CSP plants inasmuch as they are typically located in hot, arid regions lacking water- or steam-cooling resources. Alternatively, the critical temperature of the working fluid can be increased by doping sCO₂ with other fluids, hence enabling condensation at elevated temperatures of the cooling medium [3, 6–8].

The European Commission funded SCARABEUS project [9] aims to demonstrate the potential of using CO₂ blends for large-scale plants in the order of 100 MW_e. The use of selected blends that lead to higher critical temperatures enables condensation at elevated temperatures, which would increase the conversion efficiencies of supercritical CO₂ power cycles in CSP plants to values of around 50%. Hence, the cycle efficiency can be increased by up to 6 percentage points compared to a simple recuperated CO₂ cycle depending on the cycle configuration of choice and

(Martin T. White), amb1@us.es (Antonio Muñoz), andrea.paggini@bakerhughes.com (Andrea Paggini), marco.ruggiero@bakerhughes.com (Marco Ruggiero), ds@us.es (David Sánchez), a.sayma@city.ac.uk (Abdulnaser I. Sayma)

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3 the nature of the selected blend. In this regard, the SCARABEUS consortium has investigated several chemical com-
4 pounds as possible additives to sCO₂. Amongst these, three candidate dopants have been found to be particularly
5 interesting: Titanium Tetrachloride (TiCl₄, [10]), Hexafluorobenzene (C₆F₆, [11]) and Sulphur Dioxide (SO₂, [12]).
6 Using these dopants enables thermal efficiencies higher than 50% for minimum cycle temperatures (condenser outlet)
7 as high as 50 to 55°C and for a turbine inlet temperature of 700°C [3]. Furthermore, this high thermal performance
8 can be achieved with these blends using relatively simple cycle layouts, namely simple recuperated for TiCl₄, pre-
9 compression for C₆F₆ and recompression for SO₂. These configurations do not require the addition of inter-cooling
10 and re-heating processes; features that seem to be essential to enhance the performance of pure sCO₂ cycles for CSP
11 applications [13] even if they also increase the system capital cost [14]. As a consequence, the use of CO₂-based
12 blends seems to be a very promising means to simultaneously increase cycle efficiency and reduce capital costs.

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19 Supercritical CO₂ power cycles are associated with turbomachinery of a small physical size due to the high density
20 of the working fluid and the low-pressure ratios of the cycle. This could result in more compact turbomachinery, with
21 lower manufacturing, installation and maintenance costs. However, given that sCO₂ turbines operate at high inlet
22 pressures and temperatures, typically between 20 and 25 MPa [15] and 400 and 800°C [16] respectively, they do face
23 some design and operational challenges. Their performance is highly affected by clearance, windage and frictional
24 losses which are typically associated with a compact turbine design, alongside the high density and low kinematic
25 viscosity of the working fluid. The novelty of the working fluid also introduces some uncertainty regarding the
26 suitability of existing design models. Consequently, developing accurate and robust design and performance analysis
27 tools is an important step towards developing new designs, and several studies on this topic have been published for
28 different turbine scales and architectures. Multiple designs have been presented for sCO₂ radial turbines with a power
29 rating of 100-200 kW [17], 50-85 kW [18], 1.5 MW [19, 20] and 10 MW [21], while other authors have focused on
30 designing axial turbines for up to 15 MW [16, 20, 22, 23]. Fewer studies have focused on developing designs for
31 large-scale axial turbines with net power outputs around 100 MW power rating [24], and no studies have previously
32 considered blends. Conceptual designs have also been developed for axial turbines with power ratings of 246 MW,
33 450 MW, 645 MW and turbine efficiencies of 92.9%, 90% and 90% have been predicted respectively [25–27].

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43 To explore the feasibility and operation of the CO₂ cycle and to test key components, several test rigs have been
44 developed, which includes the development of experimental turbine prototypes with up to 8 MW power output [28–
45 33]. Within the group of developed prototypes, there is a single 1 MW axial turbine, whilst the rest have been of
46 the radial turbine configuration. It has been found that sCO₂ turbines experience several operational challenges due
47 to the compact geometries, high density and low kinematic viscosity of the working fluid compared to air. This
48 results in challenges related to the design of the seals and bearings, particularly for small-scale demonstrators which
49 are associated with high rotational speed and the increased potential for rotordynamic instability. On a different
50 note, the high inlet temperature can pose challenges related to material selection, alongside challenges related to the
51 throttle control and turbine stop valve, since the valves are placed at the highest temperature point in the cycle [34].
52 Furthermore, structural and mechanical considerations have been found to be highly significant for dense working
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3 fluids such as sCO₂ [35]. Specifically, supercritical CO₂ is expected to result in higher aerodynamic loads compared
4 to air and steam turbines, partly due to the large pressure differences experienced across the turbine, but also because
5 of the high density of the fluid. Ultimately, these considerations can introduce constraints that reduce the feasible
6 turbine design space; hence, it becomes important to consider structural and mechanical design aspects throughout
7 the design process to ensure feasible turbine designs are obtained.
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11 Previous studies have focused on the conceptual design of turbomachinery and the development of testing facilities
12 for CO₂ based plants, with an emphasis on radial turbine configurations with a reduced power rating. Comparatively,
13 the current study, and the SCARABEUS project more generally, is concerned with the use of sCO₂ blends within
14 large-scale CSP plants (100 MW_e) that utilise an axial turbine. Given that the turbine efficiency significantly affects
15 the overall plant performance, it is important to ensure that high efficiency axial turbine designs can be achieved for
16 the optimal blend and cycle conditions that result in the highest cycle thermal efficiency. Therefore, the aim of this
17 paper is to study the impact of adopting different sCO₂-based blends on the turbine flow path design, and to assess
18 the achievable aerodynamic performance whilst accounting for practical mechanical and rotordynamic constraints.
19 Moreover, the paper aims to assess the sensitivity of the turbine design to the working fluid selected and to the
20 boundary conditions resulting from cycle optimisation.
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24 The novelty of this work lies in achieving the stated aim by introducing both mechanical and rotordynamic design
25 constraints within a mean-line aerodynamic design model to restrict the maximum bending stress acting on the blades
26 and the axial flow path length. Ultimately, the results from this study provide the first indication that a high-efficiency
27 turbine with an efficiency in excess of 92% can be achieved for a 100 MW_e power cycle operating with sCO₂-based
28 blends.
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32 The paper is structured as follows: an overview of the thermodynamic cycle modelling used to define the bound-
33 ary conditions for the turbine design is presented in Section 2. The turbine design methodology is summarised in
34 Section 3, which includes details relating to the aerodynamic design process alongside the mechanical design con-
35 siderations that apply for large-scale axial turbine. The results are presented and discussed in Section 4, where the
36 effect of the selected blend and imposed cycle boundary conditions on cycle and turbine performance are evaluated
37 (Section 4.1 & 4.2). Finally, the main conclusions of this study are presented in Section 5.
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45 46 **2. Cycle modelling**

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48 In order to study the impact of adopting different sCO₂-based blends on the turbine flow path design, cycle sim-
49 ulations were carried out using Thermoflex, which is a commercial software [36] selected for its widely-recognised
50 reliability. The simulations were conducted for a wide range of possible blends with the aim of defining a set of
51 turbine boundary conditions to be considered in the turbomachinery analysis.
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55 Thermal efficiency (η_{th}) is taken as the main figure of merit for cycle performance, although a detailed comparison
56 of other performance metrics based on both first and second law analyses can be found in previous publications by
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the authors [3, 37]. Thermal efficiency is expressed as the ratio of cycle specific work W_s to the enthalpy rise across the primary heat exchanger Δh_{PHX} , where the latter is a direct indicator of the heat recovery potential of the cycle (a lower Δh_{PHX} implies a larger heat recovery internal to the cycle):

$$\eta_{th} = \frac{W_{turb} - W_{compr}}{\dot{m}_{turb} \Delta h_{PHX}} = \frac{W_s}{\Delta h_{PHX}} \quad (1)$$

Three different chemical compounds are taken into account to produce CO₂ blends, namely Hexafluorobenzene (C₆F₆), Titanium Tetrachloride (TiCl₄) and Sulphur Dioxide (SO₂), and their main thermophysical properties are provided in Table 1. These dopants are chosen due to their good availability and the potential performance enhancement. In particular, a preliminary screening carried out by the SCARABEUS consortium has revealed that using C₆F₆, TiCl₄ and SO₂ resulted in the largest enhancement in cycle performance among more than thirty chemical compounds [8, 11, 12]. It is worth noting that the three selected dopants present different thermodynamic behaviour, particularly in terms of critical pressure and molecular complexity¹. However, they all have a critical temperature significantly higher than that of pure CO₂, which is a key feature required for to enable working fluid condensation at a minimum cycle temperature up to 50-60°C. A brief overview of potential safety hazards for the three selected dopants, developed according to standard 704 of the National Fire Protection Association, is presented in Table 1. The use of both TiCl₄ and SO₂ might face some potential limitations because of the corrosion effects due to the high reactivity of TiCl₄ with air moisture and the formation of H₂SO₄ when SO₂ combines with water. This is currently being investigated by the SCARABEUS consortium (more information about the utilisation of SO₂ can be found in [12]). Despite this, it is worth highlighting that the health hazards posed by SO₂ or TiCl₄ are very similar to, and potentially even lower than, those of other fluids commonly employed in CSP plants, such as Therminol VP1 (a common heat transfer fluid in parabolic-trough power plants), or in air-conditioning and refrigeration systems, such as ammonia, propane and R-1234yf [12]. More information about these compounds can be found in previous publications by the authors [3, 6]. Focusing on other environmental considerations, these dopants present virtually no ozone depletion or global warming potential and they are not included in the lists of ozone-depleting and green-house gases by the United States Environmental Protection Agency (EPA, [40, 41]). According to EPA, very high concentrations of Sulphur Dioxide may present some issues related to the formation of acid rain [42], but two observations can be made in this regard. Firstly, high concentrations of SO_x are typically produced from the exhaust/stack gases from combustion processes. However, no combustion takes place within the SCARABEUS CSP plant, and hence the only source of SO₂ released to the environment is through leakage from the system and these can be minimised in rotating machinery by the utilisation of dry gas seals [43]. Secondly, such leakages could be virtually eliminated in the near future as a result of the adoption of hermetically sealed turbomachines. Accordingly, the environmental impact of the selected dopants considered within SCARABEUS is deemed minimal.

¹The molecular complexity of a fluid is directly related to the molecular structure and the degrees of freedom of the atoms in its molecule, and it can be considered proportional to the specific heat [38]. In this work, it has been estimated as $(T_c/R) \cdot (dS/dT)_{T_R=0.7}$, according to [39](p.109).

The thermal stability of the dopants is currently being experimentally investigated within the SCARABEUS consortium. A summary of the main results is presented in Table 1. Titanium Tetrachloride (TiCl_4) shows very promising results, with thermal degradation observed only for temperatures above 700°C . Currently, no detailed information is available for CO_2 and SO_2 , which are currently being tested, although several references in the literature indicate that this blend is thermally stable for temperatures higher than 700°C [44]. On the contrary, C_6F_6 has been found to show clear signs of thermal degradation for temperatures above 600°C ². For this reason, turbine inlet temperatures exceeding this temperature are not considered for this dopant.

Table 1: Dopants thermophysical properties (columns 2 to 6) and hazard according to NFPA 704 [46] (columns 7 to 10).

Chemical Compound	MW [kg/kmol]	T_{cr} [$^\circ\text{C}$]	P_{cr} [bar]	Molecular Complexity [-]	Thermal Stability	Health Hazard	Flammability	Chemical Reactivity	Special Hazard
CO_2	44.01	31.06	73.83	-9.324	$>700^\circ\text{C}$	2	0	0	Simple Asphyxiant
SO_2	64.06	157.60	78.84	-8.230	$>700^\circ\text{C}$	3	0	0	-
C_6F_6	186.06	243.58	32.73	12.740	$<625^\circ\text{C}$	1	3	0	-
TiCl_4	189.69	364.85	46.61	1.922	$>700^\circ\text{C}$	3	0	2	React with water

Previous studies have demonstrated that the selection of the best cycle layout depends strongly on the nature of the dopant employed [3]. For this reason, simple recuperated, *precompression* and *recompression* cycles are considered in this paper, for $\text{CO}_2/\text{TiCl}_4$, $\text{CO}_2/\text{C}_6\text{F}_6$ and CO_2/SO_2 respectively. This selection is based on earlier studies which confirmed that these configurations are capable of better exploiting the potential of each dopant. The three cycles, whose layouts are provided in Figure 1, are considered here in transcritical configuration due to the condensing characteristics of the proposed plant concept. A simple recuperated cycle sets a direct constraint on turbine exhaust pressure, which is constrained by the condensation pressure that is defined from the minimum cycle temperature. Even if this is not a problem for the $\text{CO}_2/\text{TiCl}_4$ blend, which is characterised by an extremely high recuperative potential, it degrades the thermal performance when using $\text{CO}_2/\text{C}_6\text{F}_6$ and CO_2/SO_2 blends. Thus, the *precompression* and *recompression* configurations have been considered, which are minor variations of the simple recuperated cycle that involve splitting the internal heat recovery process in two (i.e., through low and high-temperature recuperators) and the installation of an additional compressor in the cycle.

In the *recompression* layout, a recompressor is added at the outlet from the low-pressure LTR to enhance heat recovery by balancing the heat capacity rate of the two streams [47]. As for the *precompression* cycle, a precompressor is installed in the low-pressure stream between the low and high-temperature recuperators (LTR and HTR). This helps to overcome the constraint imposed by the condensation temperature on the turbine exhaust pressure, thereby increasing the specific work of the cycle. It is worth noting that these configurations were proposed around 50 years ago by Gianfranco Angelino for power cycles running with pure CO_2 [47].

²This threshold temperature was obtained by the University of Brescia and Politecnico di Milano within the SCARABEUS project [45]

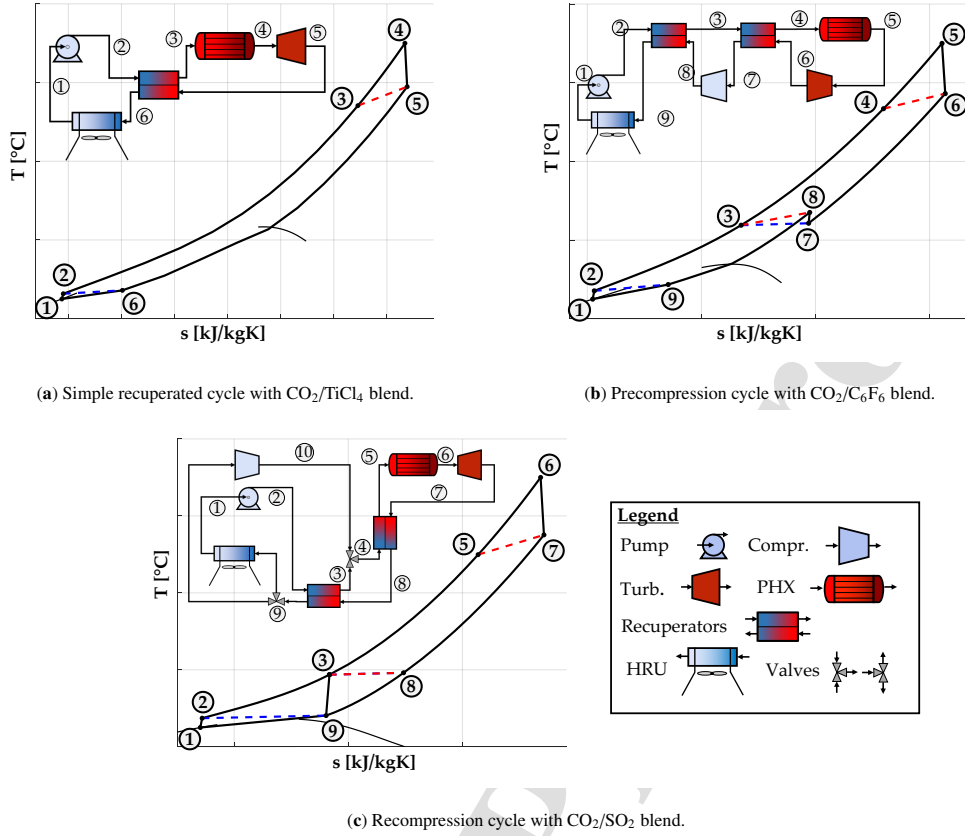


Figure 1: Cycle layouts considered in the analysis (adapted from [48]).

To assess the influence of dopant concentration on cycle performance and turbine design, a sensitivity analysis was carried out considering this parameter (see Table 2). This analysis aims to explain the underlying thermodynamic behaviour of each cycle configuration considered in order to identify the most promising operating conditions. To do so, the following molar fraction X_i ranges are defined for each dopant: 10-20% for C_6F_6 , 14-24% for TiCl_4 and 30-40% for SO_2 . In each case, eleven different molar fractions are considered, at 1% intervals (e.g., 10-11-12...20% for C_6F_6 case), and then a reduced number of representative cases are identified and employed as boundary conditions for the turbine analysis (the criteria used in this selection are reported in Section 4.2.1).

The molar fraction ranges are obtained starting from the lower bound (i.e., minimum allowable dopant fraction), which is strongly dependent on the nature of the chemical compound considered. The criterion used to define the lower bound for each dopant is that the difference between the minimum cycle temperature (T_{min}) and the critical temperature of the resulting blend (T_{cr}) must be equal to or higher than 30°C . This 30°C temperature gap is a conservative assumption made to ensure that the compression process is not carried out in close proximity to the critical point (for more information, see [12]). In the present study, T_{min} is set to 50°C , which means that the resulting T_{cr} must be equal to or higher than 80°C ; this corresponds to a minimum dopant molar fraction of 10%, 14% and 30% for

C₆F₆, TiCl₄ and SO₂ respectively. The different values are caused by the heterogeneous thermodynamic behaviour of the blends considered, which is caused by each dopant leading to a different critical point. It is worth noting that dopants with higher critical temperatures yield wider, and more pronounced, pressure-temperature envelopes and critical loci curves. A graphical representation of this is shown in Figure 2, where the critical points of the three blends are presented together with an indication of the aforementioned 30°C temperature gap and the resulting minimum dopant molar fractions considered in this study. The critical loci curves, along with the thermophysical properties of all blends, have been obtained with the standard Peng-Robinson Equation of State³. The corresponding Binary Interaction Parameters (K_{ij}), provided in Table 2, have been obtained by regression of experimental VLE (Vapour Liquid Equilibrium) data available within the Aspen library [50–52].

Table 2: Set of dopant specifications employed: range of molar fraction (X_i), Equations of state (EoS) and Binary Interaction parameter (K_{ij}).

Dopant	X_i [%]	EoS	K_{ij}
TiCl ₄	14-24	Standard Peng-Robinson	0.0704
C ₆ F ₆	10-20	Standard Peng-Robinson	0.16297 - 0.0003951 T[K]
SO ₂	30-40	Standard Peng-Robinson	0.0242

Further information regarding the computational environment can be found in one of the authors' previous works [3]. In the current study, a common set of boundary conditions and assumptions for key system components are employed, as summarised in Table 3. A gross power output of 100 MW_e is considered, while two different turbine inlet temperatures are taken into account: 550°C to represent a state-of-the-art value for solar towers, and 700°C, which is representative of next-generation CSP plants. Additionally, a sensitivity analysis on the maximum cycle pressure is carried out, which is varied between 250 and 350 bar.

Table 3: Boundary conditions and specifications of turbomachinery and heat exchangers.

PIT	TIT	P_{max}	η_{is} [%]	ΔT_{min}	ΔP_{heater}	ΔP_{cond}	ΔP_{rec} [%]
[°C]	[°C]	[bar]	Pump/Turb/Compr	[°C]	[bar]	[bar]	Low P / High P
50	550/700	250	88 / 92 / 89	5	1.5	1	1 / 1.5

³Recent publications by the SCARABEUS consortium identified PC-SAFT as the best Equation of State to estimate the thermo-physical properties of CO₂/SO₂ blends under real gas conditions (close to the critical point) [12, 49]. Nevertheless, the boundary conditions of the turbine in the present paper correspond to thermodynamic behaviour that is very close to that of an ideal gas, with compressibility factors ranging from 1.01 to 1.05 [12]. Bearing this in mind, the utilisation of Peng-Robinson EoS in this manuscript is not a concern in terms of accuracy.

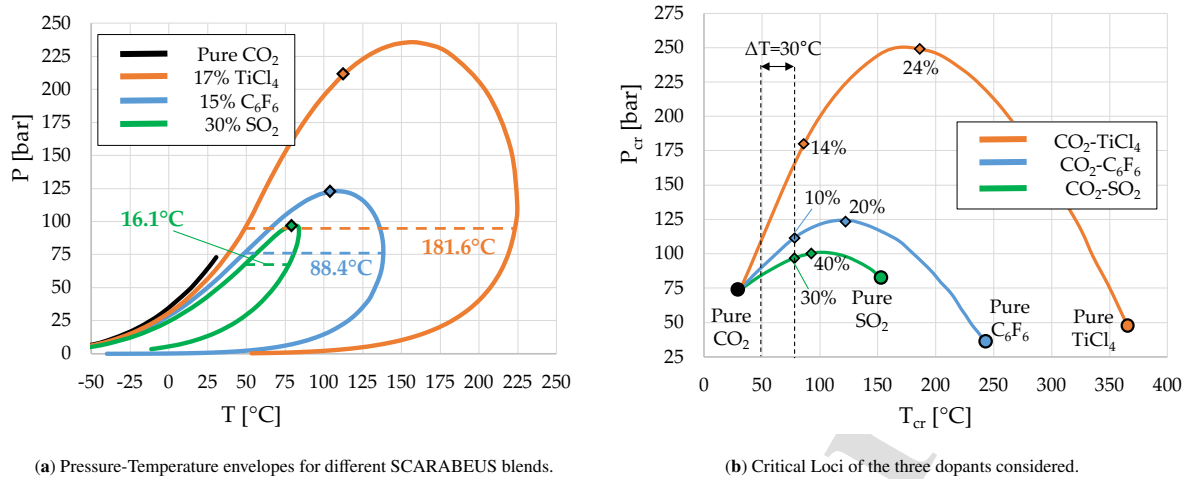


Figure 2: Pressure-Temperature envelopes for three different blends and pure CO₂ (left) and critical loci for the three dopants (right), adapted from [12]. In Figure (a), critical points are represented by markers while temperature glides for a bubble temperature of 50°C are indicated with dotted lines and their numerical values are reported in the labels

3. Turbine design methodology

To design the turbine aerodynamic flow path, a multi-stage mean-line design approach has been implemented. The model used in the current study builds on an earlier model, and full details of the approach can be found within one of the authors' previous works [53], alongside the details provided in in Appendix A. In summary, within the previous model the steady-state mass, energy, and momentum equations were solved at each station within the turbine at the turbine mean diameter. Designing the flow path at a constant mean-diameter results in a hub diameter that decreases from the turbine inlet to the turbine exhaust, and this results in an increase in the radius ratio along the turbine. As a result, turbine blades with a larger chord size are required to limit the stresses on the blade roots, which in turn has a knock-on effect since larger chord sizes result in larger roots and introduce additional challenges relating to the stiffness and rotordynamics of the rotor. Therefore, the previous design methodology [53], has been updated to enable the flow path to be constructed assuming a fixed hub diameter and a variable mean diameter, which reduces the impact of these potential rotordynamic and mechanical challenges. The design model assumes repeating stages, and for a given set of design inputs the blade geometry, velocity triangles and thermodynamic properties can be obtained for each turbine stage; further details on the design variables are provided later in this section. To evaluate the aerodynamic performance of the turbine, the design tool is integrated with the Aungier [54] loss model to obtain the total pressure loss coefficients for the stator and rotor of each stage. This loss model has been found by the authors to be the most suitable for sCO₂ turbine design [53]. The losses considered in the model include profile, secondary flow, tip clearance and trailing edge losses [54]. In line with the thermodynamic cycle analysis, the thermodynamic properties for the blends are obtained using the standard Peng Robinson equation of state (EoS) using consistent

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3 binary interaction parameters.
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5 In addition to evaluating the aerodynamic turbine performance, mechanical and rotordynamic design constraints
6 are introduced into the mean-line design methodology. This ensures only technical feasible turbine designs are pro-
7 posed, which in turn enables a fair comparison of the achievable turbine performance for the different dopants and
8 corresponding cycle conditions (i.e., composition, pressures, temperatures and mass-flow rate). The main mechanical
9 and rotordynamic constraints are introduced based on industrial experience and are formulated from a number of key
10 design parameters that can be easily assessed and controlled throughout the mean-line design process. The rationale
11 for the mechanical design can be summarised as follows:
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- 16 • Synchronous designs with a rotational speed of 3,000 RPM (i.e., 50 Hz grid frequency) are selected for a plant
17 power with a net power output of 100 MW sCO₂, due to the difficulty of incorporating a gearbox for such
18 turbine scales.
19
- 20 • Considering that the expanding fluid is characterised by a large power density, it is assumed that the bending
21 stresses generated by the expansion are more critical than the centrifugal stresses generated by blade rotation.
22 Thus, the target in the mean-line design is to keep the static bending stresses under a suitable limit. For the pre-
23 liminary design phase a limit of < 130 MPa has been set based on industrial experience considering alternating
24 and centrifugal stresses that are consistent with sCO₂ applications.
25
- 26 • The bending stress limit is fixed at a constant value for all stages, regardless of the different operating tem-
27 peratures encountered by each stage. This assumption is reasonable since the blade materials identified for this
28 application are all nickel-based alloys, which do not exhibit significant degradation in the mechanical properties
29 of interest within the operating range of the whole turbine (inlet to exhaust).
30
- 31 • The chords of the airfoils of each blade row are scaled targeting bending stresses within the limit established.
32 Static stresses are calculated assuming a constant dimensionless second moment of area of the airfoil and
33 without considering any stress intensification factor, where this factor was considered in the establishment of
34 the bending stresses threshold.
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- 36 • To allow the preliminary sizing of the blade root, and to subsequently estimate the rotor stiffness parameter,
37 a preliminary value for the airfoil chord length is selected (< 100 mm). The rotor stiffness is an essential
38 parameter driving the rotordynamic behaviour of the turbine.
39
- 40 • The number of stages and the estimation of the chord length allows an estimation of the overall length of the
41 flow path. Longer flow path designs are associated with smaller hub diameters and since weight is proportional
42 to the flow path length and to the hub diameter squared, it could be anticipated that increasing the number of
43 stages may not increase cost. However, since the overall cost of the turbine is an essential criterion within the
44 SCARABEUS project a cost analysis is included in a later section of this paper.
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- The estimation of the overall length of the flow path enables a preliminary assessment of rotordynamic stability within the mean-line design with the introduction of the slenderness ratio (SR); this is defined as the ratio of the bearing span to the hub diameter. The limiting value for the slenderness ratio has been established based on the results of detailed rotordynamic assessments carried out for other similar turbines for supercritical CO_2 applications (< 9).

Within the multi-stage axial turbine design model, a constant enthalpy drop is assumed across each stage, whilst a constant value for the loading coefficient (ψ), flow coefficient (ϕ), degree of reaction (λ), trailing edge to throat ratio (t/o) and pitch to chord ratio (s/c) of each stage is assumed. These assumed values are listed in Table 4. These parameters are set based on well established turbomachinery design practices, and whilst it is true that a further increase of turbine efficiency may be achieved through additional refinement of these parameters, one can expect the designs obtained under these assumptions to result in practically feasible designs that result in high efficiencies. More specifically, the loading and flow coefficients are selected to allow for an optimum turbine aerodynamic performance based on the Smith chart [55], while the trailing edge to throat ratio is selected to reduce the trailing edge losses based on the specified range in the literature [56]. Finally, the pitch to chord ratio is set based on recommendations within the literature [57]. The axial spacing between the turbine stages, and the radial tip clearance gap, have been specified as a percentage of the upstream pitch and tip diameter respectively.

Alongside the specified design parameters, an initial assumption for the number of rotor blades (n_{blades}), number of stages (n_{stages}), total-to-total efficiency (η_{tt}) and stator enthalpy loss coefficient (λ_N) is specified for each case. This allows the velocity triangles and thermodynamic properties along the flow path to be obtained. Following this, the blade geometry can be obtained for each stage based on the specified pitch-to-chord ratio, which includes the chord length (c), hub diameter (D_{hub}), blade height (h) and pitch (s). Using the Aungier loss correlations, the total pressure loss coefficients are then predicted [54] and these are converted to enthalpy loss coefficients using the correlations defined in Ref [58]. The mean-line design is then repeated using the updated values for λ_N and the total-to-total efficiency of each stage (η_{tt}). Once the system of equations converges, the design can be evaluated based on the specified rotordynamic and mechanical constraints to ensure that $\sigma_{bending}$, c and SR are within the threshold limits. If the design does not meet the specified criteria, the number of blades ($35 < n_{blades} < 100$) and number of stages are adjusted manually until the mechanical and rotordynamic design constraints are met. As a general example, the chord length should be increased (and the number of blades decreased accordingly to maintain the same solidity) to reduce the bending stresses and the number of stages should be reduced to allow for a reduced slenderness ratio. A more detailed description of the design methodology is provided in [Appendix A](#).

The turbine design model has been verified and cross-checked with published numerical and experimental studies in previous work by the authors [53]. Specifically, this covers different working fluids including air, sCO_2 and R245fa, with power rating between 144 kW and 10 MW. A good agreement is obtained for the blade dimensions and flow angles, alongside the predicted total-to-total efficiency, with maximum percentage differences of 1.3% and 1.2% in

the total-to-total and total-to-static efficiency respectively within the four selected verification cases. Further details are also presented in [Appendix A](#).

Table 4: Mean-line turbine design parameters

Decision variables	Description	units	Value
N	Rotational speed	[RPM]	3000 (50 Hz motor)
k_s	Surface roughness	[mm]	0.002
ϕ	Stage flow coefficient	[-]	1 [55]
ψ	Stage loading coefficient	[-]	0.5 [55]
Λ	Degree of reaction	[-]	0.5 [55]
t/o	Trailing edge thickness to throat ratio	[-]	0.05 [56]
s/c	Pitch-to-chord ratio	[-]	0.85 [57]

4. Results and discussions

4.1. Cycle analysis

In this section, the results obtained for variable dopant concentration, maximum cycle pressure (P_{max}) and turbine inlet temperature (TIT) are discussed. This discussion is driven by the impact on thermal efficiency, with the objective to select the cases with highest efficiency for the associated turbine flow path design.

Figures 3 to 5 present the trend of thermal efficiency (η_{th}) as a function of the molar fraction and maximum pressure for $TiCl_4$, C_6F_6 and SO_2 respectively, using a combined surface and contour map. The first important observation is that the simple recuperated cycle with $TiCl_4$ is the only cycle whose thermal efficiency is significantly affected by the variation in P_{max} and X_i . For this system, η_{th} ranges from 41.5% up to 45.5% at 550°C TIT and from 48 to 51.5% at 700°C. On the contrary, the thermal efficiency of the precompression cycle with C_6F_6 is barely affected by changes in maximum pressure and molar composition, with values in the range 42.75-43.15% at 550°C. Finally, the recompression cycle with SO_2 exhibits more intermediate behaviour, with thermal efficiency in the order of 43.5-44.5% and 50.3-51.5% at 550°C and 700°C respectively, showing only a slight dependence on both P_{max} and X_i .

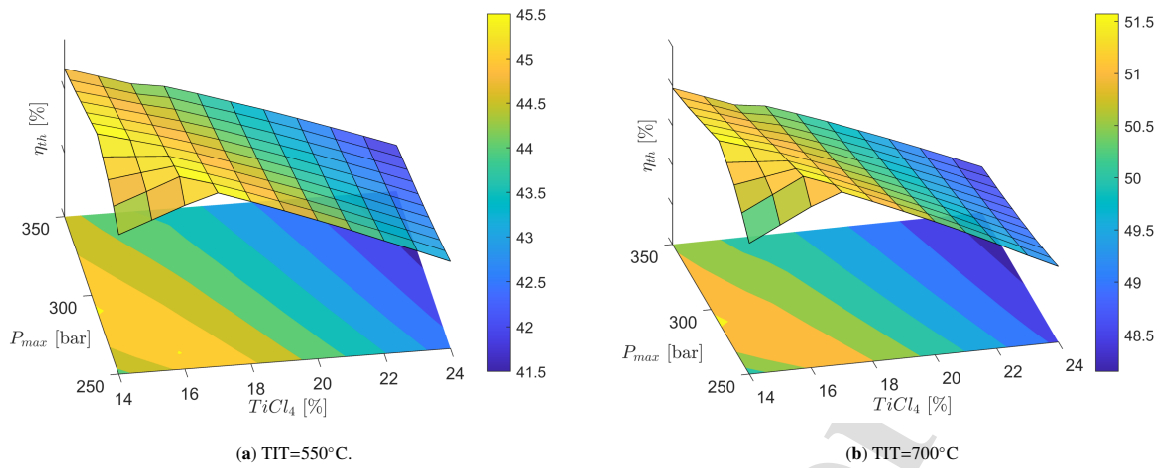


Figure 3: Thermal efficiency of a simple recuperated cycle operated with $CO_2/TiCl_4$ blend as a function of maximum cycle pressure and dopant molar fraction. Two turbines inlet temperatures are considered.

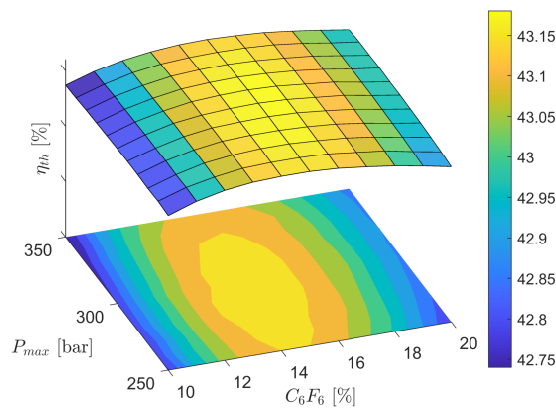


Figure 4: Thermal efficiency of a precompression cycle operated with CO_2/C_6F_6 blend as a function of maximum cycle pressure and dopant molar fraction, considering a turbine inlet temperature of $550^\circ C$ (results at $700^\circ C$ are not reported due to the limited thermal stability of this blend).

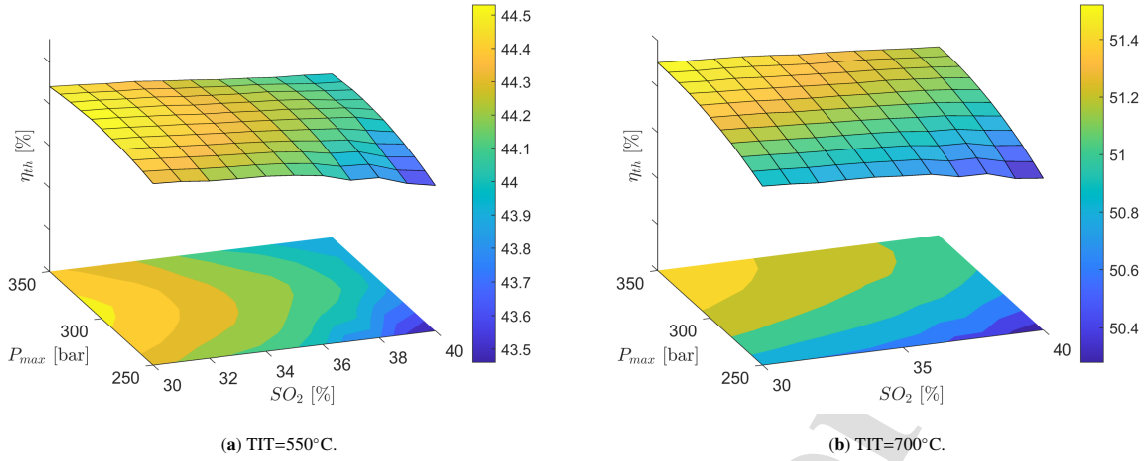


Figure 5: Thermal efficiency of a recompression

cycle operated with CO_2/SO_2 blends as a function of maximum cycle pressure and dopant molar fraction. Two turbines inlet temperatures are considered.

Other interesting observations can be made by focusing on the optimum molar composition (i.e. the molar fraction of dopant that yields peak cycle efficiency). For $\text{CO}_2/\text{TiCl}_4$ blend, the molar fraction varies significantly with maximum cycle pressure, from 18% at 250 bar down to 14% for 350 bar, though its dependence on TIT is very weak. At both temperature levels (550°C and 700°C), peak thermal efficiency values are achieved at mid- to low molar fractions and pressures while efficiency is lowest on the top-right corner of the contour map (high P_{max} and X_i). The situation changes drastically for CO_2/SO_2 blend, which achieves optimum performance for dopant concentrations around 30%, regardless of the inlet pressure and temperature. Interestingly, considering the contour maps, the optimum P_{max} is found to depend on the temperature considered, shifting from 310 bar to 350 bar when TIT is increased from 550°C to 700°C. A thorough explanation of this pattern, based on a 2^{nd} -law analysis, is provided in [48]. Nevertheless, from a practical standpoint, the interest in operating at such high pressures may be offset by the technical limitations derived from the need for bulkier, more expensive equipment, which may not be compensated for by the limited η_{th} gain. Therefore, a thorough thermo-economic analysis will be required to identify the optimum cycle operating conditions.

The dissimilar scenario for each dopant is a result of adopting different cycle layouts for the different blends. This is better understood if thermal efficiency is expressed as the ratio of cycle specific work W_s to the enthalpy rise across the primary heat exchanger Δh_{PHX} , see Eq. (1). For a closed recuperative cycle, operating with a given working fluid composition, an increase in pressure ratio (PR) results in higher values of W_s & Δh_{PHX} . On the one hand, W_s is enhanced due to the higher turbine expansion ratio (ER). On the other hand, a higher ER also leads to a lower turbine outlet temperature, which directly affects the PHX inlet, thus increasing Δh_{PHX} . The higher pressure ratios come not only from a higher P_{max} but also from the higher X_i dictated by the condensing nature of the transcritical layouts investigated in this study. In such systems, the pump inlet pressure ($P_{in,pump}$) is set by the minimum cycle

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3 temperature ($T_{min}=50^{\circ}\text{C}$) and a higher concentration of dopant implies a lower pump inlet pressure, brought about by
4 the higher critical temperature and pressure of the blend [3]. This results in higher cycle pressure ratios if a constant
5 maximum cycle pressure is considered, and this become even more evident when P_{max} and X_i are increased at the same
6 time. However, in this case the change in working fluid composition leads to significantly different thermodynamic
7 properties which consequently affect the heat recovery potential; this leads to an overall drop of W_s and Δh_{PHX} , and a
8 significant rise in the working fluid mass flow rate [3]. In both cases, the thermal efficiency of the investigated cycle
9 is determined by the trade-off between the variations observed in specific work, and the heat recovery potential as a
10 consequence of the higher cycle pressure ratio. Therefore, in order to understand the reasoning between the different
11 trends of η_{th} shown in Figures 3a to 5a, a deeper analysis of the effect of varying the PR on W_s and Δh_{PHX} for each
12 system is necessary.
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19 For this purpose, two different scenarios are analysed: variable P_{max} for constant blend composition and variable
20 blend composition for constant maximum cycle pressure. In the first case, the trends of the different metrics of interest,
21 namely η_{th} , W_s , Δh_{PHX} , \dot{m} , $P_{in,pump}$, PR and ER, are presented in Figures 3 to 5 as a function of P_{max} and normalised
22 with respect to the value corresponding to the lowest P_{max} in the analysis. In the second case, the dependence of these
23 parameters on dopant concentration for a given P_{max} is shown in Figures 3b to 5b. This analysis has only been carried
24 out for a turbine inlet temperature of 550°C to limit the length of this section. In fact, a similar scenario would be
25 observed considering 700°C TIT, although it would be characterised by lower variations in Δh_{PHX} . This is due to the
26 fact that a higher TIT enables higher turbine exhaust temperatures, thus offsetting the aforementioned effect brought
27 by an increase in the cycle pressure ratio. This clarifies the reason behind the results presented in Figures 3 to 5 at
28 700°C ; they are very similar to those obtained at 550°C but shifted towards higher pressures.
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35 Figure 6a shows that thermal efficiency peaks at a P_{max} of around 290 bar for a simple recuperated cycle with
36 $86\%\text{CO}_2/14\%\text{TiCl}_4$. Increasing the pressure to 350 bar results in a smaller difference between the normalised W_s
37 and Δh_{PHX} and this brings about a lower η_{th} . It is observed that pump inlet pressure remains constant since constant
38 values for both T_{min} and X_i are considered. This does not apply to Figure 6b (P_{max} set to 250 bar), where a progressive
39 reduction in $P_{in,pump}$, and an increase in \dot{m} , are observed due to the higher dopant concentration. These changes bring
40 about a lower relative increase in PR than that observed in Figure 6a due to the significantly lower drop in $P_{in,pump}$
41 compared to the rise in P_{max} . This has an impact on thermal efficiency which increases initially, then peaks when the
42 molar fraction of TiCl_4 reaches 17% and finally experiences a clear drop. Once again, this can be explained by the
43 relative variations of Δh_{PHX} and W_s ; while the latter decreases almost linearly with X_i , Δh_{PHX} shows a significant
44 drop initially, followed by an evolution that is less steep. From these results, it becomes clear that the efficiency of
45 the simple recuperated cycle is strongly dependent on maximum pressure and dopant concentration. This is due to the
46 recuperated cycle layout not having any additional degree of freedom to balance the effect of sub-optimal values of
47 these parameters.
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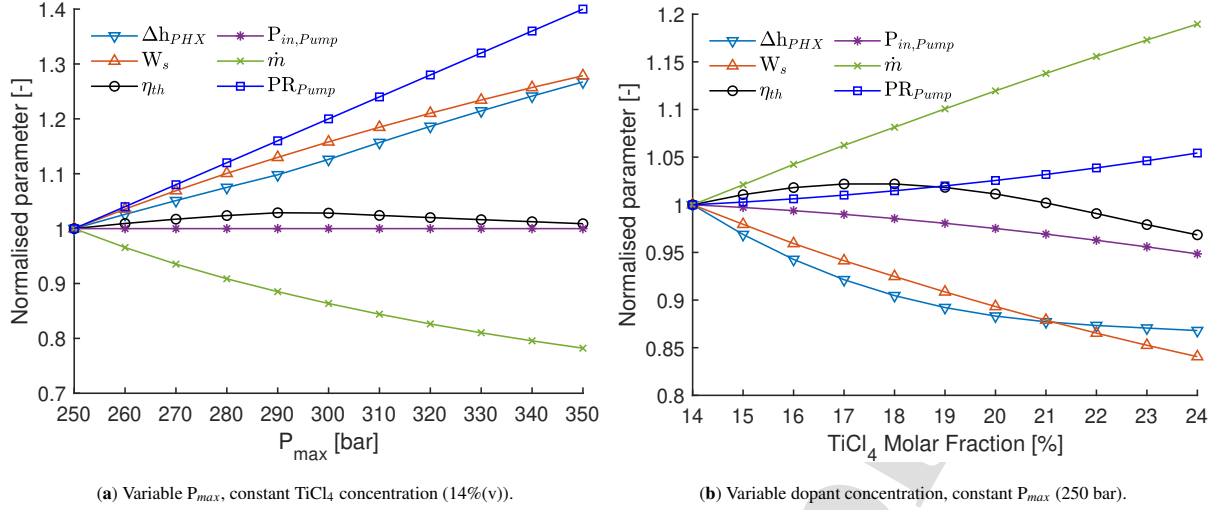


Figure 6: Relative variation of various cycle parameters as a function of maximum pressure and dopant concentration. A simple recuperated cycle operating on $CO_2/TiCl_4$ blends is considered. Turbine Expansion ratio is not plotted since it is equivalent to pump Pressure Ratio.

Contrary to the simple recuperated case, the two advanced layouts considered, namely precompression and re-compression, introduce additional degrees of freedom. As discussed in Section 2, the former layout is characterised by an additional compressor in the low pressure section that is installed in-between the two heat recuperators. This component helps to overcome the constraint set by the minimum cycle temperature on turbine exhaust pressure, hence allowing turbine expansion ratio to be optimised to yield benefits in terms of W_s (see increasing trends of ER_{Turb} and W_s in Figure 7(a)). Figure 7a shows the variation of P_{max} for a precompression cycle operating with 85% CO_2 /15% C_6F_6 . As presented in Figure 7a, the relative variation of ER is significantly different from that of PR, yielding fairly similar variations of W_s and Δh_{PHX} and subsequently a fairly constant trend for thermal efficiency. On the other hand, the slight increase in η_{th} observed in Figure 7b with dopant concentration corresponds to a lower relative reduction in W_s than in Δh_{PHX} , brought about by an increasing turbine expansion ratio.

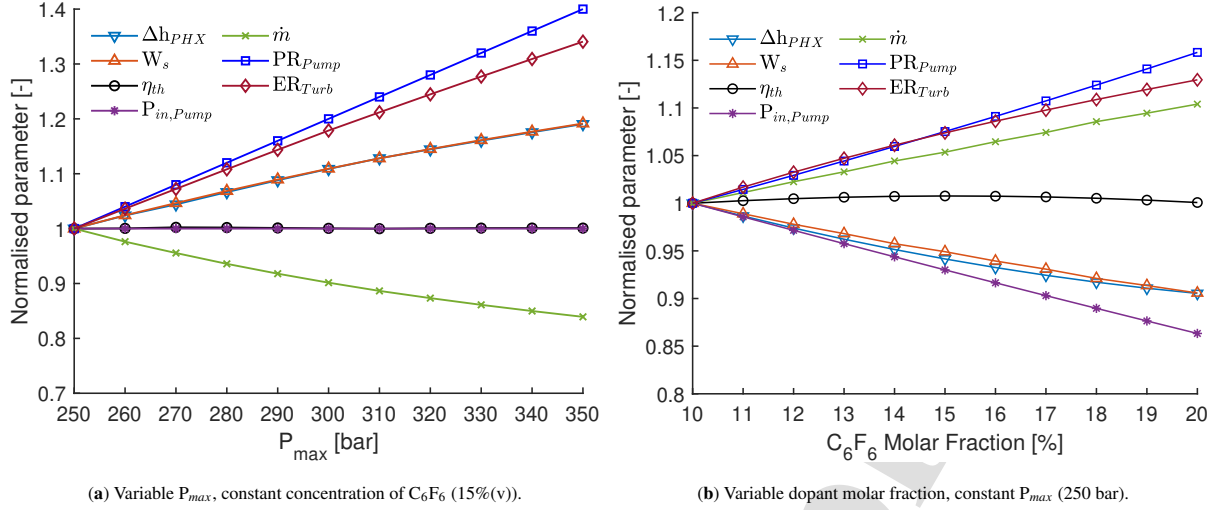


Figure 7: Relative variation of various cycle parameters as a function of maximum pressure and dopant concentration. A precompression cycle operated with CO_2/C_6F_6 is considered.

The recompression cycle does not aim to significantly increase specific work, but rather to improve the regenerative potential of the cycle in order to increase efficiency. To this end, the amount of working fluid circulating through the high-pressure/low-temperature side of LTR is reduced. Ultimately, this helps to balance the heat capacity rates of the two streams in this heat exchanger, thus reducing the irreversibility of the heat transfer process and increasing thermal efficiency. This is observed by comparing the results in Figures 6a to 8a, which applies to a recompression cycle running with 70% CO_2 /30% SO_2 . In the latter plot, the relative growth of Δh_{PHX} and W_s is very similar and yields almost constant thermal efficiency with a very weak dependence on P_{max} . Similarly, the slight reduction in η_{th} , observed in Figure 8b, is a result of the very similar relative deviations experienced by Δh_{PHX} and W_s , which is in turn brought about by the opposing effects of the split-flow factor and $P_{in,Pump}$.

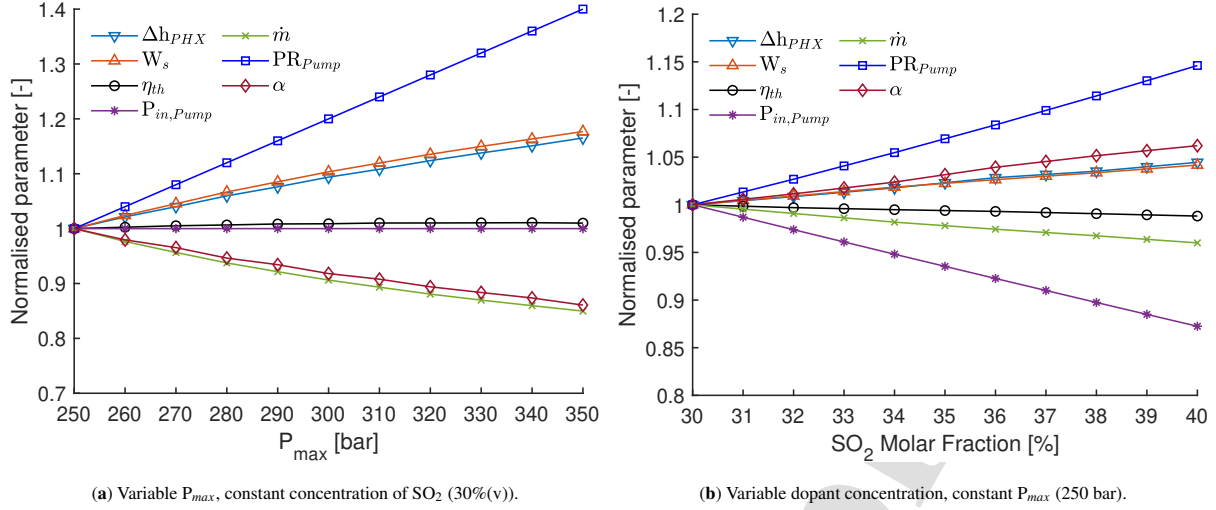


Figure 8: Relative variation of various cycle parameters as a function of maximum pressure and dopant concentration. A recompression cycle running on CO_2/SO_2 is considered. Turbine Expansion ratio is not plotted since this is equivalent to pump Pressure Ratio.

The behaviour of the cycles is strongly dependent on the thermodynamic characteristics of the blends. Blends of $CO_2/TiCl_4$, for instance, are characterised by a very wide PT-envelope (i.e., a large temperature glide, see Figure 2a), which is linked to a significant difference between the critical conditions of the two constituent compounds. A positive consequence of this is that working fluid condensation starts inside the recuperator and is not limited to the HRU (condenser). Hence, this is the main reason for the extraordinary heat recovery potential of this system [3]. On the negative side, this prevents the adoption of layouts incorporating split-flow options such as the recompression cycles, and limits the beneficial effects brought by precompression [3]. On the contrary, CO_2/SO_2 blends are characterised by very narrow PT envelopes, corresponding to low temperature glides, and this avoids condensation of the working fluid within the recuperator. As a result of this, these blends perform very poorly in a simple recuperated cycle but they are particularly suitable for the recompression layout. In this regard, it is worth noting that the (limited) drop in η_{th} observed in the bottom-right corner of Figure 5 is brought about by a significant increase in the temperature glide of the CO_2/SO_2 blend, caused by the extremely high X_i , which prevents the efficient operation of the split-flow feature. In such circumstances, the split-flow ratio is forced to take sub-optimal values to shift the inlet to the compressor away from the two-phase region (see the change in slope of the split-flow ratio trend in Figure 8b for X_i higher than 35%), which leads to a lower thermal efficiency of the cycle.

4.2. Turbine design and analysis

4.2.1. Definition of candidate boundary conditions

Once the optimum working fluid composition and maximum cycle pressure levels are identified for each blend, a series of representative boundary conditions are defined to study their impact on turbine design. Firstly, the optimum P_{max} for each blend is selected, according to the results shown in Figures 3 to 5. This corresponds to 300 bar for C_6F_6

(550°C case only) and 310 and 350 bar for SO₂, for 550°C and 700°C respectively; for TiCl₄, 290 bar is considered regardless of TIT. Secondly, five different values of molar fraction are defined for each dopant, including the optimum and minimum/maximum values. The five molar fractions are defined for both 250 bar and optimum P_{max} , and this is done for both 550°C and 700°C TIT (with the exception of C₆F₆, for which only 550°C is considered).

A dual approach is adopted to select the five molar fractions. If the optimal molar fraction X_i of dopant (i.e., the one achieving maximum η_{th}) falls between the minimum and maximum values, the remaining two cases (for a total of five sets of boundary conditions for turbine design) are selected as the arithmetic mean between the minimum and optimum values and between the optimum and maximum values respectively. For example, this is the case for a simple recuperated cycle operating with CO₂/TiCl₄ at TIT=550°C, for which the optimum X_i is 17%, and this falls within the allowable range of 14% to 24%; in this case, the other two points considered are 15.5% and 20.5% (see Table B.9).

If, on the other hand, the optimum molar fraction coincides with the minimum value, the other three points result from evenly distributing the entire range of molar fractions. This is the case of the recompression cycle operating with a CO₂/SO₂ blend, whose optimum X_i is 30%. In this case, the cases selected for turbine design are 30%, 32.5%, 35%, 37.5% and 40% (see Tables B.9 and B.10). It is worth noting that some of these molar fraction values were not considered in the previous section, where X_i took integer values only.

In summary, a set of sixty different cases are thus identified, and successively employed as input data for the turbine design process. The detailed set of specifications, along with turbine inlet and outlet conditions, can be found in Appendix B. The set is divided into four cases defined by means of different combinations of turbine inlet temperature and maximum cycle pressure. *Case A* refers to 550°C and 250 bar, *Case B* to 700°C and 250 bar, *Case C* to 550°C and the optimum P_{max} (which depends on the system considered) and *Case D* to 700°C and optimum P_{max} .

As a final comment, it is worth remarking that, even if the present paper focuses specifically on the turbine design, the thermal performance of precompression and recompression cycles strongly depends on the efficiency of the compressor included in such configurations. The design of this equipment, which requires further investigation due to the high novelty of the working fluid employed, will be undertaken and disclosed in future work.

4.2.2. Exploration of the design space for the three candidate blends

Using the results from Section 4.2.1 the achievable turbine performance has been initially evaluated at a turbine inlet temperature and pressure of 550°C and 250 bar respectively, and at the minimum molar fraction for the three blends (14%, 10% and 30% for CO₂/TiCl₄, CO₂/C₆F₆ and CO₂/SO₂ respectively). These conditions were selected to allow an initial exploration of the design space, before then conducting further investigations into the sensitivity of the turbine performance to increasing the pressure, temperature and molar fraction. Table 5 summarises the cycle conditions for the three candidate blends considering a gross power output of 100 MW_e and the assumptions specified in Table 3.

Table 5: Boundary conditions for the three candidate blends at 550°C

Blend	X_i [%]	\dot{m} (kg/s)	P_{out} (MPa)	PR (-)	η_{th} (%)	Cycle configuration
CO ₂ /TiCl ₄	14	1485	9.8	2.47	44.4	Recuperated
CO ₂ /C ₆ F ₆	10	1098	6.5	3.69	42.8	Precompression
CO ₂ /SO ₂	30	1016	6.9	3.42	44.3	Recompression

In this section, a comparison of the performance of the flow path designs obtained for each blend is presented. Initially, four stage turbine designs were selected for the three candidate blends to limit the blade peripheral speed to 180m/s with the assumption of a constant enthalpy drop across each stage. A summary of the designs, including details of the 1st and last stages of the 4-stage flow path is presented in Table 6 for the three candidate blends.

Owing to the different thermodynamic properties of the candidate dopants, and also variations in the chosen cycle configuration, different values for the turbine stage specific work were obtained for each blend composition. As a result, large differences in the hub diameters and bending stresses were obtained. The 70%CO₂/30%SO₂ blend results in the largest hub diameter and the smallest gas bending stress as shown in Figure 9. On the contrary, the smallest hub diameter and the highest bending stresses are attributed to the 86%CO₂/14%TiCl₄ blend. For the CO₂/TiCl₄ flow path the blade count has been lowered to keep the bending stresses within the specified limit. Increasing the blade count for this flow path would result in bending stresses exceeding the 130 MPa static bending stress limit; although the same logic applies for the CO₂/C₆F₆ and CO₂/SO₂ designs. Concerning the aerodynamic performance, the turbine design for CO₂/TiCl₄ achieves the highest efficiency compared to either the CO₂/C₆F₆ and CO₂/SO₂ designs, which is due to larger aspect ratio blades, smaller hub diameters and a smaller radial tip clearance gap. All three blends resulted in a slenderness ratio that is well within the specified design limit which indicates rotordynamic instability is of no concern. This also indicates there is scope to increase the flow path length, with the goal of increasing the number of stages and increasing efficiency.

Table 6: Flow path design details for the CO₂ blends for a fixed number of stages.

Parameter	CO ₂ /TiCl ₄		CO ₂ /C ₆ F ₆		CO ₂ /SO ₂	
	1 st stage	last stage	1 st stage	last stage	1 st stage	last stage
Number of stages [-]	4		4		4	
Hub diameter [mm]	876.2		1115.8		1145.5	
Bending stress [MPa]	126.9	126.7	88.4	129.3	77.7	128.0
Number of rotor blades	63	52	95	86	95	95
Radial tip clearance [mm]	0.67	0.71	0.81	0.86	0.83	0.87
Aspect ratio [-]	0.70	0.95	0.50	0.99	0.48	0.97
Slenderness ratio [-]	4.16	4.16	3.03	3.03	2.93	2.93
Total-to-total efficiency [%]	91.05		88.91		88.36	

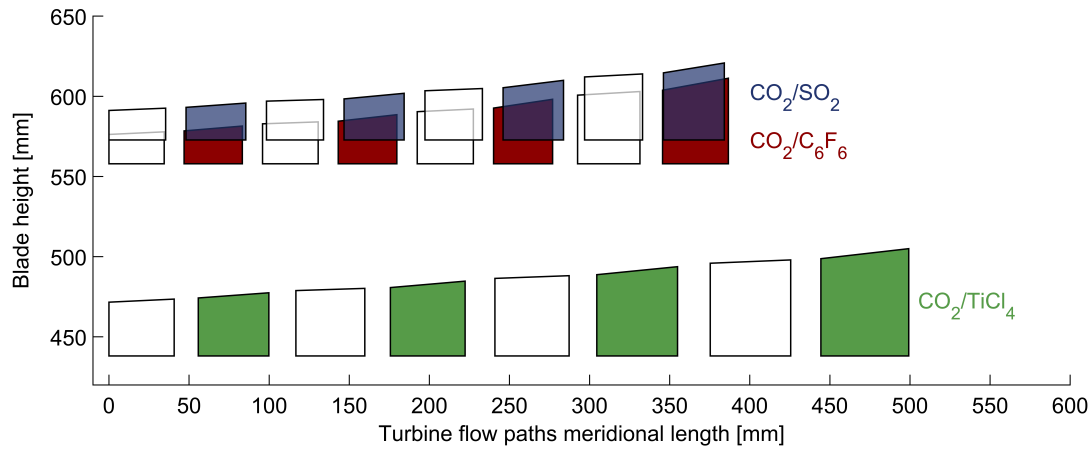


Figure 9: Turbine flow path meridional view for four-stage turbine designs for $\text{CO}_2/\text{TiCl}_4$, $\text{CO}_2/\text{C}_6\text{F}_6$ and CO_2/SO_2 blends; unfilled and filled shapes represent the stator and rotor blades respectively

To enable a fairer comparison between the three flow path designs, the effect of increasing the number of stages within the range of 4 to 14 stages was investigated for the three design cases. In the following set of results, the turbine performance is investigated based on the operating conditions specified in Table 5, which corresponds to the minimum molar fraction value for each blend. The analysis aims at examining the effect of a reduced hub diameter (D_{hub}), which is the result of increasing the number of design stages (n_{stages}), on the gas bending stress on the rotor blades ($\sigma_{bending}$), the isentropic efficiency (η_{it}), and the slenderness ratio (SR). In this set of results, the designs are modified for each design case to keep the gas bending stress with the threshold limit, with the rotor blade count ranging between 35 and 95. Given that the highest rotor bending stresses are experienced by the last turbine stage, which is due to the combination of a reduced density, enlarged flow area and increased blade heights, the bending stress values presented correspond to this specific stage. The results are summarised in Figures 10a to 10d.

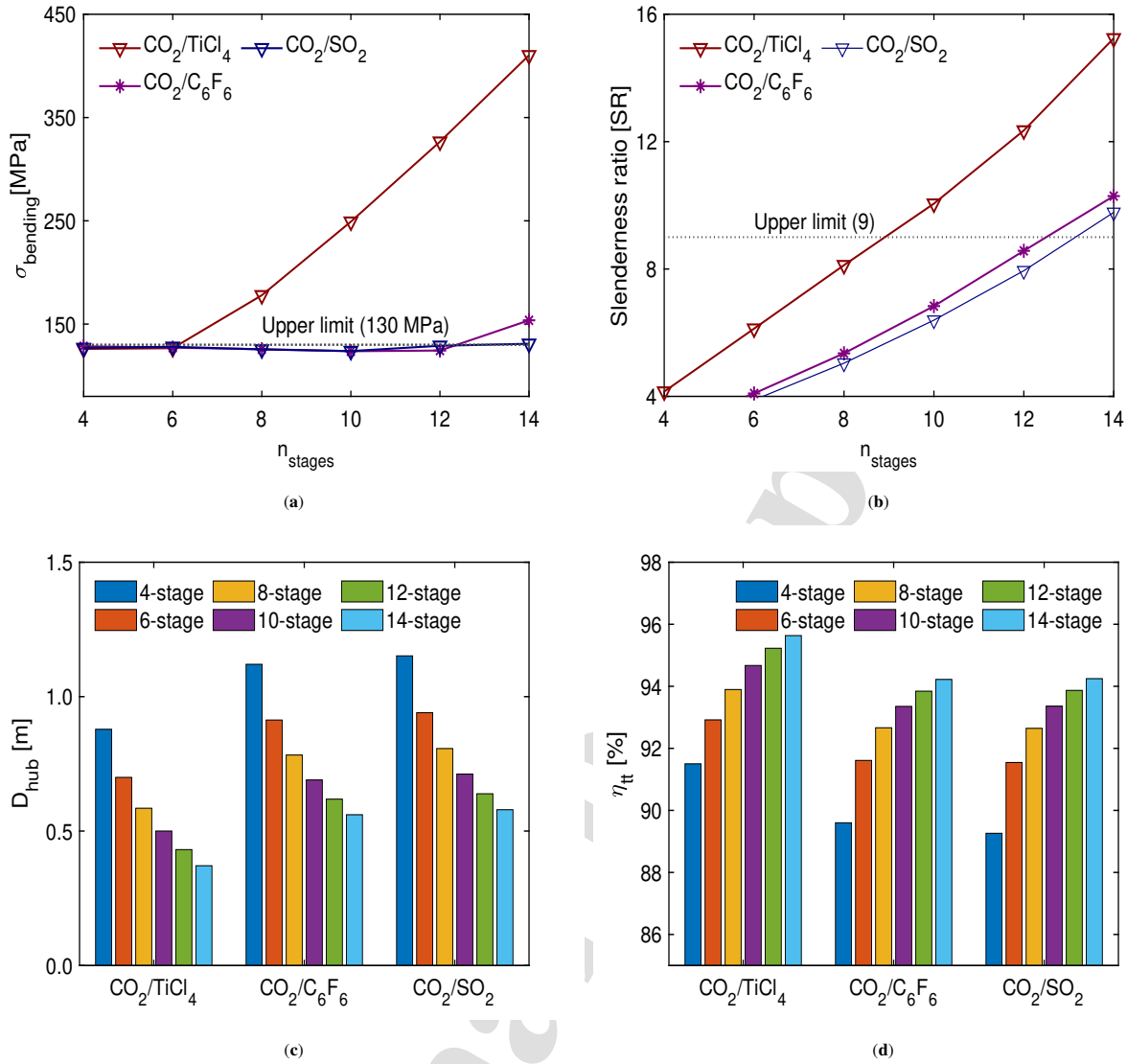


Figure 10: Number of stages [n_{stages}] versus (a) rotor bending stress [$\sigma_{bending}$] for the last turbine stage; (b) slenderness ratio [SR] for CO₂/TiCl₄, CO₂/C₆F₆ and CO₂/SO₂ blends; (c) total-to-total efficiency [η_{tt}]; (d) hub diameter [D_{hub}] for CO₂/TiCl₄, CO₂/C₆F₆ and CO₂/SO₂ working blends and between 4 and 14 turbine stages.

In view of the implemented design hypothesis, within which the designs are obtained at a constant rotational speed of 3000 RPM and loading coefficient of 1, the number of stages dictates that both the blade peripheral speed and the hub diameter, and this is a function of the specific isentropic enthalpy drop for a given blend and set of operating conditions. The smallest hub diameter is achieved for CO₂/TiCl₄ and the largest for CO₂/SO₂. Increasing the number of stages to 14 increases the overall total-to-total efficiency to 95.6% and 94.2% for CO₂/TiCl₄ and CO₂/SO₂ respectively. This is compared to initial respective efficiencies of 91.05% and 88.36% for the four-stage design. This

increase in the number of stages is associated with a reduction in the hub diameter and the blade peripheral speed, which results in higher efficiency due to reducing the secondary flow losses. The reduction in the blade peripheral speed enables to produce designs with longer blade heights and hence, this results in smaller chord length to blade height ratio and reduced secondary flow losses. Furthermore, less tip clearance losses are experienced with the long flow path designs as a results of the reduced the clearance gap size which is defined as a constant ratio of the tip diameter.

Increasing the number of stages also results in a higher slenderness ratio for all three-flow path designs, with the highest ratio obtained for the $\text{CO}_2/\text{TiCl}_4$ case. Moreover, to enhance the aerodynamic efficiency whilst achieving a design that complies with the rotor bending stress limit, it is necessary reduce the number of blades within the range of 95 to 35, as shown in Figure 11. Reducing the number of rotor blades results in a larger blade pitch, leads to longer chord lengths and smaller bending stress (both tangential and axial) on the blades. For the $\text{CO}_2/\text{TiCl}_4$ flow path, increasing the number of stages above six, whilst, at the same time, reducing the number of blades to 35 (the lower limit) results in bending stress that are above the threshold limit of 130 MPa. Therefore, the $\text{CO}_2/\text{TiCl}_4$ design should be limited to six stages in order to meet the constraints imposed on the slenderness ratio and bending stress. However, for both $\text{CO}_2/\text{C}_6\text{F}_6$ and CO_2/SO_2 , the number of stages can be increased up to 12 stages without exceeding the maximum rotor bending stress of 130 MPa. Moreover, the slenderness ratio can be kept below 9 and the number of blades is above or equal to the minimum value of 35.

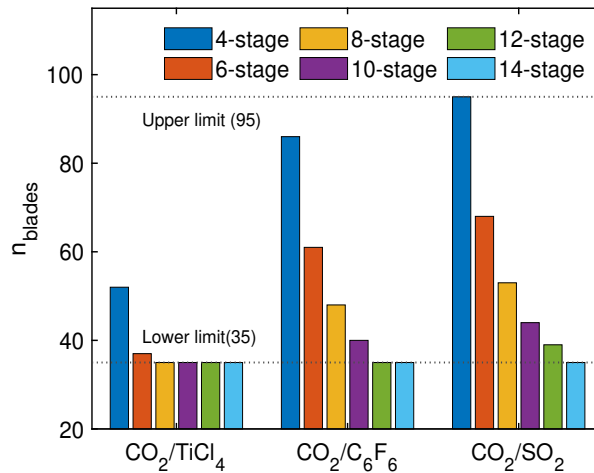


Figure 11: Number of rotor blades for the last turbine stage [n_{blades}] of turbines design for $\text{CO}_2/\text{TiCl}_4$, $\text{CO}_2/\text{C}_6\text{F}_6$ and CO_2/SO_2 with 4-14 turbine stages.

Based on the results presented in this subsection, it is possible to select the optimal number of stages, and hence hub diameter, that obtains the highest efficiency for a specified set of turbine boundary conditions. This number of stages provided the higher aerodynamic efficiency, whilst keeping the rotor bending stresses and slenderness ratio

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3 within the specified threshold limit. However, it should be noted that each pair of blend and boundary conditions
4 results in an optimal flow path design with a different number of stages and a different number of rotor blades.
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7 4.2.3. Sensitivity of efficiency to cycle conditions 8

9 The previous analysis was completed at the minimum blend fraction (X_1) and at an inlet temperature and pressure
10 of 550°C and 250 bar respectively. This section aims to investigate the effect of changing the thermodynamic boundary
11 conditions, namely the turbine inlet temperature (T_{inlet}) and pressure (P_{inlet}) and dopant concentration (X_i) on the
12 achievable turbine efficiency for a turbine design that meets the imposed mechanical and rotordynamic constraints.
13 To do this, the remaining turbine design boundary conditions, namely the mass flow rate (\dot{m}), pressure ratio (PR) and
14 molar fractions are taken from the results obtained from the thermodynamic cycle analysis. In the following set of
15 results, as reported in Figures 12a to 12c, axial turbine designs are produced at a total inlet temperature and pressure
16 of 550°C & 250 bar (*Case A*), 700°C & 250 bar (*Case B*), 550°C & P_{opt} (*Case C*) and 700°C & P_{opt} (*case D*). This is
17 completed at different molar fractions ranging from 14 to 24%, 10 to 20%, and 30 to 40% for CO₂/TiCl₄, CO₂/C₆F₆
18 and CO₂/SO₂ respectively.
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25 For the CO₂/TiCl₄ blend, changing the boundary conditions of turbine design by increasing the inlet temperature
26 from 550 to 700°C results in a lower rotor bending stresses, and allows for a larger number of stages, smaller hub
27 diameters and higher turbine efficiencies, whilst keeping the slenderness ratio within the defined limit as indicated
28 in Figure 12a. On the other hand, less significant effects are obtained when turbine inlet pressure is increased from
29 25 MPa to P_{opt} for the same inlet temperature. As for the effect of molar fraction, increasing this from 14 to 24%
30 results in a lower turbine efficiency (η_t), which is due to the increased bending stresses; hence to keep $\sigma_{bending}$ within
31 the specified limit, the stage number should be reduced or the number of blades should be reduced and the blade
32 chord length increased. Increasing the dopant concentration results in a lower enthalpy drop across the turbine stage
33 and thus a larger mass flow rate is needed to produce the same plant power output. This means that larger tangential
34 stresses are applied on the rotor blades. Nevertheless, if increasing the dopant concentration [X_i] allowed for producing
35 designs with the same number of stages, a higher total-to-total efficiency would be obtained as experienced with X_1
36 & X_2 and X_3 & X_4 at 550°C & 250 bar (*Case A*). The feasibility of these designs is not addressed in this paper
37 inasmuch as assessing the mechanical integrity of the flow path requires a more detailed analysis which is beyond the
38 criteria identified for screening purposes at the mean-line design stage. It is worth highlighting that the discontinuity
39 experienced in the turbine efficiency with respect to the molar fraction is the result of integer decision variables,
40 namely the number of stages and number of blades, which must be adjusted in order to comply with the specified
41 mechanical and rotordynamic limits. For example, for the 550 °C and 250 bar case with CO₂/TiCl₄, the number of
42 stages is equal to 6 for a molar fraction of 14 and 15.5%, but as the molar fraction is increased to 17 and 20.5% the
43 number of stages must be decreased to 5 to comply with the imposed constraints.
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55 For the CO₂/SO₂ flow paths, increasing the inlet temperature from 550 to 700°C has a less significant effect on
56 turbine efficiency and results in trends that are contradictory to those observed for CO₂/TiCl₄. Specifically, a small
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increase in efficiency is obtained for the low pressure case compared to the reduction in efficiency for the P_{opt} case. Increasing the inlet temperature for the CO_2/SO_2 blend results in a lower slenderness ratio for the same number of stages, and allows for a larger number of stages (Figure 12c). However, as discussed in the previous section, the CO_2/SO_2 flow path design allows for a larger number of stages than the $\text{CO}_2/\text{TiCl}_4$ case, and as a result increasing the number of stages further, beyond a certain limit, results in a less significant efficiency enhancement. This is due to the small change in hub diameters that results from increasing the number of stages, which is due to the small change in blade peripheral speed that is experienced.

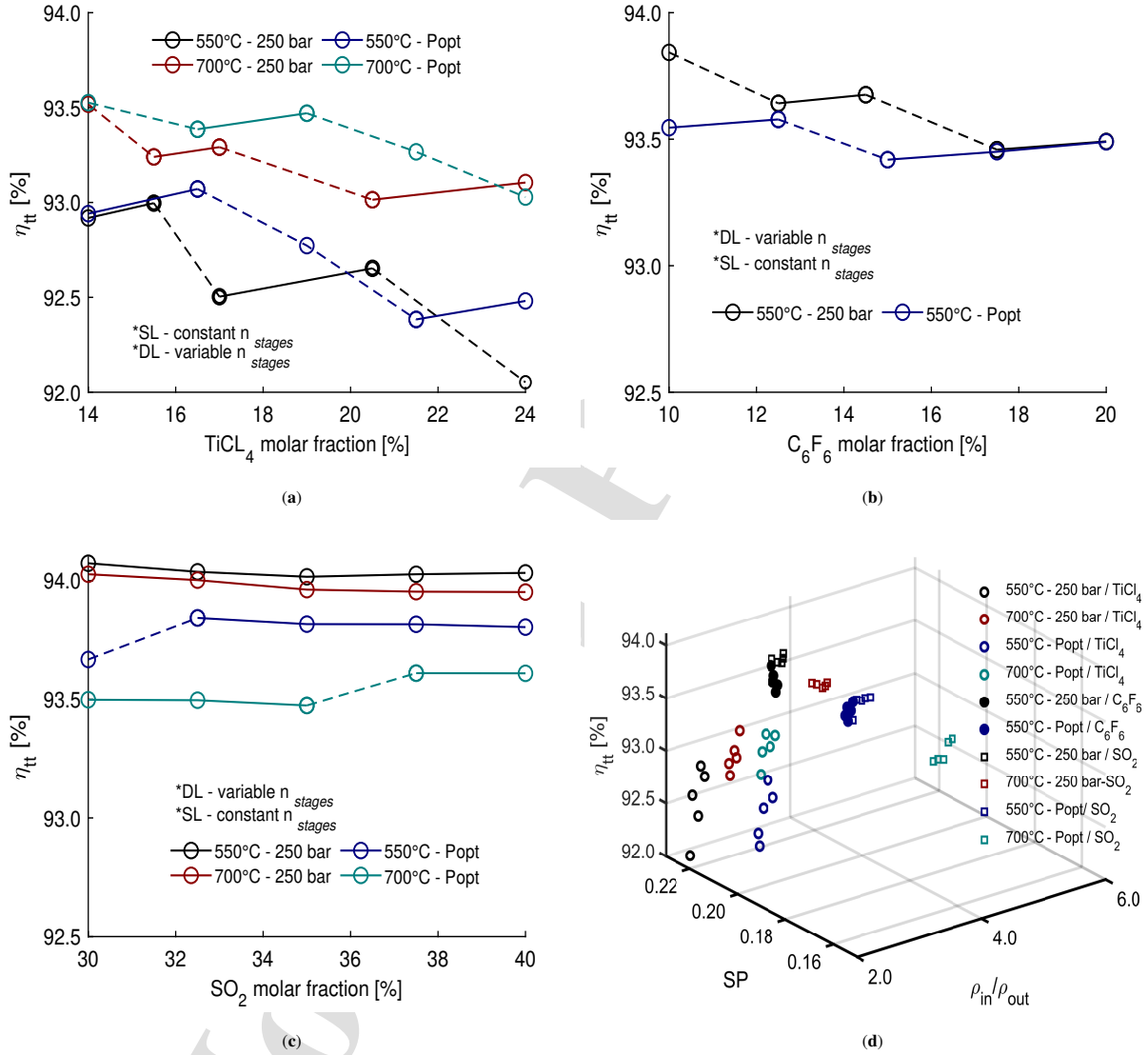


Figure 12: Total-to-total efficiency (η_{tt}) versus dopant concentration for (a) $\text{CO}_2/\text{TiCl}_4$, (b) $\text{CO}_2/\text{C}_6\text{F}_6$, and (c) CO_2/SO_2 .

** P_{opt} : is the optimum maximum pressure for each cycle

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4 To analyse the effect of increasing the temperature from 550 to 700°C, and setting turbine inlet pressure to P_{opt}
5 for the CO₂/SO₂ flow paths, the turbine size parameter and volumetric expansion ratio are introduced. This is done
6 to highlight the effect of the working fluid properties, cycle parameters and turbine size on the achievable turbine
7 efficiency. The turbine size parameter is defined as $SP = \sqrt{\dot{V}_{out}}/\Delta H_s^{0.25}$, where ΔH_s is the isentropic enthalpy drop
8 and \dot{V}_{out} is the volumetric flow rate at the outlet. The volumetric expansion ratio is defined as (ρ_{in}/ρ_{out}) , where ρ_{in}
9 and ρ_{out} are the fluid densities at the turbine inlet and outlet respectively. For the low pressure cases of all blends, the
10 resulting size parameters obtained are rather similar, although there are some differences in the volumetric expansion
11 ratio. Contrary to the CO₂/TiCl₄ case, increasing inlet temperature for the high-pressure case results in lower turbine
12 efficiencies for the CO₂/SO₂ flow paths due to the significant reduction in turbine size parameter (SP), alongside the
13 increase in volumetric expansion ratio, as indicated in Figure 12d. For the two blends examined, a maximum absolute
14 efficiency difference of 0.88% is obtained due to changing the molar fraction in the CO₂/TiCl₄ flow path at 700°C and
15 250 bar. This confirms that high efficiency turbines can be designed within the SCARABEUS project for the three
16 candidate working blends over the range of boundary conditions examined.
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20 In the cycle optimisation, the optimum dopant concentration was found to be 17, 14.5 and 30% for the 550°C
21 and 250 bar inlet condition (*Case A*), for the CO₂/TiCl₄, CO₂/C₆F₆ and CO₂/SO₂ blends respectively. These values
22 changed to 17 and 30% for 700°C and 250 bar (*Case B*) operating with CO₂/TiCl₄ and CO₂/SO₂ blends respectively.
23 However, the turbine mean-line design indicates that optimal turbine efficiency is obtained at different molar fractions
24 and this corresponds to 15.5, 10, 30% for Case A, and 14 and 30% for Case B for the same blends. Consequently,
25 it can be observed that different optimum molar fractions are obtained from the perspective of cycle performance
26 and turbine performance. For example, for the CO₂/TiCl₄ case, designing the turbine at the optimum cycle molar
27 fraction results in an absolute turbine efficiency drop of 0.52 and 0.23% compared to the optimum cycle design point
28 for cases A and B, respectively. On the other hand, if the optimum cycle thermal efficiency is compared against the
29 one calculated with the molar fraction that maximises the turbine efficiency, a drop of 0.5 and 1.05 percentage points
30 is observed for cases A and B, respectively. A similar analysis for CO₂/C₆F₆ yields an absolute drop of 0.16%
31 in the turbine efficiency for *case A*; the corresponding drop in cycle efficiency is 0.36 percentage points. Ideally, the
32 optimal molar fraction should be identified through a coupled cycle-turbine design activity, whereby the cycle and
33 turbine are simultaneously optimised. However, due to the complexity of the turbine design process, which includes
34 multiple-stages and the need to manually iterate integer design variables to bring the turbine design within the imposed
35 mechanical and rotordynamics, such an approach has not been adopted; such an approach could be explored in future
36 research. Nonetheless, it is worth remembering that this behaviour exists. However, for the purposes of this current
37 study, it is considered most suitable to design the turbine for the optimal molar fraction that maximises the thermal
38 efficiency of the cycle.
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42 Regarding turbine performance, the CO₂/SO₂ flow path designs achieve the highest efficiencies at an inlet tem-
43 perature and pressure of 550°C and 250 bar and 700°C and 250 bar respectively. Similarly, the CO₂/C₆F₆ flow path
44 designs achieve the highest efficiencies at an inlet temperature and pressure of 550°C and 250 bar. However, the
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3 CO₂/TiCl₄ flow path achieved the highest total-to-total efficiency (η_{tt}) at an inlet temperature and pressure of 700°C
4 and P_{opt} . It is evident that increasing the inlet pressure for the CO₂/SO₂ blend at an inlet temperature of 700°C results
5 in a smaller size parameter compared to the CO₂/TiCl₄ case. Therefore, the CO₂/TiCl₄ flow path is the best performing
6 for the 700°C and P_{opt} case compared to the other flow paths, as indicated in Figures 12d.
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10 To further elaborate on the performance of the axial turbines operating with the different candidate blends, the
11 change in specific work, blend molecular weight, bending stresses and mass-flow rate are presented in Figures 13a
12 and 13b at the five different molar fractions. These figure are obtained at a turbine inlet temperature and pressure
13 of 550°C and 250 bar respectively (case A). For the CO₂/TiCl₄ case, increasing the molar fraction of dopant (X_i)
14 results in smaller hub diameters, taller blades and higher bending stress for the same number of stages (Figure 13b).
15 This confirms the more significant reduction in the number of stages experienced by the CO₂/TiCl₄ case with the
16 increasing concentration of dopant, compared to both CO₂/C₆F₆ and CO₂/SO₂. This is attributed to the significant
17 increase in the mass-flow rate required to achieve the same net power output from the plant, which is due to the lower
18 specific work of the CO₂/TiCl₄ blend compared to CO₂/C₆F₆ and CO₂/SO₂. The relative increase in mass flow rate
19 with dopant concentration is much larger for TiCl₄ than for the other dopants, as indicated in Figure 6, 7 and 8b.
20 Although increasing the molar fraction of dopant, and hence the molecular weight of the blend, results in a lower
21 specific work for CO₂/C₆F₆ and CO₂/TiCl₄, a slight increase is experienced in the CO₂/SO₂ case. Consequently,
22 increasing the molar fraction results in designs with a lower number of stages for the CO₂/TiCl₄ and CO₂/C₆F₆ flow
23 paths, which is necessary to allow for rotor bending stress and slenderness ratio within the specified limits; as a result
24 more discontinuities are observed in the efficiency trends as shown in Figure 12a and 12b. However, for the CO₂/SO₂
25 case, increasing the molar fraction results in turbine designs with a larger number of stages, which is due to the larger
26 enthalpy with increasing dopant concentrations, as indicated in Figure 13a. This effect has been discussed in detail in
27 a previous work by some the current authors [6].
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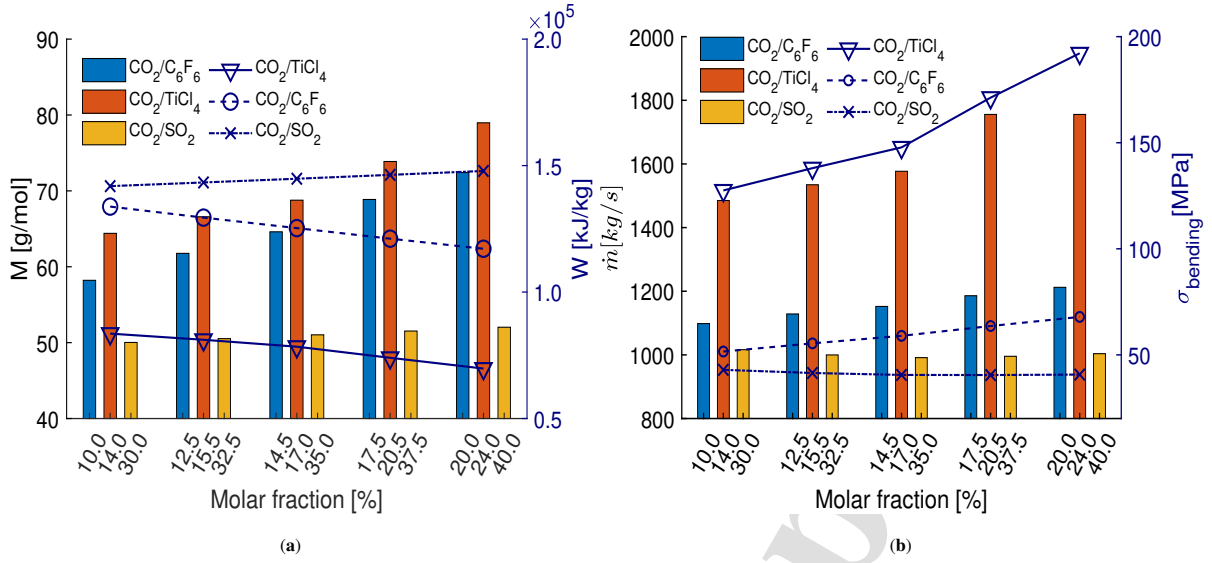


Figure 13: Molar fraction of dopant (X_i) versus (a) molecular weight (M) and specific work (W), (b) mass flow rate (\dot{m}) and rotor bending stresses ($\sigma_{bending}$) with the same number of stages

4.2.4. Efficiency trends for the most technically feasible cycle

According to the health and environmental considerations discussed in Section 2, alongside the current state-of-the-art in CSP power cycles, a precompression cycle operating with $\text{CO}_2/\text{C}_6\text{F}_6$ at 550°C could be considered to be the one of the most technically feasible cycles. The analysis in this subsection focuses on this cycle in more detail, and aims to examine how the achievable turbine efficiency is influenced by the target inlet pressure and blend composition.

The contours of the optimal number of stages and the corresponding turbine isentropic efficiency are reported in Figures 14a and 14b for dopant concentrations ranging between 10 and 20% and turbine inlet pressures ranging between 240 and 300 bar. For the same molar fraction, increasing the inlet pressure results in a larger number of stages, and a lower turbine efficiency due to the increased pressure ratio and reduced mass flow rate. Similarly, for a fixed number of stages, increasing the molar fraction of dopant results in a lower turbine isentropic efficiency, where a molar fraction of 10% is found to yield highest overall turbine isentropic efficiency. Thus, for the $\text{CO}_2/\text{C}_6\text{F}_6$ blend, an increase in both the molar fraction and turbine inlet pressure results in a maximum drop in turbine efficiency of 0.4 points. Nonetheless, these results confirm that for the range of operating conditions considered, it is still possible to design a turbine flow path that can achieve a high isentropic efficiency.

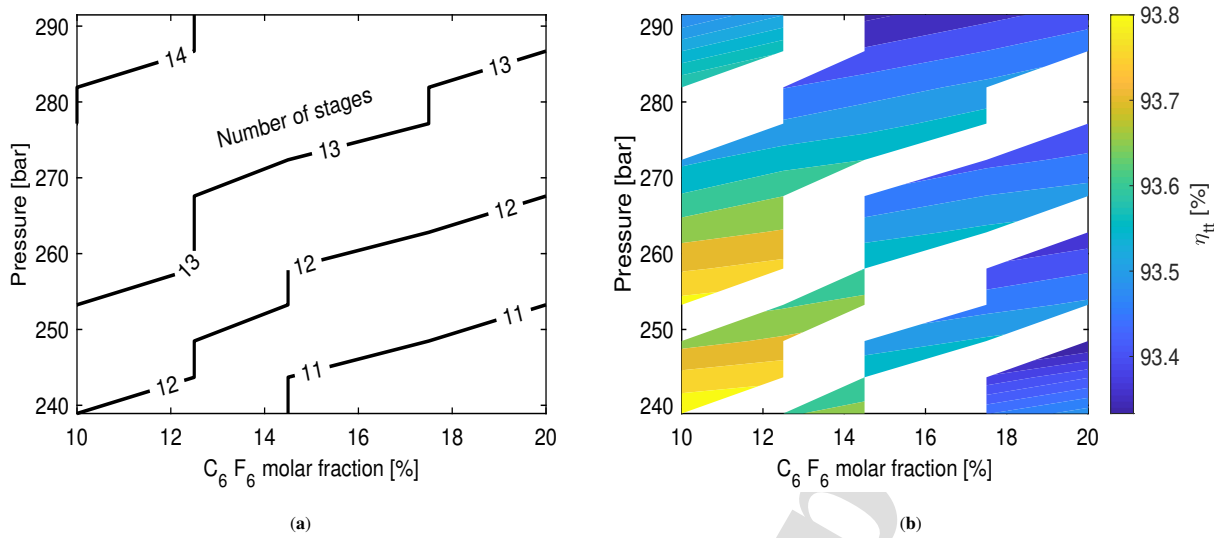


Figure 14: Contours of the optimal (a) number of stages contours, (b) and total-to-total efficiency [%] for $\text{CO}_2/\text{C}_6\text{F}_6$ flow paths at a turbine inlet temperature of 550°C at different turbine inlet pressures and dopant concentrations. Results are generated assuming a 100 MW_e power plant.

4.2.5. Remarks about the turbine design for CO_2 blends

In summary, for the sCO_2 blends considered, a total-to-total turbine isentropic efficiency above 92% can be achieved. This is considered an important milestone within the SCARABEUS project, and is a promising result for developing the technology further. Moreover, it is worth reiterating that, in comparison with the reference cycle design, where an overall turbine efficiency was assumed to be equivalent to 92%, better cycle performance can be obtained for the updated flow path efficiency. On this point it should however be noted that the current study is concerned with providing an assessment for the flow path performance and does not account for the additional losses experienced with the turbine, such as inlet, bearing, balancing drum, and throttle and discharge losses that would further reduce the turbine efficiency below the results obtained here. Having said this, it is worth noting that most of these losses scale with the same parameters that influence turbine efficiency; for example, balancing drum and bearing losses are expected to be higher with larger hub diameters. On the contrary, throttle losses can be safely assumed to be low regardless of the specific flow path designs given that the size of the valves is typically chosen targeting fluid velocities that yield similar losses. Nevertheless, these losses will have to be quantified in later design stages.

In this study, fixed values for the turbine design parameters were assumed. Thus, whilst flow path efficiencies above 92% were obtained, further enhancement in turbine performance may be possible through an extension of the optimisation process to account for the optimisation of aerodynamic design variables including pitch-to-chord ratio (s/c), flow coefficient (ϕ), loading coefficient (ψ) and degree of reaction (Λ). Optimisation for those parameters may result in further variations in the turbine design. In this regard, additional analysis has been carried out by the authors to investigate the effect of changing these design parameters on the aerodynamic turbine performance and the

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3 flow path design. This work is on-going, but the main conclusions will be summarised here. Specifically, a parametric
4 study was carried out for the $\text{CO}_2/\text{C}_6\text{F}_6$ blend operating within a precompression cycle at an inlet temperature of 550°C .
5 Changing both the loading and flow coefficients was found to have the most significant effect on the flow path designs
6 compared to the other design parameters (Λ and s/c). Increasing the loading coefficient over the range from 0.8 to
7 1.5, at a fixed flow coefficient, pitch-to-chord ratio and degree of reaction of 0.5, 0.85 and 0.5 respectively, resulted in
8 a reduction in the number stages from fourteen to five stages to keep the bending stresses within the threshold limit
9 (130 MPa). This led to a reduction in efficiency of around 4 percentage points over the examined loading coefficient
10 range. On the contrary, increasing the flow coefficient, at a fixed loading coefficient, pitch-to-chord ratio and degree
11 of reaction of 1.0, 0.85 and 0.5 respectively, resulted in lower bending stresses. An efficiency enhancement by up
12 to 2.0 percentage points was obtained as a result of increasing the flow coefficient (ϕ) from 0.3 to 0.7; where the
13 number of stages increased from six to thirteen stages. Changing the the degree of reaction and pitch-to-chord ratio
14 was found to have less significant effects on the flow path design and performance compared to both the flow and
15 loading coefficients. Ultimately, changing the loading and flow coefficients simultaneously resulted in a maximum
16 efficiency of 93.8%, which was obtained at values of ψ & ϕ of 0.8 and 0.6 respectively. This allows for an efficiency
17 enhancement of 0.2% compared to the base-line design where fifteen design stages are required compared to eleven
18 stages for the baseline design case. It is worth mentioning that the 0.2% increase in the turbine efficiency is considered
19 within the margin of accuracy of mean-line flow path design.

20
21 It is evident that high turbine efficiency is achieved for designs that are able to accommodate a large number of
22 stages; for example 10 to 12 stages can be accommodated for the $\text{CO}_2/\text{C}_6\text{F}_6$ flow path design at 550°C and 250 bar
23 over a molar fraction range from 10 to 20%. However, it is also important to consider the effect that increased number
24 of stages may have on the cost of the turbine. This is another essential criterion for the development of sCO_2 power
25 blocks for CSP plants technologies, and a particular objective of the SCARABEUS project.

26
27 In practice, the overall cost of the turbine is driven by its overall size, which is a function of the turbine diameter
28 and of the axial length. Whilst increasing the number of stages results in a larger axial length, it also results in a
29 smaller hub diameter. Noting that weights of the major components, such as rotor and casing, are proportional to the
30 length, but proportional to the hub diameter squared, it may be anticipated that a turbine designed for a smaller hub
31 diameter and a larger axial length could be cheaper compared to a turbine designed for a larger hub diameter and a
32 smaller axial length (low number of stages). This hypothesis is aligned with common industry experience (e.g., steam
33 turbines) if similar classes of materials are employed for the major components; in this case, the tacit equivalence
34 between weights and costs is a reasonable assumption. However, if the major components adopt different materials
35 whose cost per kilogram is extremely different, which is the case for nickel based alloys compared to conventional
36 steels, the assumption may not hold.

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38 In this regard, a preliminary direct material cost analysis has been carried out for different flow path designs to
39 compare the cost associated with machines with a small number of stages to machines with large number of stages.
40 The analysis has been carried out for turbine designs produced with different number of stages within the range of 4
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3 to 14 stages was investigated for the CO₂/SO₂ blend. The cost analysis is developed based on industrial experience
4 and the methodology is presented in authors previous work [59] but the main conclusions will be summarised here.
5 Several assumptions have been made within the preliminary cost analysis methodology to allow for easily evaluating
6 the flow path cost using the mean-line design outputs. In brief, only the direct material cost has been considered
7 in this analysis and the overall cost of the machines with a low number of stages is estimated with respect to the
8 cost of the 14-stage 80%CO₂/20%SO₂ flow path. Figure 15 reports the cost of a range of designs with respect to
9 the fourteen-stage case. The highest cost difference for all machines, with respect to the reference case, is due to
10 the contribution from the inner casing; which accounts for almost 65% of the total $\Delta cost$ for the 4-stage design.
11 Ultimately, this analysis indicates that the 14-stage design results in savings of almost 1.8 M€ with respect to the
12 4-stage machine. Examining Figure 15 further indicates that as the number of stages increases, the cost difference
13 compared to the reference 14-stage design reduces. Specifically, designing the turbine with more than 8-stages results
14 in a direct material cost that only differs by around 0.1 M€ compared to the reference design. This is due to the more
15 similar radial dimensions of the machine (i.e., hub diameter) rather than the increase in the axial dimension obtained
16 for the 14-stage design. Nonetheless, this increase in the direct material cost is considered insignificant bearing in
17 mind that cost pricing is set based on a conservative estimates; where in reality some of the used nickel based alloys
18 are expected to cost higher than the assumed values.
19

20 The preliminary direct material cost analysis indicated that machines with a large number of stages are financially
21 feasible compared to the machines with a small number of stages. Although it is worth noting that the operating
22 expenditure (OPEX) should be added to the overall machine cost to quantify the effect of efficiency differences of
23 the machine over the lifespan of the entire plant. In this regard, the four-stage machine results in a total-to-total
24 efficiency (η_{tt}) that is almost 6% less than the 14-stage machine, and assuming the same thermal input into the cycle,
25 would reduce power output by around 9 MW. By considering the operating expenditure (OPEX) for all machines, the
26 machines with less number of stages, and a lower η_{tt} , are expected to result in higher OPEX compared to the machines
27 with a larger number of stages.
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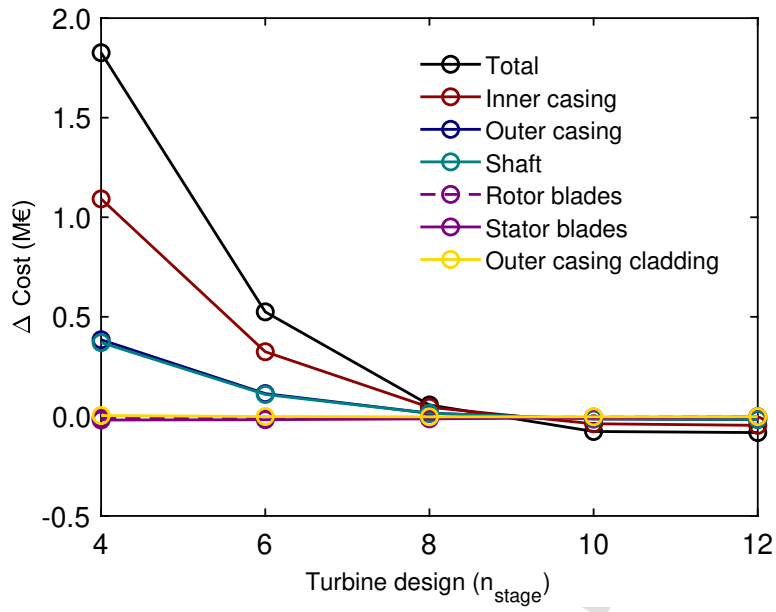


Figure 15: Direct material cost differences associated with the different turbine designs with respect to the CO₂/SO₂ 14-stage design [59]

5. Conclusions

Mean-line flow path designs for a large-scale axial turbine, for installation in a 100 MW_e CSP plant, were presented for different blends based on carbon dioxide, namely CO₂/TiCl₄, CO₂/C₆F₆ and CO₂/SO₂, and for different boundary conditions. The mean-line aerodynamic design was integrated with mechanical and rotordynamic constraints to limit the maximum stress acting on the blades and the length of the shaft for rotordynamic stability. The design tool was verified against case-studies from the literature for air, sCO₂ and organic Rankine cycle (ORC) turbines to ensure the suitability of the design tool for different working fluids. A maximum percentage difference of 1.5% and 1.2% in the total-to-total and total-to-static efficiency, respectively, was observed.

To study the impact of adopting different sCO₂-based blends on the turbine flow path design, multiple flow path designs were produced for different cycle operating conditions, where different turbine inlet temperatures, turbine inlet pressures and molar fraction were considered. The turbine flow paths were designed with the goal of achieving maximum aerodynamic efficiency, while meeting imposed mechanical and rotordynamic considerations. Designs with a large number of stages were found to result in higher turbine efficiencies; this corresponds to designs with reduced hub diameters due to keeping a fixed synchronous rotational speed. These designs showed to be financially feasible compared to short flow path designs based on the conducted preliminary cost analysis results. Among the examined blends, it was found that using the CO₂/TiCl₄ blend resulted in the shortest flow-path length compared to both CO₂/C₆F₆ and CO₂/SO₂. Furthermore, for the three CO₂ blends investigated it was possible to obtain a flow path with an overall total-to-total efficiency in excess of 92%. This is considered promising for the future of CO₂ plants. This proves that using CO₂ blends can result in high efficiencies across the range of the boundary conditions and molar fractions considered. Hence, a high component efficiency is achievable, which will help realise the thermodynamic potential of the proposed cycle designs.

Finally, the sensitivity of the turbine design to the three blends was assessed for optimised cycle conditions. This was completed for two different turbine inlet pressure and temperature levels, ranging between 250 & 350 bar and defined at 550 & 700°C respectively, and for five different molar fractions for each blend. Despite each blend showing a different level of sensitivity to the inlet temperature, pressure and molar fraction, all the flow path designs obtained were found to achieve a high aerodynamic efficiency, which is in excess of 92%, whilst meeting the rotordynamic and mechanical constraints. Moreover, a cycle efficiency greater than 50% was achieved for all the investigated blends at an inlet temperature of 700°C. Ultimately, it is concluded that designing the turbine for the optimal molar fraction that maximises the thermal efficiency of the cycle is a worthwhile endeavour.

Nomenclature

Acronyms

CFD	Computational fluids dynamics
Cond.	Condenser

1	
2	
3	CSP Concentrated Solar Power
4	
5	EoS Equation of State
6	
7	ER Expansion Ratio
8	
9	HRU Heat Rejection Unit
10	HTRec High Temperature Recuperator
11	
12	LCOE Levelised Cost of Energy
13	
14	LTRec Low Temperature Recuperator
15	
16	ORC Organic Rankine cycle
17	
18	PHX Primary Heat Exchanger
19	
20	PR Pressure Ratio
21	
22	Rec. Heat Recuperator
23	
24	SCARABEUS Supercritical Carbon dioxide/Alternative fluids Blends for Efficiency Upgrade of Solar power plants
25	
26	sCO ₂ Supercritical Carbon Dioxide

Greek Symbols

25	λ_N Stator enthalpy loss coefficient [-]
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27	λ_R Rotor enthalpy loss coefficient [-]
28	
29	Δh Enthalpy rise [kJ/kg]
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31	η_{th} Thermal efficiency [%]
32	
33	η_{tt} Total-to-total efficiency [%]
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35	Λ Degree of reaction [-]
36	
37	ϕ Flow coefficient [-]
38	
39	ψ Loading coefficient [-]
40	
41	ρ Gas density [kg/m ³]
42	
43	σ bending stress [MPa]

Roman Symbol

42	\dot{m} Mass flow [kg/s]
43	
44	c Chord length [m]
45	
46	D Diameter [m]
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48	h Blade height [m]
49	
50	n number of stages/rotor blades [-]
51	
52	o Throat opening [m]
53	
54	s Blade pitch [m]
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56	t Trailing edge blade thickness [m]
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58	TIT Turbine Inlet Temperature [°C]
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60	W_s Specific Work [kJ/kg]
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3 X_i Molar fraction of dopant [%]
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5 Y Total pressure loss coefficient [-]
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7 Subscripts

- 8 blades rotor blades
9
10 hub at the hub
11
12 in inlet
13
14 max maximum
15
16 opt optimum
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18 PHX Primary Heat Exchanger
19
20 stage turbine stages
21
22 turb compression
23
24 turb turbine

24 Acknowledgements

25
26 The SCARABEUS project has received funding from the European Union's Horizon 2020 research and innovation
27 programme under grant agreement N°814985.
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Appendix A. Turbine design methodology

A full description of the turbine design methodology is presented in this section, although the method largely builds on the authors previous work [53]. An iterative design process is implemented to obtain the turbine design at a constant hub diameter. The design process starts with assuming a constant enthalpy drop across the stage ($\Delta h_{0(stage)}$), loading coefficient (ψ) of the first design stage, flow coefficient (ϕ) and degree of reaction (Λ). Based on this, the peripheral blade speed at the rotor inlet and the axial flow velocity through the whole machine are obtained:

$$U = \sqrt{\frac{\Delta h_{0(stage)}}{\psi}} \quad (\text{A.1})$$

$$C_a = U_2 \times \Phi \quad (\text{A.2})$$

The relation between total enthalpy and static enthalpy at the rotor inlet and exit and the degree of reaction definition can be expressed as:

$$h_{02} = h_2 + \frac{1}{2} C_2^2 \quad (\text{A.3})$$

$$h_{03} = h_3 + \frac{1}{2} C_3^2 \quad (\text{A.4})$$

$$\Lambda = \frac{h_2 - h_3}{h_{01} - h_{03}} \quad (\text{A.5})$$

The absolute velocity components C_2 and C_3 are expressed as a function of the axial (C_a) and tangential velocity components (C_w) as:

$$C_2 = \sqrt{C_a^2 + C_{w2}^2} \quad (\text{A.6})$$

$$C_3 = \sqrt{C_a^2 + C_{w3}^2} \quad (\text{A.7})$$

The ratio between the inlet blade speed and outlet blade speed (R) is assumed to be equal to U_2/U_3 . Using Equations A.3 - A.5, the degree of reaction can be expressed as:

$$\Lambda = \frac{\Delta h_0 - \frac{1}{2} C_2^2 + \frac{1}{2} C_3^2}{\Delta h_0} \quad (\text{A.8})$$

hence,

$$\Delta h_0 (1 - \Lambda) = \frac{1}{2} C_2^2 + \frac{1}{2} C_3^2 \quad (\text{A.9})$$

Using Equations A.6 - A.7, this can be expressed as:

$$\Delta h_0 (1 - \Lambda) = \frac{1}{2} (C_a^2 + C_{w2}^2) - \frac{1}{2} (C_a^2 + C_{w3}^2) \quad (\text{A.10})$$

The tangential velocity component at the rotor outlet can then be obtained from:

$$C_{w3} = \sqrt{C_{w2}^2 - 2\Delta h_0 (1 - \Lambda)} \quad (\text{A.11})$$

The enthalpy drop across the stages is defined as:

$$\Delta h_0 = U_2 C_{w2} + U_3 C_{w3} \quad (\text{A.12})$$

Substituting Equation A.11 in the definition of the angular momentum (Equation A.12) enables calculating the tangential velocity components at the inlet and outlet of the rotor blades (C_{w2} & C_{w3}). Therefore, the flow angles can be obtained as follows:

$$\alpha_3 = \tan^{-1} \frac{C_{w3}}{C_a} \quad (\text{A.13})$$

$$\alpha_2 = \tan^{-1} \frac{C_{w2}}{C_a} \quad (\text{A.14})$$

$$\beta_2 = \tan^{-1} [\tan \alpha_2 - U_2/C_a] \quad (\text{A.15})$$

$$\beta_3 = \tan^{-1} [\tan \alpha_3 - U_3/C_a] \quad (\text{A.16})$$

Following this, velocities at the inlet and the outlet of the stator and rotor blade rows can be calculated (Equations A.17 - A.20) and deviation angles can be obtained using the approach described by Ainley and Mathieson [57].

$$C_2 = \frac{C_a}{\cos \alpha_2} \quad (\text{A.17})$$

$$W_2 = \frac{C_a}{\cos \beta_2} \quad (\text{A.18})$$

$$C_3 = \frac{C_a}{\cos \alpha_3} \quad (\text{A.19})$$

$$W_3 = \frac{C_a}{\cos \beta_3} \quad (\text{A.20})$$

With the velocities fully defined, the thermophysical properties at the different turbine stations can be obtained through the equation of state:

$$[P, T] = f(h, s) \quad (\text{A.21})$$

$$[\rho, c_p, k] = f(P, T) \quad (\text{A.22})$$

At this stage, the flow areas can be obtained as a function of the density and the axial velocity, which is assumed to be constant across all the design stages. Following this, the hub diameter, mean diameter and diffusion angle can be calculated and U_3 can be updated. The process can then be reiterated until convergence. For the subsequent stages after the first stage, the axial velocity and enthalpy drop across the stage are known from the earlier stage and hence the process is initiated with the assumed degree of reaction, blade velocity U_2 and ratio $R = U_2/U_3$.

The aerodynamic performance of the turbine stage should be evaluated to predict the total-to-total turbine efficiency as defined in Equation A.23:

$$\eta_{tt} = \left[1 + \left(\frac{\zeta_R W_3^3 + \zeta_S C_2^2 \frac{T_3}{T_2}}{2(h_{01} - h_{03})} \right) \right]^{-1} \quad (\text{A.23})$$

where C and w are the absolute and relative velocities and ζ_S and ζ_R are the enthalpy loss coefficients for the stator and rotor respectively. Within the mean-line design context, losses are introduced in the form of stagnation pressure loss coefficients for the stator and rotor. These are defined as follows:

$$Y_S = \frac{p_{01} - p_{02}}{p_{02} - p_2} \quad (\text{A.24})$$

$$Y_R = \frac{p_{03,rel} - p_{03,rel}}{p_{03,rel} - p_{3,rel}} \quad (\text{A.25})$$

To calculate the total-to-total turbine efficiency (η_{tt}), the stator and rotor pressure loss coefficients (Y_S & Y_R) are converted to enthalpy loss coefficients using the expressions:

$$\zeta_R = Y_R \times (1 + 0.5(k M_3^2)) \quad (\text{A.26})$$

$$\zeta_S = Y_S \times (1 + 0.5(k M_2^2)) \quad (\text{A.27})$$

where k is the specific heat ratio, and M_2 and M_3 are the absolute rotor inlet and relative rotor outlet Mach numbers respectively. Stagnation pressure loss coefficients for the stator and rotor (Y_S & Y_R) are obtained by quantifying the energy losses that the working fluid experiences during the expansion in the stator and rotor blade rows using the Aungier loss model [54]. The design process can be summarised into the following steps and using the flow chart in Figure A.16.

1. Assume ϕ , ψ , λ for the first design stage.
2. Define t/o , s/c , t_{cl} , k_s .
3. Assume the number of rotor blades (n_{blades}), number of stages (n_{stages}).
4. Assume the total-to-total turbine efficiency (η_{tt}), stator loss coefficients (ζ_S), $R = U_2/U_3$.
5. Blade angles and velocity triangles are calculated.
6. Flow thermodynamic properties including pressure (P), temperature (T), density (ρ), speed of sound, the ratio of specific heats (k) and viscosity (ν) are obtained using Simulis [60].
7. Obtain detailed blade geometry including, blade heights, annulus area, chord and axial chord length, blade pitch and throat-to-pitch ratio (o/c).
8. Estimate annulus losses and hence stage and turbine efficiency.
9. Obtain R and U_2 and re-iterate until the residual error between the assumed and calculated values satisfies the specified criteria.
10. Obtain turbine efficiency (η_{tt}) and re-iterate until the residual error between the assumed and calculated efficiency satisfies the specified criteria.

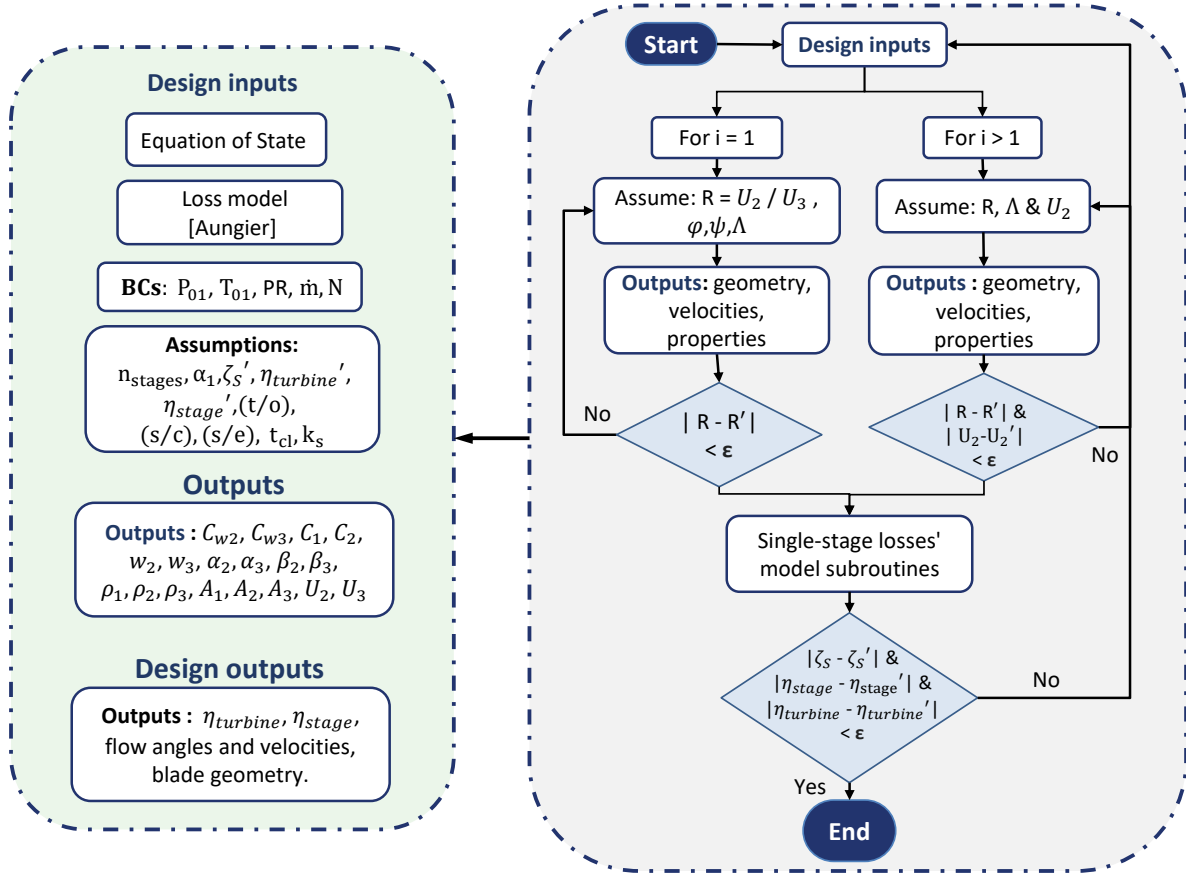


Figure A.16: Flow chart of a multi-stage axial turbine design methodology at constant hub diameter.

11. Calculate the tensile centrifugal and gas bending stresses on the turbine blades.

The designs are then evaluated from both the rotordynamic and mechanical perspective to ensure that $\sigma_{bending}$, C and SR are within the threshold limits. If the design does not meet the specified criteria, then the number of blades ($35 < n_{blades} < 100$) and the number of stages should be modified manually until the mechanical and rotordynamic design constraints are met (Figure A.17); for example, the chord length should be increased, and the number of blades decreased accordingly to maintain the solidity, in order to reduce the bending stresses. The number of stages should also be reduced to bring the slenderness ratio within the specified limit.

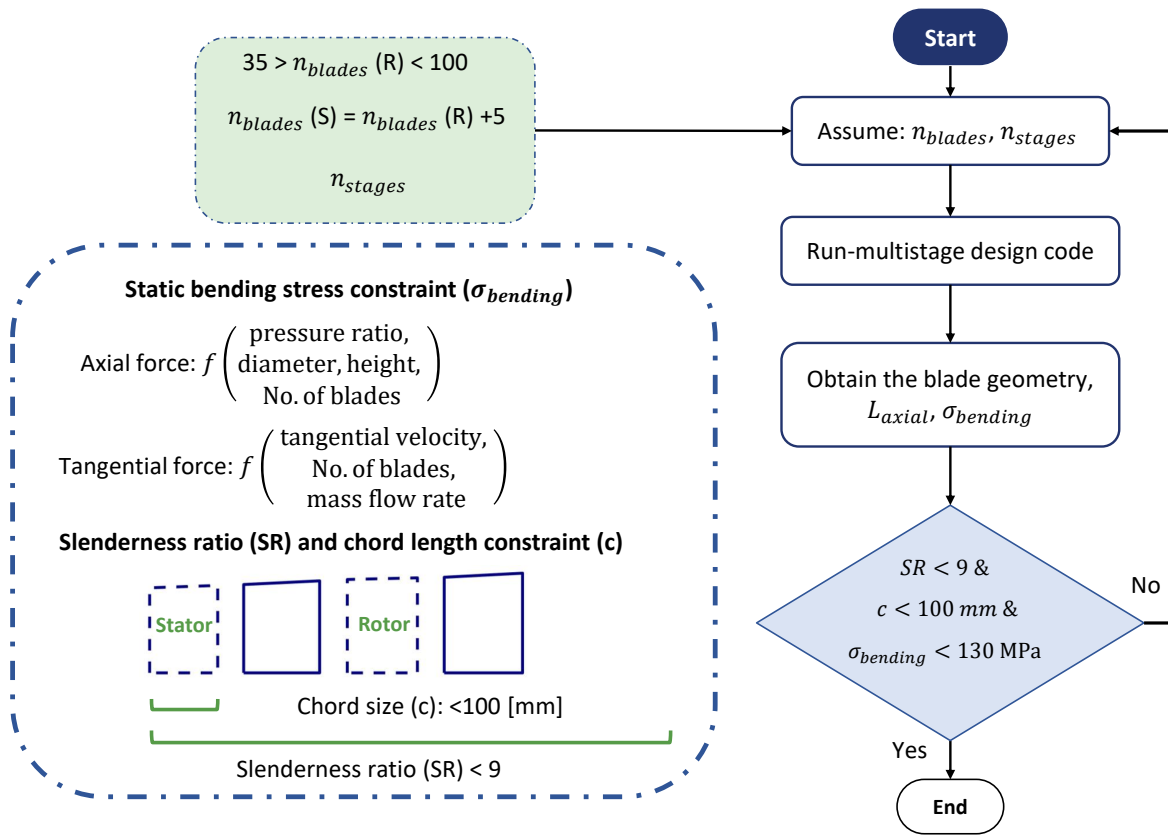


Figure A.17: Flow path optimisation methodology considering mechanical and rotordynamic design criteria.

The turbine design model has previously been verified against cases from the literature operating with conventional working fluids, such as air, and non-conventional working fluids including $s\text{CO}_2$. The design tool has been verified for a 140 KW air, 10 MW $s\text{CO}_2$ and 440 & 1520 KW organic Rankine cycle (ORC) to ensure the suitability of the design tool for different working fluids. The results of both verification cases were reported in the authors previous work [53], but a summary of the results is shown in Table A.7 & A.8 . Ultimately, a good agreement is obtained for both the geometric parameters as well as the total-to-total efficiency. Specifically, for the four selected verification cases the maximum percentage differences in the total-to-total and total-to-static efficiency were 1.3% and 1.2% respectively.

Table A.7: Verification results of the Loss models versus the experimental data and CFD simulations for the 140 kW air turbine [53].

Parameter	Symbol	AN [53]	EXP. Data [61–63]	CFD [64]
Stator outlet absolute flow angle [°C]	α_2	69.53	69.84	68.45
Stator outlet relative flow angle [°C]	β_2	6.58	7.13	4.82
Stator outlet absolute velocity [m/s]	C_2	156.78	170.8	153.84
Absolute Mach at Stator outlet [-]	M_2	0.42	0.457	0.412
Static pressure at Stator outlet [bar]	P_2	1.10	1.111	1.108
Static temperature at Stator inlet [K]	T_2	357.15	357.4	357.4
Static temperature at Stator outlet [K]	T_3	346.45	347.17	347.06
Rotor outlet relative flow angle [°C]	β_3	68.79	68.75	67.07
Rotor outlet absolute flow angle [°C]	α_3	0.73	2.45	7.58
Rotor outlet relative velocity [m/s]	W_3	151.53	166.3	157.51
Static pressure at rotor outlet [bar]	P_3	0.98	0.994	0.983
Static temperature at rotor outlet [K]	T_3	336.52	337.86	336.60
Stator mean radius [mm]	r_{2m}	186.42	181.5	181.5
Rotor mean radius [mm]	r_{3m}	186.42	185	185
Stator inlet blade height [mm]	h_1	88.1	89.2	89.2
Stator outlet (rotor inlet) blade height [mm]	h_2	95.79	97	97
Rotor outlet blade height [mm]	h_3	103.91	103	103
Number of Stator blades [-]	n_N	28	29	29
Number of rotor blades [-]	n_R	30	30	30
Stator loss coefficient [%]	ζ_S	6.2	3.79	5.82
Rotor loss coefficient [%]	ζ_R	7.5	9.08	6.66
Total-to-total stage efficiency [%]	η_{tt}	92.83	91.62	93.32

Table A.8: Verification results of the axial turbine design for air and sCO₂ and ORC turbines [53].

Parameter	Description	Aungier [53]	Results [23, 61, 62, 65]
140 kW air turbine			
ζ_S (%)	Nozzle kinetic energy loss coefficient	0.062	0.038
ζ_R (%)	Rotor kinetic energy loss coefficient	0.074	0.091
η_t (%)	Total-to-total efficiency	0.928	0.916
Difference (%)	η_{tt} (%) with respect to Exp.Data	1.310	-
10 MW sCO₂ turbine/ [1st turbine stage]			
ζ_S (%)	Nozzle kinetic energy loss coefficient	0.037	-
ζ_R (%)	Rotor kinetic energy loss coefficient	0.072	-
η_t (%)	Total-to-total turbine efficiency	0.920	0.916
Difference (%)	η_{tt} (%) with respect to Exp.Data	0.437	-
440 kW ORC turbine			
Y_T	Total loss	0.183	0.180
η_{ts} (%)	Total-to-static efficiency	0.896	0.891
Difference (%)	η_{ts} (%) with respect to Exp.Data	0.561	-
1520 kW ORC turbine			
Y_T	Total loss	0.446	0.444
η_{ts} (%)	Total-to-static efficiency	0.865	0.855
Difference (%)	η_{ts} (%) with respect to Exp.Data	1.169	-

Appendix B. Candidate boundary conditions for turbine design

This annex presents the entire set of specifications employed in the turbine mean line design. More information regarding the selection criteria are provided in Section 4.1. A graphical representation of the different operating conditions considered is provided in Figures B.18 to B.20, employing the same surface and contour plots previously discussed in Section 4.1 (Figures 3 to 5). Optimum cases (font in bold in tables) are represented by star markers, and the remainder by circles.

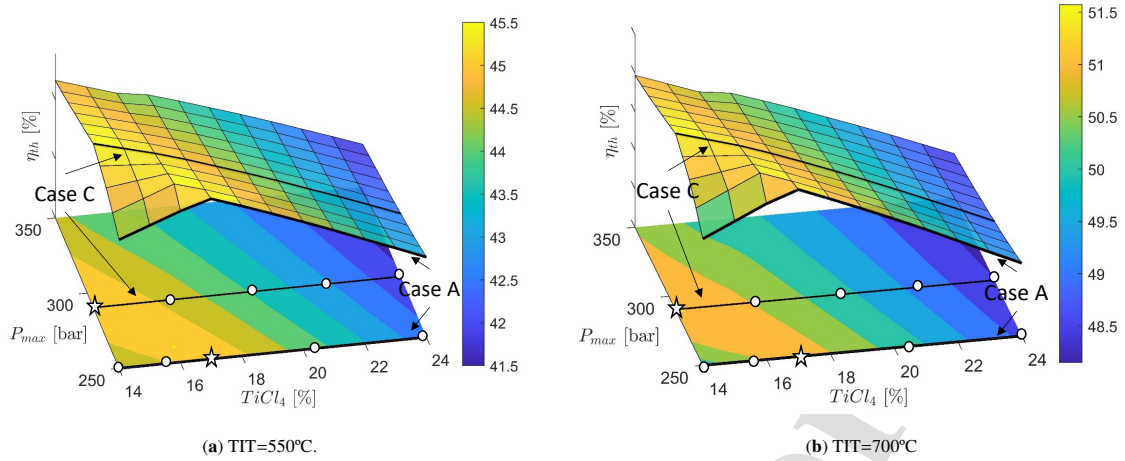


Figure B.18: Thermal efficiency of a simple recuperated cycle operated with $\text{CO}_2/\text{TiCl}_4$ blends as a function of maximum cycle pressure and dopant molar fraction. Two turbine inlet temperatures are considered. The operating conditions employed in turbine design as identified by markers, the different Cases by black solid lines.

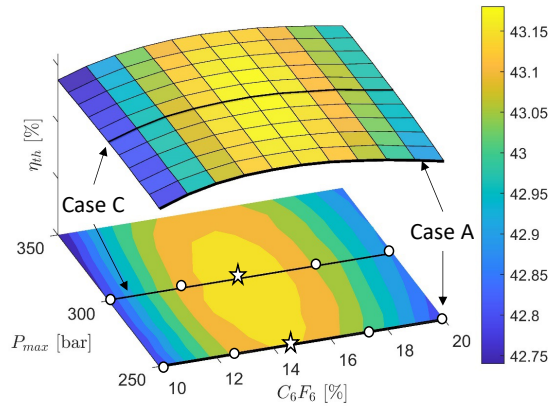


Figure B.19: Thermal efficiency of a precompression cycle operated with $\text{CO}_2/\text{C}_6\text{F}_6$ blends as a function of maximum cycle pressure and dopant molar fraction, considering a turbine inlet temperature of 550°C (results at 700°C are not reported due to the limited thermal stability of this blend).

The operating conditions employed in turbine design as identified by markers, the different Cases by black solid lines.

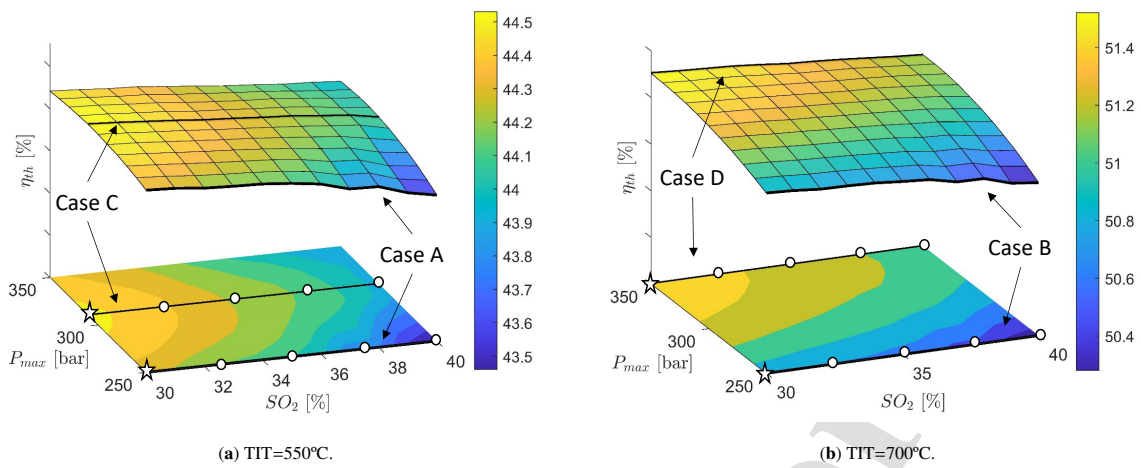


Figure B.20: Thermal efficiency of a recompression

cycle operated with sCO_2/SO_2 blends as a function of maximum cycle pressure and dopant molar fraction. Two turbines inlet temperatures are considered. The operating conditions employed in turbine design as identified by markers, the different Cases by black solid lines.

Table B.9: Complete set of specifications employed for turbine design (Cases A and B). The results for precompression cycle with CO₂/C₆F₆ at 700°C are not reported due to the limited thermal stability of this blend

		Case A (TIT = 550°C, Pmax = 250 bar)					Case B (TIT = 700°C, Pmax = 250 bar)				
CO ₂ /TiCl ₄	Thermal Efficiency [%]	44.35	44.92	45.42	44.13	42.71	50.28	50.84	51.33	50.21	48.89
	TiCl ₄ molar fraction [%]	14	15.5	17	20.5	24	14	15.5	17	20.5	24
	Turbine mass flow [kg/s]	1485	1535	1577	1677	1756	1174	1210	1241	1312	1367
	Turbine Inlet T [°C]	550	550	550	550	550	700	700	700	700	700
	Turbine Inlet P [bar]	242.6	242.6	242.6	242.6	242.6	242.6	242.6	242.6	242.6	242.6
	Turbine Outlet P [bar]	98.13	97.66	97.14	95.40	93.44	98.13	97.66	97.14	95.40	93.44
	Total turbine isentropic enthalpy drop [kJ/kg]	90.36	87.65	85.14	80.24	76.08	109.80	106.68	103.80	98.25	93.59
	Total-to-total turbine efficiency [%]	92.92	93.00	92.50	92.65	92.05	93.52	93.24	93.29	93.01	93.10
CO ₂ /C ₆ F ₆	Thermal Efficiency [%]	42.81	43.12	43.17	43.08	42.87	-	-	-	-	-
	C ₆ F ₆ molar fraction [%]	10	12.5	14.5	17.5	20	-	-	-	-	-
	Turbine mass flow [kg/s]	1098	1129	1152	1186	1212	-	-	-	-	-
	Turbine Inlet T [°C]	550	550	550	550	550	-	-	-	-	-
	Turbine Inlet P [bar]	238.9	238.9	238.9	238.9	238.9	-	-	-	-	-
	Turbine Outlet P [bar]	64.63	62.33	61.48	58.81	57.53	-	-	-	-	-
	Total turbine isentropic enthalpy drop [kJ/kg]	143.38	139.01	134.47	130.29	125.94	-	-	-	-	-
	Total-to-total turbine efficiency [%]	93.84	93.64	93.68	93.46	93.49	-	-	-	-	-
sCO ₂ /SO ₂	Thermal Efficiency [%]	44.32	44.21	44.11	43.82	43.46	50.87	50.79	50.71	50.54	50.28
	SO ₂ molar fraction [%]	30	32.5	35	37.5	40	30	32.5	35	37.5	40
	Turbine mass flow [kg/s]	1016	999.9	991.3	995.6	1004	780.8	772.8	760.4	760.0	761.8
	Turbine Inlet T [°C]	550	550	550	550	550	700	700	700	700	700
	Turbine Inlet P [bar]	238.9	238.9	238.9	238.9	238.9	238.9	238.9	238.9	238.9	238.9
	Turbine Outlet P [bar]	69.93	67.75	65.60	63.47	61.35	69.93	67.75	65.60	63.47	61.35
	Total turbine isentropic enthalpy drop [kJ/kg]	151.87	153.53	155.18	156.84	158.51	184.14	186.32	188.50	190.70	192.92
	Total-to-total turbine efficiency [%]	94.07	94.04	94.02	94.03	94.03	94.03	94.00	93.96	93.95	93.95

Table B.10: Complete set of specifications employed for turbine design (Cases C and D). The results for precompression cycle with CO₂/C₆F₆ at 700°C are not reported due to the limited thermal stability of this blend

		Case C (TIT = 550°C, Pmax = Popt)					Case D (TIT = 700°C, Pmax = Popt)				
CO ₂ /TiCl ₄	Thermal Efficiency [%]	45.55	44.86	44.02	43.09	42.13	51.57	50.96	50.21	49.97	48.53
	TiCl ₄ molar fraction [%]	14	16.5	19	21.5	24	14	16.5	19	21.5	24
	Turbine mass flow [kg/s]	1316	1387	1455	1521	1571	1032	1084	1132	1178	1212
	Turbine Inlet T [°C]	550	550	550	550	550	700	700	700	700	700
	Turbine Inlet P [bar]	281.4	281.4	281.4	281.4	281.4	281.4	281.4	281.4	281.4	281.4
	Turbine Outlet P [bar]	98.13	97.33	96.22	94.79	93.44	98.13	97.33	96.22	94.79	93.44
	Total turbine isentropic enthalpy drop [kJ/kg]	104.07	98.84	94.36	90.52	86.93	126.80	120.79	115.67	111.33	107.30
	Total-to-total turbine efficiency [%]	92.94	93.07	92.77	92.38	92.48	93.53	93.39	93.47	93.27	93.03
CO ₂ /C ₆ F ₆	Thermal Efficiency [%]	42.80	43.10	43.17	43.07	42.89	-	-	-	-	-
	C ₆ F ₆ molar fraction [%]	10	12.5	15	17.5	20	-	-	-	-	-
	Turbine mass flow [kg/s]	987.7	1016	1046	1073	1101	-	-	-	-	-
	Turbine Inlet T [°C]	550	550	550	550	550	-	-	-	-	-
	Turbine Inlet P [bar]	286.7	286.7	286.7	286.7	286.7	-	-	-	-	-
	Turbine Outlet P [bar]	66.13	64.28	63.47	60.68	58.91	-	-	-	-	-
	Total turbine isentropic enthalpy drop [kJ/kg]	159.57	153.64	146.93	143.49	139.15	-	-	-	-	-
	Total-to-total turbine efficiency [%]	93.55	93.58	93.42	93.45	93.49	-	-	-	-	-
CO ₂ /SO ₂	Thermal Efficiency [%]	44.53	44.42	44.29	44.16	43.95	51.52	51.44	51.31	51.23	51.1
	SO ₂ molar fraction [%]	30	32.5	35	37.5	40	30	32.5	35	37.5	40
	Turbine mass flow [kg/s]	907.8	903.0	892.0	888.8	879.9	649.7	645.9	639.2	636.2	634.7
	Turbine Inlet T [°C]	550	550	550	550	550	700	700	700	700	700
	Turbine Inlet P [bar]	296.3	296.3	296.3	296.3	296.3	334.5	334.5	334.5	334.5	334.5
	Turbine Outlet P [bar]	69.93	67.75	65.60	63.47	61.35	69.93	67.75	65.60	63.47	61.35
	Total turbine isentropic enthalpy drop [kJ/kg]	175.15	176.34	177.53	178.73	179.95	229.37	230.77	232.17	233.60	235.06
	Total-to-total turbine efficiency [%]	93.67	93.84	93.82	93.82	93.80	93.50	93.50	93.47	93.61	93.61

Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

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