

## Thermodynamic and turbomachinery design analysis of supercritical Brayton cycles for exhaust gas heat recovery

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1 Thermodynamic and turbomachinery design analysis of supercritical  
2 Brayton cycles for exhaust gas heat recovery

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5 **Abstract**

*Significant amount of energy is wasted in engine systems as waste heat. In this study, the use of supercritical Brayton cycles for recovering exhaust gas heat of large-scale engines is investigated. The aim of the study is to investigate the electricity production potential with different operational conditions and working fluids, and to identify the main design parameters affecting the cycle power production. The studied process configurations are the simple recuperated cycle and intercooled recuperated cycle. As the performance of the studied cycle is sensitive on the turbomachinery design and efficiencies, the design of the process turbine and compressor were included in the analysis. Cycles operating with CO<sub>2</sub> and ethane resulted in the highest performances in both the simple and intercooled cycle configurations, while the lowest cycle performances were simulated with ethylene and R116. 18.3 MW engine was selected as the case engine and maximum electric power output of 1.76 MW was simulated by using a low compressor inlet temperature, intercooling, and high turbine inlet pressure. It was concluded that working fluid and the cycle operational parameters have significant influence not only on the thermodynamic cycle design, but also highly affects the optimal rotational speed and geometry of the turbomachines.*

6 **Keywords:** Supercritical Brayton Cycle, Waste heat recovery, Organic fluid, Energy efficiency,  
7 Turbomachinery design

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## Nomenclature

### *Latin alphabet*

$P$	power	kW	s	isentropic
$c_p$	specific heat capacity	kJ/kgK	c	cycle/compressor
$h$	specific enthalpy	kJ/kg	comp1	compressor 1
$q_m$	mass flow rate	kg/s	comp2	compressor 2
$q_v$	volumetric flow rate	m <sup>3</sup> /s	wf	working fluid
$p$	pressure	bar	in	inlet
$T$	temperature	°C	out	outlet
$n$	rotational speed	rpm	e	electricity
$b$	blade height	m	eg	exhaust gas
$s$	specific entropy	kJ/kgK	h	heater
$D$	turbine diameter	m	hub	blade hub
$Re$	Reynolds number	-	tip	blade tip
$x$	Pressure rise factor		t	turbine

### *Greek alphabet*

$\eta$	efficiency	-	pass	passage loss
$\phi$	heat rate	kW	0	turbine stator inlet
$\Pi$	pressure ratio	-	1	turbine stator outlet/rotor inlet
$\varsigma$	loss factor	-	2	turbine rotor outlet
$\kappa$	velocity ratio	-	0'	compressor rotor inlet
$\mu$	dynamic viscosity	Pas	1'	compressor rotor outlet
$\varepsilon$	recuperator effectiveness	-		

### *Abbreviations*

CIT	Compressor inlet temperature
SBC	Supercritical Brayton Cycle
ORC	Organic Rankine cycle
CO <sub>2</sub>	Carbon dioxide
WHR	Waste heat recovery
MDM	Octamethyltrisiloxane
R116	Hexafluoroethane

## 1. Introduction

During the last decades, several methods to increase efficiency and reduce emissions in different types of energy production processes have been studied and developed intensively. Converting waste heat into electricity has been identified as one of the most promising ways in achieving significant efficiency improvements and emission reductions in power production systems and industrial processes[1]. Despite the recent improvements in energy efficiency of large-scale engine power plants and marine engine systems, a large portion of the fuel power is still wasted in the process in a form of waste heat. When considering the waste heat recovery (WHR) in engine systems, the exhaust heat utilization contains the largest potential for improving energy efficiency of the whole system, due to the relatively high temperature level and large amount of waste heat, when compared to the other waste heat streams from the engine. Thus, most of the research efforts related to WHR in engine systems have been concentrating on the utilization of the exhaust gas heat[2].

The potential of recovering waste heat with different technologies has been intensively studied for engine systems at different power scales. The most widely used types of waste heat recovery systems are the conventional steam Rankine cycle or organic Rankine cycles (ORC) using an organic fluid as the working fluid. The use of ORC systems has been preferred instead of conventional steam Rankine cycles especially in low power output or low temperature waste heat recovery systems[3]. Kalina cycle using a mixture of water and ammonium as the working fluid has been also considered as suitable technological option for high temperature waste heat recovery in engine power plants[4] and in large ships [5]. Bombarda et al. [4] evaluated that approximately 10 % increase in power output in large-scale diesel engine systems can be achieved by converting exhaust heat into electricity by using Kalina cycle or ORC. Uusitalo et al. [6] investigated the recovery of high temperature waste heat in large-scale gas fired engines by using ORCs and it was estimated that the waste heat recovery system was capable to produce about 10 % increase in the power plant power output. One of the most important steps in designing a waste heat recovery is the selection of working fluid. Uusitalo et al. [7] investigated the use of different hydrocarbons, siloxanes, and fluorocarbons in ORCs. In general, fluids with relatively high critical temperature (in a range from 250 to 350 °C), such as siloxanes with heavy molecules and high critical temperature hydrocarbons were considered as the most potential candidates for high temperature applications when considering the power output and cycle efficiency. Lai et al. [8] investigated the use of different fluids including alkanes, aromates and linear siloxanes in high temperature ORCs. They evaluated cyclic hydrocarbon cyclopentane as the most suitable fluid candidate for about 300 °C heat carrier temperature level by taking into account several evaluation criteria. Fernandez et al.[9] investigated the use of different siloxanes in high temperature ORC applications and they concluded that the simple linear siloxanes MDM and MM represent high system performance and also ensure fluid thermal stability. Branchini et al. [10] suggested the use different performance indexes

44 including cycle power output, expansion ratio, mass flow rate ratio, and heat exchange surface for evaluating  
45 the most suitable working fluid for the considered heat recovery application. The working fluid not only  
46 have an effect on the cycle performance but it has also a significant impact on the sizing and suitable  
47 technological solutions for the process main components and cycle layout[11]. It has been also shown that  
48 there is significant potential for increasing the cycle power output of WHR systems by adopting supercritical  
49 fluid conditions. Schuster et al. carried out an optimization for a supercritical ORC and identified more than  
50 8 % increase in system efficiency when compared to subcritical process[12]. Supercritical fluid conditions  
51 for a WHR ORC were also studied by Gao et al. [13]. They concluded that the turbine inlet pressure and  
52 temperature highly affects not only the cycle performance but also the turbomachinery size.

53 Alongside with the use of different types of ORC and Rankine cycles, the use of supercritical Brayton  
54 cycles(SBC) have been considered and investigated for various applications in the recent times. When  
55 comparing the operational principles of SBC and ORC or other Rankine technologies, the main difference is  
56 that in a SBC the working fluid remains at supercritical conditions thorough the whole cycle and the fluid  
57 is compressed with a compressor instead of a pump. Unlike in the high temperature ORCs, the use of low  
58 critical temperature fluids are preferred instead of high critical temperature fluids in SBCs. Especially, SBC  
59 systems using CO<sub>2</sub> as the working fluid have been studied and developed intensively, although no commercial  
60 products are yet available based on this technology. The main advantages of using supercritical CO<sub>2</sub> as the  
61 working fluid are the high thermodynamic efficiency, high stability at high temperatures, non-toxicity and  
62 non-flammability of the working fluid as well as the high power density, which results in reduced component  
63 sizes when compared to other type of power cycles[14]. The most potential applications for supercritical  
64 CO<sub>2</sub> cycles have been identified to be concentrating solar power plants[15] and future nuclear reactors[16].  
65 Ahn et al. [17] and Li et al. [18] reviewed the literature related to the current research and development  
66 of supercritical CO<sub>2</sub> cycles. In both papers it was recognized that there are 12 different cycle layouts  
67 that have been proposed and investigated in the literature, ranging from a simple regenerative cycle to  
68 more complex cycles with several turbomachines and heat exchangers installed at different parts of the  
69 process. Al-Sulaiman and Atif[19] studied different cycle layouts for supercritical Brayton cycles utilizing  
70 solar energy. Their results showed that out of different cycle layouts, the highest power outputs were reached  
71 with a recompression cycle, in where the flow is splitted and the compression is divided into two stages. In  
72 their study, the simple regenerative cycle represented also high cycle efficiencies for the studied application.  
73 The use of supercritical CO<sub>2</sub> in waste heat recovery applications has been also considered and investigated.  
74 Chen at al. [20] compared the use of a transcritical CO<sub>2</sub> cycle and ORC using R134a as the working fluid  
75 for recovering low temperature (about 150 °C) waste heat. Their results indicated that slightly higher  
76 power output could be reached when using CO<sub>2</sub> cycle and that the system using CO<sub>2</sub> as the working fluid  
77 is more compact, when compared to the studied ORC system. More recently, system using supercritical  
78 CO<sub>2</sub> as the working fluid for recovering exhaust heat of marine gas turbines was investigated[21]. The

79 results showed significant increase potential in the ship energy system thermal efficiency at both full-load  
 80 and part-load operational conditions. Wang and Dai [22] studied the waste heat recovery potential by using  
 81 transcritical CO<sub>2</sub> and ORC cycles for recovering waste heat recovery from the cooling energy of recompression  
 82 supercritical CO<sub>2</sub> cycle. They concluded that the second law efficiencies of these two WHR technologies  
 83 were comparable.

84 The high performance of the turbomachines is important for reaching high efficiency for a SBC system.  
 85 In [23], it was estimated that the turbomachines operating with supercritical CO<sub>2</sub> have compact size and  
 86 can reach over 90 % efficiency. Similar conclusions were also given related to the compressor design in[24]  
 87 regarding large scale power systems operating with supercritical CO<sub>2</sub>. Conboy et al. [25] concluded based  
 88 on results from a small scale experimental setup that despite the turbine and compressor are performing  
 89 reasonably well there are significant heat losses and losses due to frictional drag when the size of the  
 90 turbogenerator is small, but these losses can be significantly reduced in the future commercial-scale SBCs.  
 91 It has been also shown that there are high variations in the fluid properties near the critical point and near  
 92 the pseudocritical line which affects especially on the compressor design for such a system. In [26] the use  
 93 of a water pump derived compressor was investigated for compressing supercritical CO<sub>2</sub> as the density of  
 94 the fluid is high and the fluid is nearly incompressible close to the critical point. Lee et al. [27] investigated  
 95 experimentally operation of a compressor with supercritical CO<sub>2</sub> and concluded that very high uncertainty  
 96 on performance measurement was observed due to the high property variations near the critical point. An  
 97 example on the variation in isobaric specific heat near the critical point is presented for CO<sub>2</sub> in Fig. 1.

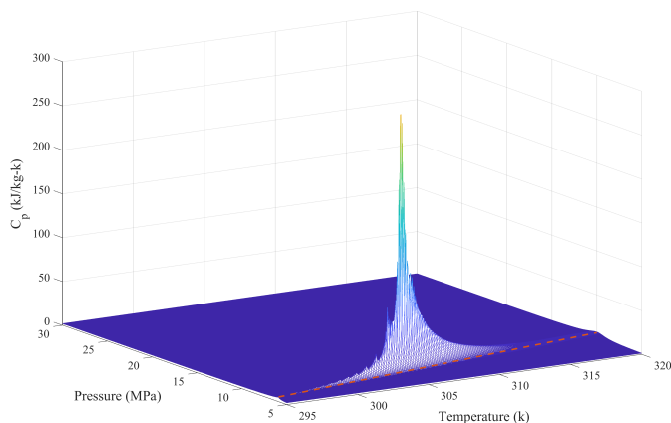


Figure 1: Variation in the fluid isobaric specific heat near the critical point and pseudocritical line. The pseudocritical line is illustrated as dashed line.

98 In principle, supercritical Brayton cycles could employ a variety of different low critical temperature  
 99 fluids as their working fluid. Unlike in the field of ORC research, only few studies have been considering

100 the use of some other fluids than CO<sub>2</sub> in SBCs. In [23] several potential fluid candidates were listed and  
101 discussed, but no further thermodynamic analysis was carried out with these different fluids. Rovira et  
102 al. [28] investigated the factors affecting the performance and design of supercritical Brayton cycles. They  
103 concluded that if the ratio of heat source temperature and heat sink temperature is moderate or low, the  
104 cycle specific work notably increases if the gas compression begins close the critical point conditions. They  
105 also considered other fluids alongside with CO<sub>2</sub> as potential fluid candidates, namely xenon, R41, Ethane,  
106 R410a, and R13 but no further analysis was carried out. In addition, closed Brayton cycles using mixtures of  
107 carbon dioxide and hydrocarbons have been identified and proposed to be a potential solutions for increasing  
108 the cycle efficiency and power output[29]. In addition, Jeong et al. [30] studied the possibility to increase the  
109 efficiency of SBC by mixing different fluids with CO<sub>2</sub>. The studied fluids were nitrogen (N<sub>2</sub>), oxygen (O<sub>2</sub>),  
110 helium, and argon and they concluded that the highest system efficiency was reached by using a mixture  
111 of CO<sub>2</sub> and Helium. The system efficiency was observed to decrease with the other studied fluids when  
112 compared to the cycle efficiency when using pure CO<sub>2</sub>.

113 The literature review shows that different technologies for recovering exhaust heat and converting it  
114 into electricity have been intensively studied in the recent years and most of the research efforts have  
115 been concentrating on the development of ORC technology, especially at the low power or temperature  
116 levels. The previous studies on using SBCs in different applications have shown great potential related to  
117 this technology, especially, due to the high cycle efficiencies and compact sizes of the process components.  
118 However, the potential of using supercritical Brayton cycles for recovering high temperature waste heat from  
119 large scale engines has not been investigated and identified. The scientific novelty and the main objectives  
120 of this research is to investigate and evaluate the power production potential from high temperature exhaust  
121 heat of a large-scale engine by using closed Brayton cycles adopting supercritical fluids. As the previous  
122 research and development work of SBCs has been mainly concentrating on systems having significantly  
123 high temperatures, large power scale, and using CO<sub>2</sub> as the working fluid, an interesting research question  
124 arises on could some other low critical temperature fluid be more suitable and effective choice for this type  
125 of energy conversion cycles instead of CO<sub>2</sub>. The system is thus, studied by using different low critical  
126 temperature fluid candidates and the main operational parameters affecting on the cycle power output are  
127 investigated and highlighted. In addition, as the literature review also showed that the system efficiency  
128 is highly dependent on the turbomachines performance and design, the results of centrifugal compressor  
129 and radial turbine design analysis, as well as turbine loss evaluation with different fluids and operational  
130 parameters are presented and discussed in this paper.

## 131 2. Cycle configurations and numerical methods

132 A simple recuperated cycle configuration as well as an intercooled and recuperated cycle configuration  
133 were selected for the SBC analysis. In the studied cycles the working fluid is at supercritical state thorough  
134 the process and recuperator is included in studied cycle layouts for preheating the fluid entering the heater.  
135 Similar simple cycle configuration has been used for example in the experimental facility presented in[31]  
136 and in the intercooled cycle a second compressor and intercooler have been added between the compressor  
137 stages. The main components of the studied cycles as well as the simplified process diagrams are presented  
138 in Fig. 3a and b. It should be noted that also several other cycle configurations have been proposed in  
139 the literature(e.g. in[17, 18]) for SBCs, representing improvements in the cycle efficiency, especially when  
140 operating at very high temperatures. However, the temperature and power level adopted in this study are  
141 rather low, following that the use of more complex cycle architectures were not considered. For example the  
142 recompression cycle allowing to maximize the heat transfer in system recuperators, was not considered in  
143 this study as it was observed that in this application the cycle performance is not as sensitive on the heat  
144 transfer in the recuperator as it is in higher temperature applications (results presented and discussed in  
145 Fig. 7a and b). In addition, the cycle configurations selected for this study are well comparable in terms of  
146 complexity to the typical WHR ORC systems.

147 The SBC simulations were carried out by using four different fluids that were selected and evaluated as  
148 the most suitable fluid candidates among the considered fluids. The selection of the fluid candidates was  
149 based mainly on the critical temperature of the fluid that has to be slightly below or close to the studied  
150 compressor inlet temperatures. This ensures supercritical fluid state thorough the cycle and allows to reach  
151 high cycle performance under the studied conditions. The studied fluids are namely, carbon dioxide (CO<sub>2</sub>),  
152 ethane, ethylene, and hexafluoroethane (R116). The molecular formula, molecular weight, critical properties  
153 and flammability of the studied fluids are summarized in Table 1. In addition to the studied fluids, sulfur  
154 hexafluoride was also evaluated as suitable candidate for the studied system, but due to the insufficient  
155 thermodynamic data for calculating the turbine losses available in [32], this fluid was not included in the  
156 final analysis presented in this paper.

157 The exhaust gas temperature of 354 °C and exhaust gas flow rate of 30.2 kg/s were used in the analysis  
158 as the heat source input values. The studied exhaust gas temperature level and flow rate were selected  
159 based on the exhaust values of a modern 4-stroke gas fired engine, having the power output of 18.3 MW[33].  
160 The exhaust gas thermal energy was assumed to be wasted in the engine system without a heat recovery,  
161 meaning that there is no usage for the heat power and the target is to maximize the electricity production  
162 of the studied engine system. Thus, the conversion of exhaust gas heat into electricity is assumed to directly  
163 increase the from fuel to usable energy efficiency. It was also assumed that the studied WHR system has no  
164 effect on the gas engine performance.



Table 1: Properties of the studied working fluids.

Fluid	Molecular formula	$M$ , [kg/kmol]	$T_{crit}$ , [ $^{\circ}C$ ]	$p_{crit}$ , [bar]	flammability
Carbon dioxide	$CO_2$	44.0	30.95	73.8	non-flammable
Ethane	$C_2H_6$	30.1	32.15	48.7	flammable
Ethylene	$C_2H_4$	28.1	9.15	50.42	flammable
Hexafluoroethane (R116)	$C_2F_6$	138.0	19.85	30.5	non-flammable

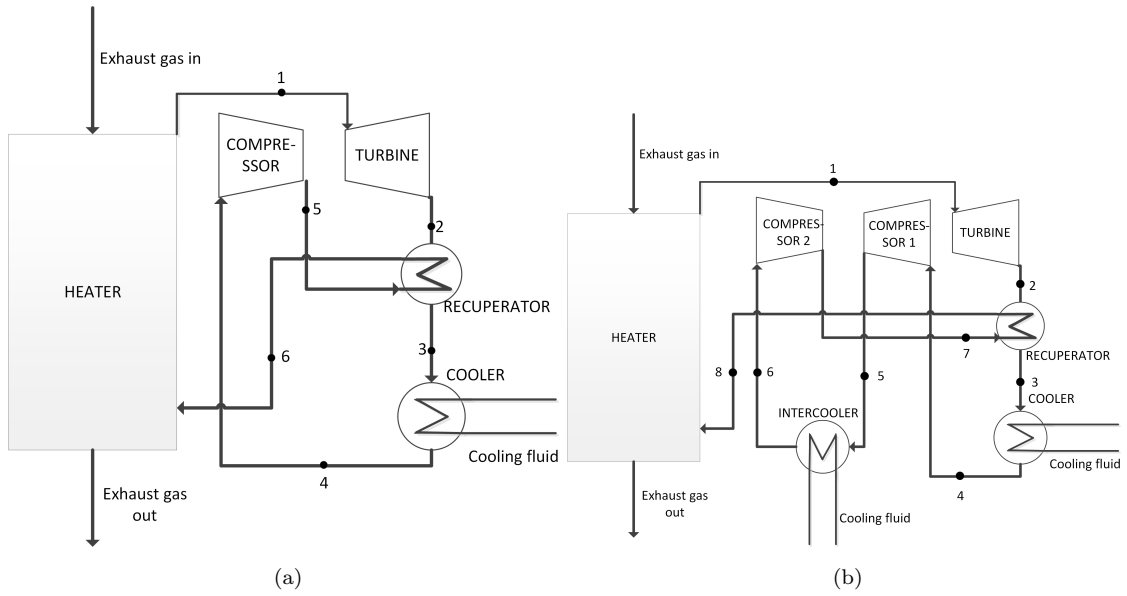


Figure 2: Simplified process diagrams of the studied recuperated simple SBC and intercooled SBC.

## 165 2.1. Cycle analysis

166 The process simulations were carried out by using a cycle analysis tool developed at Lappeenranta  
 167 University of Technology capable for analyzing closed Brayton cycles. The calculation is based on the general  
 168 calculation principles of closed Brayton cycles and the fluid thermodynamic state at the each process node  
 169 was defined by using a commercial thermodynamic library Refprop[32] containing accurate properties and  
 170 equations of states for the studied fluids. The energy and continuity equation were solved at the inlet and  
 171 outlet of each process component based on the given input parameters. The thermodynamic cycle model  
 172 uses the working fluid, component efficiencies, turbine inlet state, compressor inlet state and the heat source  
 173 values as the input parameters and solves the unknown properties at different process nodes. No pressure or  
 174 heat losses in the system piping and in the heat exchangers were included in order to simplify the analysis.

175 The main equations used in the SBC analysis are presented in the following. The heat rate extracted

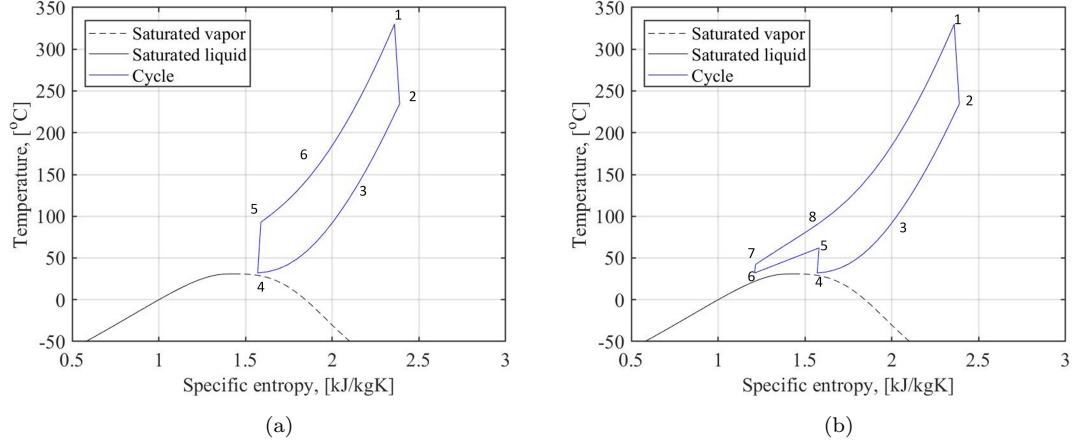


Figure 3: Example of the studied supercritical Brayton cycles on T-s plane. (a) is for simple cycle and (b) is for intercooled cycle. In both cycles, CO<sub>2</sub> is used as the working fluid and the turbine inlet pressure of 200 bar and the compressor inlet temperature of 32 °C is used.

176 from the exhaust gas to the working fluid was solved as,

$$\phi_h = q_{m, eg} c_{p, eg} (T_{eg, h, in} - T_{eg, h, out}). \quad (1)$$

177 The working fluid mass flow rate was solved by using the energy balance of the heater as

$$q_{m, wf} = \frac{\phi_h}{(h_{h, out} - h_{h, in})}. \quad (2)$$

178 The turbine outlet enthalpy was solved by using the definition of turbine isentropic efficiency,

$$h_{t, out} = h_{t, in} - \eta_{t, s} (h_{t, in} - h_{t, out, s}). \quad (3)$$

179 in which  $h_{t, out, s}$  was solved based on the isentropic expansion from the turbine inlet state to the turbine  
180 outlet pressure.

181 The mechanical power of the turbine was calculated as

$$P_t = q_{m, wf} (h_{t, in} - h_{t, out}). \quad (4)$$

182 The compressor outlet enthalpy was solved by using the definition of compressor isentropic efficiency,

$$h_{c, out} = h_{c, in} + \frac{(h_{c, out, s} - h_{c, in})}{\eta_{c, s}}. \quad (5)$$

183 in which  $h_{c, out, s}$  was solved based on the isentropic compression from the compressor inlet state to the  
184 compressor outlet pressure.

185 The mechanical power of the compressor was calculated as

$$P_c = q_{m,wf}(h_{c,out} - h_{c,in}). \quad (6)$$

186 The electric power output of SBC was calculated as,

$$P_e = \eta_g(P_t - P_c). \quad (7)$$

187 The recuperator effectiveness defining the temperature change in the recuperator was used for calculating  
188 the fluid temperature at the recuperator hot side outlet. The recuperator effectiveness was defined as,

$$\varepsilon = \frac{(T_{hot,in} - T_{hot,out})}{(T_{hot,in} - T_{cold,in})}. \quad (8)$$

189 The cold side outlet state was solved from the energy balance of the recuperator. The cycle efficiency  
190 is determined by using the net electric power output from the system and the heat power that is extracted  
191 from the exhaust gases to the working fluid in the heater.

$$\eta_e = \frac{P_e}{\phi_h}. \quad (9)$$

192 The main parameters that were used in the cycle analysis are summarized in Table2. The exhaust gas  
193 temperature at the heater outlet was varied depending on the cycle operational conditions by following the  
194 criteria that the temperature difference between the exhaust gas and working fluid does not exceed the  
195 minimum limit of 20 °C at the cold end of the heater. The maximum temperature at the cycle side has been  
196 selected based on the temperature level of the exhaust gases and it has been used for all the studied fluids in  
197 order to evaluate the thermodynamic cycles in a comprehensive way. It should be noted, that the selected  
198 maximum turbine inlet temperatures above 300 °C can be close to the thermal stability threshold with some  
199 organic fluids[34]. The maximum pressure in the cycle of 400 bar was adopted in the cycle analysis and  
200 the simulations were carried out by using different turbine inlet pressures in order to investigate the effect  
201 of cycle pressure level on the cycle performance and turbomachinery design. However, it should be noted  
202 that the highest studied pressure levels are significantly higher when compared to the more conventional  
203 power systems and the very high pressure level could lead to difficulties in material strength and sealing  
204 of the system. The compressor inlet pressure of 0,5 bar higher than the critical pressure of the fluid was  
205 used and critical temperature slightly higher than the critical temperature of the fluid were used in the  
206 simulations, in order to ensure supercritical fluid conditions at the compressor inlet. According to Angelino  
207 and Invernizzi[35] this type of cycle reaches the highest performance when the compressor inlet condition is  
208 close to the critical point of the fluid. The validation of the cycle analysis code is presented in Section *Cycle*  
209 *and turbomachinery code validation*.

Table 2: Process simulation parameters.

Cooler outlet temperature/compressor inlet temperature	30,50, [°C]
Generator efficiency	95, [%]
Exhaust gas temperature	354, [°C]
Exhaust mass flow rate	30.2, [kg/s]
Minimum temperature difference in the heater	20, [°C]
Maximum turbine inlet temperature	330, [°C]
Maximum turbine inlet pressure	400, [bar]
Compressor inlet pressure	$p_{\text{crit}} + 0.5$ , [bar]

### 210 3. Turbine and compressor design analysis

211 The turbine type for the analysis was selected to be a radial turbine and compressor type was selected to  
 212 be a centrifugal compressor as this type of turbomachines have simple structure and can reach high efficiency  
 213 in small-capacity applications. Radial turbines have been used for example in an experimental system for  
 214 supercritical CO<sub>2</sub>[36, 37] and this type of turbines are also widely used in ORC applications e.g.[38, 39].  
 215 Centrifugal compressors have been considered in several studies for compressing supercritical CO<sub>2</sub> and has  
 216 been also used in experimental facilities[40]. Examples of a radial turbine and centrifugal compressor rotor  
 217 geometries are shown in Fig. 4a and b.

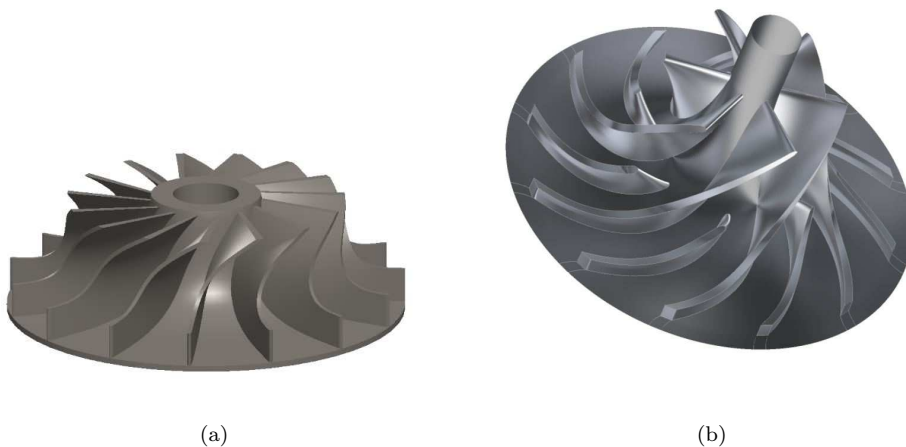


Figure 4: Examples of radial turbine (a) and centrifugal compressor (b) geometries.

218 The turbomachinery design is based on the design principles presented by Balje[41] and Rohlik[42]. The  
 219 suitable turbine rotational speed was calculated by setting the specific speed  $N_s$  as an input value in the  
 220 analysis and by using the working fluid flow rate and isentropic enthalpy change that were solved in the  
 221 cycle design analysis. The specific speed can be defined as

$$N_s = \frac{\omega q_{v2}^{0.5}}{\Delta h_s^{0.75}}. \quad (10)$$

222 The rotational speed was calculated by using  $N_s = 0.6$  which is close to the optimal value for radial  
 223 turbines, which is about 0.4 - 0.8 according to the design guidelines [41, 42]. The same equation can be used  
 224 for compressors for defining the specific speed but in this case, the volumetric flow rate at the compressor  
 225 rotor inlet is used.

226 The turbine design is based on solving the suitable geometry by using velocity triangles consisting of three  
 227 vectors, namely the absolute velocity  $c$ , peripheral velocity  $u$  and relative velocity  $w$ . A schematic example  
 228 shape of a velocity triangle at the turbine rotor inlet is presented in Fig.5. The expansion was divided  
 229 equally for turbine stator and rotor. For the turbine stator, efficiency of 90 % was used for estimating the  
 230 enthalpy at the stator outlet. The enthalpy at the stator outlet was calculated as,

$$h_1 = h_0 - \eta_{st}(h_0 - h_{1s}). \quad (11)$$

231 and the absolute flow velocity  $c_1$  at the stator outlet was calculated by using the stator inlet and outlet  
 232 enthalpy

$$c_1 = \sqrt{2(h_0 - h_1)}. \quad (12)$$

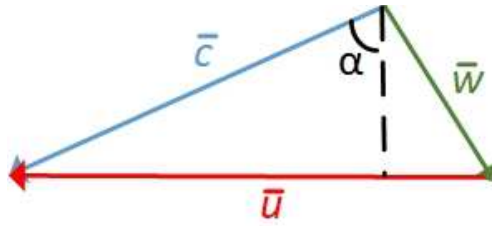


Figure 5: A schematic example of velocity triangle at the rotor inlet.

233 The optimal absolute flow angle  $\alpha$  at the rotor inlet was selected as a function of the specific speed by  
 234 following the principles presented in[42]. The velocities at the rotor inlet  $u_1$  and  $c_{u1}$  are solved by using  
 235 the absolute flow angle and the total enthalpy change over the turbine. The tangential component of the  
 236 absolute velocity  $c_{u1}$  was solved from the rotor inlet velocity triangle and the peripheral velocity  $u_1$  was  
 237 solved by using the Euler turbomachinery equation in where the rotor discharge flow was assumed to be  
 238 axial,

$$u_1 = \frac{\Delta h_t}{c_{u1}} \quad (13)$$

239 The turbine diameter can be calculated as,

$$d_1 = \frac{u_1}{\pi n} \quad (14)$$

240 The rotor inlet blade height was calculated by using the continuity equation. The rotor diameter and  
 241 blade height at the rotor outlet are calculated by using the diameter ratios  $d_{2tip}/d_1$  and  $d_{2hub}/d_{2tip}$  that  
 242 were defined by following the guidelines of Rohlik[42].

243 In the turbine loss analysis the stator loss, rotor passage loss, and the disk friction loss were calculated  
 244 for each turbine design. The turbine rotor disk friction loss and passage loss were evaluated according to  
 245 Daily and Nece [43] and Balje [44]. These models were selected for the study as similar loss correlations have  
 246 been previously used for estimating turbomachinery losses for radial turbines operating with supercritical  
 247 CO<sub>2</sub>[45]. The disk friction loss was evaluated by using the following equations

$$\Delta h_{df} = 0.5f(\rho_1 + \rho_2)D_1^2 \frac{u_1^3}{16q_{m,wf}} \quad (15)$$

248 in where,

$$Re = \rho_1 u_1 \frac{D_1}{2\mu_1} \quad (16)$$

$$f = \frac{0.0622}{Re^{0.2}} \quad (17)$$

250 .

251 The rotor passage loss was evaluated by using the following equation

$$\Delta h_{pass} = \varphi^{1.75} \frac{(1 + \kappa)^2}{8} \varsigma u_1^2 \quad (18)$$

252 in where,

$$\varsigma = 0.88 - 0.5\varphi \quad (19)$$

$$\kappa = \frac{c_{r1}}{c_{r2}} \quad (20)$$

$$\varphi = \frac{c_{r1}}{u_1} \quad (21)$$

253 The total loss in the turbine is defined as

$$\Delta h_{loss} = \Delta h_{df} + \Delta h_{pass} + \Delta h_{stator} \quad (22)$$

and the turbine efficiency is defined as

$$\eta_t = \frac{\Delta h_s - \Delta h_{loss}}{\Delta h_s} \quad (23)$$

The incidence loss was not taken into account in the analysis since only different turbine design points were studied and zero incidence for the flow at rotor inlet was assumed at the design condition. In addition, tip clearance loss was not included since there is only little information in the literature on the suitable loss correlations and methods for accurately calculating the tip clearance loss for radial turbines, especially with non-conventional and supercritical working fluids. Thus, the results presented in this study can slightly overestimate the turbine isentropic efficiency, especially with turbines having small blade heights at the rotor inlet. However, in the experimental work by Dambach et al. [46] it was concluded that the tip clearance loss with radial turbines is less significant when compared to axial turbines. The radial turbine design code and predicted losses were compared and validated against radial turbine designs available in the literature and this validation and comparison is presented in the following section.

A simplified compressor design was also included in the analysis to evaluate the compressor size and geometry for the studied system. The compressor geometry was calculated for different fluids and operational conditions by using the Sandia Laboratory experimental setup main compressor[40] as the reference compressor design. The compressor geometry analysis was carried out only for the simple cycle configuration with different fluids in order to limit the number of the studied cases. However, the compressor design for the intercooled cycle was included for CO<sub>2</sub> in order to compare the compressor design in simple and intercooled cycle. The compressor loss calculations were not included in the analysis. The working fluid flow rate and compressor inlet and outlet conditions were used as the input values for defining the compressor geometry. In addition, the compressor rotational speed was set to equal value as were gained in the turbine design for the respective conditions as the turbine and compressor were assumed to be assembled on the same shaft. This resulted in compressor specific speeds in the range of 0.6-1.0 in the simple cycle layout that can be considered to be in a feasible range for centrifugal type compressors[41]. In the design, the shape of the velocity triangle at the compressor wheel outlet was defined by giving the velocity ratios  $c_{r1'}/u_{1'}$  and  $c_{u1'}/u_{1'}$  as well as diameter ratios  $d_{0'tip}/d_{1'}$  and  $d_{0'hub}/d_{1'tip}$  as inputs. These ratios were defined and selected based on the reference compressor design[40] and were kept constant thorough the study for different fluids and operational conditions. The compressor diameter and blade height at the impeller inlet and outlet were solved by using the same methods as were applied and described for the turbine design.

### 3.1. Cycle and turbomachinery code validation

SBC cycle model was validated against data available in the literature. For the cycle code validation, the simulation results of a transcritical CO<sub>2</sub> cycle presented by Kim et al. [47] were used as the reference case. The turbine inlet pressure and temperature, outlet pressure, isentropic efficiency, and recuperator

286 effectiveness were set to the same values as were used in[47]. The main results of this comparison are  
 287 presented in Table 3 for the simple cycle configuration. The fluid compression calculation was validated and  
 288 compared against the design values of the main compressor of the Sandia laboratory experimental setup[36].  
 289 The results of the comparison are presented in Table 4. In this comparison, the fluid state at the compressor  
 290 inlet, compressor outlet pressure, fluid mass flow rate and compressor efficiency were set to the equal values  
 291 as in the reference[36].

Table 3: Cycle code validation.

	$\Delta T$ [K]	$\Delta T$ [K] [47]	$\Delta h$ [kJ/kg]	$\Delta h$ [kJ/kg] [47]
Expansion	151.0	151.0	169.9	169.9
Cooler	33.6	34.2	221.5	222.7
Heater	301.6	302.5	371.9	373.1
Recuperator hot side	395.5	394.7	450.1	449.0
Recuperator cold side	259.2	258.3	450.1	449

Table 4: Compressor calculation validation.

	$P$ [kW]	$\Delta T$ [K]
Sandia main compressor	49	17.8
Sandia main compressor [36]	51	19.0
dev	2	1.2

292 The turbine design code was validated and the results are compared against different radial turbine  
 293 designs for non-conventional working fluids available in the literature. The design comparison is carried  
 294 out for three different radial turbine designs using siloxane MDM, CO<sub>2</sub> at supercritical state and R245fa  
 295 as the working fluids. In the comparison presented in Table 5, the turbine inlet temperature and pressure,  
 296 outlet pressure, and fluid flow rate were set to the same values as in the literature references. In addition,  
 297 the turbine design specific speed, absolute flow angle  $\alpha_1$ , flow acceleration in the turbine stator, and the  
 298 degree of reaction, were set to the same values as were presented in the references if this information was  
 299 available. If the information was not given in the references, these values were selected in order to have the  
 300 turbine design results as close as possible to the turbine values presented in the references. Turbine wheel  
 301 dimensions, rotational speed, power output, and efficiency were calculated by using the developed turbine  
 302 design code and the results were compared against the turbine dimensions and performance given in the



303 literature references.

Table 5: Comparison of the turbine design code results and the turbine dimensions and performances available in the literature.

	fluid	$D_{rot}$ , [mm]	$n_{rot}$ , [rpm]	$P_t$ [kW]	$\eta_t$ [%]	$N_s$ -	$\alpha$ [deg]
[39]	R245fa	$\approx 125$	20 000	32.7 (electrical)	82 (max)	-	-
Turbine design code	R245fa	136.3	21 788	36.0 (mechanical)	86.5	0.45	72
Dev %	-	9.04	8.94	-	5.5	-	-
[48]	MDM	144	31 455	13.0	76	0.49	69.4
Turbine design code	MDM	146.0	31 348	12.6	79.5	0.44	69.4
Dev %	-	1.4	-0.3	-2.8	4.6	-	-
[36, 37]	CO <sub>2</sub>	67.6	75 000	178	87	-	-
Turbine design code	CO <sub>2</sub>	66.2	75 474	176.7	86.2	0.36	75
Dev %	-	-2.1	0.6	-0.7	-0.9	-	-

304 The comparison shows that the obtained results are well in line with the used turbine design references,  
305 especially when considering the turbine diameter and rotational speed. Some deviations can be observed  
306 in the predicted turbine isentropic efficiencies, and power outputs with all the turbines. The smallest  
307 deviations were found for the turbine operating with supercritical CO<sub>2</sub> and the highest deviations in the  
308 power output and efficiency predictions were observed with the turbines operating with MDM and R245fa.  
309 However, the maximum deviations of less than 10 % were obtained for all the studied parameters. Overall  
310 it can be concluded that the applied turbine design method can be considered to be suitable for qualitative  
311 and preliminary evaluation on the effect of using different fluids and cycle operating conditions on turbine  
312 efficiency and geometry, as the same method is systematically implemented for the radial turbine design  
313 with all the studied fluids and conditions thorough the analysis. Overall, the validation of both the cycle  
314 and turbine design codes show good agreement when compared to the selected literature references.

315 The validation of the compressor design code is presented in Table 6. The flow rate through the com-  
316 pressor, compressor inlet and outlet state, and the design rotational speed were set to the equal values as  
317 were used in[40]. In general, the designed compressor wheel has diameters and blade height close to the  
318 values of the reference compressor. The deviation in the impeller outlet blade height was 0.3 mm and the  
319 maximum deviation out of the studied diameters was 0.5 mm.

Table 6: Comparison of the compressor design code results and the centrifugal compressor design available in the literature.

	fluid	$D_{1'}$ [mm]	$D_{0'hub}$ [mm]	$D_{0'tip}$ [mm]	$b_{1'}$ [mm]
[40]	CO <sub>2</sub>	37.4	18.7	5.1	6.8
Compressor design code	CO <sub>2</sub>	37.2	18.6	5.6	6.5

## 320 4. Results and Discussion

321 In this section the main results of the study are presented. First, a sensitivity analysis on different process  
 322 parameters is carried out by using CO<sub>2</sub> as the working fluid. Second, the results of the effect of different fluids  
 323 and operational parameters on the power production potential and efficiency are presented and discussed.  
 324 In this thermodynamic analysis, the turbomachinery isentropic efficiencies are kept constant for all the  
 325 fluids and operational parameters. Third, the design and loss evaluation on the process radial turbine and  
 326 centrifugal compressor with different fluids and operational conditions are presented and discussed.

### 327 4.1. Sensitivity analysis of main process parameters with CO<sub>2</sub>

328 The sensitivity of the cycle performance on the main process parameters were studied first with CO<sub>2</sub>  
 329 as the working fluid. The studied parameters are the compressor and turbine efficiency, turbine inlet  
 330 temperature and the recuperator effectiveness. The results presented in the following were obtained by  
 331 using the simple cycle configuration and compressor inlet temperature of 50 °C. The turbine inlet pressure  
 332 was varied between 100 bar to 400 bar and the turbine inlet temperature was varied from 270 °C to 330 °C  
 333 in the analysis. The results of the effect of turbomachinery efficiency on compressor power consumption and  
 334 turbine power output are presented in Figure 6a and b. The compressor power consumption was calculated  
 335 for a single compressor without intercooling. The result of the sensitivity of turbine inlet temperature on  
 336 the cycle performance is presented in Figure6c. In these simulations turbomachinery efficiencies of 85% were  
 337 adopted.

338 The results show that the compressor power consumption and turbine power output are highly sensitive  
 339 on the efficiency of the turbomachines. The effect of the turbine or compressor efficiency are more pronounced  
 340 as the turbine inlet pressure is high, when compared to a cycle designed for lower pressure ratio. Thus,  
 341 for achieving a high efficiency and net power output for the studied system, it is of high importance that  
 342 both the compressor and turbine can be operated with high efficiency. The results of the effect of turbine  
 343 inlet temperature show that the higher the turbine inlet temperature, the higher the cycle power output.  
 344 Thus the turbine inlet temperature of 330 °C was used in the following analysis which is 24 °C less than

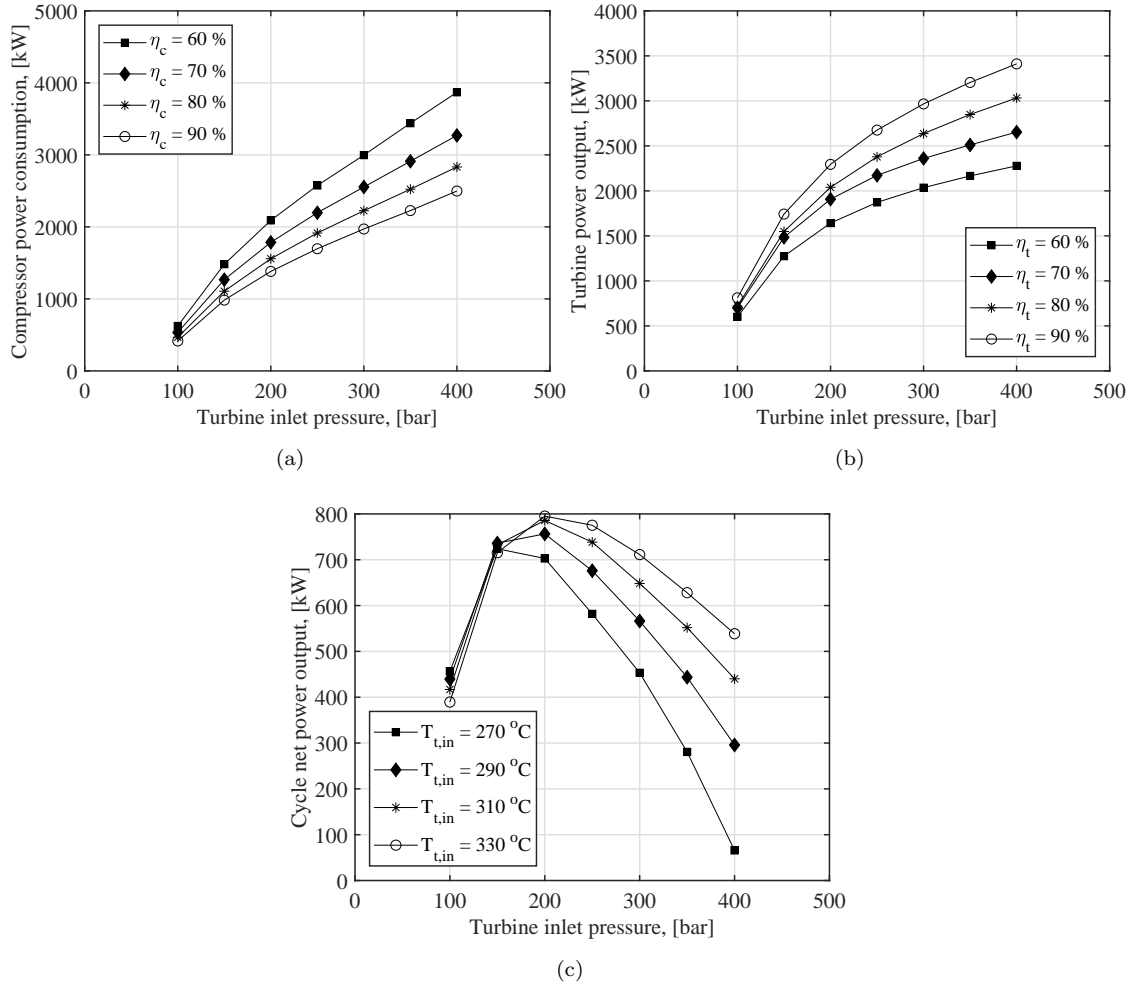


Figure 6: Effect of compressor efficiency on compressor power consumption (a), turbine efficiency on turbine power output (b), and turbine inlet temperature on cycle net power output (c).

345 the temperature level of the exhaust gases. This was estimated to ensure sufficient temperature difference  
 346 between the heat source and working fluid at the hot end of the heater.

347 The sensitivity of recuperator effectiveness on the cycle power output and the effect of the recuperator  
 348 effectiveness on the heat source temperature at the heater outlet are presented in Figures 7a and b. The  
 349 analysis on the effect of recuperator effectiveness on power output show that the recuperator effectiveness  
 350 has only minor effect on the cycle power output with the applied method. This can be explained that  
 351 in the cycle analysis the heat source temperature at the heater outlet was defined by using the minimum  
 352 temperature difference between the heat source and working fluid. Thus, as the recuperator effectiveness is  
 353 increased the heat source temperature at the heater outlet has to be also increased in order to maintain the  
 354 required temperature difference between the heat source and the working fluid. This results in a lower heat

355 rate in the heater but increases the amount of heat transferred in the recuperator. Thus, it was concluded  
 356 that the benefit of using a high recuperator effectiveness in the cycle is not as significant in this application,  
 357 as have been presented in the literature for higher temperature applications.

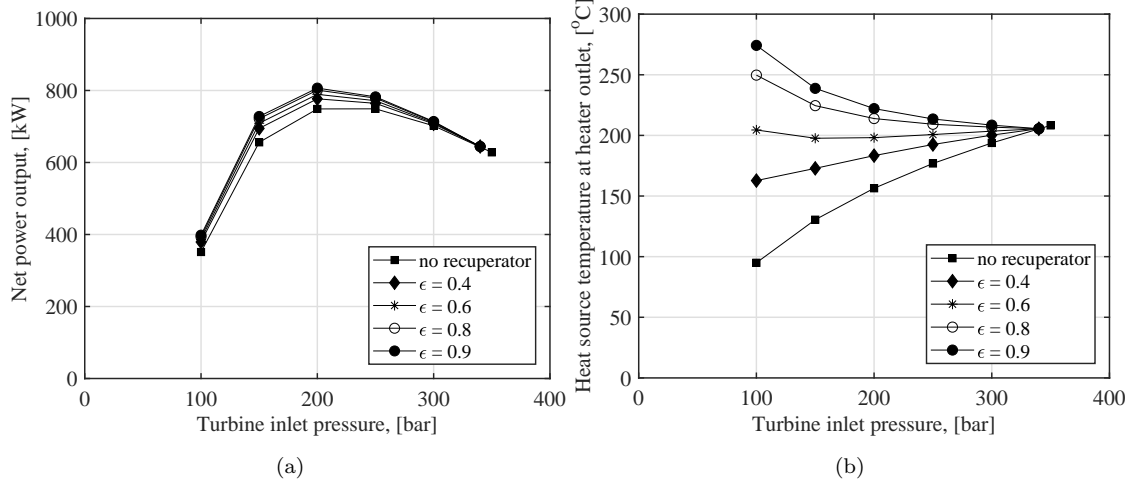


Figure 7: Effect of recuperator effectiveness on cycle net power output (a) and heat source temperature at the heater outlet(b).

358 In addition to the above presented results, the effect of the pressure level between the Compressor 1 and  
 359 Compressor 2 on the intercooled cycle performance was studied by using  $\text{CO}_2$  as the working fluid. The  
 360 pressure rise in the compressor 1 was defined as

$$p_{comp1,out} = x(p_{comp1,in} * p_{comp2,out})^{0.5} \quad (24)$$

361 and the results obtained for different  $x$  values are presented in Fig.8a and b. Based on the obtained results,  
 362 the pressure level between the Compressor 1 and Compressor 2 has an effect on the cycle power output,  
 363 especially when using the higher CIT of  $50^{\circ}\text{C}$ . For both studied cases a higher cycle power output was reached  
 364 when the Compressor 1 pressure ratio is lower when compared to the pressure ratio of the Compressor 2.  
 365 However, by designing the pressure ratio of both compressors to be equal ( $x = 1$ ), the power as well as the  
 366 wheel dimensions of Compressor 1 and Compressor 2 are in the same order of magnitude that was considered  
 367 as beneficial for the turbomachinery design for such a system. Thus,  $x = 1$  was used in the intercooled cycle  
 368 analysis in the following.

#### 369 4.2. Results of the cycle analysis

370 The results of the cycle analysis for the simple cycle configuration and intercooled cycle configuration are  
 371 presented in the following. The results were obtained by using turbine and compressor efficiency of 85 % that  
 372 were selected based on previous research works on supercritical  $\text{CO}_2$  turbomachinery[23, 17, 36, 47]. The  
 373 maximum degree of recuperation of 0.7 was used and the simulations were carried out by using compressor

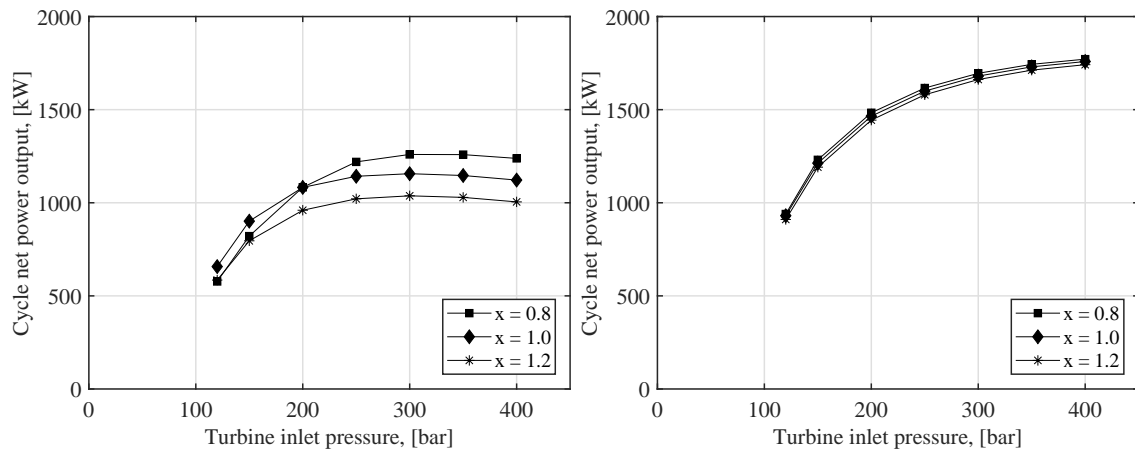


Figure 8: Effect of compressor 1 outlet pressure on the power output of intercooled SBC. Results presented in (a) were obtained by using CIT of 50 °C and (b) were obtained by using CIT of 31 °C.

374 inlet temperatures (CIT) of 30 °C and 50 °C in order to study the effect of the compressor inlet temperature  
 375 on the cycle performance. With the lower temperature conditions slightly higher temperatures of 31 °C and  
 376 33 °C were used for CO<sub>2</sub> and ethane, respectively, in order to maintain the fluid at supercritical state at  
 377 the compressor inlet.

378 The results of the power output are presented in Figures 9a-d and cycle efficiency in Figures 10a-d with  
 379 different turbine inlet pressures and with different fluids.

380 The use of CO<sub>2</sub> as the working fluid resulted in higher electric power outputs in all the studied cases  
 381 when compared to the other fluids and ethane reached the second highest performances. In general, the use  
 382 of intercooling in the cycle and low compressor inlet temperature results in highest cycle performances. The  
 383 maximum electric power output of 1759 kW was simulated with CO<sub>2</sub> by using the lower compressor inlet  
 384 temperature and turbine inlet pressure of 400 bar. The maximum electric power output of 1156 kW was  
 385 obtained by using the compressor inlet temperature of 50 °C and turbine inlet pressure of 300 bar. These  
 386 values correspond to 9.6 % and 6.3 % of the gas engine power output. This maximum power production  
 387 potential is slightly lower when compared to the use of ORC technology for recovering exhaust heat of  
 388 large-scale engines according to the previous studies e.g. [4, 6]. Corresponding maximum power outputs  
 389 are about 440 kW and about 150 kW lower with ethane when compared to the results with CO<sub>2</sub>. The use  
 390 of ethylene and R116 as the working fluids resulted in lower maximum cycle performances when compared  
 391 to ethane and CO<sub>2</sub>. The turbine inlet pressure, resulting in the highest power output, is dependent on  
 392 the compressor inlet temperature, cycle configuration and working fluid. With the lower compressor inlet  
 393 temperature, the highest power outputs were simulated with the highest turbine inlet pressures between 300  
 394 bar to 400 bar, with CO<sub>2</sub>, ethane and R116. When ethylene is used as the working fluid, the maximum  
 395 power output was simulated by using a lower turbine inlet pressure close to 200 bar. With the higher

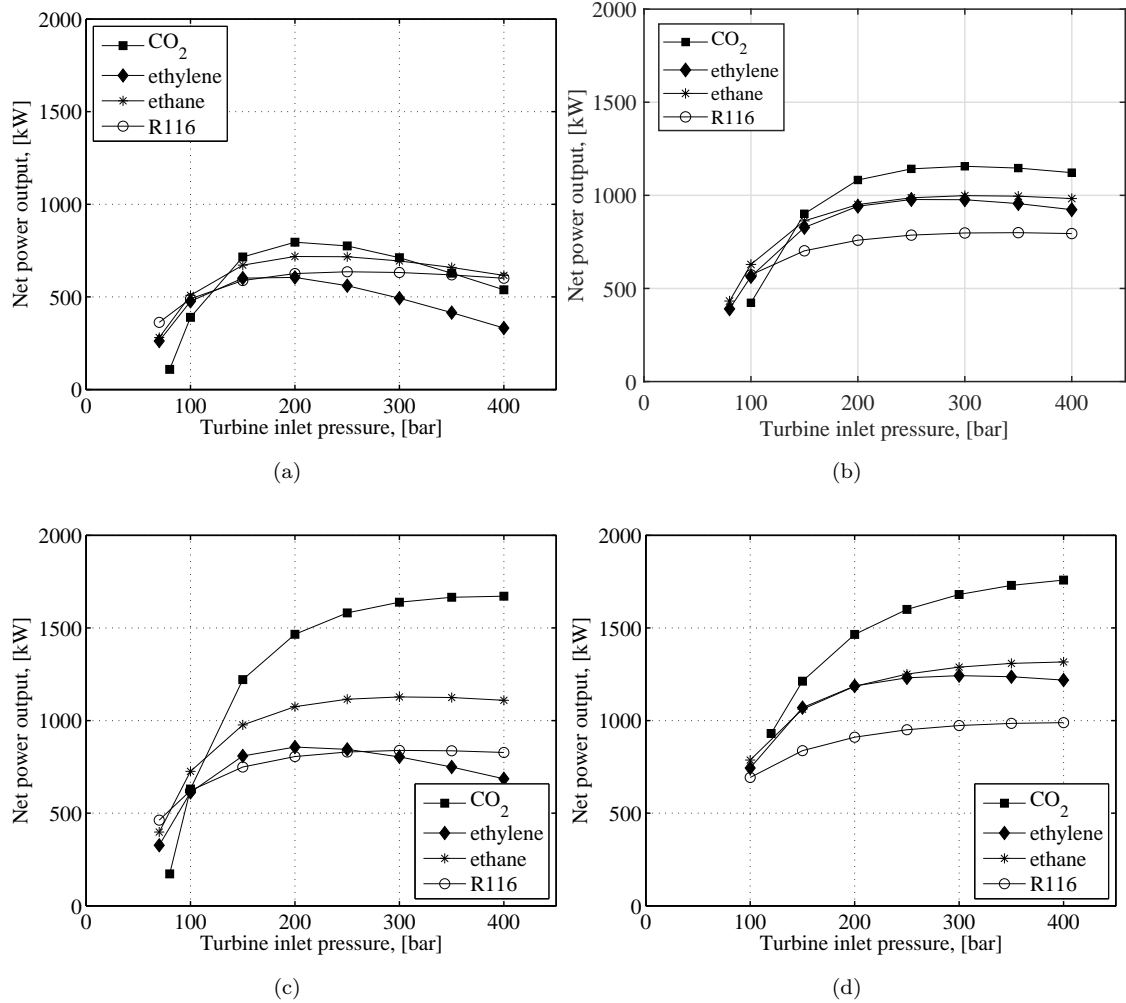


Figure 9: Effect of turbine inlet pressure on SBC power output. Results presented in (a) are for simple cycle and (b) for intercooled cycle with CIT of 50 °C. Results presented in (c) are for simple cycle and (d) for intercooled cycle with CIT of 30 °C.

396 compressor inlet temperature, the turbine inlet pressure resulting in the highest power outputs is lower  
 397 with all the studied fluids when compared to the cycle with the lower compressor inlet temperature. The  
 398 maximum cycle efficiencies above 20 % were simulated with CO<sub>2</sub> and ethane by using the lower compressor  
 399 inlet temperature and high turbine inlet pressure, whereas the maximum cycle efficiencies close to 15 %  
 400 or slightly above 15 % were simulated for all the studied fluids with the compressor inlet temperatures of  
 401 50 °C. It should be noted that for reaching the low compressor inlet temperature, resulting in the highest  
 402 performances, a cooling fluid with a low temperature has to be available for the cycle. Thus, to reach the  
 403 lower compressor inlet temperature is not possible in hot climates and in applications in where cooling fluid  
 404 temperatures below 30 °C are not available.

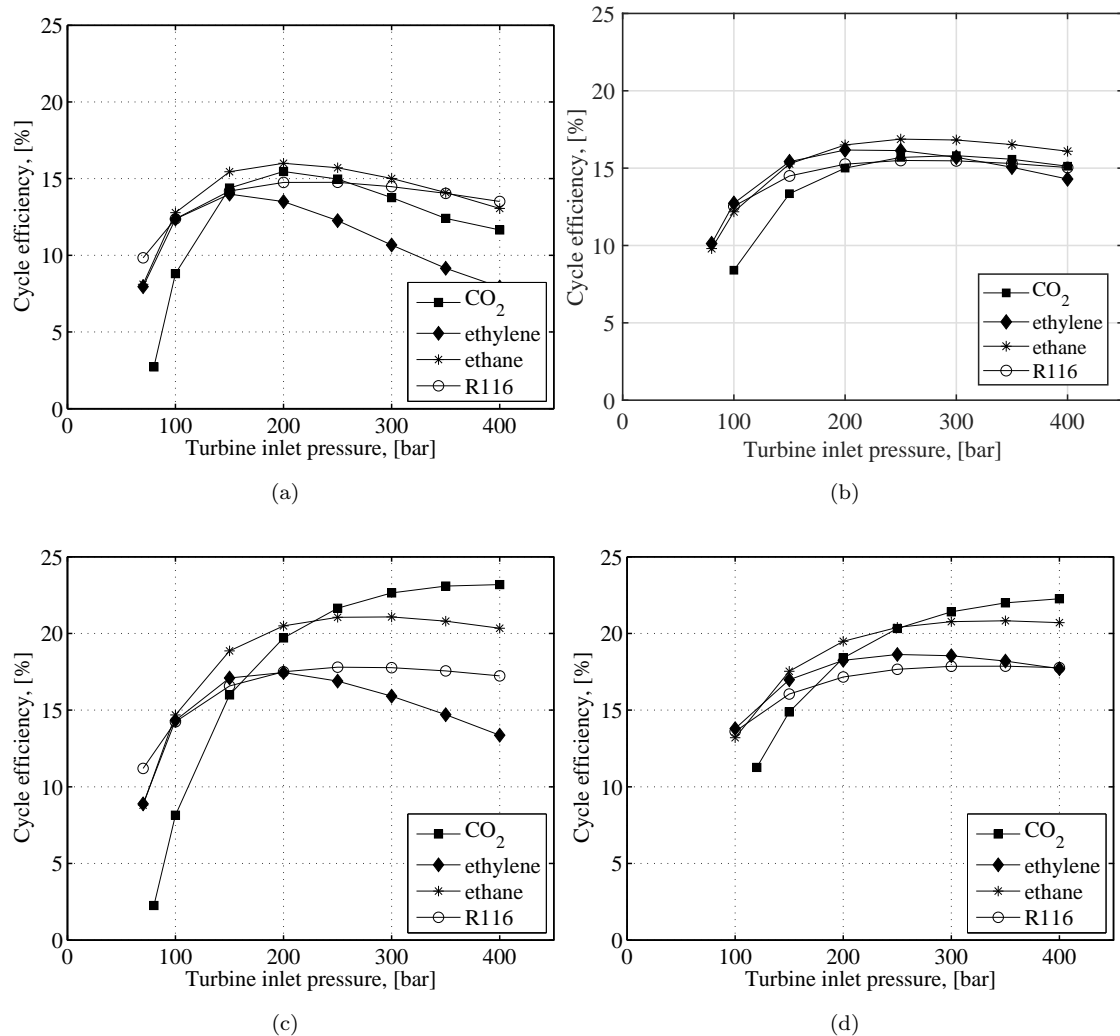
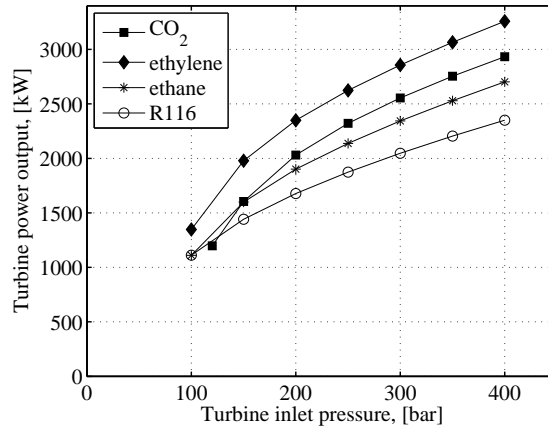


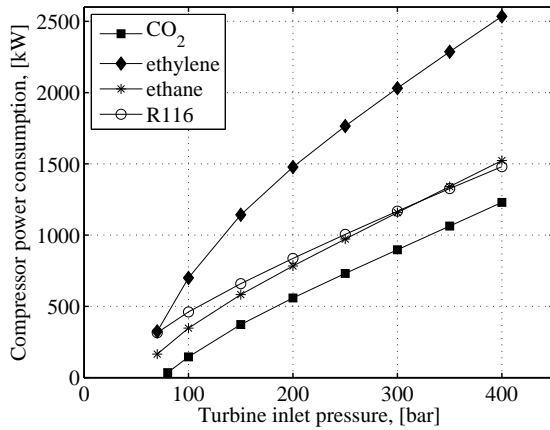
Figure 10: Effect of turbine inlet pressure on SBC efficiency. Results presented in (a) are for simple cycle and (b) for intercooled cycle with CIT of 50 °C. Results presented in (c) are for simple cycle and (d) for intercooled cycle with CIT of 30 °C.

405 The results of the turbine mechanical power output and the power consumption of the fluid compression  
 406 are presented in Figures 11a-c. These results were obtained by using the lower compressor inlet temperature.  
 407 The cycle using ethylene as the working fluid results in the highest turbine mechanical power. However,  
 408 the power consumption of the compressor with this fluid is significantly higher when compared to the  
 409 other studied fluids. This mainly explains the low cycle power output when using ethylene as the working  
 410 fluid. CO<sub>2</sub> represents the second highest turbine power and in addition, the power consumption of the  
 411 compressing the fluid is significantly lower when compared to the other studied fluids, which results in  
 412 high cycle performances. With all the studied fluids, the intercooling between the compressors reduces  
 413 the compression power consumption, which mainly explains the higher cycle performances when using the

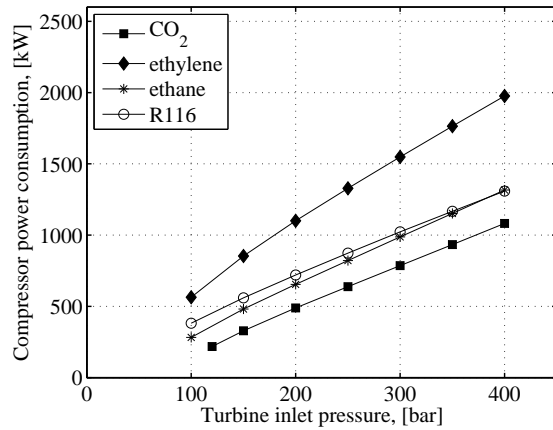
414 intercooled cycle configuration.



(a)



(b)



(c)

Figure 11: Effect of turbine inlet pressure on turbine power output (a), and compressor power consumption (b) and (c). (b) is for single stage compression and (c) is for the intercooled compression. The simulations were performed by using the lower CIT.

415 The results of the heater heat rate for the studied cases are presented in Figures 12a-d. Based on the  
 416 simulation results the system using CO<sub>2</sub> as the working fluid can extract higher amount of heat from the  
 417 heat source when compared to the other studied fluids, especially in the simple cycle configuration. The  
 418 differences in the heater heat rates can be explained by the deviations in the working fluid temperatures at  
 419 the heater cold end with different fluids, cycle configurations, and cycle operating pressures. For example,  
 420 as presented earlier the use of ethane as the working fluid resulted in comparable or slightly higher cycle  
 421 efficiencies when compared to the cycles operating with CO<sub>2</sub> but the cycle power outputs were significantly  
 422 lower because of the lower capability to extract heat from the exhaust gases in the heater. In general, as the



423 turbine inlet pressure increases, higher amount of heat power can be extracted from the heat source in the  
 424 heater. The high turbine outlet temperature and high heat transfer in the system recuperator can explain  
 425 the lower heat rate in the heater if a low turbine inlet pressure is adopted. Consequently, this leads to higher  
 426 exhaust gas temperature at the heater outlet and reduces the heater heat rate, when compared to the cycles  
 427 adopting higher pressure ratio over the turbomachines. The use of intercooling and low compressor inlet  
 428 temperature increases the amount of heat that can be transferred from the exhaust gases to the working  
 429 fluid.

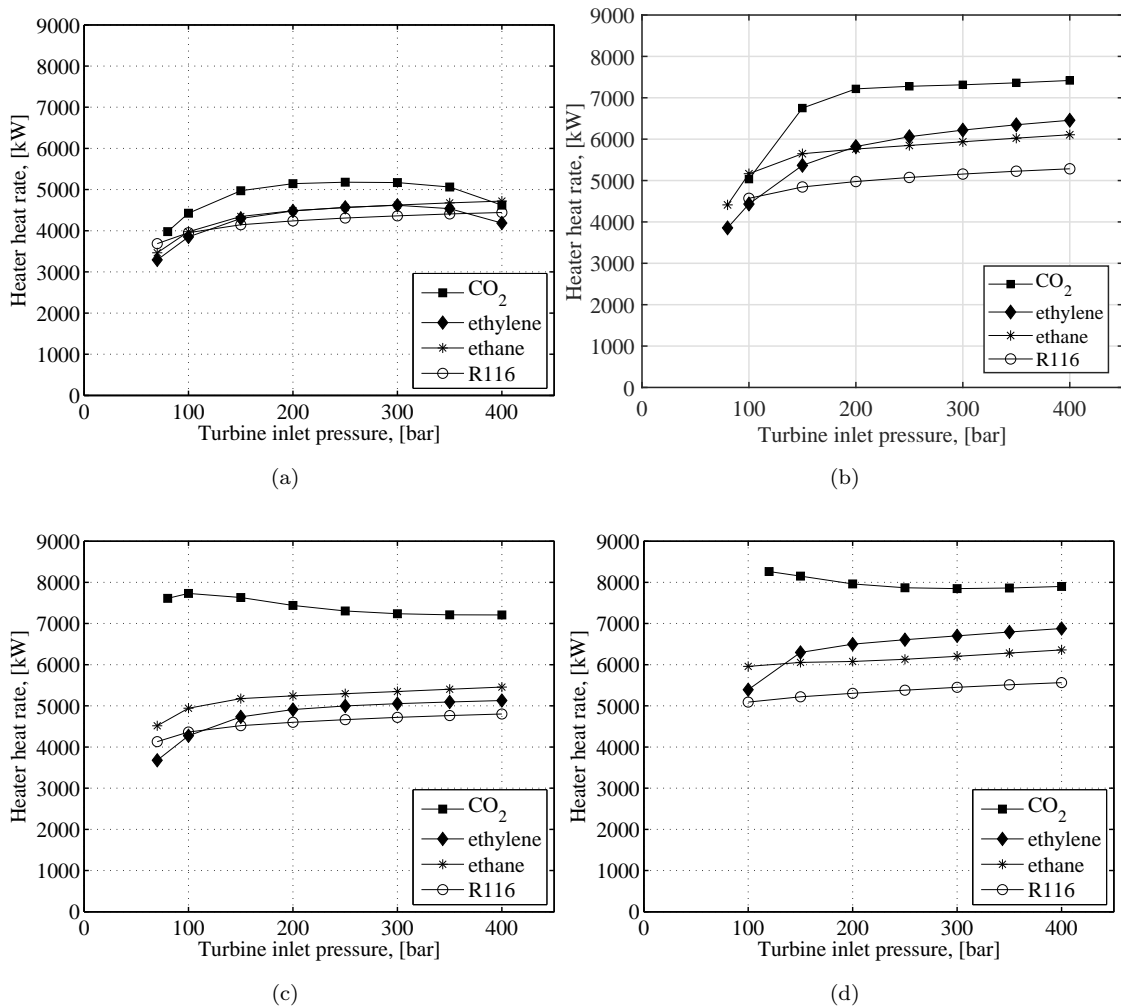


Figure 12: Effect of turbine inlet pressure on heater heat rate. Results presented in (a) are for simple cycle and (b) for intercooled cycle with higher CIT. Results presented in (c) are for simple cycle and (d) for intercooled cycle with lower CIT.

430 The results of cycle mass flow rates and fluid enthalpy change in the heater are presented in Figure  
 431 13. These results were obtained by using the simple cycle configuration and the lower compressor inlet  
 432 temperature. From the studied fluids, R116 represents the highest mass flow rates of above 30 kg/s. The

433 lowest working fluid mass flow rates less than 15 kg/s were simulated with ethane and ethylene. The observed  
 434 deviations in the mass flow rates can be explained by the differences in the fluid enthalpy change in the  
 435 heater as well as by the differences in the heater heat rates with different fluids. The fluids ethylene and  
 436 ethane have the highest enthalpy change in the heater of the studied fluids. The working fluid mass flow  
 437 rate is slightly lower and enthalpy change in the heater is higher with all the studied fluids when a high  
 438 turbine inlet pressure is adopted in the cycle, in a comparison to the use of a lower turbine inlet pressure. It  
 439 was observed that the cycle configuration and compressor inlet temperature do not have a significant effect  
 440 on the working fluid mass flow rate or on the heater heat rate.

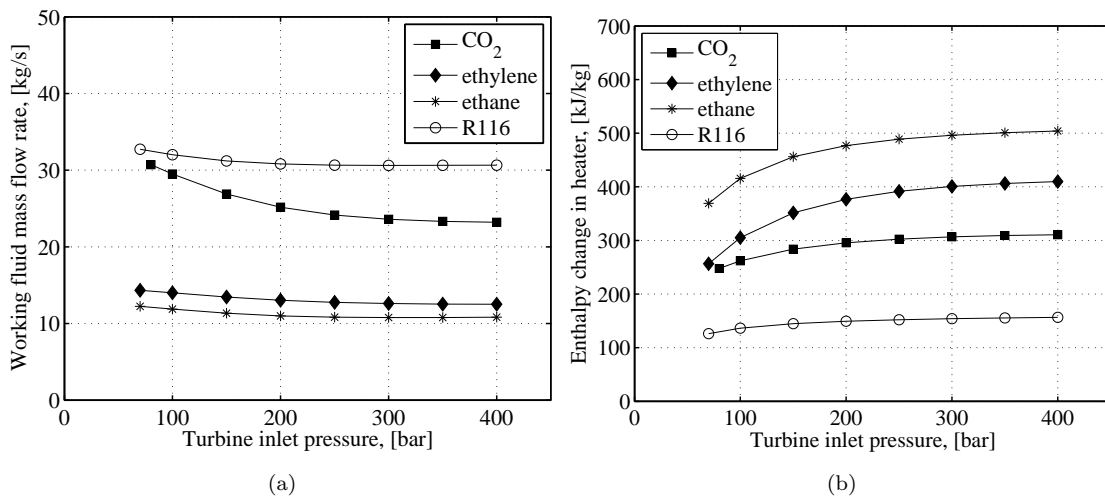


Figure 13: Effect of turbine inlet pressure on working fluid mass flow rate (a) and fluid enthalpy change in heater (b). Results are presented for simple cycle with lower CIT.

441 The results of the cycle analysis are summarized in Table 7 showing the main process parameters resulted  
 442 in the highest cycle performance for each of the studied case and each fluid.

#### 443 4.3. Turbomachinery design analysis

444 As were observed in the sensitivity analysis, the cycle power output is highly sensitive on the efficiency  
 445 of the cycle turbomachines. Thus, the turbomachinery design and turbine losses were studied in detail. The  
 446 turbine efficiency prediction, turbine geometry and rotational speed were calculated for different operational  
 447 conditions and fluids by combining the thermodynamic cycle model and the turbine design model. The  
 448 turbine design was carried out by using the simple cycle configuration and CIT of 50 °C, but the selected cycle  
 449 configuration and CIT have only minor effect on the turbine design. The simplified diagram representing  
 450 the combined cycle and turbine calculation method is presented in Figure 14.

451 The results of the turbine rotational speed, rotor diameter, blade height at the turbine rotor inlet, and  
 452 Mach number at the stator outlet are presented in Figures 15 a-d for different fluids and turbine inlet

Table 7: Summary of cycle analysis results representing the conditions with the highest simulated power output.

CO <sub>2</sub>	Simple, CIT=50°C	Simple, CIT=31°C	Intercooled, CIT=50°C	Intercooled, CIT=31°C
$P_e$ , [kW]	796.7	1671.6	1156.1	1758.6
$\eta_e$ , [%]	15.5	23.2	15.8	22.3
$p_{t,in}$ , [bar]	210.0	400.0	300.0	400.0
$\Pi_t$ , [-]	2.8	5.4	4.0	5.4
$p_{t,out}$ , [bar]	74.3	74.3	74.3	74.3
$q_m$ , [kg/s]	27.3	23.2	23.3	22.8
$P_c(\text{total})$ , [kW]	1536.6	1229.9	1397.2	1082.1
$P_t$ , [kW]	2375.2	2989.4	2614.2	2933.2
$\phi_h$ , [kW]	5156.4	7209.4	7313.6	7900.3
$T_{eg,h,out}$ , [°C]	205.5	146.4	143.4	126.5
Ethylene	Simple, CIT=50°C	Simple, CIT=30°C	Intercooled, CIT=50°C	Intercooled, CIT=30°C
$P_e$ , [kW]	612.0	857.9	980.3	1242.7
$\eta_e$ , [%]	13.9	17.4	16.0	18.5
$p_{t,in}$ , [bar]	175.0	210.0	270.0	305.0
$\Pi_t$ , [-]	3.4	4.1	5.3	6.0
$p_{t,out}$ , [bar]	50.9	50.9	50.9	50.9
$q_m$ , [kg/s]	13.3	13.0	12.6	12.5
$P_c(\text{total})$ , [kW]	1567.6	1537.0	1697.3	1570.1
$P_t$ , [kW]	2211.8	2440.3	2729.2	2878.2
$\phi_h$ , [kW]	4406.8	4933.2	6128.7	6710.3
$T_{eg,h,out}$ , [°C]	227.1	212.0	177.5	160.8
Ethane	Simple, CIT=50°C	Simple, CIT=33°C	Intercooled, CIT=50°C	Intercooled, CIT=33°C
$P_e$ , [kW]	721.2	1127.9	998.8	1316.4
$\eta_e$ , [%]	16.0	21.0	16.8	20.7
$p_{t,in}$ , [bar]	220.0	310.0	310.0	400.0
$\Pi_t$ , [-]	4.5	6.3	6.3	8.1
$p_{t,out}$ , [bar]	49.2	49.2	49.2	49.2
$q_m$ , [kg/s]	11.0	10.8	10.8	10.9
$P_c(\text{total})$ , [kW]	1263.0	1194.4	1330.0	1316.4
$P_t$ , [kW]	2022.1	2381.7	2381.4	2702.
$\phi_h$ , [kW]	4520.5	5360.4	5954.6	6357.8
$T_{eg,h,out}$ , [°C]	223.8	199.7	182.5	170.9
R116	Simple, CIT=50°C	Simple, CIT=30°C	Intercooled, CIT=50°C	Intercooled, CIT=30°C
$P_e$ , [kW]	635.9	839.0	799.8	988.9
$\eta_e$ , [%]	14.7	17.7	15.4	17.8
$p_{t,in}$ , [bar]	255.0	310.0	335.0	400.0
$\Pi_t$ , [-]	8.2	10.0	10.8	12.9
$p_{t,out}$ , [bar]	31.0	31.0	31.0	31.0
$q_m$ , [kg/s]	30.7	30.6	30.6	30.6
$P_c(\text{total})$ , [kW]	1231.7	1200.2	1317.5	1308.9
$P_t$ , [kW]	1901.0	2083.3	2159.4	2349.8
$\phi_h$ , [kW]	4314.1	4729.6	5206.1	5565.7
$T_{eg,h,out}$ , [°C]	229.8	217.8	204.1	193.7

453 pressures. With all the studied fluids, the turbine optimal rotational speed is higher and the turbine wheel  
454 has smaller dimensions as the turbine design pressure at the inlet is increased. In general, the turbine  
455 rotational speeds are high, of tens of thousands of rpm, with all the studied fluids. The highest optimal  
456 rotational speeds were obtained with ethylene and ethane, while the use of R116 as the working fluid results  
457 in turbine design with the lowest rotational speeds. The use of ethylene and ethane results in turbine  
458 geometries having the smallest turbine diameters ranging from 0.07 m to 0.12 m, while the cycles using  
459 CO<sub>2</sub> or R116 represent slightly larger turbine wheels. These deviations in the optimal rotational speeds  
460 and geometry with different working fluids are due to the differences in the enthalpy drop over the turbine

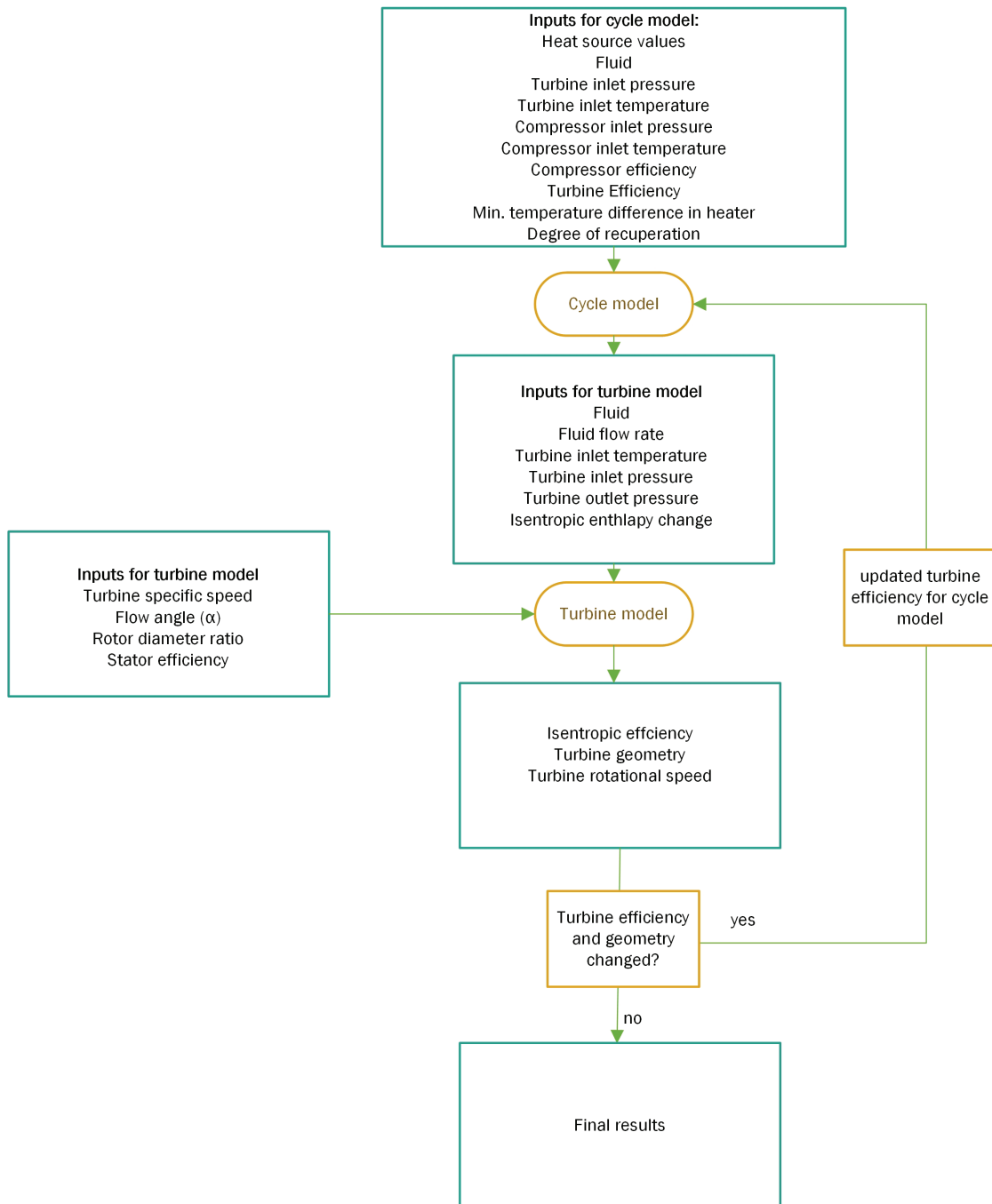


Figure 14: Simplified diagram of the combined cycle and turbine design model.

461 and different volumetric flow rates at the turbine outlet. According to the results, the designed turbines are  
 462 significantly compact, when compared to for example ORC turbomachinery(e.g [38]). This can be considered  
 463 as a beneficial feature especially in applications having restricted space for the WHR system. On the other  
 464 hand, the high rotational speed, small dimensions and high pressures will set demands and challenges in

465 the mechanical design of this type of turbogenerator, including requirements for the bearing and sealing  
 466 solutions. The turbines designed by using CO<sub>2</sub> have the highest blade heights ranging from 5 to 15 mm  
 467 depending on the turbine inlet pressure while the smallest blade heights were observed with ethane. The  
 468 small blade height at the rotor inlet can lead to increased tip clearance losses. The use of CO<sub>2</sub> also resulted  
 469 in lowest Mach numbers at the turbine stator outlet and the highest Mach numbers were observed with  
 470 R116. The high Mach number increases the losses due to the presence of oblique shock waves inside the  
 471 turbine. The flow velocity at the stator outlet was modelled to be supersonic with all the studied fluids,  
 472 especially when a high turbine inlet pressure is adopted in the cycle.

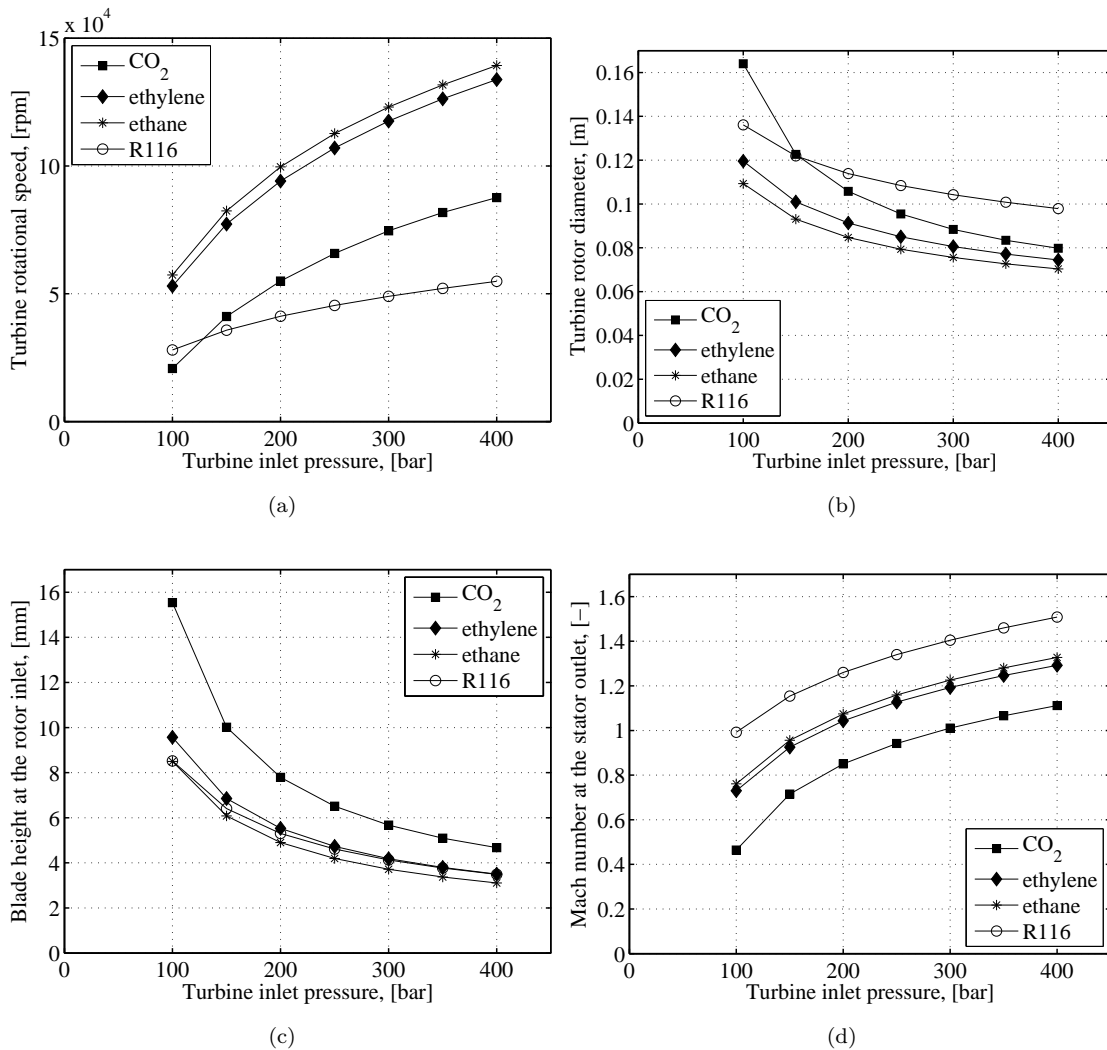


Figure 15: The turbine rotational speed (a), rotor diameter (b), blade height at the turbine rotor inlet (c), and Mach number at the stator outlet (d) with different turbine inlet design pressures.

473 The results for the predicted turbine isentropic efficiency, turbine passage loss, disk friction loss, and

474 enthalpy drop over the turbine are presented in Figures 16 a-d. The simulated turbine efficiencies were  
475 significantly high, ranging from 90.5 to 91 % for all the studied fluids. The turbine efficiency is slightly lower  
476 when a high turbine inlet pressure is used compared to a turbine designed for lower turbine inlet pressure. In  
477 addition, both the passage loss and disk friction loss were estimated to increase as the turbine is designed for  
478 a high inlet pressure, but on the other hand, also the enthalpy drop over the turbine increases. The passage  
479 loss was estimated to be more significant when compared to the disk friction loss with all the studied fluids  
480 and operational conditions. It should be noted, that in the efficiency prediction the stator efficiency was  
481 kept constant for all the fluids and operational parameters and only the passage loss and disk friction loss  
482 were included in the analysis. Thus, the turbine efficiencies presented here can be slightly over predicted.  
483 Especially with the turbine inlet pressures resulting in supersonic flow at the stator outlet, the turbine losses  
484 can be higher than presented here, due to the efficiency reductions related to the presence of shock waves.  
485 In addition, the tip clearance loss was not taken into account in the analysis, which can be a significant loss  
486 source in turbines, especially when the blade heights are significantly small at the rotor inlet.

487 The results of the compressor diameter are presented in Figures 17a and b. The blade height at the  
488 compressor wheel outlet are presented in Figures 17c and d. These results were obtained by using the simple  
489 configuration and both the higher and lower CIT. The designed compressor wheels have small diameters  
490 of less than 0.1 m in most of the studied cases and the designed compressor wheels are slightly smaller  
491 when compared to the respective turbine designs. The blade heights at the rotor outlet range from about 2  
492 mm to 5 mm, except when using a low compressor outlet pressure. In general, the higher the compressor  
493 outlet pressure the smaller the blade height and compressor diameter. The small blade height can increase  
494 especially the tip clearance loss of the compressor, resulting in low compression efficiency, when a high  
495 compressor design outlet pressure is adopted. With R116 the largest compressor wheels were obtained but  
496 on the other hand the blade height is lower with this fluid when compared to the other studied fluids.  
497 With the highest compressor outlet pressures all the studied fluids have comparable blade heights at the  
498 rotor outlet and no significant deviations between the fluids were observed. It was also observed that the  
499 compressor inlet temperature has an effect on the optimal compressor wheel diameter caused mainly by  
500 the differences in temperature and enthalpy change over the compressor. On the other hand, differences in  
501 the simulated blade heights were almost negligible when comparing the designs carried out for cycles with  
502 different compressor inlet temperatures.

503 The compressor design for the intercooled cycle was also studied with CO<sub>2</sub> as the working fluid using  
504 the lower CIT and the results are compared against the results of the simple cycle compressor design. The  
505 results are presented in Figures 18a and b. In the intercooled cycle, as the compression is divided for two  
506 compressors the compressors wheels are smaller compared to the compressor design of the simple cycle. In  
507 addition, the specific speeds of the compressors are higher, in the range from 0.8 to 1.7, compared to the  
508 simple cycle, which can lead to reduced compression efficiency in the intercooled cycle. On the other hand,

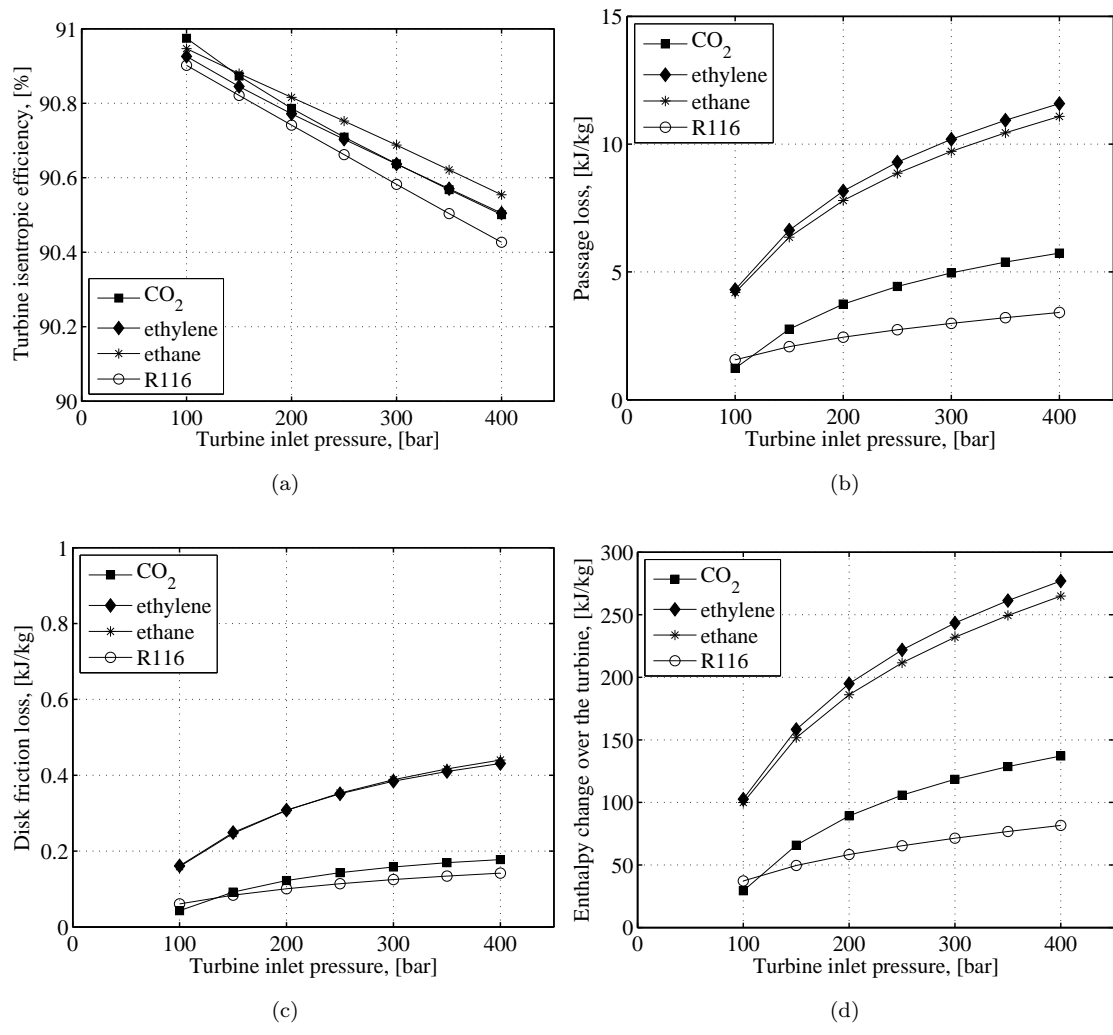


Figure 16: Predicted turbine efficiency (a), passage loss (b), disk friction loss (c), and enthalpy change over the turbine (d).

509 the blade height at compressor wheel outlet is higher when compared to the simple cycle, that can reduce  
 510 the tip leakage losses. It should be noted as a general remark related to the compressor design, that if  
 511 the compressor inlet state is close to the critical point a fluid condensation can occur in the compressor  
 512 as the fluid is accelerated and this can cause erosion of the compressor wheel and reduce the compressor  
 513 performance as a result of additional losses[49]. Thus, the lowest compressor inlet temperatures that were  
 514 used in the study might cause problems related to flow condensation, and slightly higher compressor inlet  
 515 temperatures could be considered due to this reason.

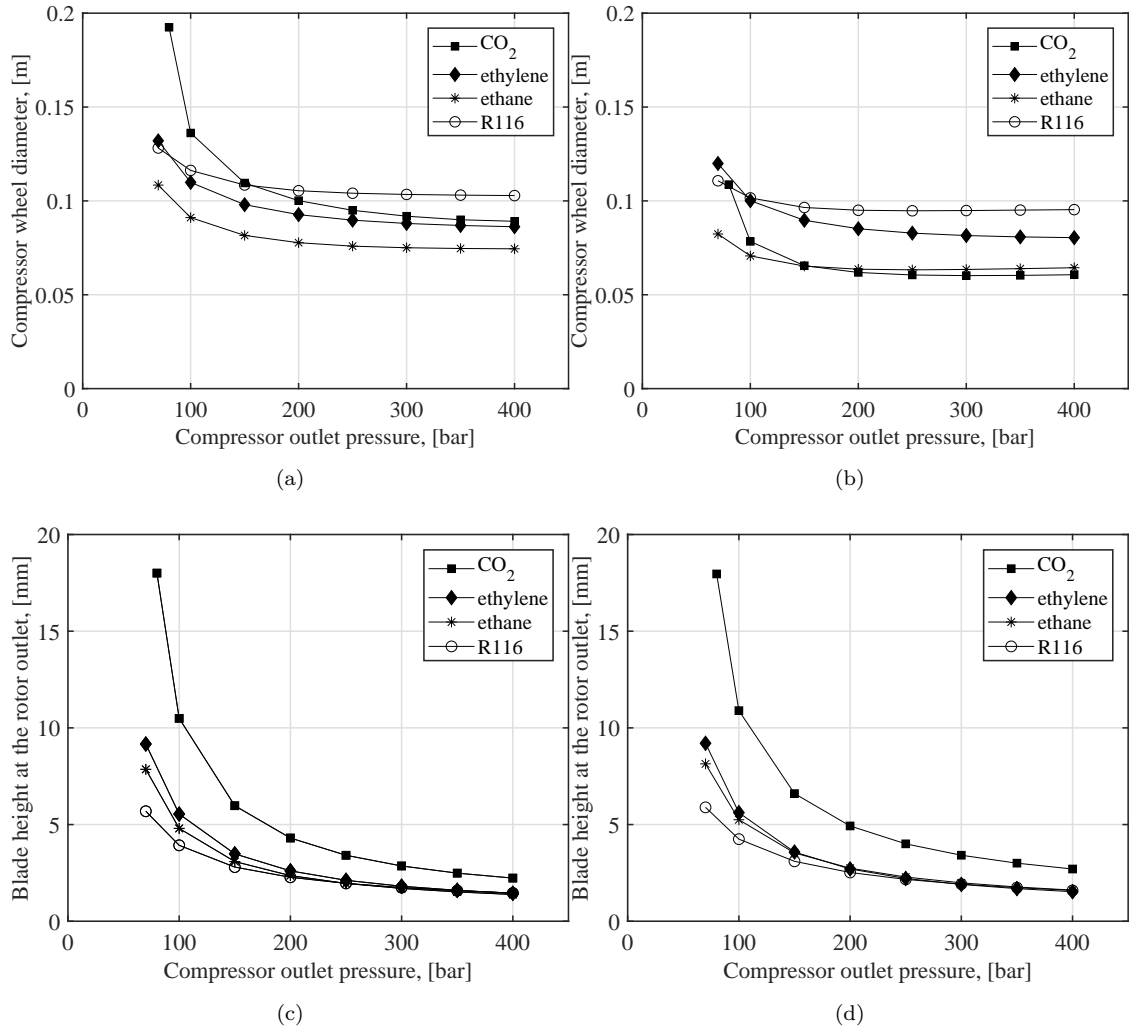


Figure 17: Compressor wheel diameter and blade height at the rotor outlet with different operation conditions and fluids. Results presented in (a) and (c) were obtained by using the higher CIT and (b) and (d) with the lower CIT.

## 516 5. Conclusions

517 The use of supercritical Brayton cycles for converting high temperature exhaust gas heat into electricity  
 518 was investigated with different working fluids and two cycle layouts. Based on this study, the use of super-  
 519 critical Brayton cycles can be considered as an attractive and efficient technological option for recovering  
 520 high temperature exhaust gas heat and for increasing the energy efficiency and reduce emissions in engine  
 521 power plants. The main conclusions drawn from the study are summarized as follows: • Supercritical Bray-  
 522 ton cycles recovering high temperature waste heat are capable for increasing energy efficiency of large scale  
 523 engines.

524 • CO<sub>2</sub> as the working fluid resulted in higher power outputs when compared to the other studied working



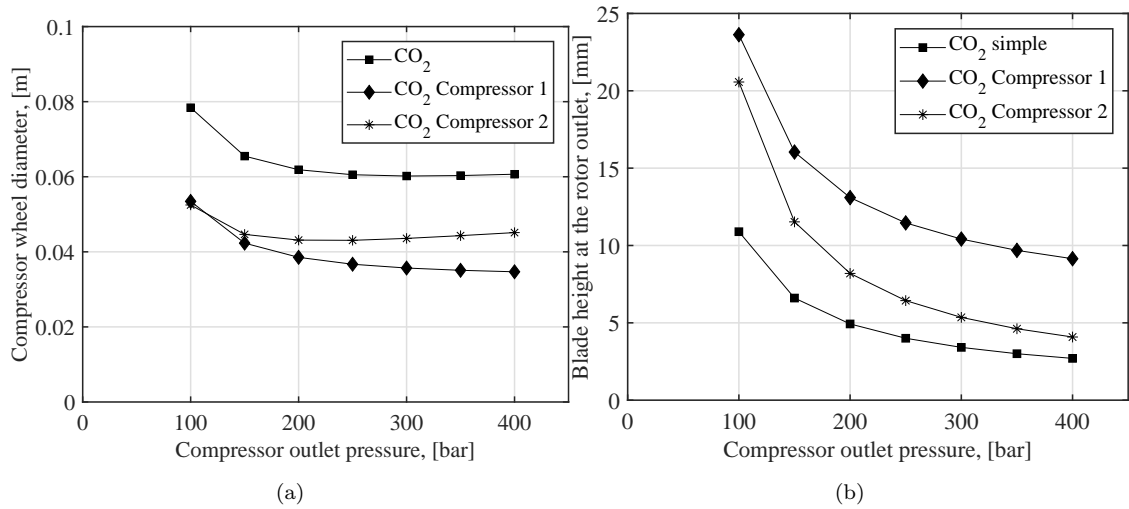


Figure 18: Comparison of compressor wheel diameter and blade height at the rotor outlet with simple and intercooled SBC. Results were obtained by using the lower CIT and CO<sub>2</sub> as the working fluid.

525 fluids. The maximum power output of 1759 kW was simulated by using intercooled cycle layout and low  
 526 compressor inlet temperatures. The simulated maximum power output corresponds to about 9,6 % of the  
 527 engine power output.

- 528 • The use of ethane resulted in the second highest performances and R116 represented the lowest perfor-  
 529 mance among the studied cases.
- 530 • The use of intercooled cycle resulted in higher power outputs when compared to the simple cycle. On the  
 531 other hand, the cycle with intercooling is more complex when compared to the simple cycle.
- 532 • To reach high cycle performance, the system turbomachines have to be capable to operate with high effi-  
 533 ciency and low compressor inlet temperature has to be used. Based on the detailed turbine design analysis,  
 534 high turbine efficiencies of over 90 % can be reached.
- 535 • The system turbomachinery has very small dimensions and requirements for significantly high rotational  
 536 speeds of tens of thousands rpm. As the turbine inlet pressure is increased, the optimal turbomachinery  
 537 rotational speed increase and the wheel dimensions decrease. In most of the studied cycle conditions, the  
 538 use of ethane resulted in smallest turbomachinery diameters and highest rotational speeds, while the use of  
 539 R116 resulted in the largest turbomachines and the lowest rotational speeds.
- 540 • The use of significantly high turbine inlet pressure in a range of 200 bar to 400 bar is required to reach  
 541 maximum thermodynamic performance. This sets special demands and challenges for the material strength  
 542 and sealing solutions for such a system.

543

544 It was concluded that if the system turbomachines can be operated with high efficiency and low com-

545 pressor inlet temperature can be used in the cycle, the power output is comparable to the high temperature  
546 ORC technology[4, 6]. In addition, this type of WHR system can be designed to be more compact when  
547 compared to ORC technology or conventional steam turbine cycles, especially when considering the size  
548 of the turbomachinery. This can be considered as a beneficial feature, especially in applications in where  
549 there is restricted space for the WHR system installation. The main drawbacks of the studied systems can  
550 be identified to be the significantly high pressure levels that sets special demands and challenges for the  
551 material strength and sealing solutions for such a system. In addition, the high rotational speeds and small  
552 dimensions of the turbomachinery disable the use of these WHR systems in rather low power output energy  
553 systems. In fact, despite that the analysis in this paper was carried out for relatively large engine having a  
554 power output of 18.3 MW, the design of reliable turbogenerators for this size systems can be challenging,  
555 especially due to the requirements for significantly high rotational speeds and extremely high power density.  
556 Thus, it was concluded that the studied WHR cycles have the greatest potential in large scale engine power  
557 plants in where the power output is in the range of tens of MW to hundreds of MW.

558 It should be noted that thermodynamics and fluid dynamics of non-conventional and supercritical flu-  
559 ids are not yet fully understood and investigated. It should be also noted that the loss correlations and  
560 turbomachinery design methods implemented in the analysis have been initially developed for turboma-  
561 chines operating with ideal gases. Thus, the accuracy when considering the turbomachinery design and  
562 loss prediction with supercritical fluid conditions can contain high uncertainties, even though the real gas  
563 fluid properties were used in the analysis and the results were in a good agreement in the validation when  
564 compared to the different turbomachinery designs available in the literature. The authors highlight the  
565 importance of more experimental work to be carried out in the future for increasing the understanding of  
566 the main loss mechanisms, heat transfer and fluid dynamics effects of supercritical fluids and to develop  
567 more accurate performance prediction methods for the turbomachinery of this type of power systems. It is  
568 also recommended to study more complex cycle architectures for increasing the WHR system performance  
569 and to study the compressor losses and heat exchanger design with different fluids in detail in the future.

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