A Study of Working Fluids for Organic Rankine Cycles (ORCs) Operating Across and Below Ambient Temperature to Utilize Liquefied Natural Gas (LNG) Cold Energy

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Abstract: Liquefied Natural Gas (LNG) contains a significant amount of cold exergy, which is normally wasted during regasification at the receiving terminals. In recent years, organic Rankine cycles (ORCs) are proposed to exploit the LNG cold energy. This paper addresses the working fluid screening for an ORC utilizing LNG cold energy. Due to the cryogenic temperature of LNG, the condensation temperature of an ORC should be far below the ambient temperature, and the working fluid should be totally different from that for conventional ORCs operating above the ambient temperature. However, the working fluids also depend on the cycle configuration and the natural gas target pressure. In this study, 22 working fluids are investigated. A simulation-based optimization framework is proposed to compare the performance of all the candidates. The Particle Swarm Optimization (PSO) algorithm is adopted to optimize 5 and 7 dimensional search spaces for the combined systems operated across and below the ambient temperature. Promising working fluids for ORCs operated across and below the ambient temperature considering the effect of LNG target pressures are suggested based on the simulation-based optimization results. The most energy efficient working fluids are R125, R143a, R290 and R1270 for ORCs operated below the ambient temperature without waste heat utilization. For ORCs operated across the ambient temperature utilizing flue gas waste

heat from a natural gas fired power plant, R170, R134a and R290 perform better than other working fluids.

Keywords: LNG cold energy, organic Rankine cycle, working fluid selection, below ambient temperature, low-temperature waste heat

1. Introduction

A significant amount of cold energy in LNG is discarded without proper utilization at the LNG storage terminal. There are four conventional technologies for the regasification of LNG: Open Rack Vaporizer (ORV) [1], Submerged Combustion Vaporizer (SCV) [2], Ambient air-based Heating Vaporizer (AHV) and Intermediate Fluid Vaporizer (IFV) [3]. Conventional LNG regasification systems release cold energy to seawater or ambient air, which not only consumes power to drive pumps or blowers but also exerts influence on the environment and ecosystem nearby the LNG receiving terminal. In contrast, LNG cold energy can be utilized for power generation, air separation, dry ice production, and cold storage [4], etc. Power generation is a more flexible way to utilize the LNG cold exergy compared with other technologies. Organic Rankine cycles (ORCs), natural gas Direct Expansion (DE) are popular power generation technologies to utilize LNG cold exergy [5]. ORCs have been widely used for industrial waste heat recovery [6], geothermal energy utilization [7], and biomass utilization [8]. High-pressure natural gas can expand directly to target pressure to generate power. Exergy includes temperature-based exergy and pressure-based exergy [9]. The temperature-based exergy in LNG can be used as the heat sink in an ORC. The pressure-based exergy can be recovered by Direct Expansion (DE). Therefore, to exploit the exergy of LNG efficiently, ORCs and direct expansion of natural gas should be adopted simultaneously in the system.

The working fluid plays an important role in an ORC, and the topic has been studied extensively in the literature. Working fluid selection of an ORC for industrial waste heat recovery [10], engine waste heat recovery [11], geothermal energy utilization [12], solar energy utilization [13] and biomass utilization [14] has been investigated thoroughly. Saleh et al. [15] investigated 31 pure working fluids for an ORC recovering low-temperature waste heat. The ORC operates between 100℃ and 30℃ and the pressures are limited to 20 bars in this study. Lai et al. [16] compared organic working fluids, including alkanes, aromatics and linear siloxanes for high-temperature ORCs. The heat carrier inlet temperatures are assumed to be between 280℃ and 350℃. The results show that cyclopentane performs better than the other candidates. New working fluids such as R1234ze [17] and R1233zd [18] are promising alternatives to replace the conventional organic working fluids such as R245fa in ORCs. These working fluids show low global warming potential but are still very expensive [19]. It should be noticed that all these studies focus on ORCs recovering low-temperature heat and their working fluids are condensed by cooling water or air. In other words, the ORCs are operated above the ambient temperature. However, an ORC recovering LNG cold energy condensates below the ambient temperature and evaporates below or above the ambient temperature depending on the heat source. Therefore, ORCs recovering LNG cold energy operate below or across ambient temperature.

There are limited studies on working fluid selection for ORCs operating below or across ambient temperature. Lee and Han [20] proposed a multi-component working fluid ORC to recover waste heat and LNG cold energy simultaneously. They assumed the LNG evaporation pressure to be 30 bar. However, the evaporation pressure exerts great influence on the heat sink temperature level, which influences the ORC system directly. He et al. [21] studied an ORC utilizing exhaust waste heat and LNG cold energy for LNG-fired vehicles. They analyzed 5 potential working fluids, C_4F_{10}, CF_3I, R236ea, R236fa and RC318. Among them, R236fa shows the highest thermal efficiency. Rao et al. [22] investigated 16 potential working fluids for an ORC utilizing solar energy and LNG cold energy simultaneously. However, they assumed the maximum evaporation pressure of the ORC to be 20 bar, while the evaporation pressure of LNG was 30 bar. Sun et al. [23] compared different ORC configurations under several natural gas distribution pressures. However, only 4 working fluids are investigated in this study. Le et al. [24] proposed to use an ORC to recover the LNG cold energy combined with natural gas direct expansion. Propane is adopted as the working fluid in the ORC, while other working fluids are not investigated in this study. All the above studies investigated working fluid performance under given waste heat conditions or LNG regasification pressures. Therefore, these results are only applicable to the given conditions. Systematic investigation of working fluids under various conditions has not been reported yet in the literature.

There are generally two categories of working fluids, namely pure working fluids and mixture working fluids. Mixture working fluid shows higher thermal efficiency for a geothermal driven ORC in references [25] and [26]. Mixture working fluids can match well with the temperature profile of heat source due to the non-isothermal phase change. Therefore, mixture working fluids can reduce the irreversibilities in the evaporator and condenser. However, pure working fluids may also performs better than mixture working fluid as reported by Yu et al. [27]. They optimized an ORC recovering compression waste heat in an oxy-combustion power plant considering carbon capture process, and found that pure working fluid performed better than mixture working fluids in their case. Whether mixture working fluids can improve thermal efficiency or not depends on the waste heat conditions and the working fluid candidates investigated. In addition, mixture working fluids have some limitations. The heat transfer mechanism of mixture working fluids is not well known since the heat transfer coefficient of mixtures is difficult to predict. Another problem is the fractionation of the mixture in heat exchangers. To achieve large temperature glide during the phase change, the properties of the components in the mixtures should not be too similar. Thus, the fractionation is unavoidable for mixture working fluids. In summary, the mixture working fluids may suffer from the following problems [19]: (1) unknown thermodynamic properties, (2) unknown heat transfer mechanism, (3) higher equipment cost, and (4) composition shifting and fractionation.

Therefore, this study focuses on pure working fluid selection instead of mixture working fluid design. It should be noted that the pure working fluid selection is the basis of mixture working fluid design. The pure working fluid that behaves poorly for a specific ORC is probably not a good component of mixture working fluids. In addition, if a pure working fluid works well, it is not necessary to design a mixture working fluid.

In the ORC utilizing LNG cold energy, the condensation temperature is much lower compared with that of a conventional ORC, which results in totally different operating conditions. Most of the papers focus on ORCs operated above the ambient temperature. ORCs operated below and across ambient temperature are not widely studied. To the best knowledge of the authors, no systematic study of working fluid selection for ORCs operated below and across ambient temperature has been conducted. Working fluid selection for ORCs recovering LNG cold energy is quite important for the system design and merits to be investigated systematically.

2. System Description

LNG acts as the heat sink for the ORC, while the heat source, apart from the environment energy (air/seawater), could be low-temperature waste heat near the LNG terminal. Therefore, there are two types of heat sources, namely ambient energy (air/seawater) or low-temperature waste heat. In this study, seawater is assumed to be the heat source at ambient temperature. If the heat source is seawater, the ORC is operated totally below ambient temperature. In contrast, the ORC is operated across ambient temperature if waste heat is utilized simultaneously since the evaporating temperature of the ORC then should be higher than the ambient temperature.

An ORC aims at utilizing the temperature-based exergy of LNG, while Direct Expansion (DE) is an effective way to utilize the pressure-based exergy of LNG [23]. In DE, the high-pressure natural gas expands directly through an expander to generate power. Therefore, combining an ORC and DE recovering LNG cold energy simultaneously can boost the efficiency of LNG cold energy utilization significantly. The flowsheet of the combined cycle with seawater as the heat source is illustrated in Figure 1. In the ORC, the working fluid is heated to saturated or superheated vapor by the sea water and then fed to the ORC turbine. After expansion, the working fluid is condensed by LNG. In the DE, LNG is pumped to higher pressure and evaporates in the condenser of the ORC. The temperature of LNG at the outlet of the ORC condenser (LNG evaporator) is still very low. To boost the power generation from the direct expansion of natural gas, LNG is heated by seawater before being fed to the natural gas turbine. After expansion, natural gas can be used to cool down the outlet stream of the ORC turbine to reduce the heat load of the LNG evaporator and to increase the molar flow rate of the working fluid in the ORC. Finally, natural gas is heated by seawater to ambient temperature and delivered to the supplying system at the target pressure. In this process, the natural gas turbine and the ORC turbine generate power, while the LNG and ORC pumps consume power. The objective is to maximize the net power output of the system. In this flowsheet, the evaporation temperature of the ORC is below ambient temperature, thus the ORC is operating below ambient temperature. We call this system Combined ORC and DE with Seawater as a heat source (CODS) in this study.

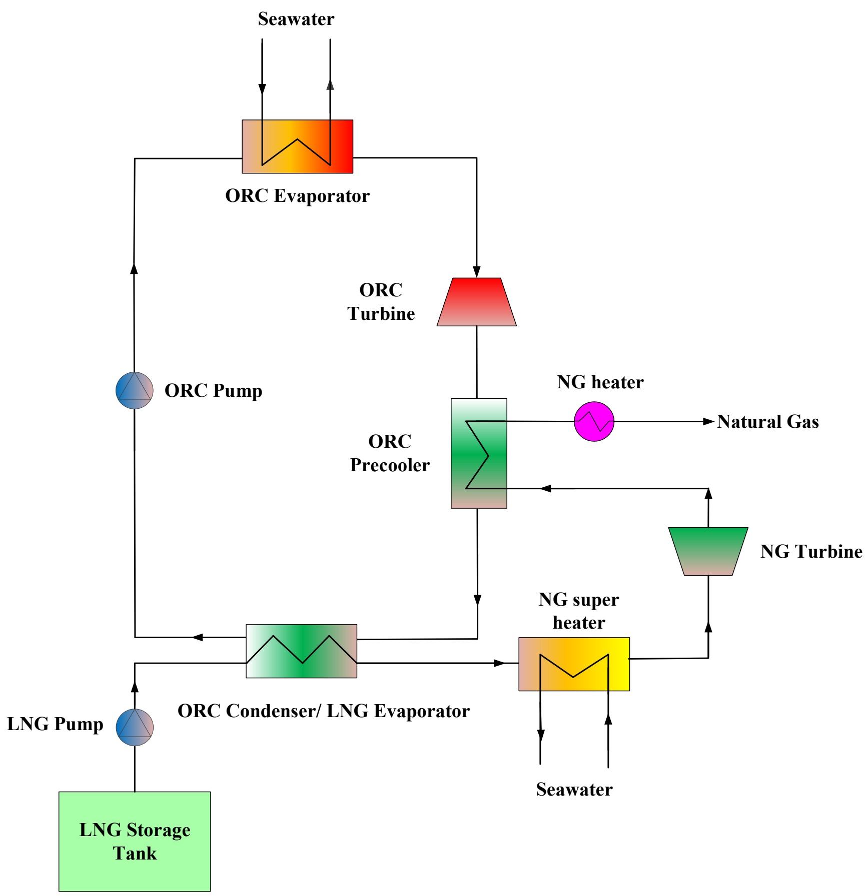

Fig. 1 Flowsheet of the Combined ORC and DE with Seawater as the heat source (**CODS**)

Similarly, if the heat source is waste heat from industry, the flowsheet of the system should be changed slightly as shown in Figure 2. The waste heat temperature from the industry is higher than the ambient temperature. In this case, seawater can be used to heat the working fluid close to the ambient temperature, and then the waste heat source heats the working fluid to a higher temperature to increase the power output of the ORC. After releasing heat to organic working fluid, the temperature of waste heat is still higher than the ambient temperature. Consequently, the waste heat can be used to heat the natural gas stream before the direct expansion. In this flowsheet, the evaporation temperature of the ORC is above the ambient temperature and the condensation temperature of the ORC is below the ambient temperature, thus the ORC is operating across ambient temperature. We call this system Combined ORC and DE with Waste heat utilization (**CODW**) in this study.

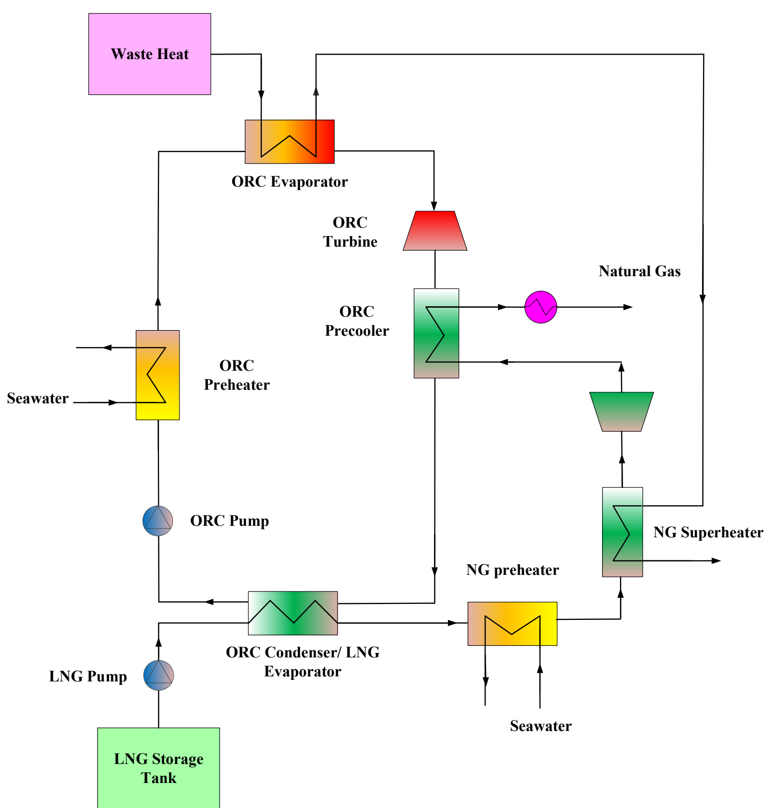

Fig. 2 The flowsheet of the Combined ORC and DE with Waste heat utilization (**CODW**)

It is obvious from a power output point of view that the ORC favors lower condensation pressure, while the DE favors higher LNG evaporating pressure. Thus, the power output of the DE is in conflict with that of the ORC, which results in a trade-off between ORC condensation pressure and LNG evaporation pressure. The ORC precoolers in both scenarios also exert great influence on both the ORC and the DE. The ORC and the DE are interacting with each other and the independent variables in this system are quite important for the optimization.

The regasified natural gas is finally delivered to the end-users. The target pressure depends on the application of the natural gas. LNG should be pumped to at least the target pressure to satisfy the specification of the end-users. The specifications of the target natural gas pressures in different applications are listed in Table 1 [28].

Table 1. Pressure specifications in different applications.

Applications	Pressure specification
Steam power stations	6 bar
Combined cycle stations	25 bar
Local distribution	30 bar
Long-distance distribution	70 bar

The working fluids and the operating conditions have considerable influence on the net power output of the system. To make a fair comparison of different working fluids, the comparison should be done under the respective optimal conditions of each working fluid. Thus, optimization of the system should be implemented while screening the working fluids. The optimal results are obtained from a simulation-based optimization framework, which will be discussed in detail in Section 4.

3. Working Fluid Preselection

Since there are many working fluid candidates, a preliminary selection is necessary to reduce the search space. The working fluids for conventional ORCs have been studied extensively in the literature. The desired working fluid should meet the requirements on environmental effects, thermophysical properties, chemical stability, etc. There are some desirable characteristics of working fluid in ORCs: (1) The working fluids should have no Ozone Depletion Potential (ODP) and low Global Warming Potential (GWP), (2) to avoid the formation of the liquid droplet at the outlet of a turbine, dry or isentropic working fluids are more favorable, (3) the working fluids should have high chemical stability, (4) non-fouling, non-corrosiveness, non-toxicity and non-flammability, and (5) easy availability and low cost. Based on these considerations, 22 working fluids are investigated as candidates for the ORC as listed in Table 2. Ahmadi et al. [29] reported that the transcritical CO_2 cycle is also an efficient way to utilize LNG cold energy and low-temperature heat. Therefore, CO_2 is also investigated in this study to make a comparison with organic working fluids. Some of them are good working fluids for a conventional ORC.

Table 2. Working fluid candidates investigated in this study

Working fluids	Chemical formula	T_c (°C)	P_c (bar)	T_s (°C) [a] at 1 bar	P_s (bar) [b] at T_0
R1150	C_2H_4	9.2	50.5	-104.20	-
R116	C_2F_6	19.9	30.4	-78.37	23.97
R23	CHF_3	25.9	48.2	-81.88	32.82
R170	C_2H_6	32.2	48.8	-88.94	30.37
R125	C_2HF_5	66.0	36.2	-48.39	9.07
R143a	$C_2H_3F_3$	72.7	37.6	-47.42	8.39
R32	CH_2F_2	78.1	57.8	-51.66	11.13
R290	C_3H_8	96.8	42.5	-42.49	6.36

R1270	C_3H_6	91.1	45.5	-48.24	7.78
R134a	$C_2H_2F_4$	101.0	40.6	-26.36	4.13
R227ea	C_3HF_7	101.7	29.1	-16.73	2.79
R3110	C_4F_{10}	113.2	23.2	-2.65	1.61
R152a	$C_2H_4F_2$	113.3	45.2	-24.20	3.72
RC318	C_4F_8	124.9	26.7	0.70	1.43
R236fa	$C_3H_2F_6$-D1	124.9	32.2	-1.15	1.56
R600a	C_4H_{10}-2	134.7	36.4	-11.96	2.19
R236ea	$C_3H_2F_6$	139.2	34.1	5.84	1.18
R600	C_4H_{10}-1	151.9	37.9	-0.77	1.48
R245fa	$C_3H_3F_5$-D1	154.1	36.4	14.66	0.83
R601a	C_5H_{12}-2	187.3	33.8	26.76	0.54
R601	C_5H_{12}-1	196.6	33.7	35.91	0.38
R744	CO_2	31.0	73.9	-88.10	44.91

Due to the low condensation temperature of the ORC utilizing LNG cold energy, there are extra factors to be considered while choosing the working fluid other than the well-known requirements for the working fluid in conventional ORCs as follows:

(I) The minimum condensation pressure is assumed to be 1 bar to avoid vacuum operation, and thus the saturation temperature at 1 bar is the minimum attainable condensation temperature. To avoid too much exergy destruction in the LNG evaporator, the saturation temperature at 1 bar should not be too high. In this study, the working fluids, whose saturation temperatures at 1 bar are greater than 0℃, are excluded for the ORCs investigated in this study. The fifth column of Table 2 lists the saturate temperatures of the working fluids at 1 bar. Promising working fluids for conventional ORC, such as R245fa, R601a and R601, are excluded due to the high saturation temperature at 1 bar as shown in Table 2.

(II) In CODS, the highest temperature of the working fluid is the ambient temperature neglecting the heat transfer temperature approach. Therefore, the saturation pressure at ambient temperature should be higher than the ambient pressure. However, to guarantee reasonable power output, the saturation pressure should be at least 2 bar to get a large enough pressure drop through the turbine. The last column lists the saturation pressures of the working fluids at ambient temperature. However, when the heat source is waste heat, this limitation is relaxed. The reason is that the waste heat can heat the working fluid to gaseous state at higher pressure.

(III) Due to the quite low temperature of the ORC recovering LNG cold energy, working fluids should not be subject to solidification [22] at very low temperature.

Based on the above analysis, R3110, RC318, R236fa, R236ea, R600, R245fa, R601a and R601 are excluded for CODS. For CODW, R3110, R236ea, R245fa, R601a and R601 are excluded. The other working fluids are investigated to screen the best working fluid for ORC in both CODS and CODW.

4. Simulation-based Optimization Framework

To make a fair and reasonable decision on the best working fluid, the performance of different working fluids should be compared under their respective optimal operating conditions. Therefore, optimization of the system should be implemented while screening the working fluids. Since the thermodynamic properties are expressed in highly nonlinear and nonconvex equations, optimization of the combined cycle is challenging for deterministic optimization algorithms. Surrogate models or simplified models are possible alternatives to replace the rigorous thermodynamic model during optimization. However, accurate thermodynamic calculations are important for reliable results. In this study, to guarantee both accurate thermodynamic properties and efficient solution of the optimization problem, we propose a simulation-based optimization framework to optimize the combined cycle.

The simulation of the process is implemented in Aspen HYSYS [30], which can provide accurate thermodynamic properties. The specifications of the simulation are as follows: Peng-Robinson Equation of State is adopted to calculate the thermodynamic properties of the working fluids. The LNG composition is taken from [20] and shown in Table 3. However, there was a small typo in the original paper. The components should be n-C_4H_{10} and iso-C_4H_{10} instead of n-C_4H_8 and iso-C_4H_8. The mass flowrate of LNG is 1620 t/h, corresponding to the Incheon LNG terminal in South Korea [20]. However, 1620 t/h is a too large number for the simulation and optimization. Therefore, the mass flowrate of LNG is assumed as 1620 kg/h in this study. The LNG is supplied at -162°C and 1 bar. The polytropic efficiency of the turbine is assumed to be 80%. The adiabatic efficiency of the pumps is assumed to be 75%. The pressure drop in heat exchangers is neglected. The seawater is able to heat the working fluid and natural gas to 10°C. The target pressure of the natural gas depends on the application as shown in Table 1 [20].

Table 3 Composition of the LNG

Component	Mole fraction
Nitrogen	0.0007
Methane	0.8877
Ethane	0.0754
Propane	0.0259
Butane	0.0056
Iso-butane	0.0045
Pentane	0.0001
Iso-pentane	0.0001
Total	1.0000

Other than the above-fixed parameters, there are many variables in the system. However, some of them are correlated and dependent variables. It is quite important to analyze the degree of freedom for the system and choose the correct independent decision variables. Since the optimization involves a multi-dimensional space formed by the key operating parameters of the combined cycle, it is challenging and computationally intensive to get the optimal operating conditions of the combined cycle. Deterministic algorithms are quite challenging due to the complex thermodynamic property calculations in this study. The inbuilt optimization capability of HYSYS is too weak to get satisfactory results. Stochastic algorithms represent a promising choice for this problem. The Particle Swarm Optimization (PSO) algorithm is adopted as the optimization engine in this study. PSO is a population-based stochastic optimization method, which is inspired by the social behavior of bird flocking [31]. Due to the nature of meta-heuristic algorithms, there is no guarantee on the global optimum solutions. Matlab and HYSYS are connected by creating a COM object through the actxserver command. The combination of rigorous thermodynamic simulation and stochastic optimization can guarantee accurate thermodynamic properties and optimal conditions. The flowsheet of the framework is shown in Figure 3.

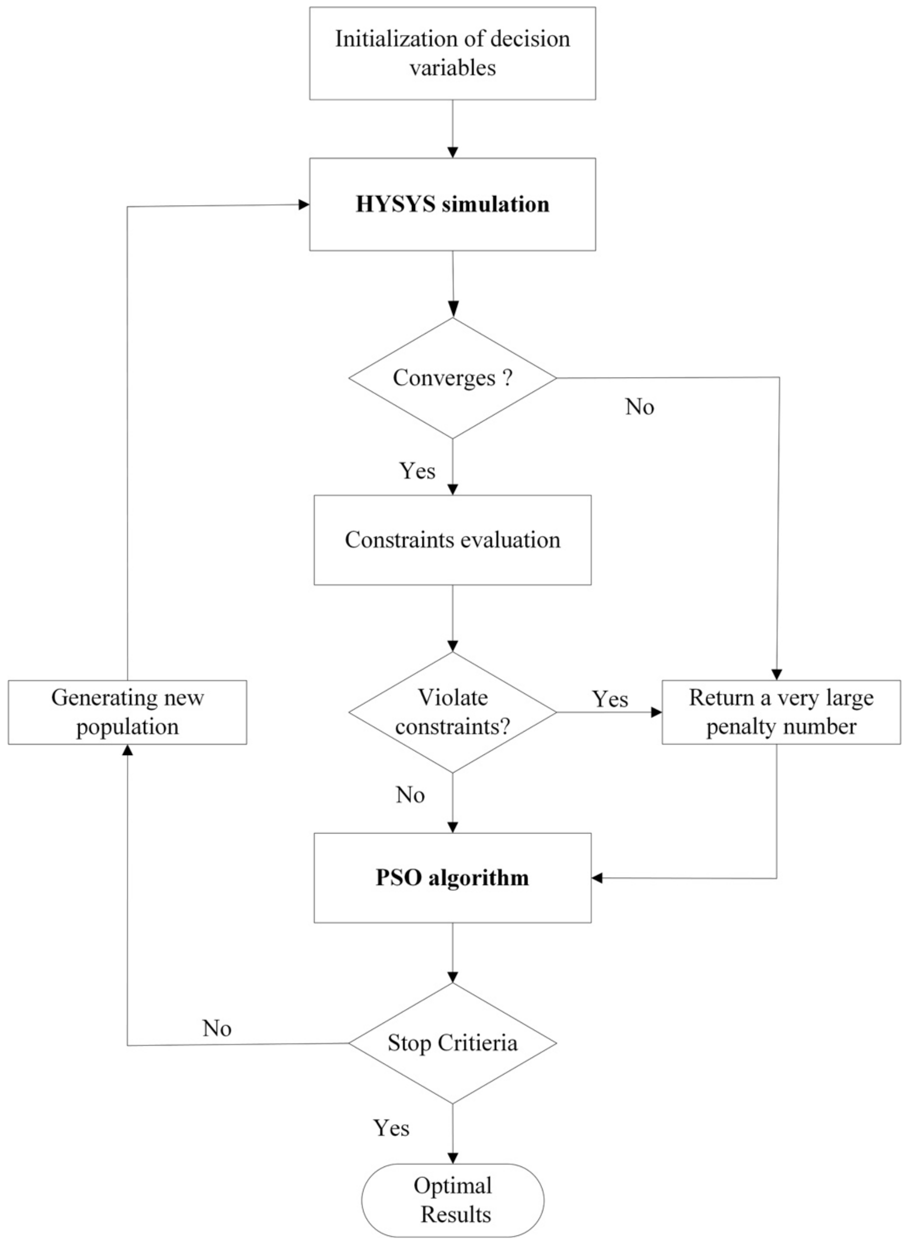

Fig. 3 Simulation-based optimization framework

The optimization model is established in Matlab. The objective function, variables, upper and lower bounds, and constraints are discussed in the following:

Objective function: Net power output of the combined cycle is chosen as the criterion to evaluate all the working fluids.

Variables: Based on a degree of freedom analysis of the system, the independent variables can be determined. In CODS, there are 5 independent decision variables, namely the condensation pressure of the ORC ($P_{orc,con}$), the evaporation pressure of the ORC ($P_{orc,eva}$), the molar flowrate of working fluid (mf_{orc}), the evaporation pressure of LNG ($P_{lng,eva}$), and the heat load of the LNG evaporator ($Q_{lng,eva}$) as shown by the variables with superscript a in Table 4. In CODW, there are two more decision variables, namely heat load of the ORC evaporator ($Q_{orc,eva}$) and heat load of the NG superheater ($Q_{ng,sh}$), which results in 7 decision variables in total. These variables are denoted with superscript b as shown in Table 4.

Variable bounds: The lower bound of the ORC condensation pressure is set as 1 bar to avoid vacuum operation. The upper bound of the condensation pressure is set as the saturate pressure at the ambient temperature in this study to guarantee the condensation process takes place below ambient temperature. However, if the critical temperature of the working fluid is lower than the ambient temperature, there is no saturation pressure at ambient temperature. In this case, the upper bound of the condensation pressure is set as the critical pressure. Therefore, the upper bound of the condensation pressure is either saturation pressure at 1 bar or critical pressure.

The lower bound of the ORC evaporation pressure is 2 bar to guarantee a large enough pressure drop in the turbine. The ORC evaporation pressure is less than the critical pressure of the working fluid since the ORCs are subcritical. However, the highest attainable temperature of the working fluid is the ambient temperature in CODS. Then the upper bound of the ORC evaporation pressure is the critical pressure or the saturation pressure at ambient temperature (if it exists). In CODW, the evaporation temperature should be above the ambient temperature. Therefore, the lower bound of the evaporation pressure is the saturation pressure at the ambient temperature, and the upper bound is the critical pressure of the working fluid.

LNG regasification pressure must be higher than the distribution pressure of the natural gas. Therefore, the lower bound of LNG regasification pressure is set as the distribution pressure of the natural gas. The upper bound of LNG pressure is set as 150 bar based on reference [32]. The lower and upper bounds for other variables are shown in Table 4. These bounds are rational for the system with LNG flowrate being 1620 kg/h.

Table 4. Lower and upper bounds for the decision variables in this study

Variables	Lower Bounds	Upper Bounds
Condensation pressure (bar)[a,b]	1	$\min\left\{P_c, P_s^{T_0}\right\}$
Evaporation pressure (bar)[a]	2	$\min\left\{P_c, P_s^{T_0}\right\}$
Evaporation pressure (bar)[b]	$P_s^{T_0}$	P_c
LNG evaporation pressure (bar) [a,b]	P_t	150
Working fluid molar flowrate (mole/s) [a,b]	10	200
LNG evaporator heat load (kW) [a,b]	10	500
ORC evaporator heat load (kW) [b]	50	400
NG superheater heat load (kW) [b]	0	300

[a] variable bounds used for CODS

[b] variable bounds used for CODW

Constraints: There are two categories of constraints in this model, namely the constraints to guarantee the normal operation of the system and the constraints to guarantee the system is economically viable.

The inlet stream of the ORC and the natural gas turbines should be totally gas.

$$\mathrm{VF}_{orc,tur,in} = 1 \qquad \text{(Constraint 1)}$$

$$\mathrm{VF}_{ng,tur,in} = 1 \qquad \text{(Constraint 2)}$$

The inlet stream of pumps should be totally liquid.

$$\mathrm{VF}_{orc,pump,in} = 0 \quad \text{(Constraint 3)}$$

The vapor fraction at the outlet of the ORC and the natural gas turbines should be greater than 0.95.

$$\mathrm{VF}_{orc,tur,out} \geq 0.95 \quad \text{(Constraint 4)}$$

$$\mathrm{VF}_{ng,tur,out} \geq 0.95 \quad \text{(Constraint 5)}$$

To guarantee the design is economically viable, the minimum approach temperature of heat exchangers has corresponding constraints. The minimum approach temperature of LNG evaporator and ORC precooler should be greater than 3°C.

$$\Delta\mathrm{T}_{lng,eva,min} \geq 3 \quad \text{(Constraint 6)}$$

$$\Delta\mathrm{T}_{orc,pre,min} \geq 3 \quad \text{(Constraint 7)}$$

For the CODW, two more constraints should be added to the model. The minimum approach temperatures of the ORC evaporator and natural gas superheater are assumed to be 3°C and 5°C respectively.

$$\Delta\mathrm{T}_{orc,eva,min} \geq 3 \quad \text{(Constraint 8)}$$

$$\Delta\mathrm{T}_{ng,sh,min} \geq 5 \quad \text{(Constraint 9)}$$

The mathematical model can be written as follows:

$$\begin{aligned}
&\max_{x\in\Omega} \quad \text{Net Power Output} \\
&\text{s.t.} \\
&\Omega = \left\{ x \;\middle|\; \begin{matrix} \text{thermodynamic model} \\ \text{flowsheet model} \\ \text{constraints 1-9} \end{matrix} \right\}
\end{aligned}$$

All the constraints are formulated using a penalty function in the Matlab model. Once any of the above constraints are violated, a large penalty is assigned to the objective function.

In this study, the large penalty is assumed to be 10e6. The swarm size is 50 and the maximum iteration is assumed to be 100 to get the results in practical time limitation. The code and PSO algorithm are implemented and run in Matlab 2014b environment on a PC with 4 cores 2.8 GHz Intel i7 CUP and 32 GB of RAM.

5. Results and Discussion

The optimization results for CODS and CODW are provided in Sections 5.1 and 5.2 respectively.

5.1 Working fluid selection for ORCs below ambient temperature

In CODS, the ORC is operated totally below the ambient temperature since both the evaporation temperature and the condensation temperature are less than the ambient temperature. Seawater can be regarded as a latent heat source because the temperature drop of seawater is very small. Yu et al. [10] investigated working fluid selection for sensible, latent and combined waste heat sources. For a latent heat source, there is no pinch limitation between the heat source and the organic working fluid. Therefore, there are no pinch temperature constraints in this case, and the working fluid is assumed to be heated to 10°C by the seawater.

Figure 4 illustrates the net power output of the system under different natural gas target pressures. It is clear that with the increase of the LNG target pressure, the net power output of the system decreases dramatically, which mainly results from the reduction of the power output from natural gas direct expansion. The numbers in the figure indicate the top 4 working fluids with respect to net power output. It is interesting that R290, R1270, R125 and R143a are the top 4 working fluids under all the target pressures.

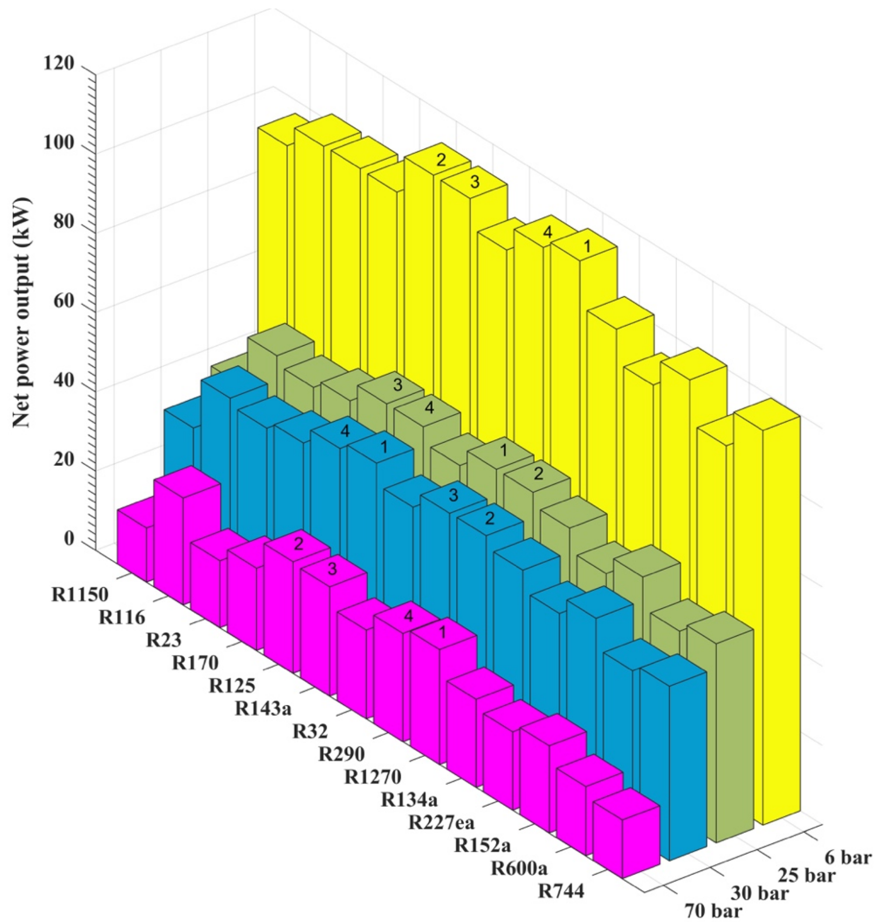

Fig. 4 Power output of working fluids under different target pressure

The detailed results of the top 4 working fluids under different target pressures are listed in Table 5. The most energy efficient working fluids are R125, R143a, R290 and R1270. It can be seen that when the target pressure is 6 bar, the condensation pressure of the ORC is 1 bar for all the top 4 working fluids. The evaporating pressure of the ORC reaches the upper bound, which is the saturation pressure at the ambient temperature. The results are consistent with the intuitive expectation. The evaporation pressure should be as high as possible to boost the power output. On the other hand, the results illustrate that superheating is not favorable in the ORC in this scenario since all optimal results indicate that vapor is saturated at the inlet of the ORC turbine. Since the seawater for simplicity is regarded as a latent heat source, it is not necessary to superheat working fluids to get better match with the sea water. It can be concluded that the favorable working fluids for an ORC utilizing LNG cold energy without waste heat utilization should have high enough saturation pressure at ambient temperature. Referring to Table 1, the top 4 working fluids has the characteristic that the saturate temperature at 1 bar is between -40 °C to -50°C. For the CODS configuration as shown in Figure 1, one could conclude that the promising working fluids are those with saturation temperatures at 1 bar between -40°C to -50°C. The reason can be explained as follows: The minimum attainable condensation temperature is the saturation temperature at 1 bar. The working fluids whose saturation temperature at 1 bar are greater than -40°C cannot attain low condensation temperature, which results in large heat transfer approach temperatures and consequently large exergy destruction in the LNG evaporator. In addition, such working fluids generally have low saturation pressure at ambient temperature as shown in Table 1, and thus generally generate less power output since the pressure ratio is small. Due to these reasons, the working fluids whose saturation temperatures are greater than -40°C do not perform well in CODS. The working fluids whose saturation temperature at 1 bar is less than -50°C can attain very low condensation temperature, but the evaporation pressure of LNG is limited by the condensation temperature of the ORC. If the condensation temperature of the ORC is very low, the evaporation pressure of LNG cannot be very high, which reduces power output from the natural gas turbine. Therefore, the lower attainable condensation temperature of the ORC does not indicate a higher overall power output of the system. The trade-off between the ORC power output and the DE power output means there is an optimal condensation pressure of the ORC. Therefore, the working fluids whose saturation temperatures at 1 bar are less than -50°C are not desirable working fluids either. With increasing natural gas target pressure (and correspondingly increasing LNG evaporation pressure), the condensation temperature of the ORC working fluid increases as well. Therefore, the net power output of the whole system decreases significantly due to power output reduction of both the ORC and the DE. It can be noticed from Table 5 that the four working fluids have condensation pressures close to 1 bar for all natural gas target pressures except for R125 and R1270 at 30 bar target pressure. Still, the net power output for these two working fluids are in line with the behavior of the other working fluids at increased natural gas target pressure. This indicates that the search space is quite complex and the problem may have multiple optimal solutions. This also reveals that with a similar net power output of the system, there may be large differences in operating conditions for the different designs. Based on the above analysis, the optimal working fluids prone to be the ones whose saturation temperature at 1 bar is in the range -50°C to -40°C. Such working fluid show both good thermal match in the LNG evaporator and acceptable ORC power output.

Table 5. The performance of top 4 working fluids under different target pressures in CODS.

Target pressure	Working fluids	W_{net} (kW)	$P_{orc,con}$ (bar)	$P_{orc,eva}$ (bar)	mf (mole/s)	$P_{lng,eva}$ (bar)	$Q_{lng,eva}$ (kW)	$\Delta T_{lng,eva,LMTD}$ (°C)	$T_{orc,con}$ (°C)	$W_{orc,tur}$ (kW)	$W_{orc,pump}$ (kW)	$W_{ng,tur}$ (kW)	$W_{lng,pump}$ (kW)
6 bar	R125	112.25	1.00	9.06	51.61	56.03	236.69	21.04	-48.39	48.59	1.22	71.93	7.05
	R143a	112.10	1.00	8.39	53.50	57.64	236.39	21.12	-47.41	48.08	1.05	72.33	7.26
	R290	111.27	1.00	6.35	57.85	62.17	241.72	22.55	-42.53	46.66	0.87	73.32	7.84
	R1270	113.65	1.00	7.77	56.99	59.00	231.17	20.39	-48.23	49.42	0.99	72.65	7.43
25 bar	R125	59.06	1.00	9.06	35.42	116.54	167.53	25.66	-48.39	33.24	0.84	41.49	14.83
	R143a	59.03	1.00	8.39	36.76	114.59	170.06	25.68	-47.41	32.99	0.72	41.34	14.58
	R290	59.79	1.00	6.35	41.28	104.31	186.37	25.61	-42.53	33.31	0.62	40.36	13.26
	R1270	59.74	1.00	7.77	39.92	130.59	162.60	26.08	-48.23	34.62	0.69	42.45	16.64
30 bar	R125	52.28	1.41	9.07	38.90	94.55	197.06	24.96	-41.07	31.08	0.89	34.09	12.00
	R143a	54.31	1.00	8.39	41.83	62.99	230.08	18.95	-47.41	37.55	0.82	25.53	7.95
	R290	53.19	1.03	6.35	40.14	121.05	179.19	26.73	-41.86	31.89	0.60	37.31	15.41
	R1270	53.29	1.44	7.77	44.02	111.39	188.74	26.31	-39.81	31.83	0.73	36.36	14.17
70 bar	R125	28.16	1.00	9.07	9.07	107.21	191.67	21.37	-48.39	29.51	0.74	13.02	13.63
	R143a	27.60	1.00	8.38	8.38	103.75	176.87	23.85	-47.41	29.23	0.64	12.19	13.18
	R290	27.35	1.01	6.36	6.36	101.43	200.96	22.39	-42.27	29.18	0.54	11.60	12.89
	R1270	29.04	1.00	7.77	7.77	116.33	167.52	25.73	-48.23	29.45	0.58	14.98	14.81

Table 6. The performance of remaining working fluids in CODW after preselection.

Working fluids	W_{net} (kW)	$P_{orc,con}$ (bar)	$P_{orc,eva}$ (bar)	mf (mole/s)	$P_{lng,eva}$ (bar)	$Q_{lng,eva}$ (kW)	$\Delta T_{lng,eva,LMTD}$ (°C)	$T_{orc,con}$ (°C)	$\Delta T_{orc,eva,LMTD}$ (°C)	$W_{orc,tur}$ (kW)	$W_{orc,pump}$ (kW)	$W_{ng,tur}$ (kW)	$W_{lng,pump}$ (kW)
R116	150.14	1.41	30.38	44.34	40.20	320.14	15.79	-71.61	26.69	88.72	4.20	70.64	5.01
R23	151.77	2.99	47.16	35.42	104.72	144.89	24.94	-60.57	38.20	59.32	2.98	108.74	13.31
R170	161.10	2.44	48.80	57.90	32.73	242.01	16.38	-70.51	25.19	103.80	5.74	67.09	4.05
R125	152.80	1.00	36.19	41.97	84.18	185.04	23.59	-48.39	31.86	81.41	4.32	86.38	10.67
R143a	160.16	1.00	37.64	46.59	74.36	191.99	26.55	-47.41	8.87	97.08	4.53	77.02	9.40
R32	145.38	1.00	37.35	23.32	105.17	129.53	49.02	-51.65	43.54	44.80	1.34	115.28	13.37
R290	155.45	1.00	42.49	38.30	86.31	185.17	34.21	-42.53	9.54	82.61	4.45	88.23	10.94
R1270	145.77	1.00	45.50	22.50	136.84	113.56	58.34	-48.23	41.60	44.61	2.56	121.15	17.44
R134a	139.88	1.00	40.54	24.40	109.92	142.19	72.11	-26.36	21.42	52.19	2.64	104.31	13.98
R227ea	129.97	1.00	29.11	23.58	106.98	100.14	100.61	-16.72	41.74	39.38	2.68	106.88	13.60
R3110	119.03	1.00	23.23	27.88	87.61	159.45	93.87	-2.64	27.74	43.37	3.40	90.16	11.11
R152a	142.11	1.00	45.00	40.89	87.60	210.48	49.10	-24.20	8.85	69.36	4.33	88.19	11.11
R236fa	126.58	1.00	32.19	21.63	96.74	141.47	101.28	-1.15	10.10	42.85	2.62	98.64	12.28
R600a	134.14	1.00	33.73	28.61	106.50	119.04	97.90	-11.96	8.69	50.57	3.38	100.49	13.54
R600	130.83	1.00	25.00	12.67	118.78	22.44	146.72	-0.76	14.24	24.70	1.08	122.33	15.12
R744	143.65	6.02	73.91	29.57	119.39	109.42	57.06	-52.52	48.52	41.14	2.82	120.53	15.20

5.2 Working fluid selection for ORCs across ambient temperature

In CODW, the ORC is operated across the ambient temperature. Since waste heat is considered in CODW, the characteristics of CODW have great influence on the system design. Therefore, it is difficult to know which working fluid performs better than others in CODW without given waste heat conditions. To decide on the optimal working fluid, the waste heat conditions have to be fixed. In this part, the waste heat source in the CODW is assumed to be the compression heat of the flue gas in a natural gas combined cycle power plant. The treated flue gas can be regarded as pure CO_2. Since the LNG mass flowrate is assumed to be 1620 kg/h, the molar flowrate of CO_2 should be 9509 kg/h based on the combustion of natural gas given in this study. The inlet temperature of compression heat is assumed to be 150°C. The target pressure of natural gas is fixed at 6 bar since the natural gas is used to fire the power plant. Since the critical temperature of R1150 is only 9.2°C, the seawater can even heat the working fluid to superheated state and the degree of superheating in the ORC evaporator will be extremely large in the CODW. For RC318, R236ea, R245fa, R601a and R601, the saturate temperature at 1 bar is greater than 0°C. These working fluids will have large exergy destruction in the LNG evaporator due to very large heat transfer approach temperature. Therefore, R1150, RC318, R236ea, R245fa, R601a and R601 are not appropriate working fluids in this scenario. The performance of different working fluids for an ORC operating across ambient temperature is shown in Figure 5. The detailed results are listed in Table 6.

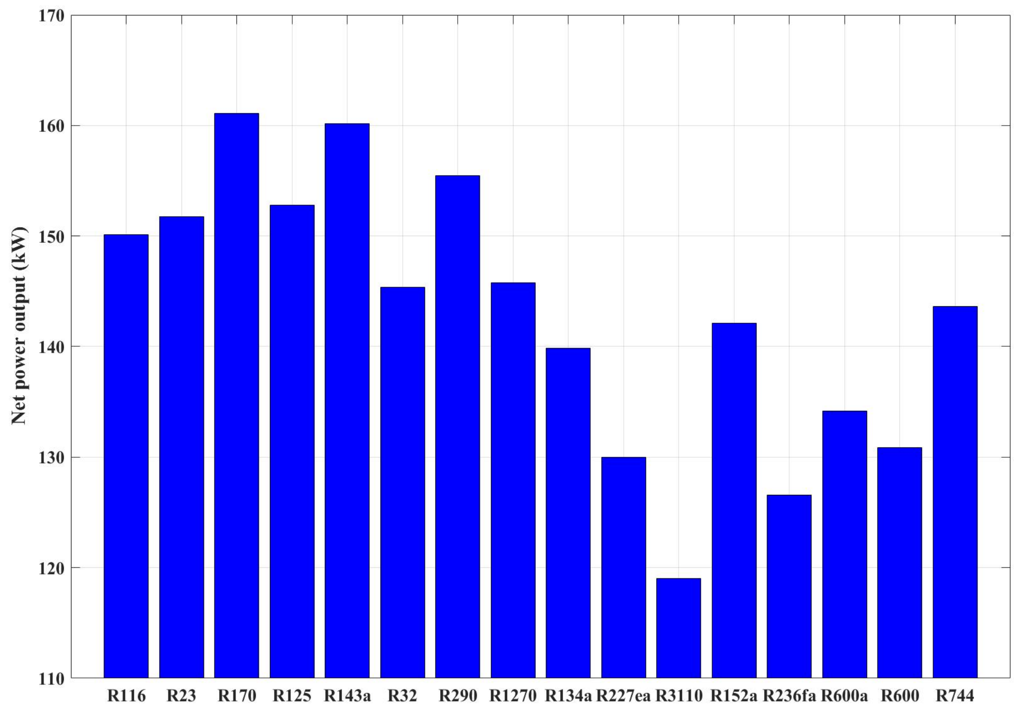

Fig. 5 Power output of working fluids in CODW

R170, R143a and R290 shows much higher net power output compared with other working fluids. The reason can be explained as follows: For working fluids with higher critical temperatures, the condensation temperatures at 1 bar are higher. Therefore, exergy destruction in the LNG evaporator will be very large due to the large heat transfer approach temperature. Similarly, the working fluids with lower critical temperature can attain lower condensation pressures, which results in smaller exergy destruction in the LNG evaporator. Since the evaporation pressure is limited by the critical pressure, the working fluids with low critical temperatures have to be superheated to a large extent to match well with the waste heat. Due to the low heat transfer coefficient for superheated gases, the capital cost of the ORC evaporator could increase significantly. As indicated in Table 6, for working fluids from R125 to R236fa the evaporation pressures are (close to) the critical pressures, which indicate that supercritical ORCs could perform better than subcritical ORCs in this scenario. R744 (CO_2) does not perform well since the evaporation pressure is limited by the critical pressure. However, supercritical ORCs are out of the scope of this study and deserves more attention in future research. In CODW, the working fluids with lower critical temperatures have to be superheated to a large extent.

Figure 6 illustrates the logarithmic mean temperature difference (LMTD) of LNG and ORC evaporators for different working fluids. With the increase of the critical temperatures of working fluids, the LMTD of the LNG evaporator generally increases because of higher condensation temperature in the ORC. On the contrary, the LMTD of the ORC evaporator generally decreases due to better thermal match for working fluids with higher critical temperature. R170, R134a and R290 can balance the LMTD of the LNG and ORC evaporators properly, therefore these working fluids perform better than other working fluids. However, the LMTD is still very large for these working fluids, which results in significant exergy destruction. This indicates that the system configuration has its own limitations and motivates the search for new system configurations. It can be inferred that one stage ORCs cannot utilize the cold energy and waste heat efficiently. Beyond the working fluid screening, new system configurations such as cascaded ORCs, series ORCs and multi-stage ORCs are promising ways to boost the exergy efficiency of the system. However, the capital cost of cascaded ORCs and series ORCs is definitely much higher. Therefore, cascaded ORCs and series ORCs with economic evaluation should be investigated in future research. For the CODW case investigated in this study, the top 3 working fluids are R170, R143a and R290.

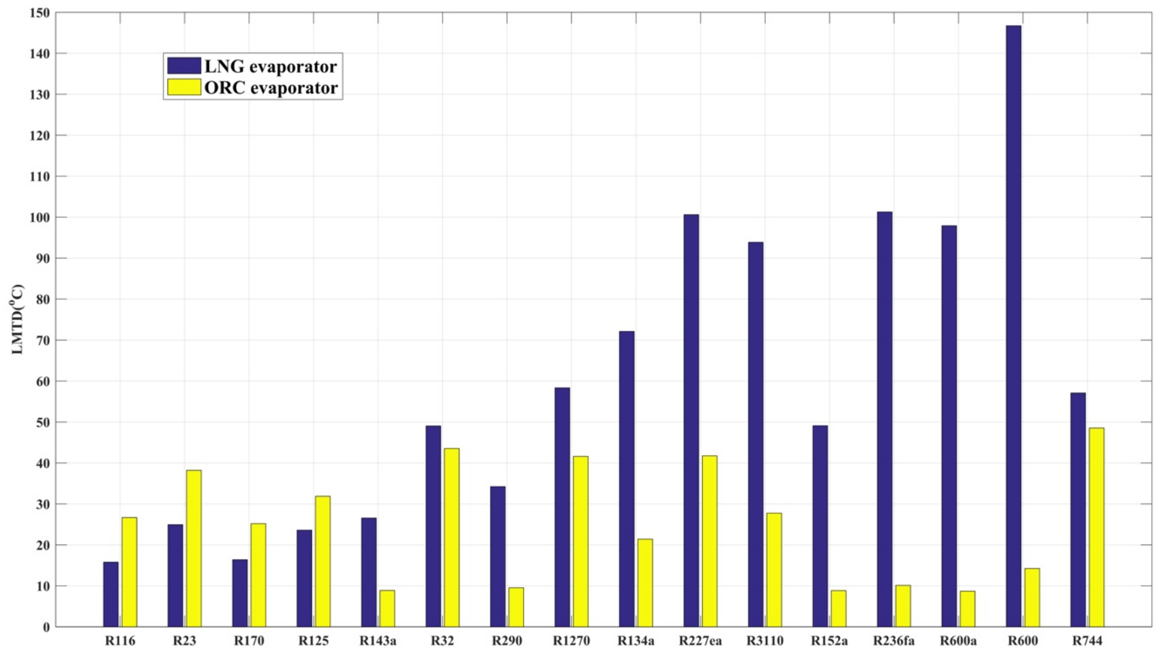

Fig. 6 LMTD for LNG and ORC evaporators in CODW

6. Conclusion

A combined single-stage Organic Rankine Cycles (ORCs) and Direct Expansion (DE) cycle recovering LNG cold energy with/without waste heat utilization are investigated in this study. The paper addresses the working fluid selection for such a combined cycle, where the ORC is operated below or across the ambient temperature. Therefore, the ORC investigated in this study is quite different from the conventional ORC system for low-temperature heat utilization. The favorable working fluids for conventional ORCs are inappropriate and even not operable due to the quite low operating temperature of the ORC utilizing LNG cold energy. A systematic investigation of the working fluids for the ORC is performed in this study. A simulation-based optimization framework is proposed based on the connection between Aspen HYSYS and Matlab. The evolutionary Particle Swarm Optimization has been adopted in this study. 22 working fluids are investigated in this study for different LNG cold energy utilization scenarios with/without waste heat utilization.

For CODS, the following conclusions are drawn:

- The top 4 working fluids under all the targets pressures of the regasified natural gas are R290, R1270, R125 and R143a.
- Working fluids whose saturation temperature at 1 bar is in the range -40°C to -50°C are promising candidates for the ORC in CODS.
- Since the top 4 working fluids are the same under different natural gas target pressures, the target pressure of natural gas has little effect on the optimal working fluids.

For CODW, the following conclusions are drawn:

- In this scenario, the heat capacity flowrate of the waste heat source has great influence on the system. The optimal working fluids depend on the waste heat conditions. Therefore, it is not possible to conclude about the optimal working fluid without knowing the conditions of the waste heat.
- For the case when flue gas compression heat in an LNG fired power plant is utilized as the heat source, the top 3 working fluids are R170, R143a and R290.
- There is still large exergy destruction in the LNG and ORC evaporators even for the top 3 working fluids. This indicates that working fluid screening can only improve the exergy efficiency to a limited extent, and new system configurations should be investigated simultaneously with working fluid selection in future research.

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Nomenclature

Symbols

mf	Molar flow rate
P	Pressure
Q	Heat load
T	Temperature
VF	Vapor fraction
x	Independent variables
Ω	Search space
η	Efficiency
ΔT	Minimum heat transfer approach temperature
T_0	Ambient temperature

Subscripts

c	Critical
con	Condensation/Condenser
eva	Evaporation/Evaporator

in	Inlet
min	Minimum
net	Net power output
ng	Natural gas
out	Outlet
pre	Precooler
pump	Pump
sh	Superheater
tur	Turbine
t	Target

Acronyms

AHV	Ambient air-based Heating Vaporizer
CODS	Combined ORC and DE with Seawater
CODW	Combined ORC and DE with Waste heat
DE	Direct Expansion
GWP	Global Warming Potential
IFV	Intermediate Fluid Vaporizer
LMTD	Logarithmic Mean Temperature Difference
LNG	Liquefied Natural Gas
ODP	Ozone Depletion Potential
ORC	Organic Rankine Cycle
ORV	Open Rack Vaporizer
PSO	Particle Swarm Optimization

SCV	Submerged Combustion Vaporizer

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