Transcritical Cycles With CO₂-based Mixtures for CSP Applications: An Overview of the SCARABEUS Findings

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Abstract. This work summarizes the methodology developed within the H2020 EU project SCARABEUS for the analysis of innovative CO₂-based mixtures used as working fluid in transcritical cycles for CSP applications. By adding a specific quantity of carefully selected dopant to CO₂ it is possible to reach a high mixture critical temperature, suitable for air cooled cycles at very high minimum temperature in hot environments with high efficiencies. Along the methodology, some results related to the design of the turbine and the heat exchangers for the innovative mixtures are presented, including a focus on the system integration between the power block and the solar plant: as such, these results can be considered as interesting research outcomes to widen the knowledge on innovative solutions for efficient power cycles. The new power cycles are foreseen to drastically increase the profitability and cut the specific cost of CSP systems with respect to the state-of-the-art.

Keywords: CO₂-Mixtures, CSP, Heat Exchanger Analysis, Innovative Power Cycles

1. Introduction

In the last few years, a growing interest within the scientific community has been recorded focusing on innovative working fluids to overcome the limits of conventional steam cycles. Supercritical CO₂ (sCO₂) cycles have been recognized as a promising alternative for efficient and compact plants [1], but their behavior is very sensitive to the cold sink temperature, with large penalizations in cycle efficiency for cycle minimum temperatures above 40-45°C, far from the critical temperature of the fluid (31°C). These conditions are easily foreseeable for concentrated solar power (CSP) applications, normally located in hot and arid region exploiting air-cooled steam cycles. An interesting approach to tackle this problem can be reached by tailoring the working fluid to the ambient conditions, increasing its critical temperature to levels around 70°C to 100°C, by operating the power cycle in transcritical conditions with a more limited compression work and a higher cycle efficiency. This concept is highlighted in
the EU H2020 project SCARABEUS [2] [3], where binary mixtures based on CO₂ are used as working fluid. Across this work some of the project results will be evidenced, emphasizing the performance increment of the innovative solution compared to conventional ones.

2. CO₂ mixtures: dopants selections and thermodynamic analysis

The selection of promising CO₂ dopants was carried out according to their foreseen thermal stability and favorable physical and chemical characteristics that were identified for the SCARABEUS CO₂ blends. In particular, an ideal mixture for the SCARABEUS concept should have: (i) a critical temperature above 70°C, (ii) high thermal and chemical stability, (iii) limited risks related to the toxicity, flammability and reactivity of the dopant. On this basis, Table 1 shows some potential working fluids (and CO₂ dopants) with their characteristics.

Table 1. List of potential working fluids and dopants investigated in the SCARABEUS project

<table>
<thead>
<tr>
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<th></th>
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</tr>
</thead>
<tbody>
<tr>
<td>CO₂</td>
<td>124-38-9</td>
<td>31.1 / 73.8</td>
<td>No / No</td>
<td>&gt; 700</td>
<td>Up to 700</td>
</tr>
<tr>
<td>C₆F₆</td>
<td>392-56-3</td>
<td>243.6 / 32.7</td>
<td>Low / Low</td>
<td>&gt; 480 (literature)</td>
<td>Up to 600 (Mixture)</td>
</tr>
<tr>
<td>TiCl₄</td>
<td>7550-45-0</td>
<td>364.6 / 46.6</td>
<td>High / No</td>
<td>&gt; 550 (literature)</td>
<td>650 (Mixture)</td>
</tr>
<tr>
<td>SO₂</td>
<td>7446-09-5</td>
<td>157.7 / 78.8</td>
<td>High / No</td>
<td>&gt; 700</td>
<td>Up to 600 (Mixture)</td>
</tr>
</tbody>
</table>

As reported in the table, the thermal stability of each mixture has been experimentally determined within the SCARABEUS project with a static method for more than 100 hours per each mixture. The process is described in Figure 1: the fresh mixture (T,P) behavior is measured before the thermal stress along an isochoric transformation, loading the mixture in a Inconel vessel. After the thermal stress, for 100 hours, if the (T,P) trend of the same isochoric process differs from the original one of the fresh mixture, the method can allow to qualitatively conclude that possible fluid thermal degradation processes have occurred.

Figure 1. SCARABEUS methodology to assess the thermal stability of a mixture

After the mixture identification and the measurement of the ideally cycle maximum temperature set by the thermal stability, a reliable equation of state (EoS) is necessary to calculate the thermodynamic properties and the vapor-liquid equilibrium (VLE) behavior of the mixture [4]. In particular, VLE data are used to identify the extension of the two-phase region at low temperature, impacting the condensation of the working fluid, and to set the cycle mini-
mum pressure at given temperature, while the EoS is exploited to assess the power cycle characteristics and, ultimately, its efficiency.

Considering the $\text{CO}_2+\text{C}_6\text{F}_6$ mixture as an example, the plot in Figure 2 (left) is reported to stress the importance of tuning the EoS with experimental data according to a simplified methodology: for each EoS, the binary interaction parameter $k_{ij}$ is retrieved to fit at best the experimental VLE data, including a set of data taken within the SCARABEUS project [5]. The same figure on the right shows the trend of isobars of interest for a thermodynamic cycle assuming a mixture composition that allow for a critical temperature of around 100°C: the difference between a s$\text{CO}_2$ cycle and the transcritical cycle with this working fluid is well evidenced, especially considering the condensation of the working fluid from 135°C and the limited temperature difference along the compression step.

![Figure 2. Behavior of the $\text{CO}_2+\text{C}_6\text{F}_6$ mixture (85% mol $\text{CO}_2$) with the PR EoS, including bubble data from literature (red dots) and data from the SCARABEUS consortium (green dots) ](image)

Analogous considerations on EoS are done for other mixtures [6], while considering the cycle for CSP applications. According to the project outcomes, conventional EoS already embedded in commercial tools like ASPEN Plus, such as the Peng Robinson and the PC-SAFT EoS, can be adopted for the SCARABEUS purposes: as a matter of fact, a reasonable level of accuracy on VLE data is evidenced when the $k_{ij}$ is optimized, allowing to effectively perform cycle calculations and to size the cycle components, which are the two major focuses of the research on mixtures as working fluids.

3. Experimental validation and heat exchanger characterization with $\text{CO}_2$ mixtures

3.1 Recuperator with innovative S-shaped and airfoil channels

At the current state-of-the-art, printed circuit heat exchangers (PCHE) are studied and designed with either straight or Zig Zag channels, especially in the s$\text{CO}_2$ field as recuperators. A small subset of literature studies deals with CFD calculations for alternative geometries (e.g. Airfoil) to improve the heat exchange and/or reduce the pressure losses [7]. However welding plates with such specific geometries using diffusion bonding process represents a challenge as contact surfaces are limited. Therefore, a compromise between the effectiveness and the manufacturing feasibility must be studied.

Within the SCARABEUS project, PCHE will be optimized by trying to replace conventional Zig Zag channels by two new geometries: S-shaped and airfoil. To do so, CFD calculations have been performed for airfoil (16 geometries) and S-shaped (8 geometries). A meth-
ontology has been developed to estimate the potential saving, by analyzing the reduction of the plates surface, considering the heat transfer coefficient and the pressure drop. In parallel, some FEA calculations were necessary to check the compatibility of the geometries with the operating conditions (220 bars and 600 °C) from a mechanical point of view: the results suggest that the configuration/arrangement have a huge impact on the mechanical stress. For example, for the operating conditions of SCARABEUS, a configuration from literature leads to a stress level which is more than 5 times the allowable value from ASME section VIII code.

Figure 3 presents the results of simulation on S-shaped and airfoil fins (considering various “S” and airfoil geometries) for the recuperator of the CO₂+C₆F₆ simple recuperative cycle, when compared with zig-zag channels, fixing the channel pressure drop at 1 bar and the UA value at 7.2 kW/K/channel. The purple bars show the reduction in heat exchange area, while the red bars the reduction in plate surface. The best solution allows to reduce the plate surface by 8% with S-shaped and by 14% for airfoils.

3.2 In-tube heat transfer enhancement for air-cooled condenser

Several internal structures are studied in literature to increase the heat transfer inside a tube [8]. Within the SCARABEUS project, considering the tubes of the air-cooled condenser, internal helical fins are found to have the best thermal performance. Microstructures have also demonstrated their efficiency but only for low Reynolds number. Internal fins were tested with thermo-hydraulic measurements at the test facility at TU Wien with 1” tubes. Two sets of experiments were performed with pure CO₂ and a mixture of CO₂+R1234ze(E) [9]. Figure 4 on the left presents the test tube adopted for the experimental analysis on heat transfer, while on the right it is reported the validation of the experimental internal convective heat transfer coefficients during condensation, measured on the CO₂ + R1234ze(E) mixture, with respect to the literature correlation of Cavallini [10], modelled with a set of transport properties tailored to this mixture [9].

Due to the good level of accuracy reached, the convective model has been adopted in the SCARABEUS project for the design of condensers. Based on the results extrapolated to a full-scale plant, an air condenser for a CO₂+mixture power cycle designed with a combination of inner microfins and groovy fins on air side could be 15% smaller and 20% less expensive than standard technologies for air-cooler of sCO₂ cycles.
3.3 Test facility at TU Wien: demonstration of the SCARABEUS concept

A test facility in Vienna will demonstrate the project feasibility using the CO2+C6F6 mixture as representative of the concept. The goal is to show the viability of circulating the mixture through a compression, a heating, an expansion and a cooling step across temperature and pressure ranges similar to the ones of a real application, ultimately by enabling the complete condensation of the working fluid at temperatures above 50 °C.

The test facility simulates a simple recuperated transcritical cycle, as shown in Figure 5. The heat is provided to the cycle by the flue gases from natural gas burner. The turbine of the cycle is emulated with an expansion valve from the maximum pressure (215 bar at design conditions), and the air-cooled condenser receives air from a ventilation system. Additional information on the characteristics of the test rig can be found in literature [11].

The test rig will be filled with working fluid twice, operating both times in “full working conditions”: initially with sCO2 and then with the mixture, whose Ts diagrams can be seen in Figure 5. The pure CO2 experiments are planned mainly to test two different PCHE designs (one with straight channels and the second with S-shaped fins) under various working conditions: mass flow rate between 0.2-0.6 kg/s, hot inlet temperature between 200-600 °C and high pressure between 80-215 bar. Then, while using the CO2+C6F6 mixture (92% molar CO2), the test rig will be operated with a minimum pressure of around 90 bar, condensing the working fluid from 106°C to 50°C, exploiting the ambient temperature as coolant.

Figure 5. Layout of test facility at TU Wien [11] and Ts diagrams of the operation with sCO2 and the CO2+C6F6 mixture
4. Turbine design and performances for CO₂ mixtures

In addition to the research on the heat exchangers for CO₂-mixtures, SCARABEUS partners focused on the design of the turbine of the cycle considering both aerodynamic and mechanical aspects: the aerodynamic design was done using a mean-line model, followed by 3D blade design and blade shape optimization using CFD simulations. The full details of the mean-line design approach implemented within this project can be found in literature [12]. Subsequently, the mechanical design was undertaken. To ensure turbine mechanical integrity, the static bending stress limit was specified to be 130 MPa, a slenderness ratio (the ratio of bearing span to hub diameter) of less than 9 was set and the number of blades in each stage was varied from 35 to 95. Due to the large scale of the plant, a direct connection between the turbine and generator was selected, where the turbine speed is set at 3000 rpm. Multiple mean-line flow path designs have been produced, at turbine inlet temperature (TIT) of 500°C and 700°C, for the CO₂+TiCl₄, CO₂+C₆F₆ and the CO₂+SO₂ mixtures spanning various dopant molar fractions and operating conditions. It was possible to obtain total-to-total efficiency above 92% and up to 94% for the three blends, showing that designs involving CO₂ mixtures can result in high efficiencies across a range of boundary conditions [13].

Based on the SCARABEUS findings on fluid thermal stability, environmental considerations, and optimized cycle analysis for the various mixtures, the CO₂+SO₂ mixture was selected to provide a complete design of the turbine for a cycle with TIT of 700°C. Therefore, a 130 MW axial turbine was designed, with an inlet pressure of 239 bar and a pressure ratio of 2.8, assuming a zero-incidence angle and the inlet flow angle, flow coefficient, loading coefficient and degree of reaction of 0, 0.5, 1.0 and 0.5 respectively. The optimum aerodynamic performance for the 80% CO₂ mixture was achieved with fourteen stages with a hub diameter of 624 mm and a total shaft length of 1.8 m. A summary of the design details of the first, seventh and last turbine stages is provided in Table 2 and the meridian view of the flow path is presented in Figure 6.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>S1</th>
<th>R1</th>
<th>S7</th>
<th>R7</th>
<th>S14</th>
<th>R14</th>
</tr>
</thead>
<tbody>
<tr>
<td>Axial chord [mm]</td>
<td>35.5</td>
<td>38.9</td>
<td>40.4</td>
<td>44.2</td>
<td>48.7</td>
<td>53.1</td>
</tr>
<tr>
<td>Hub radius [mm]</td>
<td>310.6</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Inlet tip radius [mm]</td>
<td>365.1</td>
<td>366.5</td>
<td>386.3</td>
<td>387.5</td>
<td>423.5</td>
<td>425.2</td>
</tr>
<tr>
<td>Outlet tip radius [mm]</td>
<td>366.1</td>
<td>368.0</td>
<td>387.2</td>
<td>389.8</td>
<td>424.7</td>
<td>429.0</td>
</tr>
<tr>
<td>No. of blades</td>
<td>58</td>
<td>53</td>
<td>53</td>
<td>48</td>
<td>47</td>
<td>42</td>
</tr>
<tr>
<td>Tip gap [mm]</td>
<td>-0.515</td>
<td>-</td>
<td>0.546</td>
<td>-</td>
<td>0.601</td>
<td></td>
</tr>
</tbody>
</table>

Following the 1D flow path design, the 3D blade shapes were generated with geometric parameters on the basis of a literature work on blade optimization [15], including leading-edge thickness, inlet/outlet wedge angles, airfoil curvature control points, and blade base fillet. The CFD analysis was performed using ANSYS Workbench, incorporating bladeGen, TurboGrid and ANSYS-CFX solver to generate the blade profile, mesh and simulate flow respectively. The CFD model was based on a steady-state multi-stage setup for a single flow passage, with a mixing plane interface defined between blade row solution domains. Total
pressure and total temperature and flow angles were employed to model stator inlet conditions, while static pressure is specified at the turbine outlet. The blades have also been evaluated using finite element analysis to ensure mechanical stresses are within the specified limits (i.e., the maximum stress is less than 260 MPa). It was demonstrated that using the bending stress limit applied within the mean-line design model would result in feasible turbine geometries from a mechanical design perspective. Further details about the CFD model can be found in literature. It was found that the 14-stage design of Figure 6 can achieve a total-to-total efficiency of 93.86%. The performance results showed a good agreement between the CFD and mean-line results, with a maximum difference of 0.5% observed at the design point. Moreover, off-design simulations of the turbine were carried out, showing that it can operate at a minimum allowable flow coefficient equal to 94.5% of the design flow coefficient, achieving a total-to-total efficiency of 89.2% while keeping an outlet temperature of 600 °C.

The overall turbomachinery design was finalized, including the inner and outer turbine casings, considering manufacturability constraints. The process also involved designing the main cooling streams and selecting the appropriate bearings, seals, and coupling components, reaching a comprehensive cost assessment of the turbine. The total turbine cost was estimated based on direct materials costs, incorporating actual quotations acquired from suppliers. Alternative approaches relying on cost models or correlations would have led to a significant underestimation of raw material costs, since existing cost correlations are based on models developed for steam turbines: they include factors relevant to the flow path, neglecting aspects related to the expander architecture. For the material cost estimation, it is necessary to push the limits of current technologies in the field of large casting and forgings using Ni-based alloys: accordingly, the estimated costs refer to a first-of-a-kind technology. Accordingly, it was found that the design of the 100 MW<sub>el</sub> expander should be considered an upper limit: scale-downs are feasible, but larger sizes would be challenging unless a new design concept is explored to facilitate manufacturability. Scaling up this design is also constrained by the availability of dry gas seals size, which presents a challenge for scaling up the design to accommodate larger power outputs.

Finally, the turboexpander cost for the 100MW<sub>el</sub> plant size was estimated, according to the Association for the Advancement of Cost Engineering (AACE) guidelines to be around 18 M€ in total, including the inner and outer casing, rotor, valves, and excluding the electric generator. Regarding the compatibility of the selected working fluid with the turbine material (Ni-based alloys), various issues are still to be addressed: even if only a minimal interaction with the fluid was demonstrated in exposure tests at 2000 hours at 500°C, the long-term compatibility test remains to be performed at 700°C, also to facilitate the commercialization of the SCARABEUS concept.

5. Integration of the innovative cycles in CSP environments

According to the SCARABEUS concept, the power block technology is replicable across diverse geographical contexts, each characterized by its own annual ambient temperature distribution, mainly due to the possibility to tune the critical temperature of the working fluid to any ambient temperature. The optimal configuration (i.e., cycle layout, working fluid composition, component operating conditions) of the power block has been identified through a dedicated optimization tool based on the integration of commercial (Thermoflex, SolarPILOT, System Advisor Model) and proprietary software along with a genetic algorithm optimizer. The procedure has been applied for two CSP plant categories, characterized by different TIT [16]: 550°C, employing molten salt as Heat Transfer Media (HTM) and external tubular receivers (Gen II of conventional CSP plants) and 700°C, based on solid particles and free-falling particle receivers (Gen III of CSP plants). In fact, the first generation of CSP plants (with thermal oil as HTF) is not considered in the analysis due to the low cycle efficiencies achievable.
An overview of the possible working fluids and their efficiency in solarized power cycles is presented in Figure 7 for different design ambient temperatures (i.e., locations) and for two CSP generations. Five different combinations of working fluid and cycle layout are represented: three SCARABEUS systems (the precompression cycle running on CO₂+C₆F₆, the simple recuperative cycle with CO₂+TiCl₄ and the recompression cycle with CO₂+SO₂), and two systems running on pure sCO₂ with a recompression and a partial cooling layout. This optimum combination of working mixture and cycle layout is the result of several literature works of the SCARABEUS consortium [17].

The various SCARABEUS systems consistently shows a higher cycle efficiency than the sCO₂ counterpart, particularly pronounced at elevated ambient temperatures, due to the increment in compression work far from the critical point of CO₂ (31°C). Moreover, SCARABEUS power cycles exhibit a higher adaptability to different ambient temperatures, derived from their unique capability to modify the dopant content. In fact, Figure 7 also depicts how the optimum dopant molar fraction changes with ambient temperature.

![Figure 7. Thermal efficiency as a function of design ambient temperature for five different combinations of working fluid and cycle layout. TIT of 550°C and 700°C are included](image)

The recompression cycle using CO₂+SO₂ has been used to run a complete description of the technology from the thermo-economic perspective. Off-design performance of the cycle has been estimated using Thermoflex, which has been customized with several user-defined scripts to enable the simulation of SCARABEUS-specific components. Subsequently, a computational platform within the MATLAB environment has been built for the complete solar plant. This platform employs non-physical (surrogate) models, utilizing Artificial Neural Networks to reduce the computational burden. Seville has been chosen as reference location to performance a comparison against state-of-the-art (SoA) technology based on steam turbines. The annual electricity output of a SCARABEUS CSP plant based on both Gen II and Gen III assuming base-load performance has been calculated in literature [18]. SCARABEUS plants have been benchmarked against a SoA plant also from literature [19] and compared under the same economic assumptions from this reference. The results are provided in Table 3. The cost of the SCARABEUS power block has been calculated using a combination of vendor quotes for conventional equipment and proprietary information produced during the project for the SCARABEUS-specific components.

This analysis reveals cost estimate of 1130 €/kWe and 1019 €/kWe for Gen II and Gen III power blocks, which is around 9-18% lower than the reported value for SoA plants (1240 €/kWe). The Levelized Cost of Electricity (LCoE) for SCARABEUS plants is calculated at 121 €/MWhₑ and 116 €/MWhₑ, respectively for Gen II and Gen III, which is 18% and 22% lower than SoA in Seville (148 €/MWhₑ). It is important to highlight that these figures exhibit a notable degree of uncertainty, attributed to the non-commercial nature of the components and
the financial assumptions behind these calculations. Furthermore, it is plausible that these figures could be further diminished with potential increases in the TRL.

**Table 3.** Comparison of the techno-economic performance of a steam-based (SoA) and SCARABEUS CSP plants in Seville (Spain). Costs refers to the year 2020.

<table>
<thead>
<tr>
<th>System</th>
<th>HTM</th>
<th>TIT [°C]</th>
<th>SM</th>
<th>TES Size [h]</th>
<th>Cycle Cost [€/kWe]</th>
<th>LCoE [€/MWe]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rankine, Gen II</td>
<td>Solar Salts</td>
<td>550</td>
<td>3</td>
<td>14.7</td>
<td>1240</td>
<td>148</td>
</tr>
<tr>
<td>SCARABEUS, Gen II</td>
<td>Solar Salts</td>
<td>550</td>
<td>3.26</td>
<td>17</td>
<td>1130</td>
<td>121</td>
</tr>
<tr>
<td>SCARABEUS, Gen III</td>
<td>Particles</td>
<td>700</td>
<td>3.46</td>
<td>18.2</td>
<td>1019</td>
<td>116</td>
</tr>
</tbody>
</table>

6. Conclusions

This work summarizes some of the findings of the EU-funded H2020 SCARABEUS project (ending in early 2024) on innovative CO2-based mixtures as working fluids for transcritical power cycles. The analysis starts with a knowledge of the thermodynamic characteristics of the mixtures of interest (through EoS) and their thermal stability limits. Then, the investigations continue at a component-level, underlining the impact of the CO2-dopant on the design and off-design of the heat exchangers, with a particular focus on the condenser, and the turbine. In the end, the optimal plant layout and cycle boundary conditions can be identified, for each specific mixture and TIT level. The results show that the solutions proposed are more efficient and cost-effective than both steam cycles and sCO2 solutions for the same CSP applications, especially when deployed in arid environments with high ambient temperatures.

Finally, considering the next generation technologies for solar receivers, such as solid particles receivers, receivers with advanced salts or liquid metals, the proposed power cycles propose a tailored solution that can suit the heat introduction process from the solar field, reducing the parasitic losses of steam-based SoA solutions, improving the thermal efficiency of the receiver, while at the same time maintaining a good optical efficiency of the field. Accordingly, the project clearly suggests a possible pathway forward for the scientific research into innovative power cycles for CSP systems: innovative working fluids that can be compressed in the liquid phase at temperature levels around 50°C, suitable to work up to 700°C, can really be of interest to unlock the potential of CSP.

Data availability statement

Data will be made available on request.

Author contributions


Competing 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.
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