OPTIMAL DESIGN OF SUPERCRITICAL CO₂ (S-CO₂) CYCLE SYSTEMS FOR INTERNAL COMBUSTION ENGINE (ICE) WASTE-HEAT RECOVERY CONSIDERING HEAT SOURCE FLUCTUATIONS

Jian Song  
Imperial College London  
London, UK

Yaxiong Wang  
Xi’an Jiaotong University  
Xi’an, China

Jiangfeng Wang  
Xi’an Jiaotong University  
Xi’an, China

Christos N. Markides*  
Imperial College London  
London, UK  
c.markides@imperial.ac.uk

ABSTRACT

Supercritical CO₂ (S-CO₂) cycle systems have emerged as an attractive alternative for internal combustion engine (ICE) waste-heat recovery thanks to the advantages offered by CO₂ as a working fluid, including robust performance and system compactness. The engine exhaust gases are the main available heat source from ICEs with promising thermodynamic potential for further utilisation, and whose conditions, i.e., temperature and mass flow rate, vary based on the ICE operating strategy/load. These heat source variations have a critical influence on the performance of a bottoming S-CO₂ cycle system, which needs to be carefully considered in the design stage. This paper explores the optimal design of S-CO₂ cycle systems for ICE waste-heat recovery considering heat source fluctuations as well as the probability of their occurrence as arising from actual ICE operation. A variety of heat source conditions are selected for separate designs of an S-CO₂ cycle system and performance prediction under all possible scenarios is evaluated via detailed design and off-design models, so as to select the optimal design that is able to match the heat source fluctuations and exhibit the best performance from thermodynamic and economic perspectives. The advantage of this approach relative the conventional ones that only consider one specific design condition is that it avoids either over- or under-sizing of the S-CO₂ cycle system, which also achieves comprehensive insight of the interplay between the bottoming heat recovery system and the ICE, and provides valuable guidance for further system optimisation.

INTRODUCTION

More than half of the energy through fuel combustion in internal combustion engines (ICEs) is dissipated in the form of waste heat mainly via exhaust gases and jacket water [1]. Therefore, waste-heat recovery is considered as an important pathway for ICE performance improvement, of which organic Rankine cycle (ORC) appears as an attractive solution [2-5]. More recently, supercritical CO₂ (S-CO₂) cycles have also emerged as a promising option for ICE waste-heat recovery thanks to the advantages offered by CO₂ as a working fluid, including better thermal match with the heat source, compact system structure and avoidance of working fluid decomposition under high-temperature conditions in particular for the recovery of engine exhaust gases [6,7]. S-CO₂ cycle systems also offer potential to be applied in a wide range of applications such as solar [8,9], nuclear [9,10] and geothermal energy utilisation [11,12].

Extensive research on S-CO₂ cycle systems for ICE waste-heat recovery is available, showing the growing interest in adopting this promising heat-to-power generation technology in the specific area to further enhance ICE performance. Chen et al. [13] compared the performance of supercritical CO₂ Brayton cycle and transcritical CO₂ cycle for heat recovery from automobiles via a theoretical study and the results revealed that S-CO₂ cycle had a higher efficiency thanks to the higher operating pressure. Song et al. [14] updated a single preheating S-CO₂ cycle system by adding a regeneration branch and an increase of 7% in net power output was achieved. Further to that work, a combined S-CO₂ cycle and ORC system was presented for a wide range of ICEs, with results indicating that a power output improvement of up to 40-70% could be obtained by the addition of the bottoming cycle system [15]. Hou et al. [16] analysed a combined-cycle system that coupled S-CO₂ recompression and regenerative cycles for marine engine waste-heat recovery and the system was able to offer various advantages including sufficient heat utilisation, high system compactness and low cost. Sharma et al. [17] presented a regenerative S-CO₂ recompression cycle also for shipboard applications and an increase up to 25% in engine power output at rated condition was achieved.

Most of the previous research focuses on the design and optimisation of S-CO₂ cycle systems with a specific heat source condition, i.e., fixed temperature and mass flow rate, normally at

DOI: 10.17185/dupublico/73964
the rated operating condition of the ICE. It is common that ICEs will be operated under frequent part-load conditions, which results in different heat source conditions for the bottoming heat recovery system. In other words, the S-CO₂ cycle system will be forced to operate under off-design conditions associated with the ICE load and its performance as well as the improvement in the ICE power output will be significantly influenced. Therefore, the off-design performance of the S-CO₂ cycle system needs to be considered in the design stage to avoid performance deterioration due to the mismatch between the determined system configurations (e.g., sizes and geometry of the components) and the heat source conditions, which has been rarely taken into consideration in the previous studies. This paper seeks to explore the optimal design of an S-CO₂ cycle system for ICE waste-heat recovery considering the heat source fluctuations and the probability of occurrence of such part-load conditions. All the possible heat source conditions corresponding to actual ICE operating load are selected for separate designs of the S-CO₂ cycle system and performance evaluation under all possible scenarios via detailed design and off-design models are performed, so as to select the optimal design scheme from thermodynamic and economic perspectives.

**METHODOLOGY**

**System description**

Recuperated S-CO₂ cycle system is considered in this study for waste-heat recovery from engine exhaust gases, of which the schematic diagram and the corresponding T-s diagram are shown in Figures 1 and 2. The CO₂ working fluid is firstly compressed by the compressor and heated in the recuperator by the hot CO₂ stream that flows from the turbine. CO₂ continuously absorbs heat from the engine exhaust gases and then expands in the turbine to produce power. Afterwards, CO₂ goes into the pre-cooler to be cooled down to start the next cycle.

![Figure 1: Schematic diagram of recuperated S-CO₂ cycle system for ICE waste-heat recovery.](image)

![Figure 2: T-s diagram of recuperated S-CO₂ cycle system for ICE waste-heat recovery.](image)

Thermodynamic models of the S-CO₂ cycle system can be found in the authors’ previous work [14,15] and they are omitted here.

**Turbine model**

A one-dimensional (1-D) design and off-design model of radial-inflow turbines [18,19] based on the mean-line method is used to predict the turbine efficiency, which has been employed in ORC [20] and CO₂-based systems [6,21]. In the design model, all relevant parameters, including the nozzle and rotor velocity coefficients, velocity ratio, reaction degree, wheel diameter ratio, absolute flow angle at the rotor inlet and relative flow angle at the rotor outlet, are optimised simultaneously in order to achieve the highest turbine efficiency. While in the off-design model, the geometry of the turbine determined by the design stage is provided as input and the flow characteristics as well as the working fluid parameters are predicted.

The peripheral efficiency of the radial-inflow turbine can be expressed as:

\[
\eta_p = 2 \left(\frac{\sqrt{\Omega + \varphi^2 (1 - \Omega)} - 2 \varphi \sqrt{\Omega - \Omega \cos \varphi}}{\Omega + \varphi^2 (1 - \Omega) - 2 \varphi \sqrt{\Omega - \Omega \cos \varphi}}\right)^{1/2},
\]  

Taking incidence loss, friction loss and leakage losses into consideration, the radial-inflow turbine efficiency is given by:

\[
\eta_t = \frac{w_2 \cdot \sin (\beta_i - \beta_{i,opt})}{2 \cdot \Delta h_i} \left(\frac{\rho_i + \rho_w}{\rho_i}\right)^{1/2} \left(\frac{D_i}{2}\right)^{1/2},
\]  

\[
\eta_t = \frac{K_i \cdot \left(\rho_i + \rho_w\right)}{2 \cdot m \cdot w_2^2} \Delta h_i,
\]  

\[
\eta_t = 0.4 \cdot 0.004 \cdot 0.75 \cdot 0.00023 \cdot K_i, \quad \eta_t = 0.3 \cdot (0.0004 \cdot 0.00023 \cdot K_i),
\]  

Heat exchanger models

Shell-and-tube heat exchangers are selected for the S-CO₂ cycle system, and the Bell-Delaware method [22] is used to
calculate heat transfer coefficients (HTCs) and pressure drops. The shell-side (heat source) HTC and pressure drop are given by:
\[ \alpha_s = \alpha_c \frac{G_c (\mu_u / \mu_s)^{0.14}}{P \Pr^{0.27}} j_i h_i j_i j_i , \quad (6) \]
where \( j_c, j_h, j_b, j_s \) are correction factors accounting for combined effects of bundle cut and spacing, for bundle leakage effects, for bundle bypass flow, for variable baffle spacing in the inlet and outlet sections, and for adverse temperature gradient build-up in laminar flow:
\[ \Delta P = \left \{ (N_s - 1) R_s R_i + 2 \left \{ 1 + \frac{N_{ex}}{N_{in}} \right \} R_s R_i \right \} \cdot (7) \]

The HTC of tube side with supercritical CO\(_2\) working fluid is given by (Ptukhov-Krasnoschekov-Protopopov correlation):
\[ \alpha_t = \frac{\lambda_c}{d_t} \left [ \frac{12.7(f/8)^{0.8}}{(\Pr^{0.27} - 1) + 1.07} \right ] \cdot (8) \]
\[ \left ( \frac{c_{p_t}}{c_{p_{	ext{bulk}}}^{0.35}} \right )^{-0.33} \left ( \frac{\mu_{	ext{bulk}}}{\mu_{	ext{wall}}} \right )^{0.11} \]

The total HTC of heat exchanger is given by:
\[ \frac{1}{U} = \frac{1}{i} \frac{d_i}{d_i} + \frac{d_i}{d_i} + \frac{\delta_s}{\lambda_u} \frac{d_s}{d_s} + \frac{\delta_s}{\lambda_u} + \frac{1}{\alpha_i} \cdot (9) \]

The heat exchanger area is given by:
\[ A = \frac{Q}{U \cdot \Delta T} \cdot (10) \]
where \( \Delta T \) is the log mean temperature difference (LMTD) between the hot side and the cold side.

Cost models
The module costing technique is used to calculate the bare module cost of each component, with the chemical engineering plant cost index (CEPCI) to obtain the capital cost of the systems [23]. Therefore, the specific investment cost (SIC) is calculated by Eqs. (10)-(14) with the coefficients for each component summarised in Ref. [15].
\[ C_{BM} = C_F B_{BM} = C_F (B_i + B_s F_s F_p) \cdot (11) \]
\[ \log(C_F) = K_i + K_b \log(X_i) + K_s \left [ \log(X_s) \right ]^2 \cdot (12) \]
\[ \log(F_p) = C_i + C_s \log(p_i) + C_s \left [ \log(p_i) \right ]^2 \cdot (13) \]
\[ C = \sum C_{BM} \frac{CEPCI_{2017}}{CEPCI_{2001}} \cdot (14) \]
\[ SIC = \frac{C}{W_{net}} \cdot (15) \]
where \( i \) denotes different components, \( CEPCI_{2001} = 397.0 \) and \( CEPCI_{2017} = 567.5 \) [24], which are dimensionless numbers employed to updating capital cost required to erect a power-cycle system from a past date to a later time.

The levelised cost of electricity (LCOE), which represents the present value of electricity production price considering the economic lifetime of a system and the costs incurred in the construction, operation and maintenance, is given by:
\[ LCOE = \frac{C + \sum P}{(1+i)^n} \cdot (16) \]
where \( C \) is the initial investment cost of the system, \( C_{O&M} \) is the annual operating and maintenance cost (set as 1.65% of the initial investment cost [25]), \( i \) is the discount rate (considered as 5% [25]), \( P \) is the annual power generated by the system, with an annual operation hours (set as 8000 h) and \( N \) is the expected lifetime (totally 15 years in this study).

Conditions and assumptions
An ICE with a rated power of 1000 kW [26] is selected in this paper and the heat source conditions corresponding to engine load are shown in Table 1. The temperature of engine exhaust gases changes from 540 °C to 470 °C while the mass flow rate decreases from 1.56 kg/s to 0.72 kg/s when the engine condition changes from the rated one (100%) to a part-load of 40%, which indicates significant difference among the heat source conditions.

<table>
<thead>
<tr>
<th>Load</th>
<th>100%</th>
<th>90%</th>
<th>80%</th>
<th>70%</th>
<th>60%</th>
<th>50%</th>
<th>40%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature (°C)</td>
<td>540</td>
<td>532</td>
<td>530</td>
<td>527</td>
<td>525</td>
<td>515</td>
<td>470</td>
</tr>
<tr>
<td>Mass flow rate (kg/s)</td>
<td>1.56</td>
<td>1.41</td>
<td>1.23</td>
<td>1.10</td>
<td>0.99</td>
<td>0.86</td>
<td>0.72</td>
</tr>
</tbody>
</table>

The model of the S-CO\(_2\) for ICE waste-heat recovery used in this study was developed using in-house MATLAB codes, with working fluid properties acquired from NIST REFPROP [27]. The interior-point algorithm in MATLAB’s fmincon function has been chosen as the solver to maximise the net power output under each heat source condition.

The main conditions and assumptions are given below:
(1) The minimum operating temperature and pressure of the S-CO\(_2\) cycle system are 31.5 °C and 7.5 MPa, respectively, to ensure that the working fluid is in the supercritical state; the maximum operating pressure is 20 MPa.
(2) The pinch point temperature differences in all heat exchangers in the design stage are set to 10 °C.
(3) The compressor efficiency is assumed to be 0.8 at both design and off-design conditions, which will be explored in future work by implementing detailed design and off-design models.
(4) The heat sink (cooling water) temperature is set to 15 °C and the maximum mass flow rate of the heat sink is 10 kg/s.
(5) The temperature of engine exhaust gases after heat recovery is set to be >120 °C in order to avoid acid corrosion in the corresponding pipes and heat exchangers [28].
(6) Heat losses throughout the system are neglected.
(7) All processes take place at steady state conditions.
RESULTS AND DISCUSSION

Cycle parameters as well as turbine design parameters are optimised simultaneously in the design stage to achieve the maximum net power output under each heat source condition corresponding to different ICE operating load. In other words, separate design schemes in terms of cycle parameters and components are obtained for all possible heat source conditions shown in Table 1. The maximum net power output and the corresponding SIC are shown in Figure 3, indicating that performance of the optimal designs (from a thermodynamic perspective) is closely related to the given heat source conditions. More precisely, the maximum net power output obtained from the separate designs decreases from 166 kW to 59 kW when the ICE load changes from the rated value (100%) to a part-load of 40%, while the SIC increases from 4630 $/kW to 8190 $/kW.

Figure 3: Net power output and corresponding SIC of the separate designs of S-CO₂ cycle system for ICE waste-heat recovery. Cycle parameters and turbine design parameters are optimised simultaneously to achieve the maximum net power output under each heat source condition corresponding to different ICE load shown in Table 1.

Detailed information of the separate designs for each heat source condition including turbine inlet and outlet conditions, CO₂ mass flow rate, areas of heat exchangers (recuperator, main heater and pre-cooler) and turbine efficiency are shown in Figs. 4-7, respectively. It can be seen from Figure 4 that the optimal turbine inlet and outlet pressures of the separate designs are nearly the same under different design conditions for the S-CO₂ cycle system to deliver the maximum net power output, while the optimised turbine inlet temperature decreases with the heat source temperature. Figure 5 shows that CO₂ mass flow rate corresponding to the separate designs decreases with the thermal load of the heat sources. It can be seen from Figure 6 that the main heater dominates in all designs as the density as well as the heat transfer coefficient of exhaust gases is much lower that the CO₂ working fluid, which also confirms that system compactness can be achieved as an advantage of CO₂-based systems thanks to the working fluid properties. Moreover, although the total heat exchanger area is larger with higher ICE load as well as more heat available from the engine exhaust gases, the corresponding SIC is still lower due to the high power output (see Figure 3). Figure 7 shows that the turbine efficiency is within the range of 84% to 86%, indicating the optimisation enables high-efficiency design under various heat source and operating conditions.

Figure 4: Turbine inlet and outlet conditions of the separate designs for each heat source condition corresponding to different ICE load.

Figure 5: CO₂ mass flow rate of the separate designs for each heat source condition corresponding to different ICE load.

Figure 6: Heat exchanger areas of the separate designs for each heat source condition corresponding to different ICE load.
Figure 7: Turbine efficiency of the separate designs for each heat source condition corresponding to different ICE load.

In order to select the optimal design among the schemes shown above, off-design performance of each separate design under all possible heat source conditions are evaluated via detailed off-design models. System operating parameters in the off-design stage are also optimised to achieve the maximum power output, which corresponds to the optimal control strategy in practical applications. Figure 8 shows that all separate designs experience a decrease in power output when the ICE load changes to be lower as the heat input to the S-CO$_2$ cycle system decreases. The design scheme for the rated condition (100% ICE load) provides a higher net power output under most heat source conditions, while the difference becomes smaller with lower ICE load.

Figure 8: Off-design performance of the separate designs under all possible heat source conditions.

The seven ICE operating conditions listed in Table 1 are considered as actual variations and the probability of occurrence of the ICE operating conditions will vary with different end-users as well as demand profile. Two cases are assumed to indicate the variations, i.e., one considers the same probability of occurrence for all possible conditions (equal-weighted scenario) and the other accounts for different weights for all the conditions as reported in Ref. [29], with 20.6%, 18.3%, 16.2%, 14.1%, 12.5%, 10.6% and 7.7% (different-weighted scenario), respectively.

It can be seen that the design corresponding to ICE rated load (100%) yields the maximum annual power output under both scenarios (922 MWh and 1330 MWh, respectively), and outperforms other designs significantly under the different-weighted scenario. The corresponding LCOE of the design at the rated heat source condition is the highest under the equal-weighted scenario (94 $/MWh), while it is the lowest under the different-weighted scenario (65 $/MWh). Therefore, the design at rated heat source condition is the optimal under the different-weighted scenario in terms of both thermodynamic and economic perspectives, while under the equal-weighted scenario, the design at the rated heat source condition is the optimal from the thermodynamic perspective, and the design corresponding to ICE load of 40% has the lowest LCOE of 75$/MWh.

Figure 9: Annual power output and LCOE of separate design for each heat source condition corresponding different ICE load: (a) under equal-weighted scenario, and (b) under different-weighted scenario.

CONCLUSIONS

In this paper we explore the optimal design of S-CO$_2$ cycle systems for ICE waste-heat recovery considering heat source fluctuations arising from the ICE operating load. Separate designs are presented for each heat source condition to achieve the maximum net power output. The design corresponding to the ICE rated load (100%) provides the maximum net power output of
166 kW with a corresponding SIC of 4630 $/kW, which is also the lowest among all design schemes. The off-design performance of all separate designs is evaluated at all possible heat source conditions and the design scheme for the ICE rated load is found to provide a higher net power output under most conditions. Two scenarios, i.e., equal-weighted and different-weighted, are considered in order to estimate the annual performance of the S-CO\textsubscript{2} cycle system. For the equal-weighted scenario, the design for the rated load ICE condition is the optimal from the thermodynamic perspective and the maximum annual power output reaches 922 MWh. The design for the 40\% ICE load condition yields the lowest LCOE of 75 $/MWh. The design for the rated load condition is the optimal for the different-weighted scenario with a maximum annual power output of 1330 MWh and the lowest LCOE of 65 $/MWh. The advantage of the methodology presented herein relative to conventional approaches that only consider one specific design condition is that it enables us to avoid either over- or under-sizing of the S-CO\textsubscript{2} cycle system, which also allows us to gain a more complete understanding of the interplay between the bottoming heat recovery system and the ICE, while providing valuable guidance for further system optimisation and operation.

**NOMENCLATURE**

**Symbols**

- \(B_i, C_i, K, F_M, F_P\) constants for cost models
- \(C\) cost ($)
- \(c_p\) specific heat capacity (J/kg\cdot K)
- \(d, D\) diameter (m)
- \(f\) friction factor
- \(j, R\) correction factors
- \(K_{c1}, K_{c2}\) leakage loss factor
- \(K_{f}\) friction loss factor
- \(G\) mass flux (kg/m\(^2\)\cdot s)
- \(h\) enthalpy (J/kg)
- \(i\) discount rate
- \(m\) mass flow rate (kg/s)
- \(N\) number, lifetime (year)
- \(p\) pressure (Pa)
- \(P\) power (kW\cdot h)
- \(Pr\) Prandtl number
- \(Q\) thermal load (W)
- \(q\) heat flux (W\cdot m\(^2\))
- \(Re\) Reynolds number
- \(r_i\) fouling resistance
- \(R_p\) surface roughness (m)
- \(s\) entropy (J/kg)
- \(T\) temperature (K)
- \(u\) peripheral velocity (m/s)
- \(U\) heat transfer coefficient (W/m\(^2\)\cdot K)
- \(w\) relative velocity (m/s)
- \(W\) power output (W)
- \(X\) component capacity
- \(\alpha\) heat transfer coefficient (W/m\(^2\)\cdot K)
- \(\alpha_1\) absolute flow angle in rotor inlet (°)
- \(\beta_1\) relative flow angle in rotor inlet (°)
- \(\beta_2\) relative flow angle in rotor outlet (°)
- \(\eta\) efficiency
- \(\lambda\) thermal conductivity (W/m\cdot K)
- \(\mu\) viscosity (Pa/s)
- \(\rho\) density (kg/m\(^3\))
- \(\zeta\) loss factor
- \(\phi\) nozzle velocity coefficient
- \(\psi\) rotor velocity coefficient
- \(\Omega\) reaction degree

**Subscripts**

- \(b\) bundle bypass flow; baffle
- \(BM\) bare module
- \(f\) friction loss
- \(i\) component
- \(I\) incidence loss
- \(l\) leakage loss
- \(n\) net power output
- \(opt\) optimal
- \(O&M\) operating and maintenance
- \(s\) shell side, isentropic
- \(t\) tube side
- \(T\) turbine
- \(tc\) tube rows in crossflow
- \(tcw\) tube rows in baffle window
- \(u\) peripheral
- \(w\) wall

**Abbreviations**

- CEPCI chemical engineering plant cost index
- HTC heat transfer coefficient
- ICE internal combustion engine
- LCOE levelised cost of electricity
- LMTD log mean temperature difference
- ORC organic Rankine cycle
- S-CO\textsubscript{2} supercritical CO\textsubscript{2}
- SIC specific investment cost

**ACKNOWLEDGEMENTS**

This work was supported by the UK Engineering and Physical Sciences Research Council (EPSRC) [grant numbers EP/P004709/1, and EP/R045518/1]. Data supporting this publication can be obtained on request from cep-lab@imperial.ac.uk.

**REFERENCES**


