A Novel Organic Rankine Cycle System for Heavy Duty Diesel Engines

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Abstract

Due to increasing CO_2 emissions and fuel costs there is a growing interest in heat to power conversion techniques for Heavy Duty Diesel Engines (HDDE). The use of Rankine Cycle (RC) and Organic Rankine Cycles (ORC) on long-haul HDDE is seen as a possible way to improve the overall system efficiency. The key consideration in the research and development efforts for ORCs is to investigate and identify technical paths that may improve the practicality of such a concept. For this, simple solutions are vital for a timely deployment of the technology to meet the anticipated CO_2 regulations.

To provide a potential solution, this paper presents a novel ORC system to address the shortcomings of the conventionally proposed cascade system. This novel system is a function of a new working fluid (i.e. water-propanol blend), its associated cycle operating mode (i.e. superheated expansion) and an innovative architecture (i.e. direct engine block heat recovery). Simulations conducted in Aspen HYSYS showed that the system delivered a 20% improvement in power, a 2/3rd reduction in the total heat exchanger footprint, and a reduced complexity compared to the cascade system. Implementation of this system at rated HDDE condition generated 6.9% of additional engine crankshaft power.

Keywords organic Rankine cycle; cascade system; water blend; heat recovery architecture; dual pressure system; Aspen HYSYS.

1 Introduction

In a typical HDDE up to 50% of the total fuel energy is wasted in the form of heat. Converting this waste heat into usable mechanical or electrical power is seen as a key area in the development of low carbon powertrains [1]. This is an ongoing area of intensified research, where numerous methods have been demonstrated. These methods include, but are not limited to, turbocompounding (mechanical, electrical), thermoelectric generators and fluid bottoming cycles [2, 3]. Amongst the fluid bottoming cycle options for an output capacity of less than 25 kW, ORCs using refrigerants are shown to be better adapted to a heat source quality of less than 250°C due to fluid molecular make-up [4]. On the other hand, due to the large latent heat of water, RC is favoured for a heat source quality greater than 500°C [5]. ORCs are in fact being adopted as a premier technology for long-haul HDDEs when considering conversion efficiencies, technology readiness level, impending CO₂ legislations, absolute fuel consumption, base vehicle cost, space availability and weight penalty. Key components like heat exchangers (HEX) and expansion machines (piston expanders, radial turbines) are becoming more viable due to a series of recent technological advancements and synergies with the current automotive components [6, 7]. The current market niche for ORCs is dependent on simplicity and affordability, with initial technology deployment on commercial vehicles expected in the 2020-2025 timeframe in the European Union and the United States.

This paper firstly presents the simulation results of a cascade system to form a baseline for comparison. Secondly, the shortcomings of such a system are detailed for automotive applications. Finally, to partially address the shortcomings and facilitate the introduction of ORC systems for long haul applications, a novel system is proposed and examined. The paper extends the analysis of parallel works [8]. The simulations were conducted in an advanced chemical process modelling tool, Aspen HYSYS [9]. The primary objective functions for comparison between the two systems included system power, heat transfer footprint and size of the expansion machine. For a comprehensive view, the performance aspects were based on the energy equations in all the specific points of the cycle.

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2 Baseline cascade system

The availability of exhaust heat and engine coolant heat at two vastly different qualities but similar quantity levels is usually a challenge for the application of conventional single-loop ORC setups [10]. Cascade systems which utilise independent heat recovery systems to match the specific source characteristics provide a potential solution [11]. As a result, cascade systems appear to be a preferred option for high exploitation of exhaust and engine coolant heat in the published literature, offering a reference for comparison. A cascade system consists of two different temperature level cycles. The two closed-loop cycles, the High-Temperature (HT) and the Low-Temperature (LT) cycles are interconnected at least by a common HEX. The common HEX termed 'cascade condenser' is effectively an internal heat exchanger for the system. The cascade condenser acts as a condenser for the HT cycle and as an evaporator for the LT cycle. Only the condenser of the LT cycle plays a role in dissipating heat out of the cascade system. Due to the high temperature differential across the system, need to limit exergy destruction and design considerations, two distinct working fluids are used. A higher boiling point fluid (e.g. water) is used in the HT cycle, while the LT cycle utilises a relatively lower boiling point fluid (e.g. refrigerant).



Figure 1: Cascade system (water, R245fa) (a) thermal and subsystem architecture (b) T-S diagram at the selected optimal condition (c) variation in thermal loads with HT cycle pressure (d) variation in performance with HT cycle pressure

This section presents the simulation results for the cascade system shown in Figure 1(a) using water and R245fa combination to act as a baseline for comparison. The HT cycle recovered the exhaust heat downstream of the after-treatment devices. Whereas the LT cycle recovered the engine coolant heat and the cascade heat load in series. Only engine block heat recovery was considered in this work. This is since, lubricant heat, due to piston cooling, is typically 20% of the engine block heat, and was excluded from heat recovery considerations due to low quality and quantity. The bypass lines for the two expanders with pressure reducing valves were excluded for simplicity. Furthermore, storage tanks prior to the two pumps and an exhaust flow bypass valve were also omitted.

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Table 1 summarises the modelling assumptions used for the cascade system corresponding to realistic temperatures, component efficiencies, performances and pressure losses. Table 1 also summarises the results for the 12.8 liter base engine at the rated condition [12], operating with a high efficiency Selective Catalytic Reduction (SCR) system as the only means to meet the Euro 6 oxides of nitrogen level. With a steadily increasing SCR efficiency, it is expected that Exhaust Gas Recirculation (EGR) may be phased-out by the end of the decade [1]. This will additionally offer marginal improvements in the base engine efficiency and avoid the challenges when using EGR [13].

Table 1: Base engine results, and fluid bottoming cycle assumptions and modelling overview



Engines are typically designed to operate with an engine coolant temperature of 90°C. However, recovering this heat to generate power would require relatively large heat transfer elements. It has been demonstrated that raising the coolant temperature level to a value of 115°C had no negative effect on the engine efficiency [14]. Therefore, to increase the coolant exergy content, the temperature was raised and fixed at 115°C. The condensing temperature and the temperature exiting the coolant HEX in the LT cycle were fixed at 80°C and 105°C, respectively. This resulted in an expansion Pressure Ratio (PR) and Volume Flow Ratio (VFR) of 1.7:1 and 1.9:1 for R245fa. All HEXs were modelled with a pinch point of 10°C, hence the condensing temperature for the HT cycle was also fixed at 115°C. Therefore, the system power optimisation was subjected to the parametric study of the HT cycle [8].

Figure 1(c) and 1(d) show the change in the duty of the heat transfer elements and system performance with varying HT cycle pressure. With increasing HT cycle pressure, the exhaust heat recovery decreased, while the coolant heat recovery remained constant and maximum (Figure 1(c)). Since the

temperature limits in the LT cycle were fixed, the thermal efficiency of the LT cycle was constant (Figure 1(d)). With increasing HT cycle pressure the thermal efficiency of the HT cycle and the combined cycle thermal efficiency increased (Figure 1(d)). Due to decreasing exhaust heat recovery and increasing HT cycle thermal efficiency, the cascade condensing load decreased, decreasing the load on the air cooled condenser (Figure 1(c)) and the additional fan power consumption (Figure 1(d)).

The maximum system power was achieved at a high pressure of 38.5 bar (Figure 1(d)), resulting in a PR and VFR of 20:1 and 15.7:1 for water. However, the optimal system pressure was selected as 19.5 bar. This was since the system power improvement with pressures above this value was relatively low. The cascade system at 19.5 bar offered 90% of the maximum power, but with half the PR, reducing the design intensity of the system. The system power was calculated according to equation 1 which attempts to include all the system parasitic power:

$$W_{system} = \left(W_{HT exp} + W_{LT exp} - W_{HT pump} - W_{LT pump}\right)\eta_{transmission} - W_{control} - W_{additional fan}$$
(1)

Figure 1(b) describes the T-S diagram for this optimum cascade system. The LT cycle recovered the cascade condensing load of the HT cycle to fully evaporate R245fa, which underwent a dry saturated vapour expansion. Due to the increased condensing pressure for the HT cycle, water was operated without superheat since a dryness fraction of ≈ 0.90 was maintained. The cascade system offered relatively lower maximum cycle pressures (≈ 20 bar) and relatively higher super atmospheric condensing pressures (≈ 2 bar) for both the temperature level cycles. The PR and VFR seen in the HT cycle were favourable at 10.1:1 and 8.2:1, respectively.

3 Problem definition for the cascade system

Fluid focused: The use of R245fa and water as working fluids are not without their specific challenges. R245fa presents vastly dissimilar thermodynamic and thermo-physical properties when compared to the conventional engine coolant (50% ethylene glycol, 50% water). As a result, the engine coolant loop cannot be replaced and an additional coolant HEX is required. Furthermore, R245fa has a high Global Warming Potential (GWP) of 1030 (relative to CO₂ for an integration time horizon of 100 years). Implementation of MAC Directive 2006/40/EC led to the banning of R134a (GWP 1370), and such regulations in the future may also apply to ORC systems requiring the use of fluids with GWP less than 150 [15].

Although water offers a thermally stable, non-flammable and environmentally friendly solution, the drawbacks of using water include high freezing temperature, mass flow control challenge in small capacity (< 25 kW) transient systems and lower heat recovery at HDDE exhaust temperature levels. The large latent heat drawback of water, which limits its application to higher source temperatures (> 500°C), is evident in Figure 1(b). Despite a small 10°C pinch point value, the exhaust stream was only cooled to 175°C, rather than ≈ 125 °C, till which condensation of exhaust stream can be avoided.

System focused: Over a drive cycle, a cascade system has to ensure dry vapours prior to both the expansion machines and liquid prior to both the pumps. This may present a challenge in providing combined heat recovery with maximum system power benefit. Furthermore, in long-haul HDDEs, the design condensing temperature in the air condenser will be around 70-90°C due to the cooling module design/capacity considerations. As a result, the coolant HEX and the cascade condenser will contribute noticeably towards the total heat transfer footprint and the exergy destruction in the system. Additionally, at the optimum condition (Figure 1(d)), the heat input into the LT cycle was over twice that of the HT cycle, while the thermal efficiency was less than $1/3^{rd}$. Therefore, cascade systems may be better suited to stationary large-scale output capacity units (> 100 kW), where near ambient condensing temperatures are possible, improving the LT cycle performance.

4 Proposed novel system

The challenges highlighted in Section 3, along with the relatively lower thermal efficiencies and higher investment costs associated with conventional energy conversion approaches explain why less attention has been given to engine coolant as a heat source in automotive applications. Although the increased

coolant exergy content (without detrimental effects on the base engine) is a positive direction, nonetheless, such LT sources require innovative approaches in heat recovery and/or power generation. In view of the above understanding, a study was undertaken to identify a single method which could translate to key noticeable benefits. As a result, the formulation of a new working fluid was identified as the key step in maximising the system performance, and minimising the system size and cost. The aim was to formulate a fluid that could potentially replace the conventional engine coolant loop with the ORC working fluid, and also offer suitability at HDDE exhaust temperature levels.

To meet the complex requirements for automotive applications, water blends may present an alternative avenue. Since the resurgence of fluid bottoming cycles for HDDEs is relatively new, the present research on water blends was insufficient to ascertain their suitability. As a result, an investigation of water blends to provide desired properties and characteristics by varying the water mass fractions was undertaken. The screening and evaluation methodology, presented in parallel works [8], was applied to examine over 500 documented water blends [16]. In this paper, the results of this methodology are utilised and an attempt is made to itemise the relevant fluid properties. The final selection trade-off included, frost protection, mass flow control, heat recovery, compatibility with engine construction materials, GWP, condensing pressure, thermal decomposition, heat transfer coefficient, fluid cost, health/environmental impact, heat transfer irreversibilities and net power. As a result, the use of 28% water and 72% 1-propanol by mass forming a homogeneous positive azeotrope was identified as a suitable miscible, non-reactive, water and alcohol blend. (Note hereafter referred to as W28).

To offer a more suitable system over the cascade arrangement, while exploiting high grade heat with higher cycle pressures and recovering complete engine block heat, the thermal and subsystem architecture shown in Figure 2(a) using water blends and its associated cycle operating mode is proposed. Conceptually, such a system is an adaptation of the multiple pressure level, heat recovery steam generator concept, used in coal power plants [17]. The system consists of a dual pressure level heat recovery architecture. Two pumps are utilised to generate the different subsystem pressure levels. While the expansion is either performed using two independent expansion machines or a dual pressure expansion machine (i.e. with two different pressure level inlets and one exit). The Low-Pressure (LP) loop was also the LT loop recovering the engine block heat. Similarly, the High-Pressure (HP) loop was also the HT loop recovering the exhaust heat.

The saturated liquid was pumped by the LP pump to a pressure corresponding to evaporation at 115°C (2.9 bar) and was distributed into two streams. One stream was used to recover the engine block heat directly, avoiding the use of a large coolant HEX and offering slightly higher evaporating temperature (115 vs. 105°C). The other stream was raised to the highest cycle pressure by the HP pump. The high pressure stream was preheated, evaporated and superheated in the exhaust HEX. The HP HT vapour was then expanded in the HP expander. The superheated working fluid stream exiting the HP expander was subsequently mixed with the two-phase LP LT stream exiting the engine block. The mass flow rates in the two-loops were controlled to form a dry saturated vapour after mixing. This stream was then injected into the LP expander. Although, the temperature exiting the HP expander was much higher than the stream exiting the engine block, the pressure was maintained equal. Therefore, the optimisation of the system was subjected to the parametric study of the HP loop [8].

Prior to a detailed heat transfer equipment calculation and design, the following was considered for the absolute size comparison. It was assumed that the overall heat transfer coefficient (U, W/m²°C) was similar for all the fluids. Therefore, UA (W/°C), i.e. overall heat transfer coefficient multiplied by the heat transfer area (A, m²), was considered as a first indicator for the absolute heat transfer size comparison for HEX and condenser. Although this assumption is subjected to inaccuracy, e.g. air condensers giving $\pm 20\%$ variation in the overall heat transfer coefficient between low pressure steam and light hydrocarbons [18]. Nonetheless, as it will be demonstrated later, the total system UA value will be noticeably different for the cascade and the dual pressure system to support this assumption. Similarly, VFR defined as the ratio between the volumetric flow rates at the expansion outlet to inlet was considered as a first indicator of the absolute size of the expansion machine.

For the dual pressure system, the UA value of exhaust HEX (2300 W/°C) and air condenser (6160 W/°C) were fixed at the same value as that of the optimal cascade system. The cooling air flow (16.6 kg/s) and the VFRs (8.2:1, 1.9:1) were also approximately limited to the maximum value set by the cascade system. In addition, pumping and expansion efficiencies were assumed to be constant for both the systems (given in Table 1). Although these efficiencies are a function of the working fluid properties and pressure differentials, nonetheless as a first approximation, the considered values may provide an insight into the achievable performance.

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Figure 2: Dual pressure system (W28) (a) thermal and subsystem architecture (b) T-S diagram at the constrained condition (c) variation in thermal loads with HP cycle pressure (d) variation in performance with HP cycle pressure

Figure 2(c) and 2(d) show the change in the duty of the heat transfer elements and system performance with varying HP cycle pressure. The mass flow rate was controlled to maintain the maximum W28 temperature of 250°C. This maximum selected blend temperature was over 10°C below the critical temperature of 1-propanol. In the absence of reliable thermal decomposition data for 1-propanol, subcritical temperatures and absolute temperatures limited to 250°C may avoid thermal decomposition. In practice, for all water and organic blends the flow rate has to be controlled precisely to prevent extreme temperature excursions (e.g. large superheating) and exposure lengths (e.g. heat build-up during impaired flow conditions).

With reduced water content, the exhaust heat recovery was relatively constant with increasing HP cycle pressure (Figure 2(c)). As a result, the combined thermal efficiency and system power increased (Figure

2(d)). The maximum cycle pressure was limited to 26 bar, corresponding to an HP VFR of 8.1:1. Since the cascade system recovered lower exhaust heat (120.5 vs. 141 kW) and the cascade condenser internally transferred heat in the system, it offered slightly lower air condenser load (252 vs. 268 kW). As a result, for an equal air condenser size and additional fan power consumption the condensing temperature for the dual pressure system was slightly higher (84 vs. 80°C). This resulted in a LP VFR of 2.3:1.

Figure 2(b) describes the T-S diagram for the dual pressure system at this point. If higher superheating levels can be guaranteed, the benefits of improved thermal efficiency, and hence, improved overall conversion efficiency at higher heat source temperatures (> 400°C) can be achieved. This is since the liquid fraction exiting the engine block can be increased to retain a slight superheat at LP expander inlet. Whereas at lower heat source temperature (< 300°C), the amount of superheat can be reduced so as to retain high heat recovery in the exhaust HEX, while avoiding complete evaporation inside the engine block. It is important to highlight that, compared to the engine coolant, the dual pressure system results in a relatively higher ΔT across the engine block (30 vs. 10°C) and a phase difference at the engine block exit (two-phase vs. single-phase). Such modifications although unconventional, have been experimentally demonstrated [19].

Table 2: *Key system and performance parameters for comparison between the optimal cascade and the constrained dual pressure system*

	P _{max} (HT) bar	T_{max} (HT) °C	m_{WF} (HT) kg/s	P _{max} (LT) bar	$T_{max}(LT)\circ C$	m_{WF} (LT) kg/s	Q EXHHEX kW	Q cascade cond kW	Q coolant HEX kW or engine block	Q air cond kW	W _{exp} (HT)	
Cascade system Water (HT), R245fa (LT)	19.5	210	0.05	14.3	105	1.54	120.5	106	155	252	14.7	
Dual pressure system W28 (HT, LT)	26	250	0.1	2.9	115	0.14	141	8 <u>4</u> 8	155	268	16.2	
	PR _{exp} (HT)	VFR _{exp} (HT)	$W_{exp} (LT)$	$PR _{exp} (LT)$	VFR _{exp} (LT)	UA _{ЕХН} НЕХ	UA cascade cond	UA coolant HEX	UA air cond	m cooling air kg/s	η thermal $\%$	W _{system} kW
Cascade system Water (HT), R245fa (LT)	10.1:1	8.2:1	10.6	1.7:1	1.9:1	2300	8850	11670	6160	16.6	8.6	18.4
Dual pressure system W28 (HT, LT)	9.6:1	8.1:1	12.7	2.5:1	2.3:1	2300	2. 5	877	6160	16.6	9.6	22.7

The detailed values in Table 2 (i.e. Figure 1 vs. Figure 2) then correspond to a first approximation for comparing cascade and the dual pressure system. The dual pressure system offered a 10% thermal efficiency improvement (9.6 vs. 8.6%) and a 20% power improvement (22.7 vs. 18.4 kW) compared to the cascade system. Since the dual pressure system avoided the use of the coolant HEX (11670 W/°C) and the cascade condenser (8850 W/°C), it excluded the associated HEX losses and the system UA value reduced by $2/3^{rd}$. This system is also expected to be more suited over the much more complex thermoelectric generators-ORC and ORC-Kalina cycle systems [20, 21].

It is important to point out that similarity to engine coolant properties and high engine compatibility was a primary consideration, since material changes to the engine blocks are challenging. Table 3 compares the key properties of the engine coolant with W28 and R245fa for direct engine block heat

recovery. Using engine coolant as a reference, it was noticed that W28 demonstrated a higher level of suitability. When considering density multiplied by heat capacity, as a first approximation of the fluid's heat absorption capacity, W28 displayed a higher level of similarity than R245fa (0.84 vs. 0.52). This presents a favourable case for the opportunity of replacing the conventional engine cooling loop. The properties of W28 were calculated using the Wilson property package [22]. Propyl-alcohols, like ethylene glycol also show good compatibility with common metals/alloys (e.g. aluminum, carbon steel, stainless steel, copper, cast iron), O-Ring materials (e.g. ChemRaz, EPDM, Kalrez, neoprene, Viton) and thermoplastics (e.g. acetal, NORYL, PEEK, polypropylene, PTFE) [23-25].

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At 90°C [liquid state]	Coolant	W28	R245fa	Water	Coolant	W28	R245fa	Water
Molecular weight [g/mol]	27.9	36.3	134.0	18.0	1	1.30	4.80	0.65
Mass density [kg/m3]	992	789	1129	965	1	0.80	1.14	0.97
Mass heat capacity [kJ/kg-C]	3.50	3.69	1.60	4.58	1	1.05	0.46	1.31
Mass heat of vaporisation [kJ/kg]	1738	1127	147	2283	1	0.65	0.08	1.31
Surface tension [dyne/cm]	56.1	41.9	11.1	27.9	1	0.75	0.20	0.50
Thermal conductivity [W/m-K]	0.342	0.164	0.062	0.671	1	0.48	0.18	1.96
Viscosity [cP]	0.50	0.40	0.20	0.31	1	0.79	0.39	0.63

 Table 3: Comparison of key properties for potential replacement of engine coolant

5 Expanders: The next challenge for water-blend systems

The performance of a fluid bottoming cycle strongly correlates with that of the expansion and power transfer unit. Both positive displacement expanders, in particular piston expanders, and dynamic machines, in particular radial turbines, have been suggested for automotive applications. Experimental results by Bosch on a piston expander using water have demonstrated a mechanical efficiency of 85% at 1500 rpm with inlet temperature and pressure conditions of 380°C and 32 bar [6]. For higher temperatures and pressures (400-500°C, 70-90 bar), Honda tested a swash-plate axial piston expander, which was more compact than common piston expanders [19]. Bosch also simulated a two-stage constant pressure turbine using water, delivering 10 kW with an efficiency of 65% and speed of 150,000 rpm. Additionally, the commercially available Green Turbine could also be considered for HDDEs [26]. The main characteristics of the turbine are, maximum pressure and temperature: 12 bar and 220°C, power: 15 kW, and design speed: 26,000 rpm.

Piston expanders are less cost intensive than turbines but are usually heavier. For example, a turbine with transmission weighs ≈ 25 kg, whereas a piston expander weighs ≈ 40 kg for a 25 kW capacity [6]. However, when costs are considered, radial turbines are $\approx 15\%$ more expensive to manufacture than piston expanders for capacity under 100 kW [27]. Piston expanders offer better off-design performance, permit some condensation during the expansion and show rotational speeds similar to HDDEs. Furthermore, for lower molecular weight fluids like water and W28, turbine design considerations in less than 25 kW output capacities results in lower efficiencies compared to heavier molecular weight organic fluids. The flexible operation of piston expanders provides a more practical system which outweighs the drawback of driving situations where there is no need for the recovered energy. Furthermore, developing technologies like the linear generator free piston expander, that converts mechanical energy directly into electrical energy, may lead to a practical solution for trucks with increased electrification and long-haul refrigeration trucks [28]. However, despite the recent advancements, the design of high PR, cost-effective, low-capacity, efficient water and W28 expanders remains a key challenge that has to be overcome in both the discussed systems [29].

6 Conclusions

Water and refrigerant cascade systems offer similar heat quality and quantity levels between the coolant HEX and the cascade condenser allowing complete coolant heat recovery. However, the high heat input into the low thermal efficiency section of the system, lower exhaust heat recovery, and the losses introduced due to the coolant HEX and cascade condenser showed such systems to be non-optimal for

automotive applications. The identified path to address the shortcomings of the cascade system was to formulate water-organic blends that could potentially replace the engine coolant loop, offering higher exergy input, and increased exhaust heat recovery, offering higher overall conversion efficiency. The methodology developed to screen and evaluate over 500 water blends resulted in the selection of 28% water and 72% 1-propanol with suitable trade-offs amongst the desired properties.

The proposed novel system is a function of this water blend, the superheated operating condition for the HP expander, the direct engine block heat recovery and the dual system pressure architecture. The selected cycle operating condition allowed utilising the advantages of superheating and avoided complete working fluid evaporation inside the engine block. Furthermore, the engineering challenges that may arise due to the replacement of the engine coolant to W28 are expected to be low due to the high similarity in fluid properties. The architectural advantages of the dual pressure system can provide an integrated and relatively compact engine and waste heat recovery solution for future engine platforms. This is since the system provided complete cooling of the engine block and replacement of the engine radiator to an ORC condenser.

Compared to the cascade system, the novel system showed a 20% improvement in system power, a $2/3^{rd}$ reduction in the total heat transfer footprint, and a reduced system complexity. The system efficiently exploited high temperature gaseous exhaust heat and complete engine block heat resulting in a Δ 14 g/kWh BSFC improvement. Nonetheless, accurate heat exchanger size comparison (using detailed heat transfer calculation) and achievable expansion efficiency (using expander model) remains the limitation of the presented work, and hence, a theme of focus for future works.

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