Performances of Transcritical Power Cycles with CO₂-Based Mixtures for the Waste Heat Recovery of ICE

Jinghang Liu 1, Aofang Yu 1, Xinxing Lin 2, Wen Su 1,* and Shaoduan Ou 1

1 School of Energy Science and Engineering, Central South University, Changsha 410083, China; ljhupup@csu.edu.cn (J.L.); yuaf923@csu.edu.cn (A.Y.); shaoduan@csu.edu.cn (S.O.)
2 CTG (China Three Gorges Corporation) Science and Technology Research Institute, Beijing 100038, China; lin_xinxing@ctg.com.cn
* Correspondence: suwenznsu@csu.edu.cn

Abstract: In the waste heat recovery of the internal combustion engine (ICE), the transcritical CO₂ power cycle still faces the high operation pressure and difficulty in condensation. To overcome these challenges, CO₂ is mixed with organic fluids to form zeotropic mixtures. Thus, in this work, five organic fluids, namely R290, R600a, R600, R601a, and R601, are mixed with CO₂. Mixture performance in the waste heat recovery of ICE is evaluated, based on two transcritical power cycles, namely the recuperative cycle and split cycle. The results show that the split cycle always has better performance than the recuperative cycle. Under design conditions, CO₂/R290(0.3/0.7) has the best performance in the split cycle. The corresponding net work and cycle efficiency are respectively 21.05 kW and 20.44%. Furthermore, effects of key parameters such as turbine inlet temperature, turbine inlet pressure, and split ratio on the cycle performance are studied. With the increase of turbine inlet temperature, the net works of the recuperative cycle and split cycle firstly increase and then decrease. There exist peak values of net work in both cycles. Meanwhile, the net work of the split cycle firstly increases and then decreases with the increase of the split ratio. Thereafter, with the target of maximizing net work, these key parameters are optimized at different mass fractions of CO₂. The optimization results show that CO₂/R600 obtains the highest net work of 27.43 kW at the CO₂ mass fraction 0.9 in the split cycle.

Keywords: CO₂-based mixtures; transcritical power cycles; waste heat recovery; thermodynamic analysis

1. Introduction

1.1. Background

Recently, with the rapid development of economy, the demand for energy in various industries has exploded. Although there exist many types of energy sources, such as fossil energy, solar energy, and geothermal energy, fossil energy is still dominant. So far, CO₂ produced by fossil fuel combustion has caused serious global warming, which attracts the attention of all countries in the world. Thus, it is urgent to improve the utilization efficiency of fossil fuel. As one of the major application fields of fossil fuel combustion, internal combustion engines (ICEs) consume a large amount of fossil oil every year. However, only 30–40% of the energy is converted into useful work [1], and a large amount of fuel heat is released through the exhaust gas and coolant of the vehicle. In general, the waste gas temperature of ICE can be up to 400–700 °C and the temperature of engine coolant is about 80–90 °C. Therefore, the recovery of high temperature exhaust heat can greatly improve the ICE efficiency and reduce fuel consumption. So far, various thermodynamic cycles have been proposed for efficiently recovering waste heat from ICE. Among these proposed cycles, the most representative technology is the organic Rankine cycle (ORC) [2–4], which has the advantages of simple structure and easy maintenance.
1.2. ORC

So far, there are many published pieces of literature to investigate the ORC application in ICE experimentally and theoretically. For example, with the aim to improve the ICE efficiency, Zhao et al. [5] applied ORC to recover the exhaust heat. The theoretical results indicated that the ICE output power increases by 4.13 kW. Uusitalo et al. [6] examined experimentally the influences of small-scale high-temperature ORC on the performance under different operating conditions. The experimental results showed that the maximum cycle power output is 6 kW with the turbine operating in the rotational speed range of 12,000 rpm–31,000 rpm. Furthermore, Tian et al. [7] proposed a novel ORC system and analyzed 20 working fluids’ thermo-economic performance. The results indicated that R141b, R123, and R245fa not only have the largest cycle efficiency and net work, but also possess the lowest electricity production cost. In addition to the commonly used subcritical ORC, the transcritical ORC is also considered in the ICE waste heat recovery. Being different from the subcritical ORC, the transcritical ORC makes the working fluid absorb heat at a supercritical state. For instance, Mohammadkhani et al. [8] applied a transcritical two-loop ORC to utilize the waste heat from ICE. Toluene and R143a were considered as working fluids. The simulation results showed that the system net power is 24.93 kW, and the specific investment cost is 4361$/kW. Based on the existing published literatures, Wang et al. [9] comprehensively reviewed the technology to recover the waste heat from ICE, and provided different methods of system design to improve efficiency. From the simulation results, they found that the heat recovery system can increase powertrain efficiency by 30% under specific operating conditions. However, although many researches on ORC have been conducted to recover the ICE waste heat in the last decade, the employed organic fluids are usually flammable, toxic, or of high global warming potential (GWP). In addition, at high temperatures, organic fluids are easily decomposed, thus greatly limiting the ORC efficiency improvement in the waste heat recovery of ICE.

1.3. Transcritical Power Cycle with CO₂

To address the above issues, many scholars have used CO₂ to replace the organic fluid in the field of waste heat recovery. Compared with the organic fluid, CO₂ has low GWP and exhibits high stability, with being non-flammable and non-toxic. Furthermore, because of the low critical temperature (31.1 °C), CO₂ is preferred to be applied in the transcritical Rankine cycle to recover the ICE waste heat. Compared to the ORC, the CO₂ power cycle has obvious advantages: (1) the high density of supercritical CO₂ state can greatly improve the compactness of heat exchangers, thus resulting in a smaller system footprint [10]; (2) the CO₂ power cycle can be started up quickly, and has a fast response speed [11]. This cycle is more suitable to recover the ICE waste heat. In view of these advantages, extensive research has yet been carried out to investigate the CO₂ power cycle performance in the waste heat recovery. For instance, Shi et al. [12] established an experimental system of the transcritical CO₂ power cycle to recover the diesel engines waste heat. The effects of the pressure ratio, engine speed, and pump speed on system performance were experimentally conducted. The experimental results indicated that the net work (2.05 kW) can be expected to be obtained with 1300 rpm of engine and 80 rpm of pump, and the expected thermal efficiency is 4.3% with 1300 rpm of engine and 70 rpm of pump. Li et al. [13] investigated a transcritical CO₂ power cycle with a preheater and recuperator to recover the engine waste heat, and analyzed in detail the temperature disturbance during the heating process. The results illustrated that the reduction of temperature interference can increase the cycle thermal efficiency. Meanwhile, the optimized net work increases from 14.7 kW to 19.0 kW. In addition, a transcritical CO₂ cycle test to recover low-grade waste heat was developed by Li et al. [14]. The effect of working fluid mass flow on the system performance was investigated. It was found that with the increase of working fluid mass flow, the overall system pressure increases and output power decreases. In terms of the performance comparison between CO₂ and organic fluid, Baik et al. [15] optimized the net works of transcritical CO₂ and R125 cycles to recover the low-grade heat. The results showed that
R125 performs better, with 14% higher power than CO\textsubscript{2}. Moreover, the advantage of fast response of the transcritical CO\textsubscript{2} power cycle has been studied in relevant literature\cite{16}. It was found that the response speed of a simple CO\textsubscript{2} cycle is four times faster than that of R123 cycle.

1.4. Transcritical Power Cycle with CO\textsubscript{2}-Based Mixture

For the engineering application of the transcritical CO\textsubscript{2} power cycle, there still exist many challenges. For example, due to the fact that the CO\textsubscript{2} critical temperature approaches the ambient temperature, it is very difficult to effectively condense CO\textsubscript{2} by cooling water or air, especially in the waste heat recovery of ICE. In addition, the CO\textsubscript{2} cycle pressure is relatively high, thus resulting into a high manufacturing cost and a great safety risk during the practical application. To solve the above issues effectively, CO\textsubscript{2} is proposed to mix with the organic fluid, thus forming the CO\textsubscript{2}-based mixture\cite{17}. In comparison with the pure CO\textsubscript{2}, the CO\textsubscript{2}-based mixture can increase the critical temperature to extend the condensation temperature scope of the transcritical system. Meanwhile, at the same bubble temperature, the CO\textsubscript{2}-based mixture has a lower condensation pressure than CO\textsubscript{2}. Furthermore, the mixture has advantages over the organic fluids in the aspect of safety. The relevant study\cite{18} has shown that the added CO\textsubscript{2} can effectively reduce the organic fluid flammability. By conducting experiments on the flammability limit, it was found that when the CO\textsubscript{2} molar fraction is larger than 0.3, CO\textsubscript{2}/R290 is non-flammable\cite{19}. Therefore, the researches on the transcritical cycle performance of CO\textsubscript{2}-based mixtures have aroused the interest of many scholars. For instance, Dai et al.\cite{20} applied a transcritical cycle with CO\textsubscript{2}-based mixtures to convert low-grade heat. It was found that the cycle thermal efficiency is maximized when the carbon dioxide mass fraction is about 0.5. Aiming at the geothermal water with 100--150\degree C, Wu et al.\cite{21} applied CO\textsubscript{2}-based mixtures into a transcritical cycle to produce power. Six refrigerants (R152, R161, R290, R1234yf, R1234ze, R1270) were selected to be mixed with CO\textsubscript{2}. The results revealed that the best thermo-economic performance of CO\textsubscript{2}/R161(0.3/0.7) is achieved when the CO\textsubscript{2} molar fraction is 0.3. When the condensation temperature is 10--20\degree C, the net work of CO\textsubscript{2}/R161(0.3/0.7) is increased by 14.43--50.46\% over that of pure CO\textsubscript{2}. For the utilization of low-grade heat, Chen et al.\cite{22} implemented a thermodynamic analysis on the transcritical cycle using CO\textsubscript{2}/R32 as a working fluid. The analysis results showed that CO\textsubscript{2}/R32 can achieve high thermal efficiency of 12.6--18.7\%. In terms of ICE waste heat recovery, Shu et al.\cite{23} conducted the transcritical power cycle on the waste heat recovery of ICE, based on the CO\textsubscript{2} mixture. In this cycle, a preheater and a recuperator were employed. The corresponding cycle performance of various mixtures were investigated. The results showed that CO\textsubscript{2}/R32(0.3/0.7) has the largest output work among the considered mixtures, when the condensation temperature is below 40\degree C. As for the heat transfer area, the cycle with CO\textsubscript{2}/R32(0.3/0.7) has a lower value than that of CO\textsubscript{2} cycle. Meanwhile, Shu et al.\cite{24} also studied the transcritical cycle dynamic performance with CO\textsubscript{2}-based mixtures to recover waste heat from the truck engine. It was found that as the CO\textsubscript{2} fraction increases, the system responds faster. On this basis, many scholars further studied the control strategy for the transcritical power cycle with CO\textsubscript{2}-based mixtures. Aiming at the waste heat recovery of heavy-duty diesel engines, Wang et al.\cite{25} adopted three control strategies (constant temperature, constant pressure, and optimal control strategies) to reach system stability. From the simulated results, it was found that under varying conditions of ICE, the system stability with optimal control or constant pressure control is better than that with constant temperature control. With the optimal control strategy, the system can output the highest net work.

1.5. Purpose of This Work

From the existing literatures, it can be found that only a few studies have compared the performance of different CO\textsubscript{2}-based mixtures in cycles with relatively simple structures. However, with the development of advanced cycles, for the utilization of CO\textsubscript{2}-based mixtures in the ICE waste heat recovery, additional studies are needed to further com-
pare the various CO\textsubscript{2}-based mixtures’ performance in advanced cycles. Furthermore, aiming at the condensation of the transcritical cycle to recover the ICE waste heat, most researchers \cite{24,26} just fix the condensation temperature at 20–35 °C to conduct a performance analysis. However, considering the ambient temperature, this temperature range is difficult to achieve in the mobile engine. In fact, the condensation temperature is strongly dependent on the used condensation method \cite{27}. In total, there are three methods to condense the fluid in the waste heat recovery of ICE. (1) A separate low-temperature cooling package is employed to achieve condensation. In this case, the condensation temperature of working fluid can be low to 30 °C. (2) The working fluid is condensed by the intermediate medium. The corresponding condensation temperature can range from 50 °C to 70 °C. (3) The engine coolant is employed as the heat sink of cycle. Thus, the condensation temperature can be up to 90 °C.

Aiming at the deficiencies of the existing researches, this study employs two transcritical power cycles and applies five CO\textsubscript{2}-based mixtures to recover the waste heat from ICE. The considered cycles include the recuperative cycle and the split cycle. Compared with the recuperative cycle, the split cycle can deeply recover the high-temperature waste heat. As for the CO\textsubscript{2} mixtures, five organic fluids, namely R290, R600a, R600, R601a, and R601, are selected to mix with CO\textsubscript{2}. In addition to the performance comparison of these mixtures in the two cycles, the effects of turbine inlet temperature (T\textsubscript{3}), turbine inlet pressure (P\textsubscript{h}), condensation temperature (T\textsubscript{1}), and mass fraction of CO\textsubscript{2} on system performance are discussed. On this basis, the split ratio (SR), T\textsubscript{3}, and P\textsubscript{h} are simultaneously optimized using the genetic algorithm (GA) with the objective of maximizing net work (W\textsubscript{net}).

2. Cycle Layout

In this study, two transcritical cycles, namely the recuperative cycle and split cycle, are considered. The corresponding layouts are respectively shown in Figures 1 and 2. It can be observed that besides the four basic components (working fluid pump, heater, turbine, and condenser), a recuperator is added at the pump outlet to recover the energy of the outlet fluid from the turbine in the recuperative cycle. This happens so that the cycle efficiency (\(\eta_{\text{th}}\)) and exergy efficiency (\(\eta_{\text{ex}}\)) can be increased. For the recuperative cycle, the detailed process description can be referred to in these pieces of literature \cite{28,29}. The corresponding T-s diagram is provided in Figure 3 under design conditions. Figure 3 shows that the exhaust gas outlet temperature is still as high as 253 °C. This is because there exists a large amount of recuperative heat, thus resulting in a high temperature of the working fluid entering the heater.

![Figure 1. Systematic diagram of the recuperative cycle.](image-url)
As for the split cycle, Heater 2 is added at the outlet of Heater 1 to further extract the waste heat. After being compressed in the pump, the flow is separated into two streams. One stream enters into the recuperator to conduct a heat exchange with the high-temperature fluid at the turbine outlet. Another enters Heater 2 to recover the waste heat. After being compressed in the pump, the flow is separated into two streams. One stream enters into the recuperator to conduct a heat exchange with the high-temperature fluid at the turbine outlet. Another enters Heater 2 to recover the waste heat. Thereafter, two flows are mixed at the inlet of Heater 1 to continue absorbing exhaust gas heat. The remaining processes of this cycle are similar to those of the recuperative cycle.

Figure 4 presents the corresponding T-s diagram of the split cycle under design conditions.
For the ICE, a turbocharged technology is used, and a six-cylinder engine is considered to produce waste gas. The inhaled fresh air is firstly compressed and exchanges heat with the jacket water, and then enters the cylinder to mix with the gasoline. After combustion, the generated waste gas is exhausted. The discharged gas enters the turbine to provide work for the air compressor. As shown in Figures 1 and 2, the working fluid of the power cycle is directly condensed by the air, to get the lowest condensation temperature. As for the other two condensation methods, the readers can refer to the literature [27].

3. Thermodynamic Modeling and Optimization
3.1. Thermodynamic Modeling

To compare the thermodynamic performance of CO\(_2\) mixtures in the considered two cycles, mathematical models are established. Before giving the used equations, the following assumptions are applied to simplify the modeling.

1. Without considering the variation of the system kinetic and potential energy;
2. The system operates stably and without considering the heat loss and pressure drop of pipes and components;
3. The counter-flow heat exchanger is considered in the simulation;
4. The compression and expansion processes are characterized by isentropic efficiencies.

According to the above assumptions, energy equations of each component are listed in Table 1 for the two cycles.

### Table 1. Energy equation of each component for the recuperative cycle and the split cycle.

| Components   | Recuperative Cycle | Split Cycle |
|--------------|--------------------|-------------|
| Pump         | \( W_p = m_f(h_2 - h_1) = m_f(h_{2s} - h_1)/\eta_p \) |             |
| Turbine      | \( W_t = m_f(h_3 - h_4) = m_f(h_3 - h_{4s})/\eta_t \) |             |
| Condenser    | \( Q_{\text{con}} = m_f(h_{4i} - h_1) \) |             |
| Heater1      | \( Q_{\text{Heater1}} = m_f(h_3 - h_{2i}) = m_g C_{p,g} (T_{g,in} - T_{g,mid}) \) |             |
| Recuperator  | \( Q_{\text{Re}} = m_f(h_4 - h_{4s}) \) |             |
| Heater2      | —                  | \( Q_{\text{Heater2}} = m_f(1 - SR)(h_6 - h_5) \) |
The corresponding net work and cycle efficiency are calculated by:

\[ W_{\text{net}} = W_t - W_P \] (1)

\[ \eta_{\text{th}} = \begin{cases} \frac{W_{\text{net}}}{Q_{\text{Heater}}}, & \text{Recuperative cycle} \\ \frac{W_{\text{net}}}{Q_{\text{Heater}} + Q_{\text{Heater2}}}, & \text{Split cycle} \end{cases} \] (2)

In addition to the cycle efficiency, the waste heat recovery efficiency \( \eta_r \) can be expressed as below:

\[ \eta_r = \begin{cases} \frac{Q_{\text{Heater}}}{m_f(h_{\text{g,in}} - h_g(T_0))}, & \text{Recuperative cycle} \\ \frac{Q_{\text{Heater}} + Q_{\text{Heater2}}}{m_f(h_{\text{g,in}} - h_g(T_0))}, & \text{Split cycle} \end{cases} \] (3)

Before establishing the exergy equations, the specific exergy value at each steady point \( (i) \) is calculated as \([30,31]\):

\[ e_i = (h_i - h_0) - T_0(s_i - s_0) \] (4)

where the ambient temperature \( (T_0) \) is set to be 298.15 K.

The exergy destruction \([30,31]\) of each component is presented in Table 2.

| Components | Recuperative Cycle | Split Cycle |
|------------|--------------------|-------------|
| Pump       | \( I_p = m_i(e_1 - e_2) + W_P \) | \( - \) |
| Turbine    | \( h = m_i(e_3 - e_4) - W_t \) | \( - \) |
| Condenser  | \( l_{\text{con}} = m_i(e_4 - e_1) - Q_{\text{con}}[1 - T_0/(T_{\text{average}} - 5)] \) | \( - \) |
| Heater1    | \( h_{\text{Heater1}} = m_i(e_2 - e_3) + E_{g,\text{in}} - E_{g,\text{mid}} \) | \( - \) |
| Recuperator| \( I_{\text{Re}} = m_i(e_2 - e_2 + e_4 - e_4) \) | \( I_{\text{Heater2}} = m_i(1 - SR)(e_5 - e_6) + E_{g,\text{mid}} - E_{g,\text{out}} \) |
| Heater2    | \( - \) | \( - \) |

In Table 2, \( T_{\text{average}} - 5 \) is the average temperature of the cooling medium. As for the exergy efficiency, it can be obtained by:

\[ \eta_{\text{ex}} = \begin{cases} \frac{W_{\text{net}}}{E_{g,\text{in}} - E_{g,\text{mid}}}, & \text{Recuperative cycle} \\ \frac{W_{\text{net}}}{E_{g,\text{in}} - E_{g,\text{out}}}, & \text{Split cycle} \end{cases} \] (5)

Based on the listed equations, the MATLAB platform is used for code development. The calculation flows for recuperative and split cycles are respectively given in Figures 5 and 6.
Calculation of turbine
Assume $T_4$
$h_2 = h_2 + (h_4 - h_4)$

Waste gas: $m_g, T_g, m_{in}$
Cycle: $T_3, T_1, P_h$
Coefficient: $\eta_t, \eta_p$

Calculation of pump

Yes
No

PPTD in recuperator $-15^\circ C < \Delta$

Calculation of Heater1
Calculation of condenser

Net work, parameters of states points, cycle parameters, etc

Figure 5. Thermodynamic calculation routine of the recuperative cycle.
3.2. GA Optimization

In this study, the system parameters of the two cycles are optimized by GA, due to its simplicity, versatility, and suitability for parallel processing [30,31]. Under the given ICE gas conditions, the maximum $W_{net}$ is considered as the optimization objective. For the
recuperative cycle, $T_3$ and $P_h$ are the optimization cycle variables. However, for the split cycle, $SR$ is added as the third variable for performance optimization. Figure 7 gives the flowchart of the GA. The GA encodes the randomly generated chromosomes of the initial population firstly. Then the chromosome is decoded to obtain the corresponding system parameters. According to these parameters, thermodynamic calculations are conducted. The fitness function for each chromosome corresponds to the output work. Afterwards, the temperature differences in recuperator and heaters are checked to guarantee the fact that the calculated temperature difference meets the required minimum value. If not, all chromosomes will be replaced by the next population, which are propagated by choice, intersection, and mutation operators. Thereafter, $W_{net}$ is obtained by recalculating the new generation. The optimization will finish when the genetic calculation is iterated to the maximum number of generations. Finally, the optimal parameters in the final population are substituted into the thermodynamic calculations to obtain the system efficiency and other parameters. In addition, the population size is programmed to 100 and the maximum number of generations is stated as 80.

Figure 7. Flow diagram of GA for the system parameter optimization.

4. Cycle conditions and Organic Fluid Selections

The working conditions of a six-cylinder engine are enumerated in Table 3. The outlet temperature and mass flow rate of the exhaust gas are 466 °C and 0.278 kg/s, respectively [23]. As for the gas components, due to the low contents of nitrogen oxides
and sulfides, only \( \text{CO}_2 \), \( \text{O}_2 \), \( \text{H}_2\text{O} \), and \( \text{N}_2 \) are considered. The corresponding mass fractions are 9.1\%, 9.3\%, 7.4\%, and 74.2\%, respectively.

### Table 3. Main parameters and exhaust gas components of ICE.

| Parameters                          | Values | Exhaust Gas Components | Values |
|-------------------------------------|--------|------------------------|--------|
| Fuel combustion energy (kW)         | 561.61 | \( \text{CO}_2 \) (%)  | 9.1    |
| Rated power (kW)                    | 236.50 | \( \text{O}_2 \) (%)   | 9.3    |
| Rated speed (rpm)                   | 1694   | \( \text{H}_2\text{O} \) (%) | 7.4    |
| Rated torque (N-m)                  | 1333   | \( \text{N}_2 \) (%)   | 74.2   |
| Temperature of exhaust gas (\(^\circ\)C) | 466    |                        |        |
| Mass flow of exhaust gas (kg/s)     | 0.278  |                        |        |
| Exhaust gas pressure (MPa)          | 0.10   |                        |        |

The \( \text{CO}_2 \)-based mixture is formed by \( \text{CO}_2 \) and an organic fluid. The mixture properties are strongly dependent on the selection of the organic fluid. Thus, selecting a suitable fluid is crucial to obtain a better cycle performance of the \( \text{CO}_2 \)-based mixture. In general, environmental properties have to be considered in the fluid selection. The selected fluid should be non-toxic, non-corrosiveness and stability, and have zero ozone depletion potential (ODP) and a GWP less than 150 [32].

Considering that the flue gas temperature is as high as 466 \(^\circ\)C, the traditional refrigerant is easy to decompose, so a high temperature working fluid is selected. Based on the above standards, five kinds of organic working fluids, namely R600, R600a, R601, R601a, and R290, are selected from the organic fluid library [33]. The physical parameters of these organic working fluids and \( \text{CO}_2 \) are summarized in Table 4.

### Table 4. Thermodynamic properties of the selected working fluids.

| Fluids | Molecular Mass (g/mol) | \( T_b \) (\(^\circ\)C) | \( T_c \) (\(^\circ\)C) | \( P_c \) (MPa) |
|--------|------------------------|-------------------------|-------------------------|-----------------|
| \( \text{CO}_2 \) | 44.01                  | -78.4                   | 31.1                    | 7.38            |
| R290   | 44.1                   | -42.1                   | 96.7                    | 4.25            |
| R600a  | 58.12                  | -11.7                   | 134.7                   | 3.63            |
| R600   | 58.12                  | -0.5                    | 152.0                   | 3.80            |
| R601a  | 72.15                  | 27.83                   | 187.2                   | 3.38            |
| R601   | 72.15                  | 36.06                   | 196.55                  | 3.37            |

Figure 8 shows the critical temperatures of five mixtures at different \( \text{CO}_2 \) fractions. It is found that the critical temperature decreases with the increase of the \( \text{CO}_2 \) mass fraction. At the same \( \text{CO}_2 \) fraction, the critical temperatures of five mixtures satisfy the order: R601 > R601a > R600 > R600a > R290. As for the critical pressure, Figure 9 presents the variations of these mixtures. The critical pressure firstly increases and then decreases with the increase of the \( \text{CO}_2 \) mass fraction. When the \( \text{CO}_2 \) fraction is larger than 0.2, the critical pressure satisfies the order: R601 > R601a > R600 > R600a > R290. In addition, it should be mentioned that the selected organic fluid is flammable. However, when \( \text{CO}_2 \) is used as an addition to mix with the organic fluid, the flammability will be decreased with the increase of the \( \text{CO}_2 \) fraction. According to Zabetakis’s research [19], at a \( \text{CO}_2 \) mass fraction larger than 0.3, the mixture has exceeded the combustible range of R290. Although no similar data is available for other working fluids, the flammability of these five organic fluids is similar. Thus, in this study, it is thought that the five \( \text{CO}_2 \)-based mixtures are non-flammable, when the \( \text{CO}_2 \) mass fraction is no less than 0.3.
Figure 8. Critical temperature of mixtures under different mass fractions of CO$_2$.

Figure 9. Critical pressure of mixtures under different mass fractions of CO$_2$.

Figure 10 illustrates the temperature glide variation trend with CO$_2$ mass fractions at the bubble temperature of 30 °C. It is obvious that when the CO$_2$ mass fraction increases, the temperature glide of mixture first increases and then decreases. Among the considered mixtures, CO$_2$/R290 has the lowest temperature glide, while CO$_2$/R601 has the largest value. Moreover, when the CO$_2$ mass fraction is around 0.3, temperature glides of these five mixtures reach the maximum value.
In addition to the employed CO$_2$-based mixtures, standard design conditions are also required for the thermodynamic analysis of these two transcritical systems. As listed in Table 5, in the thermodynamic calculation, $T_3$, $T_3$, and $P_h$ are set to be 30 °C, 375 °C, and 13 MPa, respectively. For the split cycle, $SR$ is assumed to be 0.7 under the basic design condition. Furthermore, isentropic efficiencies of turbine ($\eta_t$) and pump ($\eta_p$) are set to 0.7 and 0.8, respectively. Pinch point temperature differences (PPTDs) of the recuperator, Heater1, and Heater2 are all set at 15 °C. Meanwhile, to reduce the mixture flammability, the CO$_2$ mass fraction is set at 0.3.

Table 5. Standard design conditions of the two transcritical systems.

| Design Parameters                          | Set Value | Range of Variation |
|--------------------------------------------|-----------|--------------------|
| Condensation bubble temperature (°C)       | 30        | 30–90              |
| Turbine inlet temperature (°C)             | 375       | 270–390            |
| Turbine inlet pressure (MPa)               | 13        | 8.5–20             |
| Ambient temperature (°C)                   | 25        | —                  |
| Ambient pressure (MPa)                     | 0.1       | —                  |
| PPTD in Heater1 (°C)                       | 15        | —                  |
| PPTD in Heater2 (°C)                       | 15        | —                  |
| PPTD in recuperator (°C)                   | 15        | —                  |
| Pump efficiency                            | 0.8       | —                  |
| Turbine efficiency                         | 0.7       | —                  |
| Split ratio                                | 0.7       | 0–1                |
| Mass fraction of CO$_2$                    | 0.3       | 0.3–1              |

To further study the thermodynamic performance of the two cycles, sensitivity analyses are conducted on $T_3$, $P_h$, and $T_1$. Meanwhile, the effect of $SR$ on the performance of the split cycle is also discussed. As listed in Table 5, $T_3$ varies from 270 °C to 390 °C at an interval of 5 °C and $P_h$ changes from 8.5 MPa to 20 MPa. In addition, the considered range of $T_1$ is 30–90 °C. In the split cycle, $SR$ varies from 0 to 1. After that, system parameters are optimized at various CO$_2$ mass fractions (0.3–1) for the two cycles.

5. Results and Discussion

According to the conditions provided in Table 5, the recuperative cycle and the split cycle performance are derived from the established models. A synthesis of these two systems’
performances from the perspective of energy and exergy is compared. Furthermore, the effects of $T_3$, $P_h$, $T_1$, and $SR$ on the system performance are analyzed. On this basis, these parameters of the recuperative cycle and the split cycle are optimized with the maximum $W_{net}$ as the objective. Furthermore, at different CO$_2$ mass fractions, performance of these two cycles are optimized and compared. The detailed results and discussions are presented in the following subsections.

5.1. Cycle Analysis and Performance Comparison

Under set operating conditions, mixture characteristics at various state points are achieved for the recuperative and the split cycle, as listed in Tables A1 and A2 of the Appendix A for CO$_2$/R290(0.3/0.7). The corresponding T-s diagrams for the recuperative cycle and the split cycle are respectively presented in Figures 3 and 4. Based on these state properties, energy performance of five CO$_2$-based mixtures in the recuperative cycle and the split cycle are sequentially provided in Tables 6 and 7. From Table 6, it is observed that CO$_2$/R290(0.3/0.7) has the lowest turbine outlet pressure 2.88 MPa. While the highest $W_{net}$ is achieved by CO$_2$/R290(0.3/0.7) and the lowest $W_{net}$ is obtained by CO$_2$/R601(0.3/0.7). In terms of $\eta_{th}$, CO$_2$/R290(0.3/0.7) has the highest 23.74%, followed by CO$_2$/R600a(0.3/0.7), CO$_2$/R600(0.3/0.7), CO$_2$/R601a(0.3/0.7) and CO$_2$/R601(0.3/0.7). Thus, overall, CO$_2$/R290 (0.3/0.7) has the best thermodynamic performance.

Table 6. Energy performance of five mixtures in the recuperative cycle under design conditions.

| Parameters                      | CO$_2$/R290 | CO$_2$/R601a | CO$_2$/R601 | CO$_2$/R600a | CO$_2$/R600 |
|---------------------------------|-------------|--------------|-------------|--------------|-------------|
| Mass fraction of CO$_2$         | 0.3         | 0.3          | 0.3         | 0.3          | 0.3         |
| $T_{mid}$ (°C)                  | 253.35      | 283.34       | 283.92      | 269.16       | 272.39      |
| $P_l$ (MPa)                     | 3.27        | 2.95         | 3.06        | 2.88         | 3.00        |
| $m_f$ (kg/s)                    | 0.19        | 0.20         | 0.20        | 0.20         | 0.20        |
| $Q_{Heater1}$ (kW)              | 67.86       | 58.51        | 58.33       | 62.94        | 61.93       |
| $Q_{Re}$ (kW)                   | 109.07      | 125.86       | 127.40      | 116.08       | 118.54      |
| $W_t$ (kW)                      | 20.45       | 16.34        | 15.68       | 18.76        | 18.16       |
| $W_p$ (kW)                      | 4.34        | 3.89         | 3.69        | 4.21         | 4.28        |
| $W_{net}$ (kW)                  | 16.11       | 12.45        | 11.99       | 14.55        | 13.89       |
| $\eta_{th}$ (%)                 | 23.74       | 21.28        | 20.55       | 23.12        | 22.42       |
| $\eta_r$ (%)                    | 38.82       | 33.46        | 33.36       | 36.00        | 35.42       |

Table 7. Energy performance of five mixtures in the split cycle under design conditions.

| Parameters                      | CO$_2$/R290 | CO$_2$/R601a | CO$_2$/R601 | CO$_2$/R600a | CO$_2$/R600 |
|---------------------------------|-------------|--------------|-------------|--------------|-------------|
| Mass fraction of CO$_2$         | 0.3         | 0.3          | 0.3         | 0.3          | 0.3         |
| $T_{out}$ (°C)                  | 139.00      | 143.29       | 141.22      | 143.00       | 143.50      |
| $T_{mid}$ (°C)                  | 316.68      | 323.12       | 323.25      | 319.67       | 319.05      |
| $P_l$ (MPa)                     | 3.27        | 2.95         | 3.06        | 2.88         | 3.00        |
| $m_f$ (kg/s)                    | 0.25        | 0.25         | 0.25        | 0.25         | 0.25        |
| $Q_{Heater1}$ (kW)              | 48.03       | 45.99        | 45.95       | 47.08        | 47.28       |
| $Q_{Heater2}$ (kW)              | 54.95       | 55.68        | 56.35       | 54.68        | 54.33       |
| $Q_{Re}$ (kW)                   | 128.22      | 129.92       | 131.49      | 127.59       | 126.77      |
| $W_t$ (kW)                      | 26.72       | 20.53        | 19.74       | 24.04        | 22.99       |
| $W_p$ (kW)                      | 5.67        | 4.89         | 4.65        | 5.39         | 5.41        |
| $W_{net}$ (kW)                  | 21.05       | 15.64        | 15.09       | 18.65        | 17.57       |
| $\eta_{th}$ (%)                 | 20.44       | 15.38        | 14.75       | 18.32        | 17.29       |
| $\eta_r$ (%)                    | 58.90       | 58.15        | 58.51       | 58.21        | 58.12       |

For the split cycle, $W_{net}$ and $\eta_{th}$ of CO$_2$/R290(0.3/0.7) are the highest, followed by CO$_2$/R600a(0.3/0.7), CO$_2$/R600(0.3/0.7), and CO$_2$/R601a(0.3/0.7). It should be noted that CO$_2$/R601(0.3/0.7) has the largest recuperated heat 131.49 kW, but the worst thermodynamic performance. In terms of thermodynamic performance, CO$_2$/R290(0.3/0.7) is still the first choice for the split cycle. In comparison to the recuperative cycle, the split cycle
possesses a higher $W_{\text{net}}$, as shown in Table 7. This phenomenon is attributed by a higher mass flow rate in the split cycle. Meanwhile, the exhaust gas outlet temperature of the split cycle is lower than that of the recuperative cycle. For the considered five mixtures, the exhaust gas outlet temperature of the recuperative cycle ranges from 253.35 $^\circ$C to 283.92 $^\circ$C, while the split cycle has a range of 139–143.5 $^\circ$C. It means that the introduction of Heater2 can deeply recover the heat from the exhaust gas for the split cycle. Thus, by constructing advanced cycle structures, the output work can be increased and fuel combustion of ICE can be reduced.

Tables 8 and 9 respectively gives the exergy parameters of five mixtures in the recuperative cycle and split cycle under design conditions. For the exergy performance of each component, it is obvious that in the recuperative cycle, the irreversibility of the recuperator is much larger than those of other components. However, in the split cycle, the largest irreversibility is obtained by the condenser, except CO$_2$/R290(0.3/0.7). As for the total irreversibility, compared with the recuperative cycle, the split cycle has a higher value, due to the addition of Heater2. For the considered five mixtures, the irreversibility of the split cycle ranges from 27.29 kW to 33.06 kW, while the recuperative cycle has a range of 18.9 kW–19.52 kW. In terms of $\eta_{\text{ex}}$, the value of the split cycle is lower than that of the recuperative cycle for each mixture. Among the five mixtures, CO$_2$/R290(0.3/0.7) has the largest efficiency in the two cycles. The corresponding values are 45.22% and 43.55%, respectively.

### Table 8. Exergy performance of five mixtures in the recuperative cycle under design conditions.

| Parameters          | CO$_2$/R290 | CO$_2$/R600a | CO$_2$/R600 | CO$_2$/R601a | CO$_2$/R601 |
|---------------------|-------------|--------------|-------------|--------------|-------------|
| Mass fraction of CO$_2$ | 0.3         | 0.3          | 0.3         | 0.3          | 0.3         |
| $I_{\text{Heater1}}$ (kW) | 2.80        | 2.55         | 2.50        | 2.33         | 2.33        |
| $I_t$ (kW)           | 4.50        | 4.10         | 3.98        | 3.54         | 3.40        |
| $I_{\text{Re}}$ (kW) | 7.91        | 6.90         | 6.82        | 7.30         | 7.66        |
| $I_{\text{con}}$ (kW) | 3.48        | 4.54         | 4.99        | 5.06         | 5.26        |
| $I_p$ (kW)           | 0.83        | 0.81         | 0.82        | 0.75         | 0.71        |
| $I_{\text{total}}$ (kW) | 19.52       | 18.90        | 19.11       | 18.98        | 19.36       |
| $\eta_{\text{ex}}$ (%) | 45.22       | 43.50        | 42.08       | 39.61        | 38.24       |

### Table 9. Exergy performance of five mixtures in the split cycle under design conditions.

| Parameters          | CO$_2$/R290 | CO$_2$/R600a | CO$_2$/R600 | CO$_2$/R601a | CO$_2$/R601 |
|---------------------|-------------|--------------|-------------|--------------|-------------|
| Mass fraction of CO$_2$ | 0.3         | 0.3          | 0.3         | 0.3          | 0.3         |
| $I_{\text{Heater1}}$ (kW) | 1.81        | 1.77         | 1.78        | 1.73         | 1.73        |
| $I_{\text{Heater2}}$ (kW) | 5.22        | 5.00         | 4.94        | 4.90         | 4.87        |
| $I_t$ (kW)           | 5.89        | 5.26         | 5.03        | 4.45         | 4.28        |
| $I_{\text{Re}}$ (kW) | 6.94        | 6.94         | 6.87        | 7.69         | 7.96        |
| $I_{\text{con}}$ (kW) | 6.35        | 9.35         | 10.73       | 12.63        | 13.33       |
| $I_p$ (kW)           | 1.08        | 1.03         | 1.04        | 0.94         | 0.90        |
| $I_{\text{total}}$ (kW) | 27.29       | 29.35        | 30.38       | 32.34        | 33.06       |
| $\eta_{\text{ex}}$ (%) | 43.55       | 38.85        | 36.65       | 32.60        | 31.34       |

### 5.2. Effects of Key System Parameters

#### 5.2.1. Effect of Turbine Inlet Temperature

Figure 11 illustrates the changes of $W_{\text{net}}$ with $T_3$ for the two cycles. The $T_3$ is investigated in the range of 270 $^\circ$C to 390 $^\circ$C. From Figure 11a, it is found that the $W_{\text{net}}$ of the recuperative cycle tends to increase and then decrease as $T_3$ increases. This phenomenon can be interpreted based on the fact that with the increase of $T_3$, the mass flow of mixtures gradually decreases. Under a lower $T_3$, the variation of $W_{\text{net}}$ is mainly affected by the enthalpy difference; while under a higher $T_3$, the change of $W_{\text{net}}$ depends on the mass flow rate. As for the considered five mixtures, CO$_2$/R290(0.3/0.7) has the largest $W_{\text{net}}$ in the recuperative cycle, followed by CO$_2$/R600a(0.3/0.7), CO$_2$/R600(0.3/0.7), CO$_2$/R601a(0.3/0.7) and
CO₂/R601(0.3/0.7). As for the split cycle, similar trends of these mixtures are observed, and $W_{\text{net}}$ satisfies the order: CO₂/R601(0.3/0.7) > CO₂/R601a(0.3/0.7) > CO₂/R600(0.3/0.7) > CO₂/R600a(0.3/0.7) > CO₂/R290(0.3/0.7). Meanwhile, for the same mixture, the split cycle has a larger $W_{\text{net}}$ than that of the recuperative cycle. Furthermore, in these two cycles, when the organic fluids are isomers, the corresponding CO₂ mixtures perform a similar performance, such as CO₂/R600a(0.3/0.7) and CO₂/R600(0.3/0.7).

**Figure 11.** Effect of turbine inlet temperature on net work: (a) recuperative cycle, (b) split cycle.

The variations of $\eta_{\text{th}}$ with $T_3$ are shown in Figure 12. The figure presents that $\eta_{\text{th}}$ naturally increases with the increase of $T_3$ in the two cycles. Although the $W_{\text{net}}$ of the split cycle is greater than that of the recuperative cycle, the split $\eta_{\text{th}}$ is significantly lower than that of the recuperative cycle. This is due to the fact that the added Heater2 absorbs more heat from the exhaust gas in the split cycle. Among the considered five mixtures, CO₂/R290(0.3/0.7) shows the best $\eta_{\text{th}}$, followed by CO₂/R600a(0.3/0.7), CO₂/R600(0.3/0.7), CO₂/R601a(0.3/0.7), and CO₂/R601(0.3/0.7). The effects of $T_3$ on $\eta_r$ are presented in Figure 13. It can be seen that the heat $\eta_r$ decreases as $T_3$ increases. Meanwhile, being different with efficiency curves of the recuperative cycle, the curves of the split cycle among the five mixtures are more closed with each other.

**Figure 12.** Effect of turbine inlet temperature on cycle efficiency: (a) recuperative cycle, (b) split cycle.
Figure 13. Effect of turbine inlet temperature on recovery efficiency: (a) recuperative cycle, (b) split cycle.

5.2.2. Effect of Turbine Inlet Pressure

In this section, the effect of $P_h$ on the system performance is revealed by varying the pressure settings from 8.5 MPa to 20 MPa in the step of 0.5 MPa. Figure 14 shows the effects of $P_h$ on $W_{net}$ in the recuperative cycle and the split cycle. It can be observed from Figure 14(a) that in the recuperative cycle, $W_{net}$ increases as $P_h$ increases, while the growth speed gradually slows down at around 14 MPa. By comparison, the $W_{net}$ of the five mixtures is ordered by CO$_2$/R290(0.3/0.7) > CO$_2$/R600a(0.3/0.7) > CO$_2$/R600(0.3/0.7) > CO$_2$/R601a(0.3/0.7) > CO$_2$/R601(0.3/0.7). As for the split cycle, when the pressure gradually increases, $W_{net}$ increases first and then decreases, as illustrated in Figure 14(b). For the performance comparison, the split cycle has a larger work than the recuperative cycle for the same mixture. Taking CO$_2$/R600a(0.3/0.7) as an example, when $P_h$ is 16 MPa, the $W_{net}$ of the split cycle is 18.5 kW and that of the recuperative cycle is 15.42 kW. This is mainly due to a large mass flow rate of the mixture in the split cycle. The variations of $\eta_{th}$ with $P_h$ are shown in Figure 15. It can be seen that with the increase of $P_h$, $\eta_{th}$ first increases and then remains stable in the recuperative cycle and the split cycle. Different from the comparison of $W_{net}$, the $\eta_{th}$ of the recuperative cycle is higher than that of the split cycle. This can be explained by the absorption of more waste heat in the split cycle.

Figure 14. Effect of turbine inlet pressure on net work: (a) recuperative cycle, (b) split cycle.
5.2.3. Effect of Condensation Temperature

In general, there are three different cooling methods for fluid condensation in ICE [27]. The obtained $T_1$ ranges from 30 °C to 90 °C. Thus, the temperature effects on the performance of the recuperative cycle and the split cycle are analyzed. Special care should be given CO$_2$/R290(0.3/0.7). Due to the limit of critical temperature, the maximum $T_1$ is set to be 70 °C to guarantee the subcritical condensation of the mixture. Figure 17 presents the variations of the $W_{net}$ with $T_1$ in the two cycles. It is clear that the $W_{net}$ of the recuperative cycle and the split cycle naturally decrease as $T_1$ increases. Taking CO$_2$/R290(0.3/0.7) as an example, the $W_{net}$ of the split cycle decreases about 4 kW and that of the recuperative cycle decreases about 3 kW for every 20 °C rises of $T_1$. 

Figure 15. Effect of turbine inlet pressure on cycle efficiency: (a) recuperative cycle, (b) split cycle.

Figure 16a,b show $\eta_r$ curves of two cycles at different $P_h$. It is clearly seen from Figure 16a that in the recuperative cycle, $\eta_r$ increases rapidly with the increase of $P_h$. This is because the heat absorbed by Heater1 from the exhaust gas gradually increases with the increase of $P_h$. On the contrary, $\eta_r$ of the split cycle decreases with the increase of $P_h$, as shown in Figure 16b. This can be explained by the decrease of mass flow rate in the split cycle. Even so, compared with the recuperative cycle, $\eta_r$ of the split cycle is still higher, and this increase of efficiency is due to the addition of Heater2, which increases the total heat absorption of the system.
Figure 17. Effect of condensation temperature on net work: (a) recuperative cycle, (b) split cycle.

Figure 18 shows that $\eta_{th}$ of two cycles decrease with the increase of $T_1$. It is worth noting that in the recuperative cycle, when $T_1$ is lower than 55 °C, the $W_{net}$ of the considered mixtures satisfy the following order: $\text{CO}_2/\text{R290}(0.3/0.7) > \text{CO}_2/\text{R600a}(0.3/0.7) > \text{CO}_2/\text{R600}(0.3/0.7) > \text{CO}_2/\text{R601a}(0.3/0.7) > \text{CO}_2/\text{R601}(0.3/0.7)$. Meanwhile, for the considered five mixtures in the split cycle, $\text{CO}_2/\text{R290}(0.3/0.7)$ has the largest $\eta_{th}$ and $\text{CO}_2/\text{R601}(0.3/0.7)$ has the lowest efficiency when the $T_1$ range is 30–70 °C. In addition, for every 20 °C increase of $T_1$, $\eta_{th}$ of $\text{CO}_2/\text{R290}(0.3/0.7)$ in the split cycle decreases about 4%, while that of recuperative cycle is decreased by about 3%.

Figure 18. Effect of condensation temperature on cycle efficiency: (a) recuperative cycle, (b) split cycle.

The influences of $T_1$ on $\eta_r$ for the recuperative cycle and the split cycle are illustrated in Figure 19. It can be found that $\eta_r$ decreases with the increase of $T_1$ in the recuperative cycle from Figure 19a. It can be explained by the fact that the increase of $T_1$ will enlarge the recuperated heat, thus decreasing the absorbed heat in Heater1. When $T_1$ increases 20°C, $\eta_r$ of $\text{CO}_2/\text{R290}(0.3/0.7)$ in the recuperative cycle decreases about 4%. However, for the split cycle, the increase of $T_1$ affects $\eta_r$ slightly for different mixture fluids, as shown in Figure 19b. This is because that although the heat of Heater1 decreases, the heat absorbed in Heater2 continues to increase. Therefore, the total heat absorption of the split cycle varies little. Taking $\text{CO}_2/\text{R290}(0.3/0.7)$ as an example, $T_1$ increases from 30 °C to 70 °C, and $\eta_r$ decreases from 59% to 58%.
should be noted that when SR is relatively high, thus producing a basic transcritical cycle. Therefore, the effect of SR on the split cycle performance is worth investigating.

Figure 20 shows the variation curves of $W_{\text{net}}$ in split ratio within the range of 0–1. It is obvious from the figure that with the increase of SR, $W_{\text{net}}$ firstly increases and then decreases. There exists a maximal value for each mixture. This is because that at a small SR, the split cycle is close to a simple transcritical cycle, thus producing a lower $W_{\text{net}}$. Meanwhile, when SR is close to 1, the split cycle is more similar to the recuperative cycle, and the advantage of the split is weakened. It should be noted that when SR is larger than 0.8, there exists a little rise of $W_{\text{net}}$. Similarly, for the five mixtures, $W_{\text{net}}$ satisfies the order: $\text{CO}_2/R290(0.3/0.7) > \text{CO}_2/\text{R600a}(0.3/0.7) > \text{CO}_2/\text{R600}(0.3/0.7) > \text{CO}_2/\text{R601a}(0.3/0.7) > \text{CO}_2/\text{R601}(0.3/0.7)$.

Figure 19. Effect of condensation temperature on recovery efficiency: (a) recuperative cycle, (b) split cycle.

5.2.4. Effect of Split Ratio

In the above analysis, SR is set to 0.7 for the split cycle. However, in practical engineering, the SR can be manually controlled. When the value is set to 1, it represents the recuperative cycle. Meanwhile, at a SR of 0, it means that the split cycle becomes a basic transcritical cycle. Therefore, the effect of SR on the split cycle performance is worth investigating.

Figure 20 shows the variation curves of $W_{\text{net}}$ in split ratio within the range of 0–1. It is obvious from the figure that with the increase of SR, $W_{\text{net}}$ firstly increases and then decreases. There exists a maximal value for each mixture. This is because that at a small SR, the split cycle is close to a simple transcritical cycle, thus producing a lower $W_{\text{net}}$. Meanwhile, when SR is close to 1, the split cycle is more similar to the recuperative cycle, and the advantage of the split is weakened. It should be noted that when SR is larger than 0.8, there exists a little rise of $W_{\text{net}}$. Similarly, for the five mixtures, $W_{\text{net}}$ satisfies the order: $\text{CO}_2/R290(0.3/0.7) > \text{CO}_2/\text{R600a}(0.3/0.7) > \text{CO}_2/\text{R600}(0.3/0.7) > \text{CO}_2/\text{R601a}(0.3/0.7) > \text{CO}_2/\text{R601}(0.3/0.7)$.

Figure 20. Effect of split ratio on net work in the split cycle.
As for the $\eta_{th}$ in Figure 21, when SR gradually increases, $\eta_{th}$ of five mixtures increases continuously. This is because a higher ratio led to a larger recuperated heat. The total heat absorbed in Heater1 and Heater2 continuously decreases. It can be observed that when SR is 0, $\eta_{th}$ is lower than 10%. While as SR is 1, $\eta_{th}$ is higher than 20%. Figure 22 shows the variations of $\eta_{r}$ under different SR. As SR increases, $\eta_{r}$ at first barely changes and then decreases considerably. More working fluid enters Heater2 when SR is relatively small, so $\eta_{r}$ is high. After SR increases to a certain extent, the cycle is close to the recuperative cycle, so $\eta_{r}$ is reduced.

![Figure 21. Effect of split ratio on cycle efficiency in the split cycle.](image)

![Figure 22. Effect of split ratio on recovery efficiency in the split cycle.](image)

5.3. Parametric Optimization

Based on the above analysis, it can be concluded that $T_3$, $P_{th}$, $T_1$, and SR have different effects on cycle performance. However, due to the fact that $T_1$ is determined by the cooling method, $T_1$ here is set to 30 °C. For $W_{net}$ optimization of the recuperative cycle, $T_3$ and $P_{th}$ are set in the range of 240–400 °C and 8.5 MPa–20 MPa, respectively. As for the split cycle,
SR ranges from 0 to 1. On this basis, the optimization results for the recuperative cycle and the split cycle are provided in Tables 10 and 11, respectively.

Table 10. Optimized cycle parameters of the recuperative cycle.

| Parameters                  | CO₂/R290 | CO₂/R600a | CO₂/R600 | CO₂/R601a | CO₂/R601 |
|-----------------------------|----------|-----------|----------|-----------|----------|
| Mass fraction of CO₂        | 0.3      | 0.3       | 0.3      | 0.3       | 0.3      |
| T₁ (°C)                     | 30       | 30        | 30       | 30        | 30       |
| T₃ (°C)                     | 322.94   | 325.57    | 333.80   | 334.03    | 341.40   |
| P₁ (MPa)                    | 19.51    | 19.47     | 19.23    | 19.42     | 19.42    |
| Tₘid (°C)                   | 204.67   | 221.72    | 230.05   | 247.47    | 248.24   |
| P₄ (MPa)                    | 3.27     | 2.88      | 3.00     | 2.95      | 3.06     |
| mᵢ (kg/s)                   | 0.23     | 0.24      | 0.23     | 0.23      | 0.23     |
| Q₁_Heater1 (kW)             | 82.91    | 77.66     | 75.09    | 69.69     | 69.45    |
| Q₁_Heater2 (kW)             | 87.62    | 98.24     | 101.85   | 110.86    | 112.00   |
| W₁ (kW)                     | 26.76    | 24.42     | 23.34    | 20.79     | 19.88    |
| Wₚ (kW)                     | 8.43     | 8.18      | 8.06     | 7.21      | 6.86     |
| Wₙet (kW)                   | 18.33    | 16.24     | 15.29    | 13.58     | 13.01    |
| η₁ (°C)                     | 22.10    | 20.91     | 20.36    | 19.49     | 18.73    |
| ηₙ (°C)                     | 47.42    | 44.42     | 42.95    | 39.86     | 39.72    |

Table 11. Optimized cycle parameters of the split cycle.

| Parameters                  | CO₂/R290 | CO₂/R600a | CO₂/R600 | CO₂/R601a | CO₂/R601 |
|-----------------------------|----------|-----------|----------|-----------|----------|
| Mass fraction of CO₂        | 0.3      | 0.3       | 0.3      | 0.3       | 0.3      |
| T₁ (°C)                     | 30       | 30        | 30       | 30        | 30       |
| T₃ (°C)                     | 344.68   | 309.09    | 320.86   | 330.29    | 334.36   |
| P₁ (MPa)                    | 12.01    | 11.47     | 13.31    | 12.51     | 13.2     |
| SR                          | 0.67     | 0.78      | 0.66     | 0.74      | 0.63     |
| Tₘid (°C)                   | 289.47   | 256.53    | 261.17   | 277.49    | 279.40   |
| Tₜout (°C)                  | 62.83    | 100.57    | 54.18    | 107.44    | 51.40    |
| P₄ (MPa)                    | 3.27     | 2.88      | 3.00     | 2.95      | 3.06     |
| mᵢ (kg/s)                   | 0.31     | 0.38      | 0.33     | 0.33      | 0.31     |
| Q₁_Heater1 (kW)             | 56.59    | 66.88     | 65.43    | 60.34     | 59.74    |
| Q₁_Heater2 (kW)             | 69.37    | 47.73     | 63.12    | 52.20     | 69.64    |
| Qₙet (kW)                   | 140.84   | 169.23    | 122.53   | 148.56    | 121.00   |
| W₁ (kW)                     | 29.78    | 28.63     | 26.55    | 23.08     | 21.84    |
| Wₚ (kW)                     | 6.40     | 6.93      | 7.30     | 6.03      | 5.81     |
| Wₙet (kW)                   | 23.37    | 21.70     | 19.25    | 17.06     | 16.03    |
| η₁ (°C)                     | 18.56    | 18.93     | 14.97    | 15.16     | 12.39    |
| ηₙ (°C)                     | 72.04    | 65.55     | 73.53    | 64.37     | 74.00    |

For the recuperative cycle, Table 10 shows that the optimized Wₙet is substantially increased, compared to Wₙet under the basic operating condition. For instance, Wₙet of CO₂/R290(0.3/0.7) under basic operating conditions is 16.11 kW, while the optimized Wₙet is 18.33 kW. The increase of Wₙet reaches up to 13.78%. Among the five mixtures, a Wₙet of CO₂/R290(0.3/0.7) is the largest and that of CO₂/R601(0.3/0.7) is the smallest. As for the split cycle, performance is also greatly improved. From Table 11, for CO₂/R290(0.3/0.7), compared to Wₙet of 21.05 kW at basic operating conditions, the optimized Wₙet of 23.37 kW increases 11.02%. Compared with the optimization results of the recuperative cycle, the split cycle has a larger Wₙet and a higher ηₙ for the considered mixtures.

5.4. Performance Comparison at Different CO₂ Mass Fractions

Considering that the mixture properties change considerably with the CO₂ mass fraction, performance of the two cycles are further obtained at different fractions. To avoid the mixture flammability, CO₂ mass fraction ranges from 0.3 to 1.0. In this range, performance comparisons are respectively conducted under design and optimization conditions. The details are presented in the following subsections.
5.4.1. Design Conditions

Figure 23 presents the variations of $W_{\text{net}}$ with the CO$_2$ mass fraction for the recuperative and split cycles under design conditions. In Figure 23a for the recuperative cycle, it is clear that except CO$_2$/R290, with the increase of CO$_2$ mass fraction, the $W_{\text{net}}$ of the other four mixtures first increase and then decrease. This phenomenon can be explained by the temperature glides. At a lower CO$_2$ mass fraction, the temperature glide of the five mixtures is large and the $W_{\text{net}}$ is relatively small. However, with the increase of a CO$_2$ mass fraction, the temperature glide gradually decreases and the $W_{\text{net}}$ of the mixtures gradually increases. It should be noted that the $W_{\text{net}}$ of the five mixtures are equal with each other at the CO$_2$ mass fraction 0.65. When CO$_2$ mass fraction is lower than 0.65, CO$_2$/R290 exhibits the highest $W_{\text{net}}$, followed by CO$_2$/R600a, CO$_2$/R600, CO$_2$/R601a, and CO$_2$/R601. However, when the CO$_2$ mass fraction is greater than 0.65, a small difference exists for the $W_{\text{net}}$ of each mixture. As for the split cycle, the variation trend of $W_{\text{net}}$ is similar to that in the recuperative cycle. Being different with the recuperative cycle, the split cycle has an equal $W_{\text{net}}$ for different mixtures at the CO$_2$ fraction 0.7. When the fraction is less than 0.7, the highest work is still obtained by CO$_2$/R290. While, the value of net work of CO$_2$/R290 is the lowest when the fraction is higher than 0.7. In terms of the $W_{\text{net}}$ comparison between the two cycles, the split cycle always has a larger work than that of the recuperative cycle.

![Figure 23](image_url)

**Figure 23.** Net work of CO$_2$-based mixtures at different CO$_2$ mass fractions: (a) recuperative cycle, (b) split cycle.

At different CO$_2$ mass fractions, $\eta_{\text{ex}}$ of the two cycles are provided in Figure 24. It can be observed that $\eta_{\text{ex}}$ has similar curves with $W_{\text{net}}$, in terms of the variation trends and curve distributions. For the recuperative cycle, the minimum $\eta_{\text{ex}}$ 34.46% is obtained by pure CO$_2$, while the maximum efficiencies of these mixtures are obtained at different fractions. Among the five working fluids, Figure 24a depicts that when the mass fraction of CO$_2$ is 0.3, CO$_2$/R290 has the highest $\eta_{\text{ex}}$ of 45.22%. It should be noted that the equal efficiencies of different mixtures are obtained at the CO$_2$ mass fraction 0.5. For the split cycle in Figure 24b, the maximum efficiency 43.55% among the five mixtures is obtained by CO$_2$/R290 (0.3/0.7). Meanwhile, mixtures have the minimum efficiency at different mass fractions. For the considered five mixtures, the lowest efficiency are 39.85%, 38.69%, 36.65%, 32.72% and 31.45% for CO$_2$/R290(0.95/0.05), CO$_2$/R600a(0.35/0.65), CO$_2$/R600(0.3/0.7), CO$_2$/R601a(0.3/0.7) and CO$_2$/R601(0.3/0.7), respectively.
Figure 24. Exergy efficiency of CO$_2$-based mixtures at different CO$_2$ mass fractions: (a) recuperative cycle, (b) split cycle.

Figure 25 shows the variation trends of the component irreversibility with the CO$_2$ mass fraction. For the two cycles, with the mass fraction of CO$_2$ increases, the irreversibility of the recuperator increases significantly. When the mass fraction of CO$_2$ is low, the mixture has a better thermal match in the recuperator. However, opposite variations are observed for turbine in the recuperative cycle. Furthermore, for the split cycle in Figure 25b, with the increase of CO$_2$ mass fraction, the irreversibility in Heater2 increases. Due to this, the total irreversibility of the split cycle is always larger than that of the recuperative cycle.

Figure 25. Exergy destruction of CO$_2$-based mixtures at different CO$_2$ mass fractions: (a) recuperative cycle, (b) split cycle.

5.4.2. Optimization Conditions

To further compare the system performance, the maximum $W_{net}$ at different CO$_2$ mass fractions is obtained by parametric optimization. Similarly, in the optimization process, $T_1$ is set to 30°C. Considering the fact that the employed mixture has the highest critical pressure of 10.64 MPa for CO$_2$/R601, the $P_h$ ranges from 11 MPa to 20 MPa. For $T_3$, the range is 240 °C–400 °C. Furthermore, in the split cycle, $SR$ varies from 0 to 1.

Figure 26 shows the optimal $W_{net}$ of recuperative and split cycles at different CO$_2$ mass fractions. It can be noted that the $W_{net}$ of two cycles increases with the increase of the CO$_2$ mass fraction. Among the considered five mixtures, when the mass fraction of CO$_2$ is lower than 0.6, the $W_{net}$ of CO$_2$/R290 is the largest in the split cycle. Meanwhile,
it is clear that at the CO$_2$ mass fraction of 0.9, CO$_2$/R600 obtains the maximum $W_{\text{net}}$. For the recuperative cycle, as the CO$_2$ mass fraction is lower than 0.7, the $W_{\text{net}}$ of five mixtures satisfies the order: CO$_2$/R290 > CO$_2$/R600a > CO$_2$/R600 > CO$_2$/R601 > CO$_2$/R601a. Through the performance comparison, the $W_{\text{net}}$ of the split cycle is greater than that of the recuperative cycle at different CO$_2$ mass fractions for five mixtures. Moreover, the specific optimization parameters of the recuperative cycle and the split cycle are listed in Tables 12 and 13, respectively.

**Figure 26.** Optimal net work of recuperative and split cycles at different CO$_2$ mass fractions.

### Table 12. Optimal cycle parameters of the recuperative cycle at different CO$_2$ mass fractions.

| Fluids     | Parameters | 0.30  | 0.40  | 0.50  | 0.60  | 0.70  | 0.80  | 0.90  | 1.00  |
|------------|------------|-------|-------|-------|-------|-------|-------|-------|-------|
| CO$_2$/R290 | $T_3$ (°C) | 322.94| 320.69| 320.45| 324.33| 323.66| 332.79| 339.31| 353.74|
|            | $P_h$ (MPa)| 19.51 | 19.34 | 19.09 | 19.68 | 19.08 | 20.00 | 19.70 | 19.86 |
|            | $W_{\text{net}}$ (kW) | 18.33 | 18.13 | 18.11 | 18.25 | 18.24 | 18.40 | 18.33 | 18.77 |
| CO$_2$/R600a | $T_3$ (°C) | 325.57| 324.15| 320.56| 321.40| 323.95| 332.19| 339.29| 353.74|
|            | $P_h$ (MPa) | 19.47 | 19.17 | 18.96 | 19.17 | 19.23 | 19.86 | 19.67 | 19.86 |
|            | $W_{\text{net}}$ (kW) | 16.24 | 16.57 | 17.10 | 17.67 | 18.15 | 18.68 | 18.90 | 18.77 |
| CO$_2$/R600 | $T_3$ (°C) | 333.80| 329.38| 324.45| 323.27| 326.42| 336.90| 333.90| 353.74|
|            | $P_h$ (MPa) | 19.23 | 19.38 | 18.91 | 19.07 | 19.22 | 19.87 | 19.66 | 19.86 |
|            | $W_{\text{net}}$ (kW) | 15.29 | 15.86 | 16.61 | 17.39 | 18.04 | 18.62 | 18.90 | 18.77 |
| CO$_2$/R601a | $T_3$ (°C) | 334.03| 331.62| 327.22| 316.92| 322.50| 330.65| 332.79| 342.74|
|            | $P_h$ (MPa) | 19.42 | 19.79 | 19.14 | 19.90 | 19.32 | 19.56 | 19.71 | 19.86 |
|            | $W_{\text{net}}$ (kW) | 13.58 | 14.68 | 15.90 | 17.05 | 17.99 | 18.53 | 19.00 | 18.77 |
| CO$_2$/R601 | $T_3$ (°C) | 341.40| 333.92| 326.84| 326.39| 326.58| 318.00| 344.03| 353.74|
|            | $P_h$ (MPa) | 19.42 | 19.36 | 19.02 | 19.46 | 19.42 | 19.63 | 19.32 | 19.86 |
|            | $W_{\text{net}}$ (kW) | 13.01 | 14.16 | 15.52 | 16.91 | 18.05 | 18.76 | 19.04 | 18.77 |
Table 13. Optimal cycle parameters of the split cycle at different CO\textsubscript{2} mass fractions.

| Fluids     | Parameters | Mass Fraction of CO\textsubscript{2} | 0.30 | 0.40 | 0.50 | 0.60 | 0.70 | 0.80 | 0.90 | 1.00 |
|------------|------------|---------------------------------------|------|------|------|------|------|------|------|------|
| CO\textsubscript{2}/R290 | $T_3$ ($^\circ$C) | 344.68 | 338.32 | 330.55 | 361.19 | 324.35 | 323.84 | 319.98 | 321.57 |
|            | $P_h$ (MPa) | 12.01 | 12.39 | 14.48 | 17.31 | 12.84 | 15.70 | 15.98 | 17.16 |
|            | SR         | 0.67 | 0.73 | 0.69 | 0.61 | 0.71 | 0.70 | 0.68 | 0.62 |
|            | $W_{\text{net}}$ (kW) | 23.36 | 23.43 | 23.93 | 24.24 | 24.70 | 25.48 | 25.86 | 26.80 |
| CO\textsubscript{2}/R600a | $T_3$ ($^\circ$C) | 300.09 | 299.37 | 312.38 | 283.43 | 299.38 | 308.87 | 320.43 | 321.57 |
|            | $P_h$ (MPa) | 11.47 | 12.37 | 14.05 | 12.46 | 13.99 | 16.38 | 16.54 | 17.16 |
|            | SR         | 0.78 | 0.79 | 0.68 | 0.79 | 0.74 | 0.68 | 0.63 | 0.62 |
|            | $W_{\text{net}}$ (kW) | 21.70 | 22.28 | 22.91 | 24.91 | 26.01 | 26.63 | 26.95 | 26.80 |
| CO\textsubscript{2}/R600 | $T_3$ ($^\circ$C) | 320.86 | 314.91 | 321.25 | 290.38 | 303.92 | 316.46 | 313.22 | 312.57 |
|            | $P_h$ (MPa) | 13.31 | 13.57 | 13.56 | 12.60 | 15.90 | 14.61 | 15.33 | 17.16 |
|            | SR         | 0.66 | 0.75 | 0.67 | 0.72 | 0.71 | 0.66 | 0.66 | 0.62 |
|            | $W_{\text{net}}$ (kW) | 19.25 | 20.41 | 21.94 | 24.03 | 24.79 | 26.17 | 27.23 | 26.80 |
| CO\textsubscript{2}/R601a | $T_3$ ($^\circ$C) | 334.36 | 327.62 | 341.49 | 310.13 | 300.58 | 312.56 | 324.49 | 321.57 |
|            | $P_h$ (MPa) | 12.51 | 14.13 | 14.83 | 14.13 | 13.66 | 14.07 | 14.78 | 17.16 |
|            | SR         | 0.74 | 0.66 | 0.74 | 0.74 | 0.69 | 0.76 | 0.66 | 0.62 |
|            | $W_{\text{net}}$ (kW) | 17.06 | 18.37 | 20.39 | 22.61 | 24.85 | 26.76 | 27.07 | 26.80 |
| CO\textsubscript{2}/R601 | $T_3$ ($^\circ$C) | 330.30 | 336.88 | 320.03 | 285.92 | 306.95 | 286.34 | 321.87 | 321.57 |
|            | $P_h$ (MPa) | 12.30 | 14.13 | 14.83 | 14.13 | 13.66 | 14.07 | 14.78 | 17.16 |
|            | SR         | 0.74 | 0.66 | 0.74 | 0.74 | 0.69 | 0.76 | 0.66 | 0.62 |
|            | $W_{\text{net}}$ (kW) | 16.03 | 17.86 | 19.49 | 22.59 | 24.68 | 25.56 | 27.04 | 26.80 |

6. Conclusions

In this paper, two transcritical systems, namely the recuperative cycle and the split cycle, are employed to recover the waste heat of ICE. Five CO\textsubscript{2}-based mixtures namely R290, R600a, R600, R601a, and R601 are used. Based on the thermodynamic calculations, cycle performance is analyzed and compared. Key parameters including turbine inlet temperature, turbine inlet pressure, condensation temperature, and split ratio are investigated to reveal the effects on the system performance. On this basis, these key parameters are optimized to achieve the maximum net work in two cycles. Meanwhile, cycle performance of mixtures at different CO\textsubscript{2} mass fractions are compared under design and optimization conditions. From the above results, the main conclusions are drawn as follows:

- Under design conditions, in the recuperative cycle, the maximum cycle efficiency of 23.74% is obtained by CO\textsubscript{2}/R290(0.3/0.7). In addition, the largest net work of 21.05 kW in the split cycle is gained by CO\textsubscript{2}/R290(0.3/0.7). Compared with the recuperative cycle, the net work and recovery efficiency of the split cycle are much higher.

- With the increase of turbine inlet temperature, the net works of the two cycles tend to increase firstly and then decrease, while the cycle efficiency continuously increases and recovery efficiency decreases greatly. Furthermore, as the turbine inlet pressure increases, the net work of the recuperative cycle gradually increases, whereas the net work of the split cycle firstly increases and then decreases. For the effect of the split ratio, as the split ratio increases, the net work of the split cycle firstly increases and then decreases.

- Under design conditions, as the CO\textsubscript{2} mass fraction increases, the net work of mixtures except CO\textsubscript{2}/R290 shows a trend of first increasing and then decreasing in the recuperative cycle and the split cycle. However, under optimization conditions, the maximum net work increases continuously. The maximum net work of the split cycle is obtained by CO\textsubscript{2}/R600(0.9/0.1) and is 27.43 kW.

Author Contributions: Conceptualization, A.Y. and X.L.; methodology, W.S.; software, S.O.; validation, J.L., X.L. and A.Y.; formal analysis, W.S.; investigation, A.Y.; resources, S.O.; data curation, S.O.; writing—original draft preparation, J.L.; writing—review and editing, X.L.; visualization, X.L.; supervision, X.L.; project administration, W.S.; funding acquisition, W.S. All authors have read and agreed to the published version of the manuscript.

Funding: This work was funded by the National Nature Science Foundation of China, grant number 52106037 and the Provincial Nature Science Foundation of Hunan, grant number 2021JJ40755. In addi-
tion, the work was also supported by the program “Researches on key technology to optimization and
dynamic simulation of supercritical CO₂ power cycle” from China Three Gorges Corporation, grant
number 202003024 and the foundation from key laboratory of renewable energy power generation
and conversion in Fujian province, grant number KLIF-202106.

**Institutional Review Board Statement:** Not applicable.

**Informed Consent Statement:** Not applicable.

**Data Availability Statement:** Not applicable.

**Conflicts of Interest:** The authors declare no conflict of interest.

**Abbreviation**

| Abbreviation | Definition                                      |
|--------------|-------------------------------------------------|
| \( c_p \)    | Specific heat (kJ/(kg·K))                        |
| \( I \)      | Exergy destruction rate (kW)                    |
| \( W \)      | Power (kW)                                       |
| \( e \)      | The specific exergy of flow at any state point (kW/kg) |
| \( SR \)     | Split ratio                                     |
| \( E \)      | Exergy (kW)                                     |
| \( Q \)      | Heat transfer rate (kW)                         |
| \( h \)      | Specific enthalpy (kJ/kg)                       |
| \( m \)      | Mass flow rate (kg/s)                           |
| \( P \)      | Pressure (MPa)                                  |
| \( s \)      | Entropy (kJ/(kg·K))                             |
| \( T \)      | Temperature (°C)                                |
| \( \eta \)   | Efficiency (%)                                  |
| \( \Delta \) | Difference                                      |
| ICE          | Internal combustion engine                      |
| ORC          | Organic Rankine cycle                           |
| GA           | Genetic algorithm                               |
| PPTD         | Pinch point temperature difference              |
| GWP          | Global warming potential                        |
| ODP          | Ozone depletion potential                       |
| p            | Pump                                            |
| f            | Mixture fluid                                   |
| i            | A state point of cycle                          |
| Re           | Recuperator                                     |
| g            | Exhaust gas                                     |
| in           | Inlet temperature of exhaust gas                |
| mid          | Outlet temperature of Heater1                  |
| out          | Outlet temperature of Heater2                  |
| con          | Condenser                                       |
| t            | Turbine                                         |
| L            | Turbine out pressure                            |
| net          | Net work                                        |
| b            | Normal boiling point                            |
| c            | Critical state                                  |
| h            | Turbine inlet pressure                          |
| r            | Recovery efficiency                             |
| th           | Cycle efficiency                                |
| ex           | Exergy                                          |
| total        | Total heat absorbed by the system               |
Appendix A

Table A1. Thermodynamic properties of CO$_2$/R290 at different state points of the recuperative cycle under design conditions.

| State Point | P (MPa) | T (°C) | s (kJ/(kg·K)) | h (kJ/kg) |
|-------------|---------|--------|---------------|-----------|
| 1           | 3.27    | 30.00  | 1.40          | 294.91    |
| 2           | 13.00   | 40.98  | 1.42          | 317.50    |
| 2i          | 13.00   | 238.35 | 2.82          | 885.51    |
| 3           | 13.00   | 375.00 | 3.44          | 1238.91   |
| 4           | 3.27    | 316.68 | 3.51          | 1132.41   |
| 4i          | 3.27    | 59.45  | 2.25          | 564.41    |

Table A2. Thermodynamic properties of CO$_2$/R290 at different state points of the split cycle under design conditions.

| State Point | P (MPa) | T (°C) | s (kJ/(kg·K)) | h (kJ/kg) |
|-------------|---------|--------|---------------|-----------|
| 1           | 3.27    | 30.00  | 1.40          | 294.91    |
| 2           | 13.00   | 40.98  | 1.42          | 317.50    |
| 2i          | 13.00   | 301.68 | 3.12          | 1047.50   |
| 3           | 13.00   | 375.00 | 3.44          | 1238.91   |
| 4           | 3.27    | 316.68 | 3.51          | 1132.41   |
| 4i          | 3.27    | 80.09  | 2.41          | 6214.14   |
| 5           | 13.00   | 40.98  | 1.42          | 3175.04   |
| 6           | 13.00   | 301.68 | 3.12          | 1047.50   |
| 7           | 13.00   | 301.68 | 3.12          | 1047.50   |

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