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DYNAMIC ANALYSIS OF CO2-SO2 RECOMPRESSION RANKINE CYCLE USING WASTE HEAT

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ABSTRACT

Highly valuable attributes such as high efficiency and competitive capital costs are the underlying factors for the prominence of carbon dioxide (CO_2) cycles not only in theoretical fields but also in commercial applications. As a result, we are witnessing an increasing number of research projects and support for activities related to these cycles. Recently, there has been a new initiative to develop an even more promising working fluid by mixing CO_2 with certain dopants. One of them seems to be the CO_2-SO_2 mixture. Given the promising potential of this specific mixture, which seems to be exceptionally well-suited for application in transcritical cycles [1], this paper provides an overview of the early results of the transient analysis of transcritical Rankine cycle using this mixture in waste heat recovery applications (WHR).

The primary focus of this paper is to utilize the CO_2-SO_2 mixture in a 70-30 ratio for the double recuperated recompression Rankine cycle. In doing so, this study not only examines the unique characteristics of this mixture but also explores its potential applications for WHR under fluctuating operational conditions. The paper describes the modeling methodology implemented in Aspen Plus software and illustrates the key plant components transient operating conditions. By conducting the analysis of this working fluid, the paper aims to evaluate its effectiveness in harnessing waste heat, thereby contributing to the advancement of more sustainable and efficient energy solutions.

INTRODUCTION

In recent years, concerns about global warming have become increasingly pressing. These concerns particularly affect industry, as emissions from industry account for up to 40% of the world's total CO_2 emissions [2]. As a result, industries are under rising pressure to comply with regulations and meeting public expectations regarding sustainability as the market becomes more competitive and consumers lean towards environmentally friendly practices. This ultimately means that industries are facing new challenges, such as finding effective ways to reduce greenhouse gas emissions while also enhancing the efficiency of their operations. Many of these industries contain industrial processes that produce large amounts of waste heat as a byproduct of various processes. Much of this heat energy is released into the environment without being used. This implies that a promising solution to this modern problem is the implementation of waste heat recovery systems in such industrial processes. Waste heat recovery systems play a crucial role in collecting and reusing the heat generated during manufacturing operations.

Two popular ways to convert waste heat into useful energy are the Steam Rankine Cycle (SRC) and the Organic Rankine Cycle (ORC) [3-10]. Both cycles are common options for utilizing waste heat. However, a major issue with both SRC and ORC systems is their high irreversibility in the heat exchangers, which can lead to overall lower efficiency [11]. ORC systems also have limits on the temperature range in which they can operate effectively due to risk of decomposition of the organic fluid [12], resulting in lower efficiency when using certain heat sources. SRC systems often require more space, which can be challenging to manage in specific industrial environments and also tend to have larger footprint [11].

A promising alternative to these systems is the supercritical carbon dioxide (sCO_2) power cycle. This technology is gaining attention for its ability to better match the temperature of waste heat for wider range of temperatures, which leads to lower irreversibility and improved efficiency [11]. By utilizing sCO_2 in

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power generation, industries may find a more effective way to harness waste heat, thus maximizing energy recovery and contributing to sustainability efforts. Such advancements in waste heat recovery could play a significant role in the ongoing pursuit of energy efficiency in industrial processes.

In recent years, significant efforts have been made to enhance the benefits of carbon dioxide (CO_2) as a working fluid in various applications. One notable initiative is the SCARABEUS project, which has received funding from the Horizon 2020 programme of the European Commission. This project specifically investigated the effects of certain dopants added to carbon dioxide, aiming to produce a mixture that exhibits a higher critical temperature than pure CO_2. The findings from this research indicate that the CO_2-SO_2 mixture holds considerable promise, particularly for its application in concentrated solar power (CSP) systems. The process of doping CO_2 not only enables the possibility of compressing the working fluid close to its critical temperature, even in challenging hot environments where ambient temperatures may reach around 50 °C [13, 14], but it also offers significant advantages in terms of performance. This innovative mixture is anticipated to yield higher specific work output, allowing for a smaller system footprint, which is a crucial factor in the design of efficient energy systems. Furthermore, the CO_2-SO_2 mixture is expected to facilitate a greater temperature rise across the receiver, thereby enhancing the overall efficiency of CSP applications [15]. Given the promising potential of this mixture for CSP applications Morosini et al. [1] further investigates its use for transcritical cycles. However, for now there is no literature available that specifically addresses this innovative compound and its potential applications for WHR.

Based on this finding, the paper is organized as follows. In the first part, a brief description of the cycle is provided along with validation of the implemented model against accessible literature. Then, the steady-state analysis results are reported along with the thermodynamical evaluation of the cycle design point. Finally, the dynamic response of the cycle to the step change in flue gas temperature is presented and discussed.

SYSTEM DESCRIPTION

The proposed cycle layout is the recuperated Rankine CO_2-SO_2 cycle. The system is designed to recover waste heat from the flue gas produced by upstream industrial processes and convert the recovered waste heat into electrical power. The schematic layout can be seen in Figure 1.

The cycle consists of main components, which are: turbine (TURB), compressor (COMP), pump (PUMP), primary heat exchanger (PHE), low-temperature recuperator (LREC), high-temperature recuperator (HREC), and condenser (COND). For simulation purposes, there are some additional components such as a mixer (MIXER) and splitter (SPLITTER), which serve to mix and split streams accordingly. The last components visible in the layout are the flue gas valve (VEX) and cooling air valve (VA), which are used to maintain the pressure at the PHE and COND inlet respectively.

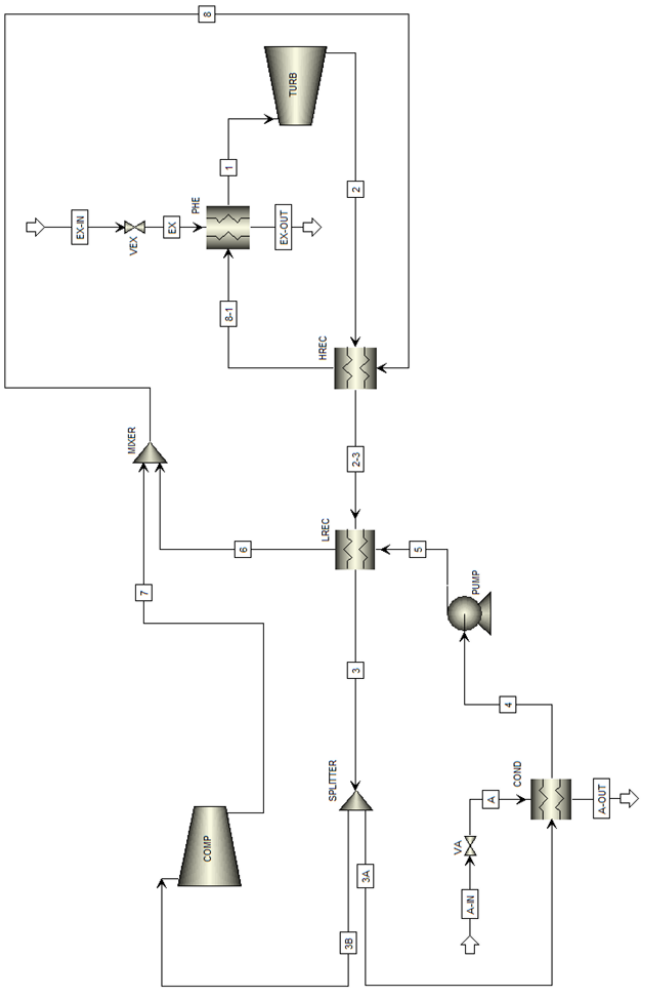

Figure 1: Schematic diagram of double recuperated recompression transcritical CO_2-SO_2 closed Rankine cycle to recover waste heat.

The waste heat recovered from flue gas is used in the PHE block to add heat to the CO_2-SO_2 working mixture. The working fluid then continues to the TURB, where it is expanded, converting its thermal energy into mechanical power. After the turbine, the HREC block is located, which helps to preheat the working fluid leaving the COMP and PUMP blocks. After HREC, there is the LREC block for further utilization of heat contained in the working fluid mixture. In the LREC block, the stream leaving HREC is used to preheat the stream leaving the PUMP. The conditions of the mixture leaving the LREC block are chosen so that the pressure and temperature are slightly above the mixture's critical conditions. The corresponding critical conditions of the mixture are (79.47 °C, 97.51 bar); the conditions of stream 3 are 83.77 °C and 68.53 bar. This approach is used to maintain the vapor phase at the compressor inlet while also minimizing the compressor work. Then, the stream is

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divided into two. One stream, 3A, enters the COND block, where the remaining heat is rejected to the environment, and the mixture is cooled down to the point that it is fully condensed and further subcooled, preventing the existence of the vapor phase. Then follows stream 4, which connects the COND outlet and PUMP inlet. The second stream after division is stream 3B, which is sent to the COMP block inlet. Both the COMP and PUMP blocks then increase the working fluid pressure. After the PUMP, stream 5 returns working fluid back to the LREC. The flow split fraction is set to be 0.33. The working fluid leaving the LREC is then mixed with the high-pressure working fluid from the COMP in the MIXER. After the MIXER, the working fluid continues to the HREC block, where it is preheated by the exhaust from the turbine. Then, the mixture enters the PHE block, where it is heated by the flue gas, reaching its maximum temperature. The fluid reenters the turbine, and the processes are repeated.

STEADY STATE MODEL VALIDATION

The suitability of Aspen Plus V14 software for modeling and predicting the performance of the cycle components under steady-state and dynamic conditions was verified by comparing the steady-state simulation results with the values obtained from Crespi et al. [15] for the closed CO_2-SO_2 recompression Rankine cycle. The comparison of steady-state results with the available literature is presented in Table 1. The steady-state predictions of the implemented model were found to agree well with the literature data, with the maximum relative difference being 0.402%. At this stage there is no available data to validate the dynamic model of double recuperated CO_2-SO_2 Rankin cycle. However, in order to obtain the most realistic results, the performance maps for turbomachinery components are used in this study.

Table 1: Comparison of the simulation results at steady state with literature obtained from Crespi et al. [15].

	Literature			Simulation			Relative difference [%]		
Cycle point	T [◦C]	P [bar]	h [kJ/kg]	T [◦C]	P [bar]	h [kJ/kg]	T	P	h
1	700	238.9	-6655.7	700	238.9	-6656.61	0	0	0.014
2	534.2	69.93	-6827.1	534.72	69.93	-6825.82	0.097	0	0.019
2-3	211.5	69.23	-7164.4	211.5	69.23	-7161.74	0	0	0.037
3	83.77	68.53	-7315.3	83.77	68.53	-7315.98	0	0	0.009
4	50	68.53	-7520.6	50	68.53	-7526.48	0	0	0.078
5	74.54	250	-7497.4	74.24	250	-7496.07	0.402	0	0.018
6	206.4	246.3	-7247.2	206.41	246.3	-7245.39	0.003	0	0.025
7	206.7	246.3	-7246.6	206.58	246.3	-7245.12	0.057	0	0.020
8	206.5	246.3	-7246.9	206.48	246.3	-7245.28	0.012	0	0.022
8-1	478.2	242.6	-6909.7	477.57	242.6	-6909.36	0.131	0	0.005

STEADY STATE MODEL

For steady-state analysis, this study utilizes data available in the existing literature to develop a cycle layout specifically scaled for WHR purposes. It is assumed that the cycle will rely on data extracted from the referenced literature source [11, 15]. This approach aims to ensure that the analysis is grounded in established research, thereby enhancing its reliability and relevance. A detailed list of values used to derive the steady-state model is presented in Table 2.

Table 2: Simulation input data obtained from the literature [11, 15].

Position	Description	Value	Units
Heat source	Temperature	380	°C
	Flow rate	100	kg/s
PHE	Cold stream outlet temperature	360	°C
	Pressure loss hot side	0.1	bar
	Pressure loss cold side	0.004	bar
TURB	Outlet pressure	69.93	bar
	Efficiency	90	%
HREC	Pressure loss hot side	0.7	bar
	Pressure loss cold side	0.13	bar
LREC	Hot stream outlet pressure	68.53	bar
	Hot stream outlet pressure	249.87	bar
	Pressure loss hot side	0.7	bar
	Pressure loss cold side	0.19	bar
SPLITTER	Split fraction	0.33	
COND	Hot stream outlet temperature	50	°C
	Hot stream outlet pressure	67.83	bar
PUMP	Outlet pressure	250	bar

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	Efficiency	89	%
COMP	Outlet pressure	249.87	bar
	Efficiency	88	%
Air cooling	Temperature	40	°C
	Flow rate	500	kg/s

The turbomachinery models used in this analysis are considered isentropic [11]. Additionally, the cement plant flue gas characteristics are specified using data from the literature [16] and can be seen in the Table 3. In this work, the REFPROP solution method is used to calculate the thermophysical properties of the working fluids. The composition of the CO_2-SO_2 working fluid is shown in Table 4.

Table 3: Flue gas composition [16].

Species	Mole fraction
CO_2	0.178
Nitrogen	0.565
Oxygen	0.075
Water	0.182

Table 4: Working fluid composition [15].

Species	Mole fraction
CO_2	0.7
SO_2	0.3

DYNAMIC MODEL

In this section, the principle of the dynamic component modeling used for the transient analysis of the proposed cycle is presented. In order to study the transient behavior of the selected cycle, a dynamic model for the entire system is necessary. The dynamic model includes all the mentioned components implemented in Aspen Plus Dynamics V14 software. Important aspect of the dynamic analysis is the volume classification in the system; for this purpose, heat exchangers are selected, as will be described later in this paragraph. Turbomachinery is treated as instantaneous blocks, meaning they have no volume. Furthermore, it should be noted that the inertial moments of the turbomachinery are not considered, and all the blocks operate with a constant rotational speed of 60 Hz. The compressor, pumps, and turbine are modeled using performance maps available from literature.

TURBINE MODEL

For the dynamic model of the turbine the data obtained from steady state analysis were used. After obtaining the input and output values of temperature and pressure for the TURB block and the efficiency specification given for the design state obtained from the literature [11], the performance maps based on data found in available literature [17] were than developed. The performance characteristics used for TURB block are presented in Figure 2.

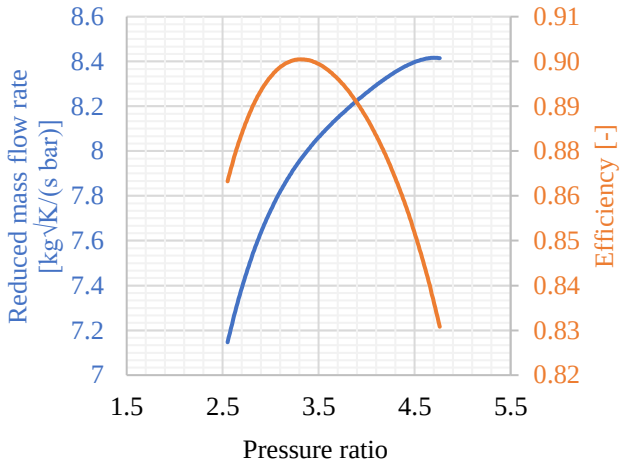

Figure 2: Turbine performance map.

COMPRESSOR MODEL

In the context of transient simulation, it is crucial to recognize the rapid fluctuations in the properties of the working fluid, around the critical point. This is particularly important for compressor since the properties at the compressor's suction are very near to the critical point. Consequently, these changes in property values have high impact on the overall performance of the system. To address this challenge effectively, it has been determined that utilizing performance maps for modeling the compressor block yields more accurate and reliable results. Firstly, the same approach as for TURB block was used. Than the performance maps, were obtained from existing literature [18] and scaled to meet the specific operating point of the simulation process. Furthermore, it should be noted that the compressor is modelled with a fixed geometry without considering variable IGV. The performance characteristics used for COMP block are presented in Figure 3.

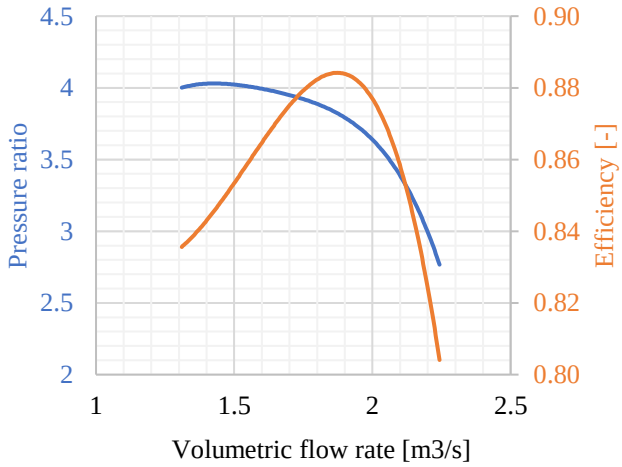

Figure 3: Compressor performance map.

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PUMP MODEL

In the case of the pump, a similar approach was used. Performance maps were developed to effectively determine the pump's operational conditions. These maps were obtained from existing literature [19] that provided information on the pump's behavior and efficiency under varying conditions. The performance characteristics used for PUMP block are presented in Figure 4.

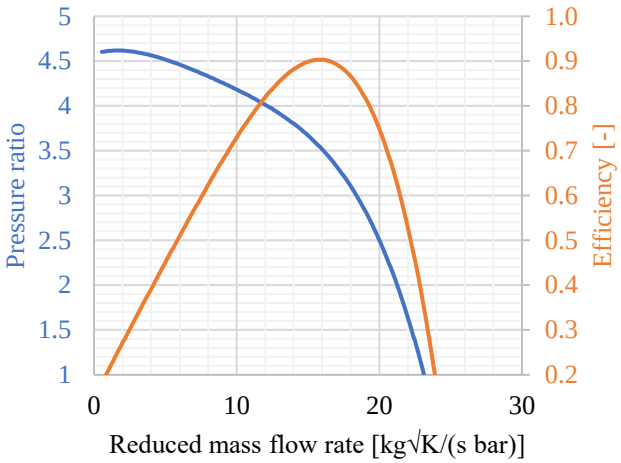

Figure 4: Pump performance map.

HEAT EXCHANGERS MODEL

In order to effectively conduct dynamic simulation analysis, it is essential to incorporate volume into the model. The heat exchangers are expected to be significantly larger than the turbomachinery components [11], which plays a crucial role in determining the overall dynamic performance of the cycle. Because of that the heat exchangers were selected to represent the volume within the system. This choice underscores their importance in optimizing efficiency, ultimately influencing the system's overall performance and reliability in various operational conditions. For purpose of this study, the data from the literature [11] were used. The volumes for all heat exchangers are reported in Table 5. The heat exchangers were modeled with a constant UA value. This overall heat transfer coefficient was derived from a steady-state simulation.

Table 5: Specified heat exchangers volume [11].

Heat exchangers	Total core volume (m^3)
PHE	12.6
HREC	11.62
LREC	11.62
COND	2.02

STEADY STATE RESULTS AT DESIGN POINT

For the purpose of this study, the upper boundary of waste heat fluctuation, specifically the maximum flow rate and maximum temperature, was adopted as a design point for the proposed WHR system [11]. This means that the system will operate at either the design point or at a mass flow rate or temperature below the design point. Results of the steady-state simulation at the design point can be found in the Table 6. The corresponding T-S diagram of the proposed cycle is reported in Figure 5.

Table 6: The list of steady-state simulation results of the WHR transcritical CO_2-SO_2 Rankine power cycle.

Cycle point	Temperature [°C]	Pressure [bar]	Enthalpy [kJ/kg]	Mass Flow [kg/s]
1	360	249.74	-7046.18	80.40
2	227.61	69.93	-7145.28	80.40
2-3	211.50	69.23	-7161.74	80.40
3	83.77	68.53	-7315.98	80.40
4	50	67.83	-7526.31	53.98
5	70.71	250.06	-7502.60	53.98
6	190.02	249.87	-7272.88	53.98
7	206.45	249.87	-7246.56	26.42
8	195.30	249.87	-7264.23	80.40
8-1	205.64	249.74	-7247.77	80.40

The results of the steady-state design point performance of the cycle show that about 16.2 MWth are recovered from the flue gas, and the electric power generated is about 4.85 MW, resulting in a cycle efficiency of about 30%. The thermodynamic results can be seen in Table 7.

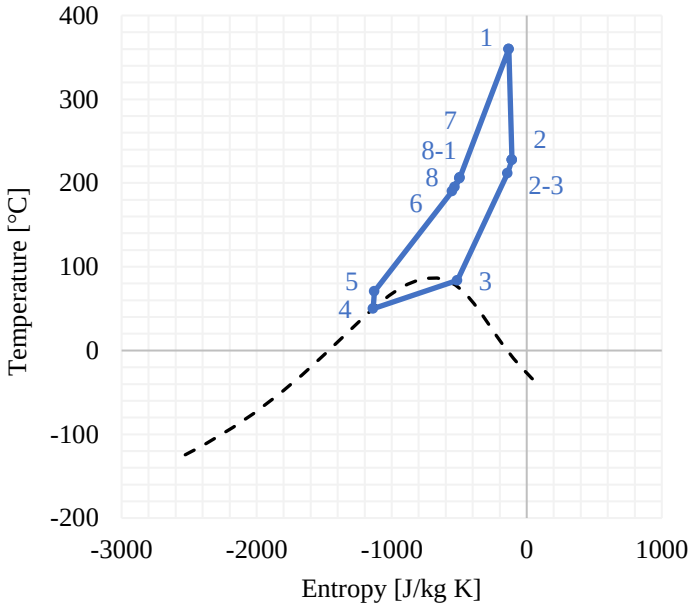

Figure 5: T-S diagram of the double recuperator recompression transcritical CO_2-SO_2 Rankine cycle.

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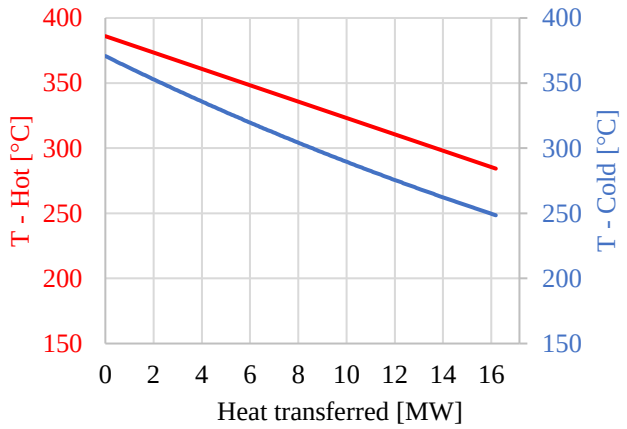
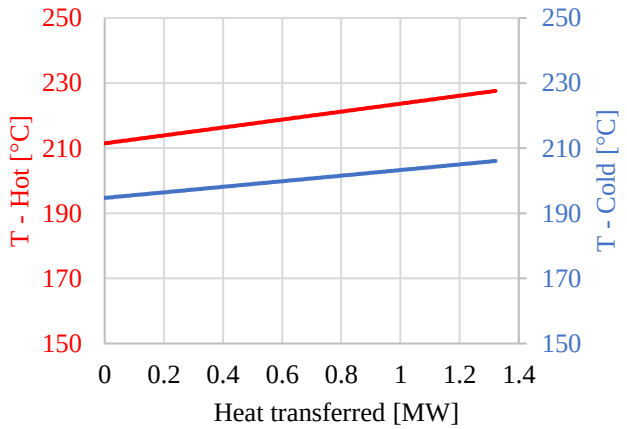
Table 7: Results of steady state thermodynamic performance of proposed WHR system

Description	Value	Units
PHE	16.21	MW
HREC	1.32	MW
LREC	12.40	MW
COND	11.35	MW
TURB	7.97	MW
COMP	1.83	MW
PUMP	1.28	MW
Cycle thermal efficiency	29.95	-
Net power output	4.85	MW

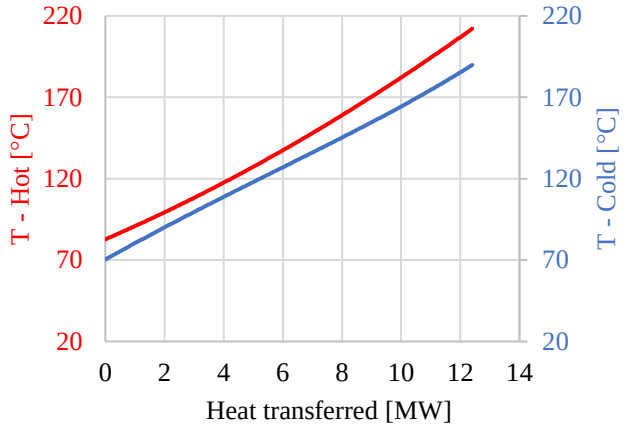
The corresponding temperature profiles of heat exchangers are illustrated in Figure 6. PHE shows an efficient matching of the temperature profile between the CO_2-SO_2 working fluid and the flue gas. This indicates a well-designed system that maximizes thermal efficiency ensuring that heat is effectively exchanged. Furthermore, the temperature profiles of both the HREC and the LREC reveal that a significantly larger portion of heat is transferred in the low temperature recuperator. This aspect emphasizes its crucial role in optimizing heat recovery processes. Additionally, the COND profiles demonstrate that the working fluid is effectively condensed ensuring that it undergoes a thorough phase change. Moreover, the fluid is further slightly subcooled within this heat exchanger enhancing overall system performance stability.



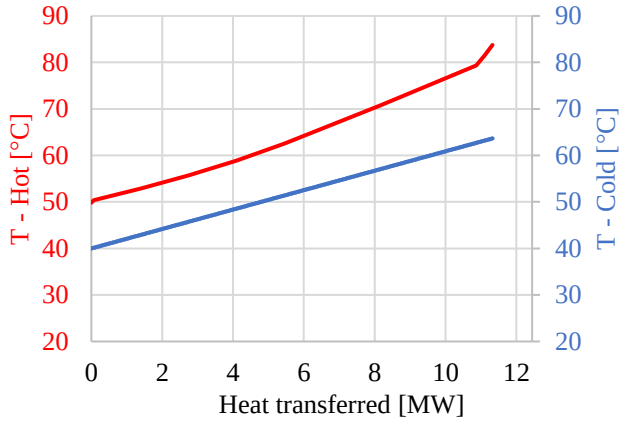
a) T-Q diagram of PHE heat exchanger.



b) T-Q diagram of HREC heat exchanger.



c) T-Q diagram of LREC heat exchanger.



d) T-Q diagram of COND heat exchanger.

Figure 6: T-Q diagrams of heat exchanger

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DYNAMIC SIMULATION RESULTS

In this paragraph, the open loop dynamic response of the modeled cycle is presented. The observed response is to a step change in the temperature of the waste heat source. The step change in flue gas temperature from the design point value (380°C) to 330°C occurs at time 100 seconds. Figure 7 shows considerable decrease in cycle efficiency due to introduced step change.

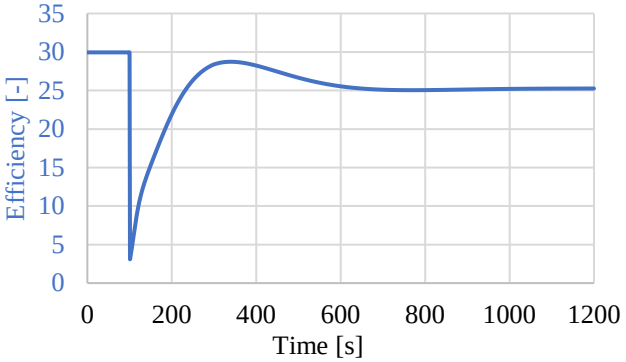

Figure 7: Dynamic response of the cycle efficiency.

The decreased temperature of the flue gas means that the working fluid cannot be heated up to the design values. As can be seen from Figure 8, the power delivered by the turbine is reduced as a consequence of the decreased temperature and pressure at the turbine inlet. The net power output drops to around 3.7 MW. The opposite is true for the compressor's power input, as it increases to about 1.96 MW. At first, though, the compressor requires less power. This is a consequence of the sudden temperature and pressure drop at the compressor inlet as can be seen in Figure 9. This change temporarily shifts the operating conditions closer to the critical point of the mixture.

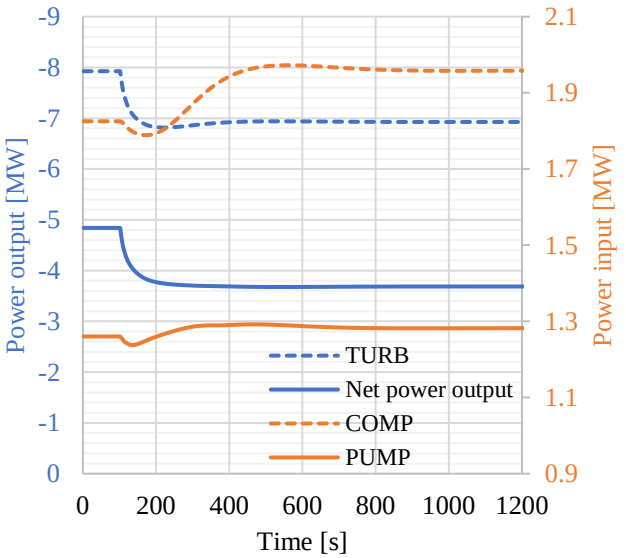

Figure 8: Dynamic responses of turbomachinery power and the net power output.

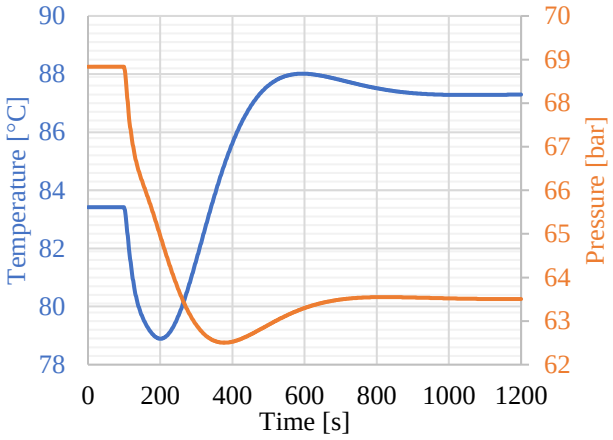

Figure 9: Dynamic response of stream 3B temperature and pressure.

Even though the conditions at the compressor inlet change, Figure 10 shows that the phase of the working fluid remains unchanged. This indicates that the compressor is able to operate even under the new cycle conditions. The same cannot be stated for the pump, as Figure 10 shows the phase change at the pump's inlet.

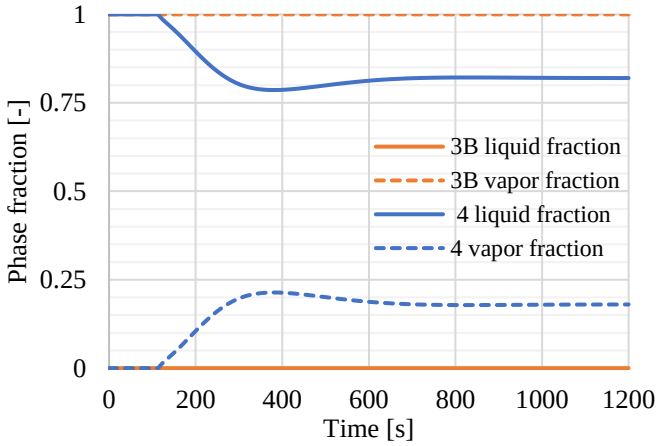

Figure 10: Dynamic responses of COMP and PUMP feed streams phase fraction.

As a result of the step change, the pressure of the stream 4 drops to around 62 bar as can be seen from Figure 11. The same Figure 11 also shows how the temperature changes relative to the bubble point temperature of the mixture. This response consequently means, that the condenser is no longer able to deliver pure liquid into the pump. This change in conditions also leads to high variation in density, as can be seen from Figure 12. These conditions are not permissible for the operation of the pump and highlight the need to implement a control strategy.

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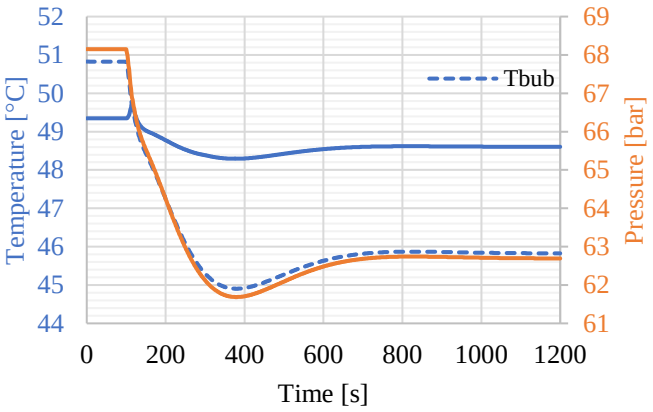

Figure 11: Dynamic response of stream 4 temperature and pressure.

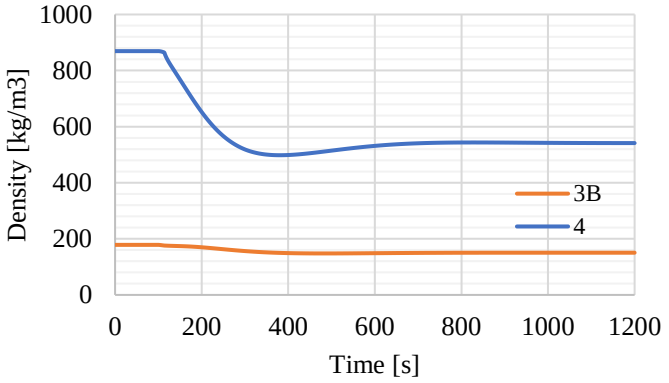

Figure 12: Dynamic responses of COMP and PUMP feed streams density.

The first proposed control strategy adjusts the fan speed in the air-cooled condenser based on pressure change in stream 3. This strategy allows to change the cooling air mass flow rate which subsequently changes the working fluid temperature at the condenser outlet allowing to shift the operating conditions and maintain liquid phase at the pump inlet. Another proposed control strategy is to introduce variable speeds for the turbomachinery (PUMP, COMP), which will allow to maintain the pressure in the cycle. The proposed control strategies will be studied during future work.

CONCLUSION

This paper has analyzed preliminary results of the utilization of a transcritical double recuperated Rankine CO_2-SO_2 cycle for waste heat recovery purposes. To obtain the design point parameters of this cycle, the data available in the literature were used. Furthermore, a steady-state simulation was performed in Aspen Plus V14 to determine the thermodynamic performance of the cycle at the design point. The cycle was designed for waste heat upper boundary conditions, specifically the mass flow rate of 100 kg/s and a temperature of 380°C. From the steady-state analysis, it was observed that the cycle is able to achieve about 30% efficiency at the design point. The efficient matching of the temperature profiles in the primary heat exchangers shows that the heat exchangers are effectively designed for this scope. For the purpose of the dynamic simulation, performance characteristics were implemented for turbomachinery equipment, and the volumes of heat exchangers were introduced into the system. The dynamic model was developed in the Aspen Plus Dynamics environment to predict the system's transient behavior under fluctuating conditions. From the observed results, it can be concluded that the cycle is not capable of handling the step change in flue gas temperature to 330°C effectively. This limitation suggests that it is essential to implement a control strategy that can adapt to varying operational conditions. Two control strategies were proposed. By implementing these controls, the cycle will be better equipped to maintain stability and performance even when subjected to mentioned changes in temperature, ultimately enhancing its overall efficiency. In light of these findings, the proposed transcritical double recuperated recompression CO_2-SO_2 Rankine cycle investigated in this study could be a promising solution for waste heat recovery purposes from industrial processes. This study also showed the importance of dynamic analysis as it contributes to the understanding of the transient characteristics of the cycle's behavior.

NOMENCLATURE

h	enthalpy (kJ/kg)
p	pressure (bar)
T	temperature (°C)
Tbub	bubble point temperature (°C)

Acronyms	
CO_2	carbon dioxide
COMP	compressor
COND	condenser
CSP	concentrated solar power
HREC	high temperature heat exchanger
IGV	inlet guide vane
LREC	low temperature heat exchanger
MIXER	stream mixer
ORC	organic Rankine cycle
PHE	primary heat exchanger
PUMP	pump
sCO_2	supercritical carbon dioxide
SO_2	sulphur dioxide
SPLITTER	stream splitter
SRC	steam Rankine cycle
TURB	turbine
UA	overall heat transfer coefficient
VA	cooling air valve
VEX	flue gas valve
WHR	waste heat recovery

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