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Thermodynamic study of a supercritical carbon dioxide Brayton cycle based on main compression intercooling configuration

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Abstract. This study presents detailed thermodynamic modeling of a supercritical Brayton cycle operating with carbon dioxide as a working fluid for electric power generation. The study incorporates a main compression intercooling configuration while elucidating the effect of operational parameters on the overall performance based on energy and exergy perspectives. The model was carefully validated with relevant authors. Moreover, two different optimization methodologies, namely particle swarm optimization and fmincom, are evaluated based on convergence criteria. The results demonstrated that the fmincom reduced the iteration time between 140 s - 180 s. The cycle pressure played a central role in the stability of the thermophysical properties of the working fluid. The energy and exergy efficiencies present a direct relation with the inlet temperature. The air cooling and regenerators represent the biggest contributor to exergy destruction, whereas the compressors featured minimal impact on the exergy degeneration. Overall, the proposed configuration demonstrated robust performance to implement with high-grade heat sources, especially in non-interconnected areas.

1. Introduction

The continuous development of power generation technologies represents a concrete solution for energy supply in non-interconnected areas where primary grids are not accessible [1,2]. Currently, several power cycles such as Rankine, Kalina, Organic Rankine (ORC), and Brayton stand as the most suitable tools to extract energy from a primary energy source [3]. Moreover, thermodynamic modeling emerges as an essential tool to unravel the feasibility of energy systems from a techno-economic perspective since it identifies the operational parameters that increase energy efficiency, maximize net power output, and reducing exergy destruction [4-6].

One of the important aspects of the operation of power cycles is the appropriate selection of the working fluid. For example, the working fluid variety in ORC applications is extensive, but they commonly represent an environmental hazard, and the adverse feasibility in high energy sources is a concrete limitation [7]. In contrast, carbon dioxide (CO₂) has demonstrated enormous advantages while implemented in Brayton cycles such as low toxicity index and inflammability, low capital cost, and most importantly, the adaptability to operate with supercritical conditions (32 °C at 3.4 kPa) compared to other fluid such like water (374 °C at 22 MPa). The last pattern enables to design of components with less complexity and size, which reflects on improving compatibility [8,9].

Precisely, supercritical CO₂ Brayton cycles (SCBC) has been implemented in several applications demonstrating its versatility with a wide range of energy sources. Padilla, *et al.* [10] found that the SCBC cycle maintains high energetic efficiencies (>50%) for concentrated solar power applications, which



demonstrates the efficacy of this energy conversion system. The authors used Python as the computational modeling environment, and the optimization was based on the Sequential Least Squares Programming (SLSQP). On the other hand, exergy analysis is an important mechanism to compare every component of the system's quality of energy while characterizing key design aspects to improve the overall conversion efficiency [11]. Marchionni, *et al.* [12] implemented a complete analysis of different SCBC configurations for waste heat recovery (WHR) applications based on energy, exergy, and economic perspectives. In this study, Matlab® software was implemented as the modeling tool due to the simplicity and robustness within the calculations and optimization tasks.

The optimization of the operational conditions of the cycle is a challenge in the development of thermodynamic modeling. However, the complexity of data and numerous variables can be simplified through the implementation of computational tools that create a friendly environment to examine the behavior of each variable. Consequently, different types of optimization methodologies have been implemented in power cycle applications to determine the best operational conditions that guarantee optimal performance [13]. Particularly, in the SCBC application, the incorporation, complete description, and optimization of the main compression intercooling (IC) configurations require a further effort to demonstrate reliable performance compared to conventional configurations.

The main contribution of this paper is to describe the thermodynamic modeling of an IC-SCBC configuration from a thermal and exergetic perspective while implementing optimization methodologies. The study incorporates detailed modeling guidelines for the advanced recompression-based SCBC configuration while characterizing the main performance metrics for energy conversion performance. Therefore, this work extends a further effort to enable a comprehensive understanding of thermodynamic modeling of energy systems.

2. Methodology

This section describes the main aspects of the IC-SCBC configuration and the thermodynamic modeling characteristics. Figure 1 depicts the schematics of the proposed cycle configuration.

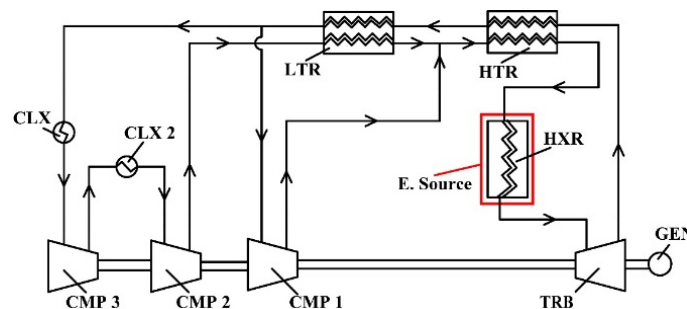


Figure 1. SCBC - main IC configuration.

Before introducing the energy and exergy analyses, it is important to define the main operational parameters that describe the overall performance. This configuration is considered an advanced SCBC configuration due to the functional complexity that is driven to enhance the overall performance. First, one of the key parameters within the configuration corresponds to the main compression ratio (r_c) that relates the pressure ratio between the turbine, which is defined in Equation (1).

$$r_c = \frac{P_{\text{high}}}{P_{\text{low}}}, \quad (1)$$

where represents the maximum and minimum pressure of the cycle, respectively. Subsequently, since the configuration comprises three compression stages, a secondary pressure ratio is derived to relate the intermediate pressure in the cycle, which is defined in Equation (2).

$$r_s = \frac{\frac{P_{high}-1}{P_{int}}}{\frac{P_{high}-1}{P_{low}}} \quad (2)$$

The following assumptions were made to characterize the thermodynamic behavior of the system. The influence of pressure drop within the turbomachinery and heat exchangers is neglected.

- Perfect insulation is considered in the cycle components.
- Both expansion and compression stages behave adiabatically.
- Energy and exergy evaluation only consider the physical and thermal contribution.
- The role of blade thickness is not accounted for the turbomachinery.
- The environmental conditions are set to 25 °C and 101 kPa for the temperature and pressure.

The optimization proposed in the study is evaluated from two different methodologies, namely particle swarm optimization (PSO) and FMINCOM, a non-linear optimization library from Matlab®. Moreover, the fluid properties database has been powered by Coolprop 3.6.0. The optimization criterion of both methodologies is described in Figure 2.

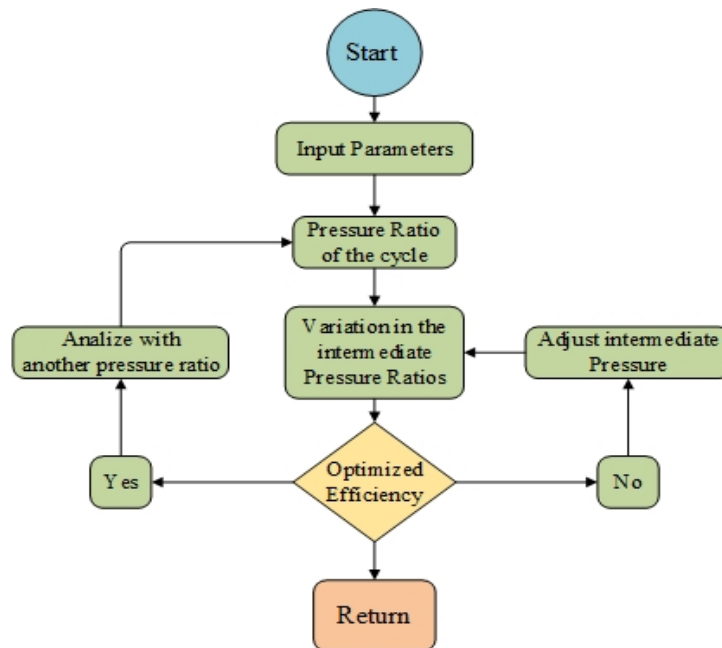


Figure 2. Optimization criteria.

Subsequently, energy and mass balance is performed in all components of the cycle to obtain an operational matrix. Therefore, the thermal efficiency (first law) is calculated with Equation (3), which is defined as the input power and the heat supplied.

$$\eta_{th} = \frac{\dot{W}_{tot}}{\dot{Q}_{in}} \quad (3)$$

The exergy balance at a component level is defined in Equation (4).

$$\sum \dot{E}_{q,in} - \dot{W}_{v,c} + \sum \dot{m}_{in} \cdot b_{in} - \sum \dot{m}_{out} \cdot b_{out} - \dot{E}_D - \dot{E}_L = 0, \quad (4)$$

where \dot{m} is the mass flow, \dot{E}_q is the heat transfer exergy rate, and b is the exergy flow. Finally, the exergy efficiency is calculated with Equation (5), where the exergy destroyed and the exergy supplied are related.

$$\eta_{II} = 1 - \frac{(\sum \dot{E}_{L,component} + \dot{E}_{D,component})}{\dot{E}_{in}} \quad (5)$$

3. Results

3.1. Model validation

The main objective of the validation section is to demonstrate that the pressure ratios can be optimized. The parameters considered for the validation are displayed in Table 1, whereas the validation results are listed in Table 2.

According to the results, the small differences presented between the proposed model and the reference could be associated with the implementation of a different fluid property database or optimization methodology, with a relative error of less than 1%. Next, the comparative assessment of the optimization methodologies is presented in Table 3. The results of the optimization comparison evaluation demonstrate that both methodologies provide similar results.

Table 1. Input data for validation.

Parameter	Value
Turbine efficiency	93%
Compressor efficiency	89%
Heat exchanger effectiveness	95%
Turbine inlet temperature	500 °C – 850 °C
High cycle pressure	25 MPa
Minimum temperature of pinch ratio	5 °C

Table 2. Thermodynamic validation of the proposed model.

Temp (°C)	Thermal efficiency		
	Present study	Padilla, <i>et al.</i> (10)	Error (%)
500	40.75	40.31	0.44
550	43.14	42.66	0.48
600	45.31	44.79	0.52
650	47.28	46.73	0.55
700	49.09	48.51	0.58
750	50.75	50.14	0.60
800	52.28	51.66	0.62
850	53.70	53.06	0.64

Table 3. Comparative assessment of optimization methodologies.

Temp (°C)	PSO		FMINCON	
	η_{th} (%)	Time (s)	η_{th} (%)	Time (s)
500	42.91	215.6	42.91	21.8
550	45.25	219.6	45.25	18.4
600	47.38	146.5	47.38	15.0
650	49.32	167.6	49.32	13.8
700	51.09	179.3	51.09	13.1
750	52.73	184.2	52.73	14.2
800	54.24	193.7	54.24	19.9
850	55.64	135.9	55.64	20.1
Total (s)		180.3		17.0

3.2. Preliminary results of the compression intercooling-supercritical carbon dioxide Brayton

Figure 3(a) shows the effect of the turbine inlet pressure (P_{high}) on the thermophysical variations of the working fluid. Moreover, Figure 3(b) displays the T-S diagram for the lowest energy inlet distribution in the cycle, which corresponds to the minimum Turbine Inlet Temperature (TIT) of 450 °C at a pressure of 25 MPa.

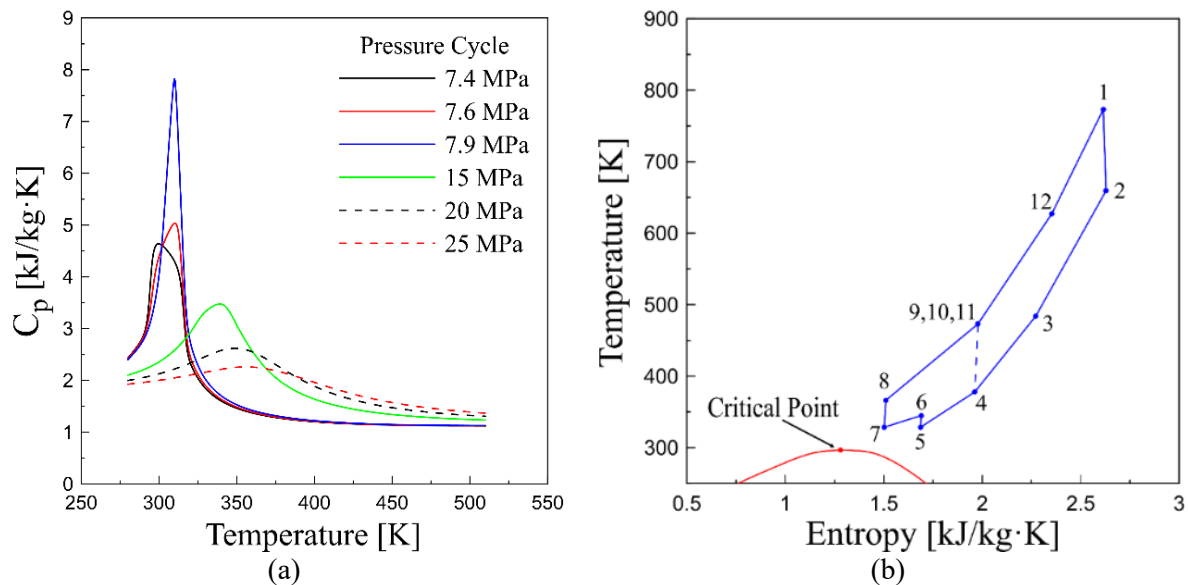


Figure 3. Characterization of the (a) heat capacity variation and (b) T-S diagram of the cycle.

According to the results of Figure 3(a), the imminent variation of the working fluid near the critical point fosters a concrete fluctuation within the calculations. Accordingly, at a pressure range of 7.9 MPa, the heat capacity ratio presents the peak values, which hinders the appropriate prediction of the cycle's overall performance. In contrast, as the pressure increases (e.g., >20 MPa), the curve features a more stable behavior along with the temperature range. Accordingly, the present study uses a P_{high} of 25 MPa. Figure 3(b) shows the T-S diagram corroborating that the cycle operates above the critical point of the working fluid. It is worth mentioning that a higher heat inlet in the cycle (higher TIT) would lift the curve.

3.3. Energy, exergy, and power generation perspectives

This section provides the general results of the thermodynamic modeling. Accordingly, both the thermal and exergy efficiencies are displayed in Figure 4(a), while the optimal pressure ratios are shown in Figure 4(b).

Based on the results, both efficiencies follow a monotonous rise as the TIT escalates, which is a direct consequence of higher net power output and lower exergy losses [14]. These results agree with similar investigations in SCBC [14,15]. Hence, Figure 4(b) demonstrates that the pressure ratios present an inverse relation. Firstly, the main pressure ratio increases sharply as a result of higher TIT. On the other hand, the secondary pressure ratio decreases as TIT escalates since higher compression work is necessary to balance the pressure of the cycle. Overall, the results corroborate that the combination of components such as intercooler, re-compressor, recuperator, and superheater used in a supercritical Brayton cycle can achieve higher thermal efficiencies than an ultra-supercritical (USC) plant, which can achieve an efficiency of about 47% operating between 732 °C - 760 °C and 35 MPa [15]. Figure 5(a) shows the exergy destruction at a component level, and Figure 5(b) displays the specific work production/consumption for the turbomachinery.

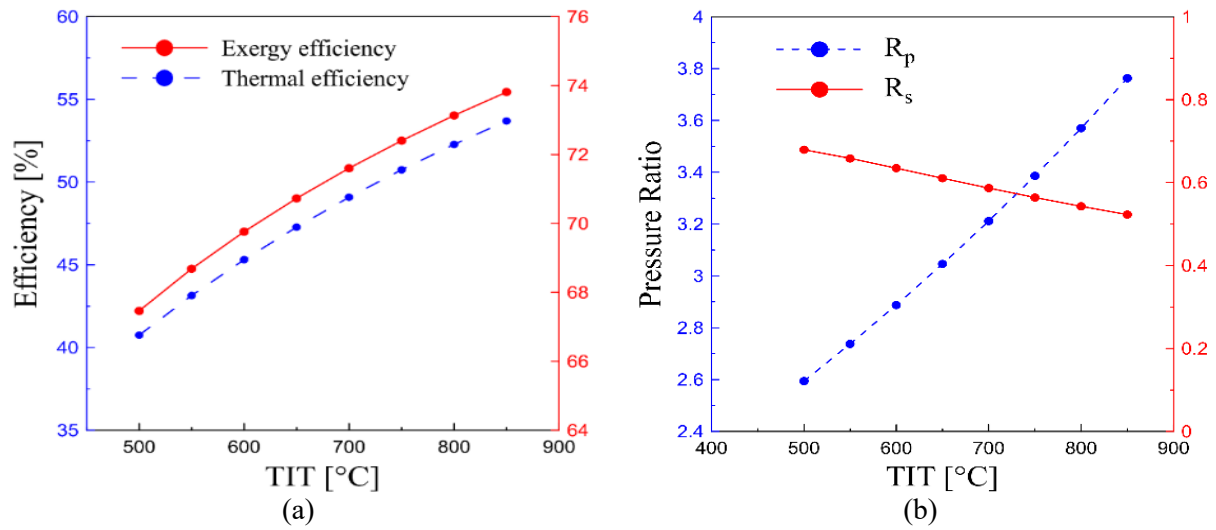


Figure 4. Results of the (a) efficiencies of the cycle and (b) optimal pressure ratios.

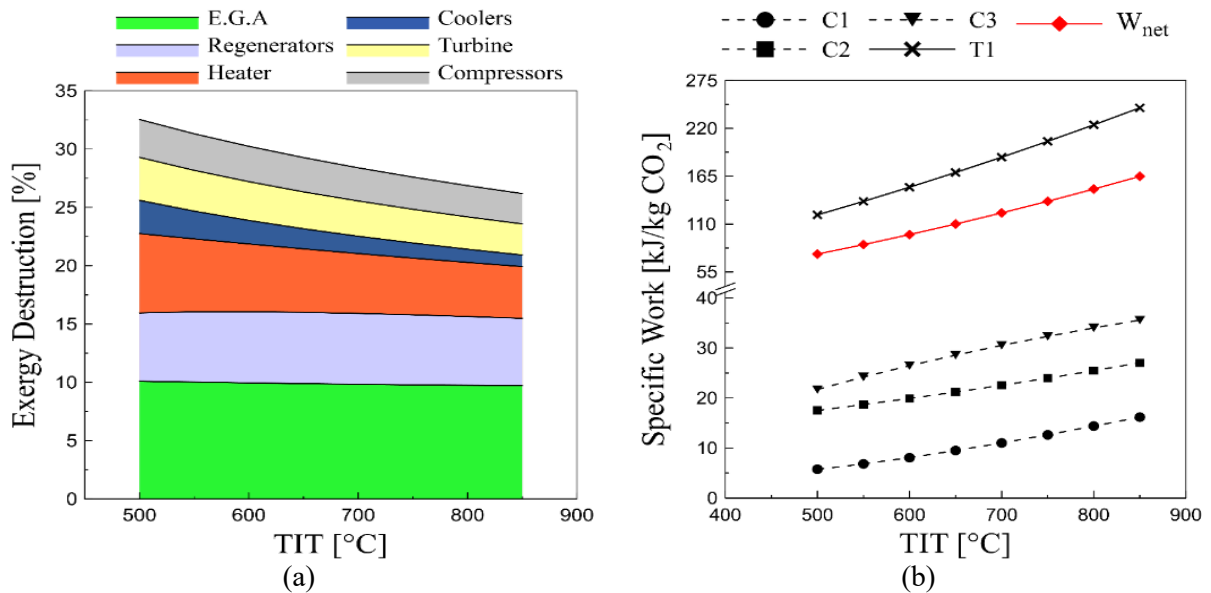


Figure 5. Results of the (a) exergy destruction and (b) power generation at a component level.

Based on the results, the exergy gained by air (E.G.A) represents the largest contributor to exergy destruction, followed by the regenerators, which can be associated with the internal irreversibilities of these components in the heat exchange [16]. Therefore, the implementation of advanced materials for the construction of heat exchangers could benefit the exergetic performance. Moreover, incrementing TIT facilitates exergy destruction reduction, which supports the results obtained from the thermal evaluation. On the other hand, the Compressors feature a minor contribution to exergy destroyed as a result of the incorporation of the cooling stages that improve the overall compression performance.

4. Conclusions

The present study outlines the thermodynamic modeling characteristics of a SCBC operating under the main compression intercooling configuration. A differential factor of the study was the incorporation of a comparative assessment for the optimization methodology. The operational performance was carefully validated, with literature references demonstrating robustness within the calculations. Moreover, the study critically evaluates the main parameters that describe the overall performance of the cycle.

The results indicated that the cycle achieves high thermal (56%) and exergy efficiencies (73%) while displaying a direct relation with the TIT. The optimal pressure ratio features an upward trend in the main ratio, whereas the second follows a sharp drop as the TIT rises. Also, it was demonstrating that P_{high} greater than 20 MPa enables stability within the prediction of the thermophysical properties of the working fluid. The specific work generation of the cycle oscillates between 56 kJ/kg - 156 kJ/kg, demonstrating the robust performance to mitigate the current challenges of non-interconnected areas.

The biggest field of opportunity in cycle optimization was found on the air cooling and regenerators as they contribute to nearly 30% - 35% of the total exergy destroyed, which further elucidates the importance of incorporating high-efficient exchangers (e.g., Printed Circuit) and advanced construction materials. Overall, the model presented and the operation characterization set a precedent for future studies that propose the integration of primary energy sources to describe the energy conversion efficiency.

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