Integrating off-design performance in designing CO₂ power cycle systems for engine waste heat recovery

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Abstract

CO₂ transcritical power cycle (CTPC) systems are a promising solution to improving engine efficiency through waste heat recovery. However, variable engine conditions often force the CTPC systems operate at their off-design conditions, where the performance may degrade due to the inefficiency of the components. Matching the system with the expected heat source variations is crucial for the commercialization of this technology. In this work, a novel design optimization framework is proposed, which considers the off-design performance under possible heat source variations at the design stage. Therefore, both the design and off-design models of the components and the system are integrated in detail in the framework, allowing simultaneous optimization of the components and the cycle parameters, and robust design of the system that could deal with the probable fluctuations on the heat sources. In particular, a detailed double-pipe model is used for the heat exchanger sizing and evaluation, and a radial-inflow turbine model based on the 1-D mean-line method for the expander sizing and performance prediction. The heat source variations are generated from the actual likely engine conditions and featured by the probability of occurrence. The results of a case study proves that the proposed framework can effectively integrate the system off-design performance when designing a system, and downsizing the equipment to match the probability of occurrence of the possible off-design operating conditions can lead to a medium-sized system that is much more favorable in terms of economic performance over its whole lifetime. The systems can not only be 50% more compact than that designed at the maximum power condition, reducing the initial investment cost to as low as 52%, but also maintain a duty ratio of as high as 90%. This design framework can be extended to the applications with transient heat sources and other cycle configurations.

Keywords: CO₂ system; system design framework; off-design analysis; radial-inflow turbine; waste heat recovery
<table>
<thead>
<tr>
<th><strong>Nomenclature</strong></th>
<th><strong>Subscripts</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$ heat transfer area (m$^2$)</td>
<td></td>
</tr>
<tr>
<td>$\lambda$ thermal conductivity (W/m·K)</td>
<td></td>
</tr>
<tr>
<td>$B_i, K_{tr}$ parameters for cost</td>
<td></td>
</tr>
<tr>
<td>$\delta$ tip clearance (m)</td>
<td></td>
</tr>
<tr>
<td>$c$ absolute velocity (m/s)</td>
<td>$\delta_w$ wall thickness of inner tube (m)</td>
</tr>
<tr>
<td>$c_p$ specific heat capacity (J/kg·K)</td>
<td>$\omega_t$ turbine rotational speed</td>
</tr>
<tr>
<td>$C_{BM}$ bare module cost ($)</td>
<td>$\sigma$ surface tension (N/m)</td>
</tr>
<tr>
<td>$C_{in}$ initial investment cost ($)</td>
<td>$\zeta$ probability of occurrence</td>
</tr>
<tr>
<td>$C_{ann}$ annual O&amp;M cost ($)</td>
<td></td>
</tr>
<tr>
<td>$C_P^0$ cost at ambient pressure and using carbon steel</td>
<td></td>
</tr>
<tr>
<td>$d$ diameter (m)</td>
<td>acid acid dew point</td>
</tr>
<tr>
<td>$\bar{D}_2$ wheel diameter ratio</td>
<td>aero aerodynamic</td>
</tr>
<tr>
<td>$F_p$ pressure factor</td>
<td>bulk bulk temperature of fluid</td>
</tr>
<tr>
<td>$F_M$ material factor</td>
<td>c cold fluid side</td>
</tr>
<tr>
<td>Fr Froude number</td>
<td>cond condenser</td>
</tr>
<tr>
<td>$f$ friction coefficient</td>
<td>cw cooling water</td>
</tr>
<tr>
<td>$G$ mass flux (kg/m$^2$·s)</td>
<td>design design condition</td>
</tr>
<tr>
<td>$h$ specific enthalpy (J/kg)</td>
<td>e equivalent</td>
</tr>
<tr>
<td>$i$ discount rate</td>
<td>f working fluid; friction</td>
</tr>
<tr>
<td>$K$ total heat transfer coefficient (W/m$^2$·K)</td>
<td>g exhaust gas; saturated gas</td>
</tr>
<tr>
<td>$L$ tube length (m)</td>
<td>gash gas heater</td>
</tr>
<tr>
<td>$l$ blade height (m)</td>
<td>G generator</td>
</tr>
<tr>
<td>$m$ mass flow rate (kg/s)</td>
<td>h hot fluid side; homogenous</td>
</tr>
<tr>
<td>$N$ expected lifetime</td>
<td>i inner diameter of inner tube</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>$P$</td>
<td>pressure (Pa)</td>
</tr>
<tr>
<td>$Pr$</td>
<td>Prandtl number</td>
</tr>
<tr>
<td>$Q$</td>
<td>heat capacity (W)</td>
</tr>
<tr>
<td>$\dot{Q}$</td>
<td>volume flow rate (m$^3$/s)</td>
</tr>
<tr>
<td>$\Delta P$</td>
<td>pressure drop (Pa)</td>
</tr>
<tr>
<td>$Re$</td>
<td>Reynolds number</td>
</tr>
<tr>
<td>$r_f$</td>
<td>fouling resistance</td>
</tr>
<tr>
<td>$s$</td>
<td>entropy (J/kg·K)</td>
</tr>
<tr>
<td>$T$</td>
<td>temperature (K)</td>
</tr>
<tr>
<td>$\Delta T_{\text{min}}$</td>
<td>minimum temperature difference (K)</td>
</tr>
<tr>
<td>$u$</td>
<td>fluid flow velocity (m/s)</td>
</tr>
<tr>
<td>$\bar{u}_i$</td>
<td>velocity ratio</td>
</tr>
<tr>
<td>$W$</td>
<td>power (W)</td>
</tr>
<tr>
<td>$\text{We}$</td>
<td>Weber number</td>
</tr>
<tr>
<td>$W_n$</td>
<td>annual energy production (MWh)</td>
</tr>
</tbody>
</table>

**Abbreviations**

- $X_{\text{ft}}$: turbulent-turbulent Lockhart-Martinelli parameter
- $x$: quality
- $\text{CEPCI}$: chemical engineering plant cost index
- $\text{CTPC}$: CO$_2$ transcritical power cycle
- $\text{DP}$: design point
- $\text{EPC}$: electricity production cost
- $\text{HEX}$: heat exchangers
- $\text{HTC}$: heat transfer coefficient

**Greek letters**

- $\alpha$: heat transfer coefficient (W/m$^2$·K)
- $\alpha_1$: absolute flow angle at rotor inlet (°)
- $\beta_2$: relative flow angle at rotor outlet (°)
- $\rho$: density (kg/m$^3$)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
<th>Acronym</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mu )</td>
<td>viscosity (Pa\cdot s)</td>
<td>LMTD logarithmic mean temperature difference</td>
</tr>
<tr>
<td>( \eta )</td>
<td>efficiency</td>
<td>LCOE levelized cost of electricity</td>
</tr>
<tr>
<td>( \varphi )</td>
<td>nozzle velocity coefficient</td>
<td>ORC organic Rankine cycle</td>
</tr>
<tr>
<td>( \psi )</td>
<td>rotor velocity coefficient</td>
<td>PPTD pinch point temperature difference</td>
</tr>
<tr>
<td>( \Omega )</td>
<td>reaction degree</td>
<td>SIC specific investment cost</td>
</tr>
<tr>
<td>( \zeta )</td>
<td>loss in turbine</td>
<td>s.t. subject to</td>
</tr>
</tbody>
</table>

WHR waste heat recovery
1. Introduction

Internal combustion engines, as one of the main power-generation devices, convert chemical energy into mechanical power. However, except 30-45% of the energy through fuel combustion to effective power [1,2], the remaining energy is mainly dissipated as waste heat through exhaust, coolant and/or intake charge air [3]. In this regard, waste heat recovery (WHR), particularly through organic Rankine cycle (ORC) technology [4], has been considered as a promising participant in improving the engine efficiency and reducing emissions [5]. More recently, CO₂ has been put into perspective as an alternative [6] to organic working fluids in ORC systems, where the thermal stability of the fluids is often a concern when dealing with high-temperature heat sources [7,8], and therefore forms CO₂ transcritical power cycle (CTPC) systems [9]. Employing CO₂ as the working fluid is associated with the notable advantages thanks to its natural and environmentally-friendly characteristics, and its good thermal stability without decomposition concerns [10]. Besides, CO₂ experiences a supercritical single-phase heating process in a gas heater when extracting energy from the heat sources, where CO₂ shows high density and low viscosity that allows compact components and system miniaturization [11,12]. Moreover, CO₂ can also prevent hardware damage and premature life caused by thermal fatigue and flow-assisted corrosion.

Research focusing on the CTPC systems as next-generation engine waste heat recovery technology has increased in the last decade. One of the main issues concerns on the system design and optimization. Chen et al. [6] compared basic CTPC and recuperative CTPC systems based on thermal efficiency and different cycle parameters such as turbine inlet temperatures, pump efficiencies and expander efficiencies were analyzed. Shu et al. [13] added both a preheater and a recuperator to a basic CTPC system to efficiently recover both exhaust and coolant energy at the rated condition of a gasoline engine. Later on, based on the parametric analysis, comprehensive selection maps [14] of four different CTPC systems were proposed in terms of net power output, exergy efficiency and electricity production cost, while Tian et al. [15] provided Pareto optimal solutions for these four systems through
a systematic multi-objective optimization based on genetic algorithm. Song et al. [16] updated a single preheating process with a regeneration branch and investigated the influences of cycle parameters on net power output. Uusitalo et al. [17] conducted parameter sensitivity analyses and highlighted the importance of the efficiencies of the turbomachines. Xia et al. [18] and Zhang et al. [19] presented a thermo-economic analysis of heat recovery systems integrated with the CO₂ systems. Liu et al. [20] optimized turbine inlet pressures for CTPC systems individually maximizing net power and exergy efficiency and minimizing costs. Liang et al. [21] integrated a recuperative CO₂ system with an ORC system to enhance the contribution of waste heat recovery system to the engine power.

All these heuristic studies regarding system design and parameter optimization contributes to the development of the CTPC systems in waste heat recovery of engines. However, a common characteristic of the aforementioned research is that only a specific heat source condition [4,13-15], normally at the rated engine condition, is selected when performing thermodynamic and thermo-economic analysis. In other words, fixed heat source conditions (temperatures and mass flow rates) are chosen to explore optimal cycle parameters and the corresponding components, and therefore the determined system is assumed to only operate at design (nominal) conditions. However, the CTPC systems are often forced to operate at off-design conditions, where the external conditions, e.g., engine conditions [22], and system operating parameters, e.g., pressures and temperatures [23], are no longer exactly the same as those at design conditions, due to the variable characteristics of the available heat sources for recovery, which are directly related to the real-life operating profiles of engines [24].

For this reason, researchers pay special attention to the off-design performance of such systems. Shu et al. [25] predicted the net power output of a CTPC system over the whole engine mapping conditions and demonstrated that system performance is quite sensitive to the heat source conditions, roughly 65% of the whole map shows infeasible if the system is designed at the rated engine condition. Similar work was conducted by Zhao et al. [26] for an ORC system although a controller was implemented. Usman et al. [27] focused on an ORC system for waste heat recovery of a light-duty
vehicle and reported that the engine power is improved by 5.8% at the vehicle speed of 100 km/h while worsened by 6.4% at the vehicle speed of 23.5 km/h. Wang et al. [28] analyzed off-design performances of four ORC systems and results show the net power is significantly deteriorated to around 40% of the designed one when engine load comes to 40%. Xie and Yang [29] simulated an ORC system under a driving cycle and concluded that thermal efficiency is as low as 3.63%, less than half of the designed 7.77%, owing to the energy fluctuation. Chatzopoulou et al. [30] evaluated off-design performance of ORC systems and reported the ORC power would be underestimated by up to 17% when excluding component off-design performance especially the expander.

Therefore, the system performance at off-design conditions significantly differs from the designed (nominal) one. The variable heat source conditions, i.e., mass flow rate and temperature, are dominant factors that force the passive waste heat recovery systems operate at their off-design conditions. Li et al. [31] predicted transient performance of CTPC systems using data-calibrated GT-SUITE models. Results suggested the improvement of the engine fuel economy could be increased from 2.3% to 4.2% if the pump and expander could be optimized at design process. Hence, instead of merely evaluating the off-design performance of a designed system, it is much more meaningful to integrate system off-design performance even during the system design phase, so as to obtain an optimal system that could operate efficiently even when it faces the possible variations of the heat sources. However, limited research takes into account the off-design performance when performing parameter determination and system design. Dyreby et al. [32,33] presented a system-level model integrating semi-empirical component models to predict the design-point and off-design operation of a supercritical CO₂ systems. Zhao et al. [34] extended the design space exploration method to design ORC systems that could match the size with the transient heat sources of driving cycles. Petrollese and Cocco [35] proposed a robust preliminary design method of solar ORC systems by considering the possible variations of the heat source and the heat sink conditions, which were featured as multi-scenarios with different probabilities.
In this work, a novel design framework is proposed for the CTPC waste heat recovery systems taking into account the off-design performance at the actual likely variations of the heat sources coming from the engines, even during the design phase. In particular, a comprehensive system-level model which is integrated with the detailed component design models and off-design models is introduced for current study. The CTPC systems are firstly designed at some design conditions and then evaluated the feasibility and off-design performance under all the possible engine conditions. The design conditions are thoroughly examined with the aim of optimizing the levelized cost of electricity (LCOE) and screening the optimal system design. In this way, the components are sized to match the probable heat source variations, eliminating the issues in relation to the extra investment costs caused by the oversized components and to the system performance degradation caused by the undersized ones. Hence, the proposed methodology can be industrial-oriented since the off-design performance are integrated during the design phase, guiding the system design towards a more practical direction.

Compared to the existing research, the major contributions of the current work are as follows.

(1) Propose a design framework for waste heat recovery systems that integrates on-/off- design optimization during the design stage. The off-design performance is initiatively involved in system design rather than merely evaluated after system design, making the system more robust when facing possible heat source variations.

(2) Integrate detailed component models in the system design model and off-design analysis model, allowing simultaneous optimization of component design and cycle operating parameters. Specifically, double-pipe heat exchanger models and radial-inflow turbine models are integrated.

(3) Demonstrate the methodology through a case study of waste heat recovery system design with variable heat sources. Different probabilities of each off-design operation are considered and compared, highlighting the usefulness of the methodology and proving that downsizing the equipment to a medium size that fits the probability of occurrence is a good choice in terms of thermo-economic performance over the whole system lifetime.
2. Modelling methodology

A robust system design framework for the CTPC systems fed by the exhaust of an internal combustion engine is proposed, which takes into account the effects of the expected variations of the exhaust, i.e., the expected off-design performance of the CTPC system, during the design phase. Both the performance of the CTPC system at the design point and at those expected off-design conditions are integrated to determine an optimal system that minimizes the levelized cost of electricity, 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. Therefore, the optimal system is not only cost-effective in terms of thermo-economic performance over its whole life cycle but also efficient at its off-design conditions, giving robustness to the system design solution. The optimization system-level model is developed in MATLAB, with fluid properties calculated from Coolprop database [36]. Fig. 1 depicts the scheme of the proposed design framework, which consists of three stages, i.e., the input stage, the design stage and the output stage.

In the first input stage, the heat source and heat sink conditions, along with the boundary conditions and the constraints are defined. Specifically, the heat source conditions (mainly the mass flow rate and the temperature) can be either the original transient profiles [31] or discrete points [34] that featured according to the raw data. It should be noticed that the range of the heat source conditions should cover those for both the system design and the off-design evaluation, i.e., the possible variations should be given. The heat sink conditions are mainly the inlet temperature and the mass flow rate of the cooling medium. The boundary conditions set the ranges of the parameters which would act as the decision variables for the cycle (such as turbine inlet pressure, turbine inlet temperature and condensation temperature) and for the components (such as fluid velocities in the heat exchangers). Constraints are those that should be satisfied for feasibility and safety in practical applications, for
example, the pressure drop limitations and pinch point temperature differences in the heat exchangers, the minimum temperature of the exhaust, and the manufacturing tolerances in the turbine.

![Diagram of the design framework integrating off-design performance at design phase.](image)

**Fig. 1.** Scheme of the design framework integrating off-design performance at design phase.

The second stage is the design stage. It is the most essential part of the framework and consists of three steps. Step 1 is the initial design optimization to determine the thermodynamic parameters at a specific design condition and estimate the initial investment cost of the system. The expander is preliminarily designed to maximize its isentropic efficiency, which returns back to the cycle calculation and allows simultaneous optimization of cycle parameters and the expander. The heat exchangers (HEX) are sized and optimized by minimizing the heat transfer areas within the allowable pressure drop. The pump can also be designed with detailed models in this step, which, however, is considered with a pre-set isentropic efficiency in the current study. After sizing the components, the initial investment cost can be estimated. The component geometric parameters are passed to the next step and act as the inputs with fixed values. Step 2 is the off-design optimization to examine the off-design operation and estimate the expected power and electricity. The possible heat source conditions
are considered, which depend on the engine conditions. The cycle operating parameters are optimized to adjust to a feasible operating condition at each new heat source condition, after which the weighted power or the overall power across the whole heat source envelope can be predicted. In this paper, we assumed the weight (probability of occurrence) of each variable heat sources for the consideration of different scenarios. Obviously, all the weights are summed to one. Step 3 is to calculate the levelized cost of electricity, which is the objective function in the overall design stage. The annual operation hours and O&M costs are assumed.

The final stage is to output the optimal system with the lowest LCOE, along with the determined design conditions, the heat exchanger geometries and the expander geometries.

The models are introduced in the following subsections in detail. It is noteworthy that the design framework can be applied to other similar systems for waste heat recovery from variable heat sources. Besides, the framework not only integrates the components models in detail but also accounts for the off-design performance evaluation in the system design. It is an embedded multi-objective optimization with the in-house coding of minimizing the LCOE in the top-level design, and at the same time minimizing the heat transfer areas while maximizing the expander efficiency in the bottom-level design at each heat source condition and each set of operating parameters (i.e., decision variables).

Ideally, the off-design performance evaluation should be embedded in the innermost layer of the codes for the design optimization on the thermodynamic parameters, which could be named as serial approach. However, it was demonstrated unnecessary and meaningless to evaluate the off-design performance of some systems if the constraints were already violated at the design point. The reasons were found as follows: (1) the constraints were checked only after finishing both the design and off-design calculation within the serial approach; (2) the decision variables of the thermodynamic parameters for the system design were randomly searched at the beginning of the optimization, which would make the system poorly designed, or even infeasible due to the constraints violation; (3) if the system was infeasible at off-design conditions, the solver would make a great effort to search the
optimal operation point and it was often the case that the solver finally converged to an infeasible point. Besides, this serial approach was also demonstrated to be quite time-consuming. Although the high-performance server (12-core Linux cluster with Xeon X5675, 48GB Ram and Nvidia Tesla K40 GPGPUs) was used, the time for finishing one-step calculation at a set of thermodynamic parameters was 3-4 hours, which inferred 50-67 days to finish the optimization if 400 points were assumed to be searched by the solver. And the time is only for getting the solution at one specific heat source condition. Therefore, an alternative approach is adopted here, which can be called parallel approach, to deal with the problem. The idea is to split the design stage into two separate optimization processes, the off-design operation is only predicted after finishing each design optimization rather than integrated in each step of design optimization. The parallel approach is not only efficient, which takes less computational time (2-3 hours to finish system design), but also able to guarantee a feasible and optimal design before off-design performance prediction.

The interior-point algorithm \textit{fmincon} in MATLAB is chosen as the solver to minimize the objective function with a number of non-linear constraints to ensure the optimum mathematical solution to be practically feasible. For those indexes to be maximized, their negative values are defined as the objective function. The \textit{multistart} structure is employed to repeatedly run the optimization from a number of different starting points to mitigate the influences of the initial value on the final solution.

\textbf{2.1. Step 1: Design optimization}

As mentioned above, the thermodynamic cycle is optimized with the detailed components design integrated during this step, as shown in Fig. 2. A basic CTPC system with four main components, i.e., a pump, a gas heater, a turbine and a condenser, is chosen for waste heat recovery of a natural gas engine. The main equations of each process (pumping, heating, expansion and cooling) can be found in Appendix A, which are based on the first law of thermodynamics.
A centrifugal pump is selected and a conservative isentropic efficiency of 0.7 [18,28] is assumed for all the systems at the design stage. Although the pump efficiency is also a critical parameter which influences cycle performance and working fluid selection [37], it is considered reasonable since the centrifugal pump technology is quite mature and it is easy to find a product that has such an isentropic efficiency.

A radial-inflow turbine is adopted because it is regarded as the suitable expansion component at the power scale of the investigated application, and it has relatively good performance at high temperatures and pressure ratios [38]. Unlike conventional method where a constant isentropic
efficiency is given, a 1-D mean-line preliminary design approach [39,40] is used to predict the maximum isentropic efficiency that could be achieved at certain cycle parameters by simultaneously optimizing several key aerodynamic and geometric parameters of the turbine. The predicted efficiency is then sent back to the cycle calculation to modify the cycle parameters [41], which allows a robust optimization of the system and avoids any overestimation or underestimation of the turbine performance that could be realized at specific conditions. The parameters optimized, i.e., the decision variables, for the turbine include the nozzle and rotor velocity coefficients, velocity ratio, reaction degree, wheel diameter ratio, absolute flow angle at the rotor inlet, relative flow angle at rotor outlet and the turbine rotational speed. Table 1 lists the general ranges of these key parameters [42,43], serving as the boundaries of each parameter during the design optimization of the objective function indicated by the turbine isentropic efficiency. A set of nonlinear constraints are also imposed that set limits to the geometric parameters of the turbine and manufacturing tolerances in practical applications. More information on the turbine design can be found in Appendix B.

Table 1. Key parameters for radial-inflow turbine design [42,43].

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nozzle velocity coefficient</td>
<td>$\varphi$</td>
<td>/</td>
<td>0.95</td>
</tr>
<tr>
<td>Rotor velocity coefficient</td>
<td>$\psi$</td>
<td>/</td>
<td>0.90</td>
</tr>
<tr>
<td>Velocity ratio</td>
<td>$\bar{u}_1$</td>
<td>/</td>
<td>0.50–0.70</td>
</tr>
<tr>
<td>Reaction degree</td>
<td>$\Omega$</td>
<td>/</td>
<td>0.40–0.65</td>
</tr>
<tr>
<td>Wheel diameter ratio</td>
<td>$\bar{D}_2$</td>
<td>/</td>
<td>0.35–0.60</td>
</tr>
<tr>
<td>Absolute flow angle at rotor inlet</td>
<td>$\alpha_1$</td>
<td>°</td>
<td>14–20</td>
</tr>
<tr>
<td>Relative flow angle at rotor outlet</td>
<td>$\beta_2$</td>
<td>°</td>
<td>25–45</td>
</tr>
<tr>
<td>Rotational speed</td>
<td>$\omega_t$</td>
<td>rpm</td>
<td>50,000–300,000</td>
</tr>
</tbody>
</table>
The gas heater and the condenser are selected as double-pipe heat exchangers due to their simple construction, low cost, pressure and temperature capabilities, low pressure drop and flow arrangement of pure counter-current [44]. The heat exchangers are sized to achieve the minimum heat transfer areas within the allowable pressure drop for both the tube side and the shell side. Therefore, the corresponding geometry is determined. The logarithmic mean temperature difference method is used to obtain the heat transfer area of each discretized section in each phase. The key part for the heat exchanger sizing is the calculation of the heat transfer coefficients. The Dittus-Boelter correlation [31] is applied to calculate the Nusselt number for the exhaust and the cooling water. The Petukhov-Kirillov correlation [45] is used for the single-phase in the condenser while a modified equation [46] is used for the heating of supercritical CO\textsubscript{2} in the gas heater. The Chen correlation [47] with a modified form of the Dittus-Boelter equation is adopted for the two-phase condensing zone. The pressure drops for single-phase fluids flowing in bare tubes are calculated by Weisbach-Darcy equation [44]. For the two-phase condensing zone, there are a range of available correlations. To avoid the differences of a certain correlation, three two-phase frictional pressure drop prediction methods, i.e., the Muller-Steinghagen and Heck correlation, the Friedel correlation and the Gronnard correlation [48], are all calculated and averaged to obtain the final pressure drop in the condensing zone. The fluid velocities are chosen as the parameters to be optimized since they directly affect the geometry of the tubes. The pressure drops of each side are considered as the constraints. Table 2 provides the relevant values. Further information on the heat exchanger calculations is reported in Appendix C.

**Table 2.** Key parameters for heat exchanger design.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exhaust gas velocity</td>
<td>(u_{s,gash})</td>
<td>m/s</td>
<td>10–50</td>
</tr>
<tr>
<td>Supercritical CO\textsubscript{2} velocity</td>
<td>(u_{t,gash})</td>
<td>m/s</td>
<td>0.5–5.0</td>
</tr>
<tr>
<td>Subcritical CO\textsubscript{2} velocity</td>
<td>(u_{t,cond})</td>
<td>m/s</td>
<td>0.5–5.0</td>
</tr>
</tbody>
</table>
Cooling water velocity \(u_s,\text{cond}\) m/s 0.5–1.0
Exhaust pressure drop limit \(\Delta P_{s,\text{lim,gash}}\) kPa 30
Cooling water pressure drop limit \(\Delta P_{s,\text{lim,cond}}\) kPa 30
CO\(_2\) pressure drop limit \(\Delta P_{t,\text{lim}}\) kPa 30

Regarding the design optimization, the objective function is to minimize the specific investment cost (SIC), i.e., the investment cost per net power output, as shown in Eq. (1). The total investment cost is evaluated by the module costing technique modified by the chemical engineering plant cost index (CEPCI) [49]. Further information about the economic analysis can be found in Appendix D.

\[
\min \ SIC = \min f \left( P_{t,\text{in}}, T_{t,\text{in}}, T_{\text{cond}}, PPTD_{\text{gash}}, PPTD_{\text{cond}} \right)
\]

\[
\begin{align*}
T_{t,\text{in}} & < T_{\text{g,in}} \\
T_{p,\text{out}} & < T_{\text{g,out}} \\
T_{\text{g,out}} & \geq T_{\text{g,acid}} \\
T_{\text{cw,mid}} & < T_{\text{cond}} \\
\Delta T_{\text{min,gash}} & \geq PPTD_{\text{gash}} \\
\Delta T_{\text{min,cond}} & \geq PPTD_{\text{cond}}
\end{align*}
\]

where \(s.t.\) means subject to; \(T_{\text{cw,mid}}\) means the cooling water temperature at the outlet of the condensing zone; the subscript ‘in’ refers to inlet and ‘out’ means outlet; ‘gash’ refers to the gas heater and ‘cond’ means condenser.

The decision variables include: the turbine inlet pressure, \(P_{t,\text{in}}\); the turbine inlet temperature, \(T_{t,\text{in}}\); the condensing temperature, \(T_{\text{cond}}\); the pinch point temperature difference in the gas heater, \(PPTD_{\text{gash}}\); and the pinch point temperature difference in the condenser, \(PPTD_{\text{cond}}\). Typically, the pinch point temperatures are pre-set as constant values, for example, 30 K for the gas heater [13-15,50] and 5 K for the condenser [15]. However, the pinch point temperature significantly influences the required heat transfer areas. The smaller the pinch point temperature, the larger the heat transfer area for the same heat capacity. Therefore, instead of setting constant values [51], the pinch point temperatures are also optimized to achieve better thermo-economic performance. Table 3 lists the values of the key
parameters for cycle optimization. The constraints include the temperature comparison between the working fluid and the secondary fluid at each discretized section to avoid cross-temperature, and the minimum temperature differences ($\Delta T_{\text{min}}$) should be greater than the pinch point temperatures.

### Table 3. Key parameters for cycle design.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Turbine inlet pressure</td>
<td>$P_{\text{t, in}}$</td>
<td>kPa</td>
<td>8,000–20,000</td>
</tr>
<tr>
<td>Turbine inlet temperature</td>
<td>$T_{\text{t, in}}$</td>
<td>K</td>
<td>500–800</td>
</tr>
<tr>
<td>Condensation temperature</td>
<td>$T_{\text{cond}}$</td>
<td>K</td>
<td>298–302</td>
</tr>
<tr>
<td>Gas heater pinch point temperature difference</td>
<td>$PPTD_{\text{gash}}$</td>
<td>K</td>
<td>20–50</td>
</tr>
<tr>
<td>Condenser pinch point temperature difference</td>
<td>$PPTD_{\text{cond}}$</td>
<td>K</td>
<td>2–5</td>
</tr>
<tr>
<td>Exhaust temperature at acid dew point</td>
<td>$T_{\text{g, acid}}$</td>
<td>K</td>
<td>393</td>
</tr>
<tr>
<td>Initial isentropic efficiency of pump</td>
<td>$\eta_p$</td>
<td>/</td>
<td>0.7</td>
</tr>
<tr>
<td>Generator efficiency</td>
<td>$\eta_G$</td>
<td>/</td>
<td>0.9</td>
</tr>
<tr>
<td>Pump motor efficiency</td>
<td>$\eta_m$</td>
<td>/</td>
<td>0.98</td>
</tr>
</tbody>
</table>

### 2.2. Step 2: Off-design optimization

In the off-design optimization, the temperatures and the mass flow rates vary with the engine conditions. Fig. 3 shows the flowchart for the off-design operation and optimization of the CTPC systems. On the CTPC system side, the geometries of the components, i.e., the heat exchangers and the turbine, are fixed. The off-design performance of the system is predicted considering the off-design performance of each component. The objective function at off-design operation can be expressed as Eq. (2) to maximize the net power output, $W'_{\text{net}}$, with the decision variables selected as: the turbine inlet pressure, $P_{\text{t, in}}$; the turbine inlet temperature, $T_{\text{t, in}}$; the exhaust mass flow rate entering the gas
heater, \( m'_{t} \) and the mass flow rate of the working fluid, \( m_{g} \). Temperatures, mass flow rates and the heat transfer areas are set as the constraints, which should be satisfied during optimization.

\[
\text{max } W_{\text{net}} = \max f \left( P_{t, \text{in}}, T_{t, \text{in}}, m_{g}^{*}, m_{t}^{*} \right)
\]

\[
\begin{align*}
T_{t, \text{in}} &< T_{g, \text{in}} \\
T_{p, \text{out}} &< T_{g, \text{out}} \\
T_{g, \text{out}} &\geq T_{g, \text{acid}} \\
T_{\text{cw,mid}} &< T_{\text{cond}} \\
\left| m_{t} - m_{t, \text{in}} \right| / m_{t} &\leq 0.01 \\
\left| A_{\text{gash}} - A_{\text{gash}} \right| / A_{\text{gash}} &\leq 0.01 \\
\left| A_{\text{cond}} - A_{\text{cond}} \right| / A_{\text{cond}} &\leq 0.01
\end{align*}
\]

where \( m_{t, \text{in}} \) means the mass flow rate achieved by the turbine; \( A \) means the heat transfer areas; the superscript denotes the parameters at off-design conditions.
For the pump, its rotational speed is adjustable to pumping required mass flow rate of the working fluid at off-design conditions. The pump off-design isentropic efficiency can be obtained according to the affinity laws [52]. A fitting formula obtained from the non-dimensional performance curves of the pump in [52] is used in this paper to predict its off-design efficiency:

\[
\eta_{p,off} = -0.7 \left( \frac{Q_{\text{off}}}{Q_{\text{design}}} \right)^2 + 1.4 \left( \frac{Q_{\text{off}}}{Q_{\text{design}}} \right) \tag{3}
\]

where \(\eta_{p,off}\) means the pump isentropic efficiency at off-design conditions; \(Q_{\text{off}}\) and \(Q_{\text{design}}\) are the volume flow rate of the working fluid at off-design condition and at design condition, respectively.
For the turbine, the nozzle and rotor geometry are fixed from the design sizing exercise. Since the detailed models need to be experimentally validated to get the accurate off-design efficiency of the turbine while no available testing data exist till now, an alternative model proposed by Chen and Baines [53] is used to predict its off-design efficiency through correlating the aerodynamic loading, which has been applied in [54]. The mass flow rate of the working fluid achieved by the turbine, $m_{\text{in}}$, at a new turbine inlet and outlet conditions must be equal to that calculated from the energy balance of the cycle, $m_i$, to within ±1%. It should be noteworthy that the choked flow would happen in the nozzle if the Mach number is higher than 1, leading to the constant mass flow rate and additional losses [55]. Therefore, the maximum allowable mass flow rate that could produce power in the turbine needs to be carefully considered. Further information on the equations used for the off-design performance prediction of the turbine are reported in Appendix B.

For the heat exchanger, the total heat transfer areas and the tube sizes are fixed. The logarithm mean temperature difference method is still applied to calculate the heat transfer areas required at off-design conditions. The same correlations described in Appendix C are adopted to calculate the heat transfer coefficients. The heat transfer areas of the gas heater at off-design conditions, $A_{\text{gash}}$, should be equal to those designed at the design point, $A_{\text{gash}}$, to within ±1%. Similarly, the heat transfer areas of the condenser at off-design conditions, $A_{\text{cond}}$, should be equal to those designed at the design point, $A_{\text{cond}}$, to within ±1%. Regarding the gas heater, the exhaust actually entering the heat exchanger is adjustable which means the exhaust can be bypassed. Regarding the condenser, the pinch point temperature and the condensation temperature at off-design conditions are set to be the same as those defined at design condition [30]. The mass flow rate of the cooling water is adjustable to meet the variable heat rejection demand at off-design conditions.
2.3. Step 3: Levelized cost of electricity calculation

After obtaining the net power output, the levelized 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, can be calculated:

\[
\text{LCOE} = \frac{C_{\text{in}} + \sum_{n=1}^{N} \frac{C_{\text{ann}}}{(1+i)^n}}{\sum_{n=1}^{N} \frac{W_n}{(1+i)^n}}
\]  

(4)

where \(C_{\text{in}}\) is the initial investment cost of the system; \(C_{\text{ann}}\) is the annual O&M costs (set as 1.65% of the investment cost [14]); \(i\) the discount rate (considered as 5% [14]); \(W_n\) the expected annual energy produced by the CTPC system, which can be obtained by the weighted net power multiplied by the expected annual operation hours (set as 7500 h [14]); \(N\) is the expected lifetime (totally 15 years [14]).

It should be noted that the CTPC system is designed for an internal combustion engine with variable operating conditions. The differences of engine fuel consumption at each condition would bring some variations in the total costs and further the LCOE, since integrating the additional CTPC system make the engine become a combined system of the engine and the waste heat recovery system. Involving the costs of the internal combustion engine and its fuel will make the calculation of the LCOE much more accurate. In current paper, these costs are temporarily ignored for the preliminary comparison of different design schemes of the CTPC system.

3. Case study

A natural gas engine of 1000 kW rated power serving in a power plant is chosen as the targeted application to implement the proposed design framework. The exhaust gas is used to feed a basic four-component CTPC system. Fig. 4(a) shows the schematic diagram and Fig. 4(b) presents the corresponding \(T-s\) diagram, with the main state denotations labelled. The basic CTPC system mainly contains a gas heater, a turbine, a condenser and a pump. Saturated liquid CO\(_2\) is pumped to a
supercritical pressure in a pump and then enters a gas heater, where it absorbs heat from the engine exhaust gas. After that, the supercritical and high-temperature CO\(_2\) expands through a turbine and produces mechanical power, which can be converted to electricity by a generator. Finally, the working fluid releases heat to the cooling water in a condenser and then return to the pump, completing a cycle.

![Diagram](image)

**Fig. 4.** The basic CTPC system: (a) schematic diagram; (b) \(T\)-\(s\) diagram.

### 3.1. Heat source conditions

The heat-balance tests were performed on the investigated natural gas engine by the manufacturer [28]. Therefore, the energy distribution under seven typical engine conditions was obtained by analyzing the effective power, the exhaust gas energy, the coolant energy and the friction power consumption. Relevant parameters were tested and recorded, with the main parameters listed in Table 4. The natural gas engine serves in a power plant where a constant speed (600 rpm in this case) is required while the engine load varies to meet different power demands. As it can be seen, the exhaust gas temperature changes from 813 K to 743 K while the exhaust mass flow rate is lowered to less than half (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%. It indicates the exhaust energy (defined as the total energy to the ambient temperature, 288 K in the
current study) decreases from 926.6 kW to 362.1 kW, with the corresponding available energy that can be recovered (defined as the total energy to the acid dew point temperature, 393 K in the current study) is lowered from 741.3 kW to 278.5 kW, showing significant differences under different engine conditions. The characteristics of exhaust energy pose great challenges for the CTPC system to be highly efficient across the whole engine condition envelope. Designing a robust system which involves the off-design performance at the design phase is quite meaningful.

Table 4. Main parameters of engine conditions.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>EC1</th>
<th>EC2</th>
<th>EC3</th>
<th>EC4</th>
<th>EC5</th>
<th>EC6</th>
<th>EC7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engine condition</td>
<td>/</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Engine power</td>
<td>kW</td>
<td>1000</td>
<td>900</td>
<td>800</td>
<td>700</td>
<td>600</td>
<td>500</td>
<td>400</td>
</tr>
<tr>
<td>Engine speed</td>
<td>rpm</td>
<td>600</td>
<td>600</td>
<td>600</td>
<td>600</td>
<td>600</td>
<td>600</td>
<td>600</td>
</tr>
<tr>
<td>Engine load</td>
<td>%</td>
<td>100</td>
<td>90</td>
<td>80</td>
<td>70</td>
<td>60</td>
<td>50</td>
<td>40</td>
</tr>
<tr>
<td>Exhaust temperature</td>
<td>K</td>
<td>813</td>
<td>805</td>
<td>803</td>
<td>800</td>
<td>798</td>
<td>788</td>
<td>743</td>
</tr>
<tr>
<td>Exhaust mass flow rate</td>
<td>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>
<tr>
<td>Exhaust energy (to 288 K)</td>
<td>kW</td>
<td>926.6</td>
<td>824.7</td>
<td>730.7</td>
<td>635.5</td>
<td>567.3</td>
<td>483.5</td>
<td>362.1</td>
</tr>
<tr>
<td>Exhaust available energy (to 393 K)</td>
<td>kW</td>
<td>741.3</td>
<td>657.2</td>
<td>581.7</td>
<td>505.2</td>
<td>450.5</td>
<td>381.9</td>
<td>278.5</td>
</tr>
<tr>
<td>Engine brake thermal efficiency</td>
<td>%</td>
<td>36.63</td>
<td>35.13</td>
<td>35.27</td>
<td>34.01</td>
<td>32.47</td>
<td>30.53</td>
<td>27.21</td>
</tr>
<tr>
<td>Exhaust energy proportion</td>
<td>%</td>
<td>33.94</td>
<td>32.19</td>
<td>32.22</td>
<td>30.88</td>
<td>30.70</td>
<td>29.52</td>
<td>24.63</td>
</tr>
</tbody>
</table>

3.2. Design point definition

Unlike most previous literature [13-16,19,28,30,38,41,50] where the heat source conditions at a certain engine condition (typically the rated engine condition) is chosen to design waste heat recovery systems, the paper comprehensively considers the probable exhaust conditions that could occur during the engine operations in most cases. Starting with the seven typical engine conditions as listed in Table 4,
the feature area of the exhaust conditions can be defined with the exhaust mass flow rate \( (m_g) \) ranging from 0.72 kg/s to 1.56 kg/s and the exhaust temperature \( (T_{\text{g,in}}) \) ranging from 740 K to 815 K. Then the feature area is gridded into 4x5 subzones, with each vertex selected as a design point. Fig. 5 shows the feature area, with 30 design points depicted with blue circles while the typical conditions depicted with red triangles (as labelled from EC1 to EC7). The design point is used for system design optimization and components sizing. The off-design performance of a designed system is individually evaluated under seven typical engine conditions (EC1 to EC7) since they have been experimentally demonstrated as the typical engine conditions, following which the expected electricity production is estimated taking into account the probability of occurrence of the engine conditions.

It is worth acknowledging that the gridding is not the best way to optimize the design point and to determine the best heat source conditions at which the CTPC system should be designed. However, the gridding allows a low computational load but still informative design results although the heat source conditions are characterized into finite combinations of the mass flow rate and the temperature. We assigned coordinates to the design points to simplify the description in the following contexts. As shown in Fig. 5, DP(1,1) indicates the exhaust conditions at the lowest temperature of 740 K and the lowest mass flow rate of 0.72 kg/s while DP(6,5) indicates the exhaust conditions at the highest temperature of 815 K and the highest mass flow rate of 1.56 kg/s. The first number reflects the exhaust temperature level while the second number the exhaust mass flow rate level, which means only the exhaust mass flow rate is different between DP(1,1) and DP(1,5).
4. Results and discussion

The design methodology proposed in this paper accounts for the off-design performance during the design phase, i.e., the possible heat source variations are considered in the system design. The overall LCOE is optimized by taking the values of the investment cost at the design step and the expected electricity production at all the possible off-design conditions. However, in the traditional system design, only a certain heat source condition is selected therefore the system is considered totally operates at the nominal condition. The thermo-economic performance is typically optimized by choosing the specific investment cost (SIC) or the electricity production cost (EPC) [14] as an objective function, which can be calculated by Eq. (D.6) and Eq. (D.7), respectively. For a better understanding of the system design optimization methodology proposed in current study, the traditional system design results without considering the off-design performance are presented first in Section 4.1 as a reference single-scenario case. Then the robust design results by adopting the newly proposed design framework are given in Section 4.2 as multi-scenario cases.
4.1. System design for totally nominal operation

The design results of totally nominal operation, i.e., without any other off-design operation, are firstly presented in Fig. 6. All the 30 design points are considered for the CTPC system design, which makes great progresses than that proposed in Ref. [28] where only one heat source condition (at EC1) is chosen for system design. The specific investment cost (SIC) is minimized at each design point.

![Fig. 6. Design results for totally nominal operation with SIC as the objective function (without off-design performance involved).](image)

As shown in Fig. 6, the CTPC system achieves different optimum of SIC at 30 design points, ranging from around 7.4 $/W to 12.0 $/W. The optimal SIC decreases significantly with the increase of the exhaust mass flow rate while it shows less variation with the change of the exhaust temperatures (at the given range investigated here, i.e., the maximum difference is 75 K). The optimal SIC is found to be obtained by completely recovering the exhaust energy, which means the outlet temperature of the exhaust is lowered to 393 K. Although both the net power output and the total investment cost of the CTPC system increase at higher exhaust mass flow, the former shows a greater increment than the latter one. For example, the net power output is increased from 27 kW to 67 kW (by a rate of 150%)
while the total investment cost is only increased from 298 k$ to 498 k$ (by a rate of 67%) when the exhaust mass flow rate changes from 0.72 kg/s to 1.56 kg/s at the temperature of 815 K. The minimum SIC among the 30 system design points is found to be 7.4 $/W at the design point of DP(6,5) where the exhaust temperature is 815 K and the exhaust mass flow rate is 1.56 kg/s. It shows that the optimal CTPC system should be designed at DP(6,5) to achieve the best thermo-economic performance if the CTPC system only operates at the design condition during its whole lifetime. The SIC is higher at other design points than that at DP(6,5), with the absolute deviations given in Table 5.

<table>
<thead>
<tr>
<th>$m_g$ (kg/s)</th>
<th>0.72</th>
<th>0.93</th>
<th>1.14</th>
<th>1.35</th>
<th>1.56</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{g,in}$ (K)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>815</td>
<td>50.2%</td>
<td>31.0%</td>
<td>13.1%</td>
<td>2.9%</td>
<td>0.0%</td>
</tr>
<tr>
<td>800</td>
<td>44.2%</td>
<td>29.7%</td>
<td>15.2%</td>
<td>4.8%</td>
<td>5.1%</td>
</tr>
<tr>
<td>785</td>
<td>50.4%</td>
<td>32.8%</td>
<td>18.9%</td>
<td>13.5%</td>
<td>3.5%</td>
</tr>
<tr>
<td>770</td>
<td>62.1%</td>
<td>38.7%</td>
<td>22.7%</td>
<td>11.6%</td>
<td>6.2%</td>
</tr>
<tr>
<td>755</td>
<td>53.0%</td>
<td>46.4%</td>
<td>25.7%</td>
<td>16.1%</td>
<td>9.6%</td>
</tr>
<tr>
<td>740</td>
<td>59.7%</td>
<td>52.4%</td>
<td>30.7%</td>
<td>19.6%</td>
<td>11.0%</td>
</tr>
</tbody>
</table>

The corresponding parameters that could achieve the optimal SIC as shown in Fig. 6 are given in Fig. 7. The optimal turbine inlet pressure is shown in Fig. 7(a). Although a range of 8,000-20,000 kPa was provided for the optimization, the turbine inlet pressure is optimized at roughly 13,000 kPa in most cases. It highlights that a moderate turbine inlet pressure is favorable in terms of the economic performance (indicated by SIC) for the CTPC system. With the rise of the turbine inlet pressure, the cycle efficiency as well as the net power output firstly increases and then decreases [6] while the total cost of the CTPC system shows an upward trend. Therefore, the specific investment cost declines first
and touches the lowest point and then climbs. The moderate turbine inlet pressure is also beneficial to the component material and the system operation.

Fig. 7(b) depicts the turbine inlet temperature. The optimal value relates to the exhaust inlet temperature and the pinch point temperature difference in the gas heater. During the optimization, the actual temperature difference between the working fluid side and the exhaust side can be either equal or greater than the given pinch point temperature difference which is optimized in the range of 20-50 K. As Fig. 7(b) suggests, the optimal turbine inlet temperature rises with the increase of the exhaust temperature. In most cases, the optimal pinch point temperature differences are in the range of 20-35 K as shown in Fig. 7(d), which can be considered as the ideal pinch point temperature of the gas heater in the CTPC system. If the pinch point temperature is too large, the system performance (especially the net power output) would be limited by the highest turbine inlet temperature it can realize.

Fig. 7(c) presents the condensation temperature. The optimal condensation temperature is around 298 K in most cases, indicating a lower condensation temperature is preferable for a cost-effective system design. It also reflects that the pinch point temperature differences in the condenser prefer a large value, e.g., 4-5 K in most of the investigated cases as demonstrated in Fig. 7(e), so that the condensation temperature can be lowered as much as possible. With the decrease of the condensation temperature (i.e., the condensation pressure), the pressure ratio across the expander is enlarged, leading to a higher power output. Besides, the heat transfer in the condenser is enhanced for both the de-superheating process and the two-phase condensation process, resulting in less heat transfer areas required for the condenser. These two effects simultaneously lower the SIC of the CTPC system.
Fig. 7. Main parameters to achieve SIC shown in Fig. 6 at each design point: (a) turbine inlet pressure, $P_{\text{t,in}}$; (b) turbine inlet temperature, $T_{\text{t,in}}$; (c) condensation temperature, $T_{\text{cond}}$; (d) pinch point temperature differences in gas heater, $PPTD_{\text{gash}}$; and (e) pinch point temperature differences in condenser, $PPTD_{\text{cond}}$.

4.2. System design accounting for off-design operation

29
In this section, the robust design results by adopting the newly proposed design framework are given as multi-scenario cases. The seven typical engine conditions (EC1 to EC7) as listed in Table 4 are considered as actual variations of the investigated natural gas engine. Therefore, the corresponding exhaust conditions are the expected variability of the heat source feeding the CTPC system. Since the probability of occurrence of the seven conditions can vary with the different end-user energy demands in the power plant, two cases are assumed to indicate the variations: one is an equal probability of occurrence of the seven conditions (Case 1), i.e., the same weight is assigned to each engine condition (around 14.3%); the other one is a different probability of occurrence of the seven conditions (Case 2), i.e., different weight is assigned to each engine condition based on the available exhaust energy (see Table 4). The pie charts in Fig. 8 present these two cases. In Case 2, the weights of the seven engine conditions from EC1 to EC7 are 20.6%, 18.3%, 16.2%, 14.0%, 12.5%, 10.6% and 7.7%, respectively.

Fig. 8. Probability of occurrence of the engine conditions: (a) same weight; (b) different weight based on exhaust available energy.
Fig. 9. Design results accounting for off-design operation: (a) LCOE under equal-weighted off-design conditions; and (b) LCOE under different-weighted off-design conditions.

Within the proposed design framework, the off-design performance is involved at the design stage. The levelized cost of electricity (LCOE) is selected as the objective function and minimized to achieve the optimum. Fig. 9 demonstrates the design results for the two cases. Unlike SIC shown in Fig. 6 where a higher exhaust mass flow rate is favorable to realize a lower SIC, the LCOE increases significantly with the rise of the exhaust mass flow rate. For example, when the exhaust mass flow rate changes from 0.72 kg/s to 1.56 kg/s at the temperature of 815 K, the LCOE upsurges from 120.4 $/MWh to 322.9 $/MWh, by a dramatic rate of 168%, if the off-design conditions are of the same weight. It demonstrates a noticeable degradation in terms of the economic performance. However, in the other case where the off-design conditions are of different weight, the LCOE increases at a lower rate of 101%, from 117.9 $/MWh to 236.7 $/MWh, indicating that the probability of occurrence of the engine off-design conditions has great influences on the economic benefit of the CTPC system.

Since the LCOE is calculated as the ratio of the discounted cash flows and the expected electricity production during the lifetime of the CTPC system, the variations of the LCOE can be explained from the perspectives of the cost and the power production. As mentioned in Section 4.1, the total investment cost of the CTPC system increases at higher exhaust mass flow rate. The electricity production is greatly influenced by the system design and also the off-design conditions. Systems designed at higher
exhaust condition (i.e., higher mass flow rate and higher temperature) tend to have larger heat transfer areas in the heat exchangers (see Fig. 10) so that they are capable to extract energy completely from the exhaust and dissipate enough heat to the cooling circuit. However, the CTPC system is oversized when the waste heat at the off-design conditions becomes less than that at the design point. The CTPC system is suffered from its incapability to operate within the feasible constraints, especially to maintain the exhaust temperature above its acid dew point temperature. The actual required heat exchanger areas at some off-design conditions are quite less than those the system provided.

**Fig. 10.** Designed heat exchanger areas at design point: (a) gas heater, $A_{\text{gash}}$; (b) condenser, $A_{\text{cond}}$.

Taking the exhaust temperature of 755 K as an example, Fig. 11 demonstrates the total heat exchanger areas required at these seven off-design conditions (from EC1 to EC7). The heat exchangers are sized during design optimization and then the tube geometries are fixed. The cycle parameters are optimized to seek a quasi-steady state that the system can realize at each off-design condition, without violating the constraints related to the cycle and component feasibility. As stated in Section 2.2, the heat transfer areas should be equal to those designed to within ±1%, which can only be considered as a feasible off-design condition. Fig. 11 shows the feasible band for each system design (filled with sparse line). Only those within the feasible band are suitable to operate safely at the corresponding design, otherwise the heat exchangers are oversized. If the mass flow rate of the working fluid were
increased to extract more heat from the exhaust, the exhaust outlet temperature would be lowered below its acid dew point, resulting in possible corrosion in the gas heater. Specifically, the system designed at DP(2,5), where the exhaust mass flow rate is 1.56 kg/s, can only operate safely at off-design conditions of EC1 and EC2 while the system designed at DP(2,1), where the exhaust mass flow rate is 0.72 kg/s, is feasible at all these seven off-design conditions, which means the system can operate continuously regardless of the possible heat source variations.

Fig. 11. Comparison of required heat exchanger areas at off-design conditions and designed heat exchanger areas at exhaust temperature of 755 K: (a) gas heater, $A_{\text{gash}}$; (b) condenser, $A_{\text{cond}}$.

Therefore, the system designed at a lower exhaust mass flow rate condition can guarantee a continuous operation at off-design conditions, which would be beneficial for the expected yearly electricity production. The duty ratio, $DR$, is defined to describe the percent time of the feasibility (or the power mode) of the CTPC system. It is calculated by the CTPC system active time divided by the total engine operating time. Fig. 12 gives the duty ratio for the two cases of the engine off-design conditions. The duty ratios of the systems designed at the exhaust mass flow rate of 1.56 kg/s are only around 30% in Case 1 and 40% in Case 2, while they are as high as 100% if the systems are designed at the lowest exhaust mass flow rate. However, it should be noted that such systems sacrifice the power
output performance at higher engine conditions. Fig. 13 gives an example of those systems designed at exhaust temperature of 755 K. The exhaust energy utilization rate in the system designed at DP(2,1) drops from 100% to 47% if the engine condition changes from EC7 to EC1, indicating an incomplete recovery of the exhaust energy. The tradeoff between the system performance and the safe and continuous operation is quite critical in the system design for variable heat sources.

Fig. 12. Design results accounting for off-design operation: (a) duty ratio under equal-weighted off-design conditions; and (b) duty ratio under different-weighted off-design conditions.

Fig. 13. Exhaust energy utilization at off-design conditions with different system designs.
Accounting for the duty ratio and the exhaust utilization rate, the expected yearly electricity production can be estimated, with the results presented in Fig. 14. The expected yearly electricity production is higher in a compact medium-size system (designed at a lower exhaust mass flow rate) than that in an oversized system (designed at a higher exhaust mass flow rate) thanks to the higher duty ratio. Besides, comparing Fig. 14(a) and (b), the differences reduce if the off-design conditions are of different weight. The expected yearly electricity production is 276.1 MWh in the case of equal-weighted off-design conditions (Case 1), which is almost the same as that (280.1 MWh) in the case of different-weighted off-design conditions (Case 2) if the system is designed at DP(2,1). However, it increases from 163.1 MWh in Case 1 to 222.3 MWh in Case 2, by a rate of 36%, if the system is designed at DP(2,5).

![Fig. 14. Design results accounting for off-design operation: (a) expected yearly electricity production under equal-weighted off-design conditions; and (b) expected yearly electricity production under different-weighted off-design conditions.](image)

The minimum LCOE in Case 1 is obtained at DP(4,1), where the exhaust temperature is 785 K and the mass flow rate is 0.72 kg/s, while it is realized at DP(5,2) in Case 2, where the exhaust temperature is 800 K and the mass flow rate is 0.93 kg/s. The minimum LCOE is roughly 117.4 $/MWh in Case 1 and 112.3 $/MWh in Case 2. Table 6 lists the optimal system design results of the main parameters, along with the results of system design for totally nominal operation. It is explicitly
demonstrated that the system design accounting for the off-design operation at the design phase can lead to much more compact systems since the heat transfer areas of both the gas heater and the condenser are less than half of those in the system designed for totally nominal operation. For example, in Case 2, the gas heater area is reduced roughly from 89 m² to 41 m² while the condenser area is lowered approximately from 38 m² to 21 m², indicating the systems can be 50% more compact than that optimized at a specific design condition (assumed to be totally nominal operation). Meanwhile, the turbine and the pump can be designed at a smaller power scale. The designed turbine power is scaled down from around 93 kW to less than 50 kW, which would result in a smaller impeller diameter. The designed pump power is reduced from 16 kW to less than 10 kW. All these lead to lower initial investment cost of the system (as low as 59%), showing great economic potential in real applications. Besides, the duty ratio of these compact systems can be as high as more than 90%, allowing a robust and continuous operation at off-design conditions. All these results prove that downsizing the equipment to match the probability of occurrence of the possible off-design operating conditions can lead to a medium-sized system that is much more favorable in terms of economic performance over its whole lifetime. Moreover, comparing Case 1 and Case 2, the best design point moves towards the engine conditions of greater weight. It can be deduced that the system should be designed right at the engine condition of EC1 if the gas engine can always operate at this condition. Therefore, integrating the off-design operation at the design stage can achieve an efficient and cost-effective system design.

**Table 6.** Optimal system design results of the main parameters.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Symbol</th>
<th>Unit</th>
<th>Case 0 *</th>
<th>Case 1 *</th>
<th>Case 2 *</th>
</tr>
</thead>
<tbody>
<tr>
<td>Design exhaust inlet temperature</td>
<td>$T_{g,\text{in}}$</td>
<td>K</td>
<td>815</td>
<td>785</td>
<td>800</td>
</tr>
<tr>
<td>Design exhaust mass flow rate</td>
<td>$m_g$</td>
<td>kg/s</td>
<td>1.56</td>
<td>0.72</td>
<td>0.93</td>
</tr>
<tr>
<td>Design turbine inlet pressure</td>
<td>$P_{t,\text{in}}$</td>
<td>kPa</td>
<td>13,824</td>
<td>13,020</td>
<td>13,064</td>
</tr>
<tr>
<td>Design turbine inlet temperature</td>
<td>$T_{t,\text{in}}$</td>
<td>K</td>
<td>747.8</td>
<td>683.2</td>
<td>700.3</td>
</tr>
</tbody>
</table>
Design condensation temperature \( T_{\text{cond}} \) K 298.7 298.2 298.2

Design pinch point temperature \( PPTD_{\text{gash}} \) K 22.1 22.9 26.1

difference in the gas heater

Design pinch point temperature \( PPTD_{\text{cond}} \) K 3.5 4.6 4.4

difference in the condenser

Design CO\(_2\) mass flow rate \( m_t \) kg/s 1.13 0.54 0.71

Gas heater heat transfer area \( A_{\text{gash}} \) m\(^2\) 89.1 29.3 40.8

Condenser heat transfer area \( A_{\text{cond}} \) m\(^2\) 38.0 15.8 21.4

Design turbine efficiency \( \eta_t \) / 0.82 0.81 0.81

Design pump power \( W_p \) kW 16.4 7.0 9.2

Design turbine power \( W_t \) kW 93.0 37.0 50.2

Design cooling water mass flow rate \( m_{cw} \) kg/s 4.43 2.86 3.56

Initial investment cost \( C_{\text{in}} \) k$ 498.4 292.5 345.3

Specific investment cost \( \text{SIC} \) $/W 7.4 / /

Expected duty ratio \( DR \) % / 100 92.3

Expected overall net power \( W_{\text{net}} \) kW 67.2 / /

Expected yearly electricity production \( W_n \) MWh / 281.2 347.0

Levelized cost of electricity \( \text{LCOE} \) $/MWh / 117.4 112.3

*Case 0 refers to the system design for totally nominal operation; Case 1 refers to the system design accounting for equal-weighted off-design operation; Case 2 refers to the system design accounting for different-weighted off-design operation.

4. Conclusions

CO\(_2\) transcritical power cycle systems have emerged as a promising technology for engine waste heat recovery. However, the economic benefit of the systems is highly related to the off-design performance, which is greatly influenced by the system design and the intrinsic variations of the heat sources. A novel design framework is proposed for a CO\(_2\) transcritical power cycle system design. The framework
not only incorporates the detailed component models but also initatively integrates the on-/off- design performance optimization at the design phase. The integrated modelling codes allow simultaneous optimization of the components and the system, with the aim of minimizing the levelized cost of electricity of the system which operates at the expected variations of the heat sources. The proposed approach improves the reliability and robustness of the waste heat recovery system design, guiding the system design towards a more practical direction.

A summary of the main conclusions from this work is given below.

(1) Without considering the off-design performance, the CO$_2$ transcritical power cycle system is suggested to be designed at a higher exhaust condition (mass flow rate and temperature) to achieve a better economic performance (in terms of the specific investment cost). Specifically, the exhaust condition of 815 K and 1.56 kg/s is preferable for the design in current work to realize the minimum specific investment cost of 7.4 $/W.

(2) With the off-design performance integrated at the design phase, a lower exhaust condition (mass flow rate and temperature) is recommended for the system design to achieve a more compact, robust and cost-effective CO$_2$ transcritical power cycle system. The minimum levelized cost of electricity of the investigated system is roughly 112 $/MWh (say designed at exhaust condition of 800 K and 0.93 kg/s). The size of the heat exchangers and the power scale of the turbine can be just half of those in the case without involving off-design performance, while the duty ratio can be as high as 90%.

(3) The probability of occurrence of the engine conditions, i.e., the heat source variations, significantly influences the design point selection. The best design point moves towards the engine conditions of greater weight.

(4) The proposed framework can effectively integrate the system off-design performance when designing a system, which proves that downsizing the equipment to match the probability of occurrence of the possible off-design operating conditions can lead to a medium-sized system that is much more favorable in terms of economic performance over its whole lifetime.
Future work aims to apply the design framework to the applications with more complex test cases, such as waste heat recovery from mobile vehicle engines with highly transient heat sources. Other cycle configurations could also be investigated for the potential system design. Besides, the framework can be improved by integrating the design models and the off-design models of the pumps, all the mechanical-to-electrical components and different type heat exchangers and expanders in detail.

**Acknowledgement**

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**Appendix A. Thermodynamic modelling of the CTPC system**

The basic equations for the thermodynamic calculation of the CTPC system shown in Fig. 4 are listed below:

Process in the pump:

$$W_p = \frac{m_t (h_{p,\text{out}} - h_{p,\text{in}})}{\eta_p} = \frac{m_t (h_{p,\text{out},s} - h_{p,\text{in}})}{\eta_p \eta_m}$$  \hspace{1cm} (A.1)

where $W_p$ is the pump power consumption; $h$ the specific enthalpy; $m_t$ the mass flow rate of the working fluid; $\eta_p$ the isentropic efficiency of the pump and $\eta_m$ the efficiency of the pump motor (typically 0.90-0.98 [56,57], set as 0.98 in current paper). The subscript ‘p’ denotes pump; ‘in’ and ‘out’ denote inlet and outlet, respectively; ‘s’ means isentropic process.

Process in the gas heater:

$$Q_{\text{gash}} = m_t (h_{\text{gash, in}} - h_{\text{gash, out}}) = m_g c_{pg} (T_{\text{gash, in}} - T_{\text{gash, out}})$$  \hspace{1cm} (A.2)

$$T_{\text{gash, in}} = m_t \frac{h_{\text{gash, x}} (T_{\text{gash, x}}, P_{\text{gash, x}})}{m_g c_{pg}} - T_{\text{gash, out}} \geq PPTD_{\text{gash}} \quad \forall T_{\text{gash, x}} \in [T_{\text{p, out}}, T_{\text{p, in}}]$$  \hspace{1cm} (A.3)
where $Q$ is the heat transfer rate; $c_p$ the specific heat capacity; $T$ the temperature. The subscript ‘g’ denotes exhaust; ‘gash’ the gas heater; and ‘x’ means each segment discretized in the heat exchanger.

Process in the turbine:

$$W_t = m_t (h_{t,in} - h_{t,out}) = m_t (h_{t,in} - h_{t,out,x}) \eta_i$$  \hspace{1cm} (A.4)

where $W_t$ is the turbine power production and $\eta_i$ the isentropic efficiency of the turbine. The subscript ‘t’ denotes the turbine.

Process in the condenser:

$$Q_{cond} = m_t (h_{out} - h_{p,in}) = m_{cw} c_{cw} (T_{cw,out} - T_{cw,in})$$  \hspace{1cm} (A.5)

$$T_{cond,x} = \frac{m_t (h_{cond,x} (T_{cond,x}, P_{in}, x) - h_{p,in})}{m_{cw} c_{cw}} - T_{cw,in} \geq PPTD_{cond}; \ \forall T_{cond,x} \in [T_{p,in}, T_{t,out}]$$  \hspace{1cm} (A.6)

$$W_{cw} = \frac{m_{cw} \Delta P_{cw}}{\rho_{cw} \eta_m}$$  \hspace{1cm} (A.7)

where $x$ is quality; $m_{cw}$ the mass flow rate of the cooling water; $\rho_{cw}$ the density of the cooling water; $\Delta P_{cw}$ the pressure drop of the cooling water side in the condenser; $W_{cw}$ is the cooling water pump power consumption [58]; the subscript ‘cw’ denotes cooling water and ‘cond’ the condenser.

Net power output, $W_{net}$:

$$W_{net} = W_t \eta_G - W_p - W_{cw}$$  \hspace{1cm} (A.8)

where $\eta_G$ is the generator efficiency, which is set as 0.9.

Thermal efficiency, $\eta_{th}$:

$$\eta_{th} = \frac{W_{net}}{Q_{gash}}$$  \hspace{1cm} (A.9)

Appendix B. Radial-inflow turbine modelling

A radial-inflow turbine is adopted as the suitable expansion component in current paper. A 1-D design and off-design model based on the mean-line method is developed for turbine performance prediction.
in the cycle calculation [41,42]. The \( h-s \) diagram (Fig. B.1) and velocity triangles (Fig. B.2) can be used to describe the model in detail. In the nozzle (from section 0 to 1), the working fluid expands with enthalpy dropping and velocity increasing. Then in the rotor (from section 1 to 2), the working fluid continues to expand and drive the rotor to rotate.

**Fig. B.1.** \( h-s \) diagram of radial-inflow turbine.

**Fig. B.2.** Velocity triangle of radial-inflow turbine.

The peripheral efficiency of the radial-inflow turbine, \( \eta_u \), is expressed as:

\[
\eta_u = \frac{u_1 \cdot c_{1u} - u_2 \cdot c_{2u}}{\Delta h_s} = \frac{2(u_1 \cdot c_{1u} - u_2 \cdot c_{2u})}{c_o^2} = 2\left(\vec{u}_1 \cdot \vec{c}_{1u} - \vec{u}_2 \cdot \vec{c}_{2u}\right)
\]

(B.1)

which can be further calculated by substituting the relative velocities based on the ideal velocity after isentropic expansion:

\[
\eta_u = 2\vec{u}_i \cdot \left(\varphi \cdot \sqrt{1-\Omega} \cdot \cos \alpha_1 - \bar{D}_2^2 \cdot \vec{u}_i + \bar{D}_2 \cdot \psi \cdot \cos \beta_2 \cdot \left[\Omega + \varphi^2 \cdot (1-\Omega) - 2\varphi \cdot \sqrt{1-\Omega} \cdot \vec{u}_i \cos \alpha_1 + \bar{D}_2^2 \cdot \vec{u}_i^2\right]^{1/2}\right)
\]

(B.2)
It is noted that the peripheral efficiency is related to several parameters, namely nozzle velocity coefficient, \( \phi \); the rotor velocity coefficient, \( \psi \); velocity ratio, \( \bar{u} \); reaction degree, \( \Omega \); wheel diameter ratio, \( \bar{D} \); absolute flow angle at rotor inlet, \( \alpha_1 \); and relative flow angle at rotor outlet, \( \beta_2 \). The general range of these key parameters for radial-inflow turbine design is summarized in Table 1.

Based on the peripheral efficiency, friction loss and leakage loss are typically taken into consideration to obtain a practical turbine efficiency.

Friction loss, \( \zeta_f \), is related to the friction effect between the working fluid and the wheel, which can be calculated as:

\[
\zeta_f = \frac{f}{1.36 \times 10^6} \cdot \frac{u_1^3}{m_l \cdot \Delta h_1} \cdot \frac{D_1^2}{v_1}
\]  

(B.3)

Leakage loss, \( \zeta_l \), denotes the loss resulted by the tip clearance between the rotor blade and the shroud, which can be calculated by:

\[
\zeta_l = \begin{cases} 
1.3 \cdot \frac{\delta}{l_m} \cdot (\eta_u - \zeta_f), & \text{if } \frac{\delta}{l_m} \leq 0.05 \\
0.05 + 0.31 \cdot \frac{\delta}{l_m} \cdot (\eta_u - \zeta_f), & \text{if } \frac{\delta}{l_m} > 0.05 
\end{cases}
\]  

(B.4)

\[
l_m = \frac{l_1 + l_2}{2}
\]  

(B.5)

where \( \delta \) is the tip clearance depending on the manufacturing technology, and \( l_1 \) and \( l_2 \) are the blade height at rotor inlet and outlet, respectively.

Therefore, the efficiency of the radial-inflow turbine predicted by the 1-D model namely 1-D turbine efficiency can be expressed as:

\[
\eta_t = \eta_u - \zeta_f - \zeta_l
\]  

(B.6)

In the presented 1-D model, the turbine efficiency is maximized by optimizing the design parameters (listed in Table 1) as well as the rotational speed, using the MATLAB’s \textit{fmincon} function.
with several constraints considering the geometric sizes. A specific efficient turbine design can be obtained under each operating condition of the power cycle system.

The off-design performance prediction in this study is based a general relationship between the aerodynamic efficiency and the velocity ratio, which was proposed by Chen and Baines [51].

\[ \eta_{aero} = 2\bar{u}_i \sqrt{1 - \bar{u}_i^2} \]  

(B.7)

In order to take the internal losses in this semi-empirical model, the efficiency of the turbine is calculated by linearly scaling the aerodynamic efficiency predicted by Eq. (B.7), based on the efficiency at design point.

**Appendix C. Heat exchanger modelling**

The double-pipe (tube-in-tube) heat exchangers are discretized into several subsections in each phase to obtain accurate fluid properties for the heat transfer area calculation. The overall heat transfer coefficient (HTC) and the corresponding heat transfer area in each subsection is calculated as:

\[
\frac{1}{K} = \frac{1}{\alpha_t \cdot d_i} + r_{ft} \cdot \frac{d_o}{d_i} + \frac{d_o}{2 \lambda_w \cdot \ln \left( \frac{d_o}{d_i} \right)} + r_{fs} + \frac{1}{\alpha_s}
\]

(C.1)

\[
A = \frac{Q}{K \cdot \text{LMTD}}
\]

(C.2)

\[
\text{LMTD} = \ln \left[ \frac{(T_{h,\text{in}} - T_{c,\text{out}}) - (T_{h,\text{out}} - T_{c,\text{in}})}{(T_{h,\text{in}} - T_{c,\text{out}}) / (T_{h,\text{out}} - T_{c,\text{in}})} \right]
\]

(C.3)

where \( K \) is the overall heat transfer coefficient; \( \alpha_t \) the HTC of the tube-side working fluid; \( \alpha_s \) is the HTC of the shell-side (annular-side) working fluid (the exhaust in the gas heater or the cooling water in the condenser); \( d_i \) the inner diameter of the inner tube; \( d_o \) the outer diameter of the inner tube; \( r_{ft} \) and \( r_{fs} \) mean the fouling factors of the tube side and the shell side, respectively; \( \lambda_w \) the thermal conductivity of the tube wall; \( A \) the heat transfer area; \( \text{LMTD} \) the logarithm mean temperature difference; \( Q \) the
heat capacity and $T$ means temperature. The subscript ‘h’ means the hot fluid; ‘c’ the cold fluid; ‘in’ the inlet and ‘out’ the outlet.

**C.1. Gas heater modelling**

Regarding the tube side (indicated by subscript ‘t’), the Petukhov-Krasnoshchekov-Protopopov correlation [46] is used to calculate the HTC for the CO$_2$ supercritical phase, $\alpha_t$:

$$\alpha_t = \frac{\dot{\lambda}_t}{d_t} \left[ \frac{(f_i/8) \Re_t \Pr_t}{12.7(f_i/8)^{0.5} (\Pr_t)^{2/3} - 1 + 1.07} \left( \frac{\bar{c}_{p,t}}{c_{p,t,\text{bulk}}} \right)^{0.35} \left( \frac{\dot{\lambda}_{t,\text{wall}}}{\dot{\lambda}_{t,\text{bulk}}} \right)^{0.33} \left( \frac{\mu_{t,\text{bulk}}}{\mu_{t,\text{wall}}} \right)^{0.11} \right]$$

(C.4)

$$\bar{c}_{p,t} = \frac{h_{t,\text{bulk}} - h_{t,\text{wall}}}{T_{t,\text{bulk}} - T_{t,\text{wall}}}$$

(C.5)

$$f_i = \begin{cases} 0.316 \frac{\Re_t}{0.25} ; & \Re_t \leq 10^5 \\ \left[ 1.82 \log (\Re_t) - 1.64 \right]^{-2} ; & \Re_t > 10^5 \end{cases}$$

(C.6)

$$\Re_t = \frac{P_d u_d}{\mu_t}$$

(C.7)

$$\Pr_t = \frac{\mu_{t,\text{bulk}} c_{p,t}}{\dot{\lambda}_t}$$

(C.8)

$$\dot{m}_t = \frac{\pi d_t^2 u_t \rho_t}{4}$$

(C.9)

The pressure drop of the CO$_2$ supercritical phase, $\Delta P_t$, is obtained by:

$$\Delta P_t = \frac{f_i L G_t^2}{2 d_t \rho_t}$$

(C.10)

where $\Re$ is the Reynolds number; $Pr$ the Prandtl number; $f$ the friction factor; $c_p$ the specific capacity; $\dot{\lambda}$ the thermal conductivity; $\mu$ the viscosity; $h$ the specific enthalpy; $\rho$ the density; $u$ the fluid velocity; $L$ the tube length; $\dot{m}$ the mass flow rate and $G$ the mass flux. The subscript ‘wall’ and ‘bulk’ represent the property of the working fluid at wall-temperature and bulk-temperature, respectively.
Regarding the shell side (indicated by subscript ‘s’), the Dittus-Boelter correlation [31] is applied to calculate the HTC for the exhaust:

\[
\alpha_s = 0.023 \frac{\dot{\lambda}_s}{d_e} \text{Re}_s^{0.8} \text{Pr}_s^{0.3} \tag{C.11}
\]

\[
d_e = d_i - d_o \tag{C.12}
\]

\[
d_o = d_i + 2\delta_w \tag{C.13}
\]

\[
\dot{m}_s = \frac{\pi (d_e^2 - d_o^2) u_s \rho_s}{4} \tag{C.14}
\]

\[
\text{Re}_s = \frac{\rho u_s d_e}{\mu_s} \tag{C.15}
\]

\[
\text{Pr}_s = \frac{\mu_s C_{p,s}}{\lambda_s} \tag{C.16}
\]

\[
f_s = \begin{cases} 
0.316 \frac{\sqrt{0.25}}{\text{Re}_s^{0.25}}; & \text{Re}_s \leq 10^5 \\
\left[1.82 \log(\text{Re}_s) - 1.64\right]^2; & \text{Re}_s > 10^5 
\end{cases} \tag{C.17}
\]

The pressure drop of the exhaust, \(\Delta P_s\), is obtained by:

\[
\Delta P_s = \frac{f_s \text{LG}^2}{2d_e \rho_s} \tag{C.18}
\]

where \(d_i\) is the inner diameter of the outer tube; \(d_e\) the equivalent diameter of the shell side and \(\delta_w\) the wall thickness of the inner tube.

**C.2. Condenser modelling**

Regarding the tube side (indicated by subscript ‘t’), the Petukhov-Kirillov correlation [45] is used for the single-phase HTC calculation of \(\text{CO}_2\) in the condenser, \(\alpha_t\):

\[
\alpha_t = \frac{\dot{\lambda}_t}{d_i} \frac{(f_t/8) \text{Re}_t \text{Pr}_t}{12.7(f_t/8)^{0.5}(\text{Pr}_t^{2/3} - 1) + 1.07} \tag{C.19}
\]

\[
\Delta P_t = -\frac{\rho_t \rho_v}{\mu_t} \frac{d_t}{2} \tag{C.19}
\]
The Chen correlation [47] with a modified form of the Dittus-Boelter equation is adopted for the two-phase condensing zone:

\[
\alpha_i = 0.023 \frac{\dot{\lambda}}{d_i} \text{Re}_i^{0.8} \text{Pr}_i^{0.4} F
\]  
(C.20)

\[
F = \begin{cases} 
1; & 1/ X_u \leq 0.1 \\
2.35(1/ X_u + 0.213)^{0.736}; & 1/ X_u > 0.1 
\end{cases}
\]  
(C.21)

\[
X_u = \left( \frac{\rho_s}{\rho_l} \right)^{0.5} \left( \frac{\mu_s}{\mu_l} \right)^{0.1} \left( \frac{1-x}{x} \right)^{0.9}
\]  
(C.22)

\[
\text{Re}_i = \frac{G_i d_i (1-x)}{\mu_l}
\]  
(C.23)

\[
\text{Pr}_i = \frac{\mu_l \rho_{pl}}{\lambda_l}
\]  
(C.24)

where \( F \) is the correction factor; \( X_u \) the turbulent-turbulent Lockhart-Martinelli parameter and \( x \) the quality. The subscript ‘l’ means the saturated liquid and ‘g’ the saturated vapor.

The pressure drop of the CO\(_2\) single-phase zone, \( \Delta P_i \), is obtained by Eq. (C.10). While for the CO\(_2\) two-phase zone, \( \Delta P_i \), is averaged by three different correlations. The first method is the Friedel correlation [48], \( \Delta P_{tp,Friedel} \):

\[
\Delta P_{tp,Friedel} = \Delta P_i \left( E + \frac{3.24FH}{\text{Fr}^{0.045} \text{We}^{0.035}} \right)
\]  
(C.25)

\[
\Delta P_i = \frac{4f_i G_i^2 (1-x)^2 L}{2 \rho_l d_i}
\]  
(C.26)

\[
\text{Fr} = \frac{G_i^2}{gd_i \rho_h^2}
\]  
(C.27)

\[
\text{We} = \frac{G_i^2 d_i}{\sigma_i \rho_h}
\]  
(C.28)

\[
E = (1-x)^2 + x^2 \frac{\rho_l f_s}{\rho_s f_i}
\]  
(C.29)
\[ F = x^{0.73} (1 - x)^{0.224} \]  
(C.30)

\[ H = \left( \frac{\rho_1}{\rho_g} \right)^{0.91} \left( \frac{\mu_1}{\mu_g} \right)^{0.19} \left( 1 - \frac{\mu_g}{\mu_1} \right)^{0.7} \]  
(C.31)

\[ \rho_h = \left( \frac{x + 1 - x}{\rho_g} \right)^{-1} \]  
(C.32)

\[ f_g = \frac{0.079}{\text{Re}_g^{0.25}} \]  
(C.33)

\[ f_l = \frac{0.079}{\text{Re}_l^{0.25}} \]  
(C.34)

where Fr refers to the Froude number; We the Weber number; \( \sigma \) the surface tension; \( \rho_h \) the homogenous density. Others are the same as described above.

The second method is the Gronnard Correlation [48], \( \Delta P_{\text{tp, Gronnand}} \):

\[ \Delta P_{\text{tp, Gronnand}} = \Delta P_l \left[ 1 + \left( \frac{dP}{dz} \right)_{Fr} \left( \frac{\rho_l / \rho_g}{(\mu_l / \mu_g)^{0.25} - 1} \right) \right] \]  
(C.35)

\[ \left( \frac{dP}{dz} \right)_{Fr} = f_{Fr} \left[ x + 4 \left( x^{1.8} - x^{4.5} f_{Fr}^{0.5} \right) \right] \]  
(C.36)

\[ f_{Fr} = \begin{cases} 1; & Fr_l \geq 1 \\ Fr_l^{0.3} + 0.0055 \left[ -\ln (Fr_l) \right]^2; & Fr_l < 1 \end{cases} \]  
(C.37)

\[ Fr_l = \frac{G_1^2}{gd\rho_l^2} \]  
(C.38)

The third method is the Muller-Steinghagen and Heck correlation [48], \( \Delta P_{\text{tp, MSH}} \):

\[ \Delta P_{\text{tp, MSH}} = G_{\text{MSH}} (1 - x)^{3/3} + bx^3 \]  
(C.39)

\[ G_{\text{MSH}} = a + 2(b - a)x \]  
(C.40)

\[ a = \frac{f_{l, MSH} G_1^2}{2d\rho_l} \]  
(C.41)
\[ b = \frac{f_{g,\text{MSH}} G_t^2}{2d_i \rho_g} \]  

(C.42)

\[ f_{l,\text{MSH}} = \begin{cases} 
\frac{64}{\text{Re}_l}; & \text{Re}_l \leq 1187 \\
0.316 \frac{\text{Re}_l^{0.25}}{\text{Re}_l}; & \text{Re}_l > 1187 
\end{cases} \]  

(C.43)

\[ f_{g,\text{MSH}} = \begin{cases} 
\frac{64}{\text{Re}_g}; & \text{Re}_g \leq 1187 \\
0.316 \frac{\text{Re}_g^{0.25}}{\text{Re}_g}; & \text{Re}_g > 1187 
\end{cases} \]  

(C.44)

Regarding the shell side (indicated by subscript ‘s’), the Dittus-Boelter correlation [31] is applied to calculate the HTC for the cooling water:

\[ \alpha_s = 0.023 \frac{\dot{\lambda}}{d_s} \text{Re}_s^{0.8} \text{Pr}_s^{0.4} \]  

(C.45)

The pressure drop of the cooling water, \( \Delta P_s \), is obtained by Eq. (C.18).

**Appendix D. Economic modelling of the CTPC system**

The total investment cost, \( C_{\text{in}} \), is evaluated by the bare module costing technique modified by the chemical engineering plant cost index (CEPCI) [49]:

\[ C_{\text{in}} = \sum C_{\text{BM}} \frac{\text{CEPCI}_{2017}}{\text{CEPCI}_{2001}} \]  

(D.1)

where \( C_{\text{BM}} \) refers to the bare module cost of each component; CEPCI\(_{2017}\) is set as 567.5 [59] and CEPCI\(_{2001}\) is 391 [49] in this study.

The bare module cost of the heat exchanger is calculated:

\[ C_{\text{BM}} = C_p^0 \cdot F_{\text{BM}} = C_p^0 \left( B_1 + B_2 F_M F_p \right) \]  

(D.2)

\[ \log \left( C_p^0 \right) = K_1 + K_2 \log \left( A \right) + K_3 \left[ \log \left( A \right) \right]^2 \]  

(D.3)

\[ \log \left( F_p \right) = C_1 + C_2 \log \left( P \right) + C_3 \left[ \log \left( P \right) \right]^2 \]  

(D.4)
where $P$ is pressure; $C_p^0$ is the cost of the component working at ambient pressure and using carbon steel; $F_M$ and $F_p$ are correction factors of the material and the operating pressure; $B$, $K$ and $C$ are the coefficients for cost calculation, as listed in Table D.1.

Similarly, the bare module cost of the working fluid pump and its motor, the expander, the generator, the cooling water pump and its motor can be obtained by:

$$\log\left(C_p^0\right) = K_1 + K_2 \log(W) + K_3 \left[\log(W)^2\right]$$  \hspace{1cm} \text{(D.5)}

where $W$ is the corresponding power or electricity in the unit of kW.

The specific investment cost, SIC, is then calculated:

$$\text{SIC} = \frac{C_{\text{in}}}{W_{\text{net}}}$$  \hspace{1cm} \text{(D.6)}

where $W_{\text{net}}$ is the net power output.

The electricity production cost, EPC, is then calculated [60]:

$$EPC = \frac{C_{\text{ann}} + i \cdot (1+i)^N}{(1+i)^N - 1} \frac{C_{\text{in}}}{W_{\text{net}} \cdot h_{\text{full-load}}^{\text{hr}}}$$  \hspace{1cm} \text{(D.7)}

where $h_{\text{full-load}}^{\text{hr}}$ is the full load operation hours per year. Other parameters are defined as the same with those in Eq. (4).

For the calculation of LCOE as shown in Eq. (4), the expected annual electricity produced by the CTPC system, $W_n$, is obtained by:

$$W_n = \sum \xi_i W_{\text{net,off},i}$$  \hspace{1cm} \text{(D.8)}

where $W_{\text{net,off},i}$ is the net power output predicted at off-design condition $i$ and $\xi_i$ means the weight or probability of occurrence of off-design condition $i$.

**Table D.1.** Cost coefficients for bare module costs estimation [35,49].
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**References**


[34] Zhao M., Canova M., Tian H., Shu G., Design space exploration for waste heat recovery system in automotive application under driving cycle. Energy 2019;176:980-90.


