- 1 An Innovative Organic Rankine Cycle System for Integrated Cooling and Heat Recovery
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6 Abstract

7 Converting a portion of the waste heat into usable power by implementing Rankine and Organic Rankine Cycles 8 (ORC) on long-haul trucks is seen as a potential way to improve the overall system efficiency. To identify 9 techno-economical heat sources across the drive cycle of a Heavy Duty Diesel Engine (HDDE), an energy and exergy analysis was performed on all the available heat streams. As a result, to recover the combined exhaust gases and 10 coolant heat, a reference cascade system was analysed. Owing to the nature of this application, a size vs. 11 12 performance optimisation was performed for the cascade system utilising water and R245fa fluid combination. Despite a 1.8% Brake Thermal Efficiency (BTE) improvement, the key consideration in the research and development efforts 13 14 for ORC systems was identified as the investigation of technical paths that may improve the practicality of such a heat-to-power conversion concept. For this, simple holistic solutions were considered vital to meet the impending CO₂ 15 16 regulations. To provide a potential solution, an innovative dual-pressure ORC system is therefore proposed to partially 17 address the shortcomings of the cascade system. This innovative system is a function of new working fluids (i.e. water blends), its associated cycle operating mode and a novel architecture (i.e. direct engine block heat recovery). A 18 19 screening and evaluation methodology applied to water-organic blends is presented. Simulations conducted in Aspen 20 HYSYS V8 showed that, compared to the reference cascade system, the proposed dual-pressure system has the 21 potential to deliver an average of 20% improvement in the system power, a 50% reduction in the total heat exchanger 22 footprint, and a reduced system complexity. These advantages bode well for an integrated and relatively compact engine cooling and exhaust heat recovery solution for future automotive HDDEs. Implementation of the proposed 23 24 system at mid-speed high-load engine operating condition increased the overall BTE from 41.4% to a maximum of 43.6%. 25

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27 Keywords

Organic Rankine cycle; Diesel engines; Energy and exergy analysis; Size and performance trade-off; Water blends;
Dual-pressure system

30

Nomenclature

A heat transfer area (m^2)

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c_p	specific heat (kJ/kg°C)
Ė	exergy (kW)
h	specific enthalpy (kJ/kg)
İ	irreversibility (kW)
'n	mass flow rate (kg/s)
M _{wt}	molecular weight (g/mol)
Р	pressure (bar)
Ż	thermal duty (kW)
S	specific entropy (kJ/kg°C)
Т	temperature (°C)
U	overall heat transfer coefficient (W/m ² °C)
Ϋ́	volume flow rate (m ³ /s)
Ŵ	power (kW)
Greek symbols	
η	efficiency
ρ	density (kg/m ³)

Δ	difference
	unerence

Abbreviations

B100	mid-speed high-load
B50	mid-speed mid-load
BTE	brake thermal efficiency
GWP	global warming potential
HDDE	heavy duty Diesel engine
HEX	heat exchanger
HP	high-pressure
HT	high-temperature
LP	low-pressure
LT	low-temperature
NFPA	National Fire Protection Association
ORC	organic Rankine cycle
PR	pressure ratio
SCR	selective catalytic reduction

UA	product of heat transfer coefficient and area (W/°C)
VFR	volume flow ratio
W28	28% water and 72% 1-propanol by mass
W47	47% water and 53% 3-ethyl-1-Butanol by mass

32 1 Introduction

The past decade has seen incremental improvements in automotive Heavy Duty Diesel Engine (HDDE) efficiency 33 34 whilst complying with the exhaust emissions standards that have been the focus for engine developments [1]. The 35 present crucial issue is the need for further engine efficiency improvements due to greenhouse emissions, impending fuel consumption regulations, increasing fuel costs and diminishing fossil fuel supplies. Key directions proposed by 36 37 researchers and engine manufacturers to develop low carbon vehicles include: new engine architectures (e.g. 38 extremely high compression ratio), powertrain efficiency enhancements (e.g. waste heat recovery) and use of 39 alternative fuels (e.g. biodiesel) [2, 3]. The HDDE is expected to remain the prime mover of choice for long-haul trucks 40 for the coming two decades due to its competitive efficiency, high power density, outstanding durability and drivability. 41 Despite the efforts to directly increase the in-cylinder engine efficiency, a significant amount of the fuel energy is lost in 42 the form of heat. As a result, heat-to-power conversion systems provide a good starting point and an attractive 43 opportunity for emissions reduction whilst using a wasted resource.

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45 There has been renewed interest in heat-to-power technologies in the automotive sector, with leading engine 46 manufacturers, research centres and original equipment manufacturers announcing their research and development 47 efforts over the decade [4, 5]. Various technologies have been proposed and are at the demonstration phase for 48 converting a portion of the waste heat into either mechanical or electrical power. These include, but are not limited to, 49 turbocompounding, thermoelectric generators and fluid bottoming cycles [6, 7]. Amongst the fluid bottoming cycle options, Organic Rankine Cycles (ORC) are being adopted as a premier technology for long-haul HDDEs when 50 51 considering conversion efficiencies, technology readiness level, impending CO₂ legislations, absolute fuel 52 consumption, base vehicle cost, space availability and weight penalty [8].

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ORC systems with different complexity levels have been examined to target a variety of heat sources in the internal combustion engine. To recover the waste heat from the charge air, engine coolant and exhaust gases, Zhang et. al. analysed the characteristics of a dual-loop cascade system in combination with two conventional refrigerants (R245fa, R134a) for a light duty diesel engine [9]. In a similar dual-loop cascade system for a large scale engine, but excluding charge air, Song et. al. utilised water for the high temperature section, however in association with a screw expander 59 for two-phase expansion [10]. While for exhaust heat recovery only, Shu et. al. selected alkanes owing to their 60 excellent thermo-physical and environmental characteristics [11].

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Adaptability of ORCs for different heat sources have led to the proposition of ORCs combined with other technologies. Shu et al. analysed a thermoelectric generator + ORC system to recover the coolant and exhaust heat [12], while, He et al. presented ORC + Kalina cycle system adding lubricant heat as the third heat source [13]. ORC systems have also been experimentally coupled to refrigeration and energy storage systems [14]. To address the mismatched demand and availability of energy, Pandiyarajan et. al. demonstrated the ability to store a noticeable level of fuel energy (10-15%) in the combined storage system, which was available at reasonably higher temperatures [15].

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69 Important components like the expansion machines and heat exchangers are becoming more viable due to the 70 synergies with the current automotive components and a series of crucial technological advancements. Both positive 71 displacement expanders, in particular piston expanders, and dynamic machines, in particular radial turbines, have 72 been suggested for automotive applications. Using simulation and experimental results, Seher et. al. showed 73 two-stage turbine and piston expander mechanical efficiencies in the region of 65-85% [16]. In addition, Yang et. al. 74 and Zhang et. al. have recently demonstrated prototypes of fin-tube and spiral-tube evaporators, respectively [17, 18]. 75 As a result, on road demonstrations have shown that ORCs have the potential to improve the fuel economy of a long-haul truck by 6% [3]. The current market niche for ORCs is dependent on simplicity and affordability, with initial 76 77 technology deployment on commercial vehicles expected during the middle of the next decade in the European Union 78 and the United States.

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80 This paper firstly presents an assessment of the various heat sources in an automotive HDDE for conversion into usable power. Secondly, the results of a cascade system to form a reference for comparison are presented as the 81 82 consequence of the size vs. performance optimisation. Thirdly, the shortcomings of the cascade system utilising water and R245fa fluid combination are detailed for transport applications. For a comprehensive understanding, the system 83 and performance parameters were based on the energy and exergy equations in all the specific points in the cycle. 84 85 Finally, to partially address the shortcomings and facilitate the introduction of ORC systems, an innovative dual-pressure ORC system is proposed and examined extending the analysis of parallel works [19]. The primary 86 87 objective functions for comparison between the reference system and the proposed system included system power, 88 heat transfer footprint and size of the expansion machines. The simulations were conducted in an advanced chemical 89 process modelling tool, Aspen HYSYS V8 [20].

91 2 Heat source assessment

The starting point of the study was the selection of a long-haul HDDE platform representative of the current and future 92 productions, followed by the identification of realistic boundary conditions and assumptions for waste heat recovery 93 94 analysis. As such, the simulation results of a 12.8-litre, 6-cylinder, single-stage turbocharged engine were utilised in 95 this study [21]. Table 1 summarises the engine parameters at the mid-speed high-load condition (i.e. 1440 rpm and 96 100% power, denoted as B100) and the relevant input variables for the heat recovery analysis. The B100 engine 97 operating condition was selected to perform a design study for the reference ORC system. The selected engine 98 platform utilised a high efficiency Selective Catalytic Reduction (SCR) system as the only means to meet the Euro 6 99 oxides of nitrogen level. With a steadily increasing SCR efficiency, it is expected that exhaust gas recirculation may be phased-out by the end of the decade [3]. This will additionally offer marginal improvements in the base engine 100 101 efficiency, and reduction in carbon deposits and engine wear [22, 23].

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The selected HDDE platform offered exhaust gas, engine coolant, charge air and lubricant heat as the four potential 103 104 sources of waste heat. Fig. 1a shows the fuel energy distribution at the B100 condition. The four sources collectively accounted for approximately 50% of the total fuel energy at the chosen speed-load point, and in fact, also over the 105 106 entire engine operating range. Fig. 1a also shows 9.8% of the fuel energy termed as uneconomical exhaust. This is since, to give a true appreciation of the recoverable exhaust energy, the usable energy content was a function of the 107 source temperature entering and leaving the specific heat exchanger. In case of the exhaust heat exchanger placed 108 downstream of the aftertreatment devices, this was 420°C at inlet and limited to a minimum of 115°C at the outlet. The 109 115°C value then provided a small safety margin prior to the exhaust gases becoming susceptible to condensation. 110 The exhaust gas composition (limited to N₂, CO₂, H₂O and O₂) was derived from the experimental results of a 111 112 single-cylinder HDDE engine [19], resulting in a specific heat value of approximately 1.15 kJ/kg°C. In addition, exhaust lines were considered non-insulated and the exhaust temperature drop of 15°C over the aftertreatment devices was 113 114 also included.

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In order to account for variations in the waste heat temperatures, the four heat streams available in the heat 116 exchangers were also assessed in terms of the exergy content [24]. The exergy content of a stream represents the 117 118 maximum possible reversible work that can be extracted from a heat engine operating between the source and ambient temperature (assumed to be 25°C). Fig. 1b shows the energy and exergy content at B100 and the mid-speed 119 mid-load condition (i.e. 1440 rpm and 50% power, denoted as B50). Charge air cooler heat and the lubricant heat due 120 to low energy and exergy contents were excluded from heat recovery considerations. Charge air heat could only be 121 considered at high load operation, but the efficient and dynamic cooling of this stream over the complete drive cycle 122 123 may be a challenge. Lubricant heat, due to piston cooling, was typically 25% of the engine coolant heat, but due to the

low quality (≈ 90°C) showed no noticeable benefit. As a result, only heat in the exhaust heat exchanger and the engine coolant heat were considered for conversion into power. Note that, conventional HDDEs are designed to operate with a mean engine coolant temperature of 90°C. To increase the coolant exergy content, raising the temperature level to a value of 115°C has also been suggested [25]. However, such a modification may result in increased NOx emissions, and additionally, increased urea consumption by the SCR system. Therefore, to assess the exergy content in this study, the coolant temperature was maintained at 90°C.

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131 3 Reference cascade system

132 3.1 Rational for the reference

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. This is principally due to the working fluid mass flow rate limitation, which either results in the underutilisation of the engine coolant heat, or liquid at the expansion machine inlet [19, 26]. Cascade systems which utilise independent heat recovery systems to match the specific source characteristics provide a potential solution [9, 10]. As a result, cascade systems appear to be a preferred option for exploitation of exhaust and engine coolant heat in the published literature, offering an appropriate reference for comparison.

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141 3.2 System overview

142 A cascade system consists of two different temperature level cycles. The two closed-loop cycles, the 143 High-Temperature (HT) and the Low-Temperature (LT) cycles are interconnected at least by a common heat exchanger. The common heat exchanger termed 'cascade condenser' is effectively an internal heat exchanger for the 144 system. The cascade condenser acts as a condenser for the HT cycle and as an evaporator for the LT cycle. Only the 145 condenser of the LT cycle plays a role in dissipating the heat out of the cascade system. Due to the high temperature 146 differential across the system, need to limit exergy destruction and design considerations, two distinct working fluids 147 are used. A higher boiling point fluid is used in the HT cycle, while the LT cycle utilises a relatively lower boiling point 148 149 fluid.

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Fig. 2a presents the simplified schematic layout of the thermal and subsystem architecture for the considered cascade system. The HT cycle recovered the exhaust heat downstream of the aftertreatment devices. Whereas the LT cycle recovered the engine coolant heat and the cascade heat load in series. The published literature indicated the suitability of water for heat source temperatures over 400°C and R245fa for heat source temperatures below 250°C [27, 28]. Hence, water and R245fa were used in the HT and the LT cycles, respectively. The bypass lines for the two

- 156 expansion machines with pressure reducing valves were excluded for simplicity. Furthermore, fluid storage tanks prior
- 157 to the two pumps and exhaust flow bypass valve were also omitted.
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Table 2 summarises the system modelling overview. The equations are presented in terms of universal state points and can be adapted for the specific components in the cascade system. Where, \dot{Q} is the thermal duty (kW), \dot{m} is the mass flow rate (kg/s), c_p is the specific heat (kJ/kg°C), T is the temperature (K), \dot{I} is the irreversibilities (kW), s is the entropy (kJ/kg°C), h is the enthalpy (kJ/kg), \dot{V} is the volume flow (m³/s), ΔP is the pressure change (Pa) and \dot{W} is the work done or absorbed (kW). Also summarised are the modelling assumptions corresponding to realistic component efficiencies, performances and pressure losses. Where, η is the isentropic efficiency and PR is the expansion pressure ratio. The analysis leading to the justification of some of these assumptions is presented in Section 3.3.

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167 For a fixed condensing temperature and a fixed minimum pinch point temperature difference in the three heat exchangers, the cascade systems net power variation was primarily a function of the parametric study of the HT cycle. 168 169 This was since the maximum coolant temperature in the LT cycle limited the maximum evaporation pressure of R245fa. As a result, Fig. 3 presents the behaviour of the cascade system with variation in the maximum system 170 pressure imposed in the HT cycle up to a value of 25 bar. With increasing HT cycle pressure, the net power in the HT 171 cycle increased (Fig. 3a). This was due to the rate of thermal efficiency increase in the HT cycle being higher than the 172 173 reduction in the quantity of exhaust heat recovered. However, with increasing HT cycle pressure, the net power in the LT cycle decreased (Fig. 3b). This was since firstly, the thermal efficiency of the LT cycle was constant due to the 174 fixed temperature limits in the LT cycle, and secondly since the heat input into the LT cycle reduced due to a reduction 175 in the cascade condenser heat load. Due to a lower heat input into the system with increasing HT cycle pressure, the 176 additional fan power consumption also decreased. Collectively, with increasing HT cycle pressure, the combined 177 system thermal efficiency and power increased (Fig. 3c). However, the rate of system power improvement at higher 178 179 pressures (above 15 bar) was limited.

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181 **3.3 Size vs. performance trade-off**

In order to quantify the practical performance improvement potential using the cascade system, a size vs. performance trade-off study was conducted for the five major system components. These being, the size of the HT expansion machine, the exhaust heat exchanger, the coolant heat exchanger, the cascade condenser and the air condenser. As a first approximation, the following was considered as an indicator of relative size variation for the heat exchangers and the air condenser. It was assumed that the overall heat transfer coefficient (U, W/m²°C) remained relatively unchanged for a particular fluid under a fixed process type. Therefore, UA (W/°C), i.e. overall heat transfer coefficient multiplied by the heat transfer area (A, m²), was considered as an indicator for the relative heat transfer size. Similarly, the PR of the expansion machine was considered as an indicator of the relative expansion machinesize for a particular fluid under a fixed process type.

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Fig. 4a shows the influence of the PR in the HT cycle on the combined expander power. The maximum combined power was achieved at a high PR value of 30:1. However, such levels of PRs are beyond the reach of any efficient single-stage expansion machine. As a trade-off, the design point pressure ratio was reduced to \approx 12:1. This was since the combined expander power improvement with PRs above this value was relatively insignificant to justify the added size and the associated costs.

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Fig. 4b shows the influence of the exhaust heat exchanger UA value on the HT expander power. There was an inflection region beyond which the UA value increased for a negligible improvement in the HT expander power. This inflection region corresponded to a minimum pinch point temperature difference of \approx 10°C. A similar pinch point value (\approx 8°C) was also observed when considering the size of the coolant heat exchanger and the cascade condenser on the LT expander power (Fig. 4c). Larger areas will lower the heat transfer irreversibilities, but have a negative impact on system packaging and cost. All the heat transfer elements were subdivided into 20 equal working fluid enthalpy change sections to minimise the numerical error in the UA value.

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Finally, Fig. 4d shows the influence of the air condenser UA value on the LT expander power. To achieve a realistic 206 207 size trade-off with this component, while also addressing the cooling demand for other components, is perhaps one of 208 the most vital modelling assumptions. This is since the performance of any fluid bottoming cycle is very sensitive to the heat rejection limit. However, due to packaging and frontal area constraints in automotive applications, overly 209 210 optimistic condensing temperatures cannot be considered as a norm. Furthermore, the rebound effect is 211 acknowledged rarely in the literature, i.e. fuel improvements may encourage the consumption of other energy forms 212 which partially offset the gains [29]. The two relevant parameters in the present application include, low ORC condensing temperature, which increase the cooling fan power consumption, and excessively large exhaust heat 213 exchanger surface area, which introduce HDDE pumping losses. Assuming that the ambient air temperature 214 increases by 10°C over the air-to-air charge air cooler, the cooling air temperature available for the cascade system 215 was 35°C. Therefore by limiting the air in the engine bay to 55°C for long-haul HDDEs, the inflection region then 216 corresponded to an average design condensing temperature of $\approx 65^{\circ}$ C (Fig. 4d). Table 2 summarises the pressure 217 218 ratio, the pinch point and the condensing temperature values selected for simulations to offer a suitable 219 techno-economical trade-off.

221 3.4 Results and discussion

Utilising the findings of the trade-off study, Fig. 2b describes the T-S diagram for the design point cascade system 222 using water and R245fa combination, while Table 3 details the key system and performance parameters to act as a 223 224 reference for comparison in further analysis. Note that the LT cycle was also the Low-Pressure (LP) cycle, and hence, the LT and LP notations were used interchangeably (this was also true for the HT cycle). The LT cycle recovered the 225 226 cascade condensing load (Pt. 6 to 4) of the HT cycle to fully evaporate R245fa (Pt. 2 to 3), which underwent a slight 227 superheated expansion (Pt. 3). Due to the low condensing pressure in the HT cycle, water was superheated to 250°C (Pt. 5) in order to maintain a dryness fraction of \approx 1 (Pt. 6). Since the coolant heat exchanger was modelled with a 228 pinch point of 8°C, the evaporating temperature of the LT cycle was fixed at 80°C (Refer to Fig. 2c for a zoomed in 229 230 view of the LT section). This resulted in a PR and Volume Flow Ratio (VFR) of 1.3:1 and 1.4:1 for R245fa, making it suited to scroll and screw expanders [30]. The VFR seen in the HT cycle was also favourable at 8.6:1, and was within 231 232 the reach of single-stage piston expanders [31]. The above mentioned positive displacement expanders have also shown successful operation with dryness fraction ≥ 0.90 [7]. 233

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The cascade system offered relatively lower maximum (10.9 bar) and minimum (0.6 bar) cycle pressures for both the 235 236 temperature level cycles. The cascade cycle generated 13.5 kW of system power, increasing the overall engine BTE 237 by 4.3%. The system power included the parasitic pump (0.6 kW) and fan power consumption (1.8 kW), along with the transmission losses (1.4 kW) for expanders and pumps. The expander (65%) and pump (55%) isentropic efficiencies 238 239 were assumed to be constant. Although these efficiencies are functions of the fluid properties and application 240 conditions, nonetheless as a first approximation, the considered values may provide an insight into the achievable performance. The system power also accounted for the base engine performance loss due to an increased 241 242 backpressure. A net reduction of 1.6 kW in engine crankshaft power was calculated when an additional backpressure 243 of 0.1 bar was introduced in the exhaust line. The exhaust heat exchanger is a potential source of inefficiency at high 244 loads, and this has to be considered during process integration. Such levels of reductions are similar to those reported 245 experimentally by Hossain and Bari [32]. It is important to highlight that, some simulation studies have shown an insignificant impact on the base engine due to the thermal physics associated with the cooling of exhaust gas stream 246 247 when utilising a well-designed heat exchanger [33, 34]. However, for more realistic cases, where the derivatives of current production components are used with the low exhaust gas guality, a reduction in the crankshaft power is more 248 249 likely. The properties of exhaust, coolant, water and R245fa were calculated using the Peng-Robinson property 250 package [35].

252 **4 Problem definition for the cascade system**

253 4.1 Fluid focused

The specific use of R245fa and water as working fluids are not without their 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 heat exchanger is suggested in the literature. Furthermore, R245fa has a high Global Warming Potential (GWP) of 1030 (relative to CO_2 for an integration time horizon of 100 years) [36]. Implementation of the recent mobile air-conditioning directive 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 [37].

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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 transient systems and lower heat recovery at practical HDDE exhaust temperature levels [7, 27]. The large latent heat drawback of water, which limits its application to higher source temperatures using conventional expansion machines, is evident in Fig. 2b. Despite a small 10°C pinch point value, the exhaust stream was only cooled to 147°C, rather than \approx 115°C, till which condensation of exhaust gases can be avoided.

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269 4.2 System focused

270 Over a complete drive cycle, a cascade system has to ensure dry vapours prior to both the expanders and liquid prior to both the pumps. This may present a challenge in providing efficient combined heat recovery for maximum system 271 272 power benefit. More importantly, the inclusion of the coolant heat exchanger and the cascade condenser contributed 273 negatively to the system irreversibilities and the heat transfer areas. Despite the size vs. performance trade-off, these two components collectively contributed 17% towards the system irreversibilities (Fig. 5a). More noticeably, these two 274 275 components collectively accounted for \approx 50% of the total heat transfer area of the system (Fig. 5b). The irreversibility equations, represented in terms of universal state points in Table 2, were used for Fig. 5a. The numerical correlations 276 277 described in Ref. [38] for calculating the heat transfer areas employing a generic pure counter-current heat exchanger were used for Fig. 5b. Additionally, at the design point, the heat input into the LT cycle was approximately twice that of 278 the HT cycle, while the thermal efficiency was only around 1/5th (Table 3). Therefore, cascade systems may be better 279 suited to stationary large-scale output capacity units (> 100 kW), where near ambient condensing temperatures are 280 281 possible, improving the LT cycle performance.

283 5 Proposed dual-pressure system

284 5.1 Method overview

The lower efficiencies and higher investment costs associated with conventional energy conversion approaches, along with the challenges highlighted in the previous section explain why relatively less attention has been given to engine coolant as a heat source in automotive applications. As a result, such LT sources require innovative approaches in heat recovery and/or power generation. In view of Fig. 5a and 5b, formulation of unique working fluids was identified as one of the key methods which could translate to noticeable benefits. 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.

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The use of water blends was considered as an alternative avenue to meet the complex requirements for automotive 293 applications. Since the resurgence of ORCs for HDDEs is relatively new, the present research on water blends was 294 insufficient to ascertain suitable blends [39]. As a result, an investigation of water blends to provide desired properties 295 296 and characteristics with varied water mass fraction was undertaken. The developed blend screening methodology, 297 presented in Table 4, was applied to examine over 500 documented water blends [40]. Justifications for the screening 298 parameters relevant to the present application are provided during the discussions in Section 5.2 and 5.3. As a result of this screening methodology, two miscible, non-reactive, water-alcohol blends were identified as suitable candidates. 299 300 These being, 28% water and 72% 1-propanol by mass (hereafter referred to as W28), and 47% water and 53% 3-ethyl-1-Butanol by mass (hereafter referred to as W47). The key thermodynamic and thermo-physical properties of 301 302 the pure organic fluids are presented in Table 5. Also included are the National Fire Protection Association (NFPA) rating on health hazard (classified from 0 to 4; 0 corresponding to minimal and 4 corresponding to severe). Both the 303 304 suggested alcohols as blend constituents offer a health hazard level of 1, this is the lowest among pure organic fluids considered in ORCs [19]. 305

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307 5.2 System overview

To offer a more suitable heat-to-power conversion unit over the cascade system, while exploiting high grade exhaust heat with high cycle temperatures and recovering complete engine block heat, the thermal and subsystem architecture shown in Fig. 6a using the identified water blends and its associated cycle operating mode is proposed. Conceptually, such a system is an adaptation of the multiple pressure level, steam generator concept, used in coal power plants. 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 is also the LT loop recovering the engine block heat directly. Similarly, the High-Pressure (HP) loop is also the HT loop recovering the exhaust heat.

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The sub-cooled liquid (Pt. 1) was pumped by the LP pump to a pressure corresponding to evaporation at 95°C and 318 was distributed into two streams. One stream was used to recover the engine block heat directly (Pt. 2), avoiding the 319 use of a large coolant heat exchanger and offering slightly higher evaporating temperatures (95 vs. 80°C). Compared 320 to the conventional engine coolant, the dual-pressure system resulted in a relatively higher ΔT across the engine block 321 and a phase difference at the engine block exit (single-phase vs. two-phase). Such modifications although 322 323 unconventional, have previously been experimentally demonstrated [5]. The use of homogenous positive azeotropic 324 blends (Table 4, property 1), as in this case, contrary to the use of zeotropic blends, then attempts to minimise the temperature rise along the engine block. In addition, use of azeotropic blends allows the use of pure fluid design 325 326 methods, reducing the design intensity of the dual-pressure system.

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328 The second stream was raised to the highest cycle pressure by the HP pump. The high pressure stream was 329 preheated, evaporated and superheated (Pt. 4) in the exhaust heat exchanger. The blends mass flow rate was 330 controlled to maintain the maximum temperature of 250°C. This maximum selected blend temperature was below the critical temperature of the pure organic constituents. In the absence of reliable thermal decomposition data for the 331 blends (Table 4, property 7), subcritical temperatures and absolute temperatures limited to 250°C may then avoid 332 thermal decomposition [41]. In practice, for all water blends the flow rate has to be controlled precisely to prevent 333 334 extreme temperature excursions (e.g. large superheating) and exposure lengths (e.g. heat build-up during impaired 335 flow conditions). The HP HT vapour was then expanded in the HP expander. The superheated working fluid stream exiting the HP expander (Pt. 5) was subsequently mixed with the two-phase LP LT stream exiting the engine block. 336 The mass flow rates in the two-loops were controlled to form a superheated vapour after mixing (Pt. 3). This stream 337 was then injected into the LP expander. Although, the temperature exiting the HP expander was much higher than the 338 stream exiting the engine block, the pressure was maintained equal. Therefore, the behaviour of the dual-pressure 339 system was subjected to the parametric study of the HP loop. Fig. 7 presents the behaviour of the dual-pressure 340 system with variation in the maximum system pressure up to 32 bar. With increasing system pressure, the exhaust 341 342 heat recovery was higher and relatively constant compared to the cascade system (Fig. 3a), while the system thermal efficiency and the system power increased. The increased exhaust heat recovery by the water blend compared to the 343 344 use of pure water was due to the reduced latent heat (Table 4, property 2).

346 **5.3 Results and discussion**

The dual-pressure system was simulated with the same UA value of the air condenser (10490 W/°C) and the exhaust 347 heat exchanger (2120 W/°C) as that in the cascade system. Although this assumption is subjected to inaccuracy in 348 relative system heat transfer size comparison, e.g. condensers giving ±20% variation in the overall heat transfer 349 coefficients between low pressure steam and light hydrocarbons [42]. Nonetheless, the overall heat transfer 350 coefficients for the fluids considered in this paper were in the order of, water > W47 ≈ W28 > R245fa. As a result, 351 when numerical correlations described in Ref. [38] for calculating the heat transfer areas were employed using a 352 generic pure counter-current heat exchanger, it was found that, the performance reduction in the exhaust heat 353 354 exchanger when replacing water with the water blends was compensated by the performance improvement in the air condenser when using water blends instead of R245fa. In addition, the dual-pressure system was also simulated with 355 the same PR for the HP expander (12:1) as that in the cascade system. 356

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Fig. 6b describes the T-S diagram for the dual-pressure system using W28 with these constraints, while Table 3 details the key system and performance parameters for the constrained dual-pressure system using both the blends (Refer to Fig. 6c for a zoomed in view of the LT section). It can be noticed that compared to water which is a highly wetting fluid (Fig. 2b), the blends were only slightly wetting under the temperature range of application (Fig. 6b). This was due to the drying nature of the pure organic constituents in the water blend (Table 4, property 4). As a result, when the blends are expanded from the saturated vapour line with real isentropic expansion efficiencies, they result in high dryness fraction at the exit.

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Due to different working fluids between the cascade system and the dual-pressure system, VFR, defined as the ratio between the volumetric flow rates at the expander outlet to inlet was considered as a first indicator of the relative size of the expansion machine. The variation in the VFR for the HP expander among water, W47 and W28 was relatively low (8.6:1-10.1:1). A relatively low VFR variation (1.4:1-1.8:1) in the LP expander was also seen among R245fa, W28 and W47. This suggested that the resulting size variation among the different HP and LP expanders will be minimal.

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The maximum cycle pressure for W28 and W47 was 14.7 and 11.1 bar, respectively. Since the cascade system recovered lower exhaust heat (123 vs. 139-141 kW) and the cascade condenser internally transferred heat in the system, it offered slightly lower air condenser load (222 vs. 236 kW). As a result, for an equal air condenser size and additional fan power consumption (1.8 kW) the mean condensing temperature for the dual-pressure system was slightly higher (66 vs. 70°C).

378 The values presented in Table 3 then correspond to a first approximation for comparing the cascade and the 379 dual-pressure system. The dual-pressure system offered an average of 20% improvement in system power. Since the dual-pressure system avoided the use of the coolant heat exchanger and the cascade condenser, it excluded the 380 associated heat transfer losses and reduced the system heat transfer footprint by 50%. Such a system is also 381 expected to be more suited over the much more complex thermoelectric generators + ORC and ORC + Kalina cycle 382 383 systems [12, 13]. Implementation of the dual-pressure system using W28 offered a system power of 17 kW, increasing the overall engine BTE by 5.3% from 41.4 to 43.2%. The resulting modified fuel energy balance for the engine + the 384 385 dual-pressure ORC system is presented in Fig. 8.

386

In addition, to assess the relative power densities of the two systems, the review conducted for ORCs (and refrigeration) systems for HDDE suggested a relative weight distribution as presented in equation 1 [19]. Note that, the fluid, valve, piping, control, tank etc. are expected to make up over 1/3rd of the total system weight. It was assumed that the power-to-weight ratio of the reference cascade system was 1. Therefore, when considering a 50% lower heat exchanger weight and a 20% higher power output, the power-to-weight ratio of the proposed dual-pressure system improved by 33%. A higher power density system bodes well for truck applications.

393

$$kW/kg_{ref} = 0.22Heatexchangers + 0.12Conderser$$
(1)
+0.2Expanders + 0.12Pumps +0.34
395

396

It is important to highlight that similarity to engine coolant properties (Table 4, property 8) and high engine 397 398 compatibility (Table 4, property 9) was a primary consideration, since design and material changes to the engine 399 blocks are challenging. Table 6 presents the relative comparison of the seven key fluid properties between the conventional engine coolant and, W28, W47, R245fa and water for direct engine block heat recovery. Using engine 400 401 coolant as a reference, it was noticed that water blends demonstrated a higher level of suitability [43]. When considering density multiplied by heat capacity, as a first approximation of the fluid's heat absorption capacity, the 402 blends displayed a higher level of similarity than R245fa (0.84-0.9 vs. 0.52). This may present a favourable case for 403 the opportunity of replacing the conventional engine cooling loop. The properties of the water blends were calculated 404 405 using the Wilson property package [35].

406

Like ethylene-glycol, propyl-alcohols followed by amyl-alcohols also show good compatibility with common metals/alloys (e.g. aluminium, brass, carbon steel, copper, stainless steel), O-Ring materials (e.g. EPDM, kalrez, natural rubber, neoprene, viton) and thermoplastics (e.g. acetal, PEEK, polypropylene, PTFE, PVDF) [19]. In addition both the blends offer freezing temperatures below -30°C (Table 4, property 3) and GWP below 20 (Table 4,

- 411 property 6). This makes these blends suitable for automotive applications from cold temperatures in North America, to
- 412 potential future regulations in Europe requiring the use of low GWP fluids in automotive ORCs.
- 413

414 **5.4** The next challenge for ORC systems

The key system and performance parameters presented in Table 3 for the water blends were constrained, and to a 415 certain extent, some of them were non-optimised in nature. The exhaust heat exchanger for both the water blends 416 417 could be considered near-optimum since they cooled the exhaust gases to 115-120°C, resulting in a pinch point of 25-30°C in the heat exchanger. Exhaust gas cooling below 115°C was considered uneconomical due to the reducing 418 419 exergy content of the heat stream and heat exchanger considerations to avoid condensation of exhaust gases. 420 However, the PR of 12:1 in the HP expander may be a variable constraining the dual-pressure system performance. This is best understood with reference to Fig. 9, which shows the effect of increasing the PR of the HP expander 421 (assuming fixed 65% isentropic efficiency). The water blends continue to offer higher combined expander power, and 422 additionally, with a marginally diverging trend compared to water up to an ultra-high pressure ratio of 20:1. As a result, 423 424 the water blends will offer a more favourable trade-off at increased PRs. Hence, after the selection of a suitable working fluid, the selection of an appropriate expansion machine is the next most important step since the 425 performance of a fluid bottoming cycle strongly correlates with that of the expansion and power transfer unit. In 426 addition. Fig. 5a also indicates that approximately 1/5th of the system losses in the cascade system were due to the 427 expanders. As a result, in automotive exhaust heat recovery applications, which correspond to high temperature 428 429 differentials between the heat source and the heat sink, the requirement of high PR, cost-effective, low-capacity and efficient expanders remains a key challenge that has to be overcome in both the discussed systems. 430

431

432 6 Conclusion

433 A practical energy and exergy analysis considering the different waste heat sources on a modern automotive HDDE 434 demonstrated the use of exhaust and coolant heat to be the most beneficial across a wide engine operating region. These two sources offer relatively similar quantity but dissimilar quality levels of heat, presenting a challenge for the 435 application of simple single-loop ORCs. The use of cascade systems appears to be a preferred solution in the 436 published literature, allowing exhaust heat recovery and complete coolant heat recovery. A size vs. performance 437 trade-off study was conducted to optimise such a cascade system using water and R245fa combination for the HT and 438 439 the LT heat recovery, respectively. However, the high heat input (226 vs. 123 kW) into the low thermal efficiency section of the system (1.8 vs. 11.5%), lower than desired exhaust heat recovery (123 vs. 141 kW), and the irreversible 440 losses (17%) and size (50%) introduced collectively due to the coolant heat exchanger and the cascade condenser 441 442 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 blends that could 444 potentially replace the engine coolant loop, offering higher exergy input, and increased exhaust heat recovery, offering 445 higher overall conversion efficiency. The blend screening methodology developed to screen over 500 water blends 446 447 resulted in the selection of 28% water and 72% 1-propanol by mass, and 47% water and 53% 3-Methyl-1-Butanol by mass with suitable trade-offs amongst the desired fluid properties. These properties included, azeotropic behaviour, 448 ultra-low freezing temperatures, near-isentropic fluid vapour curve, ultra-low GWP, high thermal stability, compatibility 449 450 with engine construction materials and low boiling point. The proposed system is a function of these water blends, the 451 limited superheated operating condition for the HP expander, the direct engine block heat recovery and the dual 452 pressure architecture. The architectural advantages of the dual-pressure system can provide an integrated and relatively compact engine and waste heat recovery solution for future HDDE platforms. This is since the system 453 provided complete cooling of the engine block and replacement of the engine cooling radiator to an ORC condenser. 454 Furthermore, the engineering challenges that may arise due to the replacement of the engine coolant to the water 455 blends are expected to be low due to the high similarity in the fluid properties. Compared to the conventional cascade 456 457 system, the innovative dual-pressure system showed an average of 20% improvement in system power and a 50% reduction in the total heat transfer footprint. This increased the system power density by 33%. The implementation of 458 the dual-pressure system resulted in a 5.3% improvement in the overall engine BTE. 459

460

This paper has attempted to include realistic component performances and a wide range of parasitic losses in the ORC system. However, the limitations of the work presented include, firstly, the absence of accurate heat exchanger size comparison by optimising the heat exchanger models, and secondly, the precise expansion efficiencies by using expander models. These two items remain a theme of focus for future works. Finally, the necessity of high PR (> 12:1), cost-effective, low-capacity (< 20 kW) and efficient expanders (> 65%) has been identified as a vital research direction.

467

468 Acknowledgements

The author would like to acknowledge the support of the Advanced Engineering Centre with respect to provision of software tools and proof-reading.

471

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574 Figure 1 (a) Fuel energy distribution at B100 (b) Energy and exergy analysis of the heat sources at B50 and B100











Figure 4 Equipment size vs. power produced trade-off for (a) HT expander (b) Exhaust heat exchanger (c) Coolant

- 611 heat exchanger and cascade condenser, and (d) Air condenser



- 630 Figure 5 Cascade system (a) Relative irreversibility distribution by system components, and (b) Relative heat transfer
- 631 size distribution by heat transfer elements

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- at the constrained point, and (c) Zoomed-in T-S diagram for the LT system section



Figure 7 Effect of the maximum system pressure in the dual-pressure system on variation in thermal loads, system

- 659 efficiency and system power using W28

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- Figure 8 Fuel energy distribution at B100 for the engine combined with the dual-pressure ORC system

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- Figure 9 Advantage when using an efficient high PR piston expander in the dual-pressure system

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Table 1 HDDE performance and the resulting variables for the heat recovery analysis

	Variable	Value and unit
	Air to fuel ratio	22.5:1
	Speed	1440 rpm
	₩ _{crankshaft}	316 kW
	$\eta_{brake\ thermal}$	41.4%
	T _{intake} manifold	60°C
	P _{intake} manifold	2.7 bar
	<i>Q</i> _{coolant}	117 kW (85-95°C)
	$\dot{Q}_{charge\ air}$	36 kW (cooled from 150 to 60°C)
	Q _{lubricant}	27 kW (85-95°C)
	T _{cooling} air inlet	35°C (secondary radiator)
	T _{cooling} air exit	55°C
	Δr _{fan} ŵ	2 JU Fa
	W fan	1 15 k l/ka°C
	m	0.4 kg/s
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/50		
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Table 2 ORC energy and exergy modelling overview and equipment performance assumptions

	Equipment	Modelling assumptions	Modelling overview
	↓↓ ↓ → ↓	$\Delta P_{all heat transfer surfaces} = 0.25 beT_{minimum pinch point} = 8-10°C$	$\begin{array}{l} \text{ar} & \dot{Q}_{heat\ exchanger} = \dot{m}_{source}\ c_{p\ source}\ (T_{inlet} - T_{exit}) \\ \dot{I}_{heat\ exchanger} = T_{ambient}\left[\dot{m}_{fluid}\left(s_{exit} - s_{inlet}\right) + \dot{m}_{source}\left(s_{exit} - s_{inlet}\right)\right] \end{array}$
		. $\eta_{fan} = 65\%$ $T_{minimum\ condesning} = 65^{\circ}\text{C}$	$ \begin{split} \dot{I}_{aircondenser} &= T_{ambient}\dot{m}_{fluid}[(s_{exit}-s_{inlet}) - \{(h_{exit}-h_{inlet})/T_{mean}\}] \\ \dot{W}_{fan} &= (\dot{V}_{air}\Delta P_{fan})/\eta_{fanandmotor} \end{split} $
	↓↓ ↓	$\begin{aligned} \eta_{expander} &= 65\% \\ PR_{HP\ expander} &= 12:1 \\ \eta_{all\ transmission} &= 93\% \\ T_{superheated} &= 250^\circ\text{C} \end{aligned}$	$ \dot{W}_{expander} = \dot{m}_{fluid} (h_{inlet} - h_{exit ideal}) \eta_{expander} \dot{I}_{expander} = T_{ambient} \dot{m}_{fluid} (s_{exit} - s_{inlet}) $
	- <u>@</u> ↑	$\eta_{pump} = 55\%$	$ \begin{split} \dot{W}_{pump} &= \dot{m}_{fluid} \left(h_{exit \; ideal} - h_{inlet} \right) / \eta_{pump} \\ \dot{I}_{pump} &= T_{ambient} \dot{m}_{fluid} \left(s_{exit} - s_{inlet} \right) \end{split} $
758		\dot{W}_{system} = ($\dot{W}_{HP\ exp}$ -	$\dot{\eta}_{system} = \dot{W}_{system} / \dot{Q}_{in}$ + $\dot{W}_{LP exp} - \dot{W}_{HP pump} - \dot{W}_{LP pump}) \eta_{transmission} - \dot{W}_{additional fan} - \dot{W}_{backpressure}$
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782 Table 3 Key system and performance parameters for the cascade system and the dual-pressure system

		Cascade system Water, R245fa	Dual pressure system W28	Dual pressure system W47
P _{system max}	bar	10.9	14.7	11.1
P _{system min}	bar	0.6	0.4	0.3
T _{system max}	°C	250	250	250
T _{system min}	°C	65	64	63
T _{evaporation} (HP)	°C	183	178	173
T _{condensation} (HP)	°C	87	-	-
PR _{expander} (HP)		12:1	12:1	12:1
VFR _{expander} (HP)		8.6:1	10.1:1	9.9:1
₩ _{expander} (HP)	kW	14.3	15.6	15.1
₩ _{pump} (HP)	kW	0.1	0.3	0.2
m _{fluid} (HP)	kg/s	0.05	0.09	0.08
$T_{evaporation}$ (LP)	°C	80	95	95
$T_{condensation}$ (LP)	°C	65	64	63
$P_{max}(LP)$	bar	7.9	1.5	1.2
$T_{max}(LP)$	°C	80	95	95
PR _{expander} (LP)		1.3:1	1.9:1	1.8:1
VFR _{expander} (LP)		1.4:1	1.8:1	1.7:1
₩ _{expander} (LP)	kW	4.5	6.7	5.7
₩ _{pump} (LP)	kW	0.5	0.1	0.1
ṁ _{fluid} (LP)	kg/s	1.29	0.11	0.09
Q _{exhaust heat exchanger}	kW	123	141	139
UA _{exhaust heat exchanger}	W/°C	2120	2120	2120
Qcascade condenser	kW	109	-	-
UA _{cascade} condenser	W/°C	8630	-	-
$\dot{Q}_{coolant\ heat\ exchanger}$	kW	117	117	117
UA _{coolant heat exchanger}	W/°C	9900	-	-
Qair condenser	kW	222	236	236
UA _{air condenser}	W/°C	10490	10490	10490
T _{air exit}	°C	55	57	57
$\dot{m}_{cooling\ air}$	kg/s	10.95	10.95	10.95
₩ _{fan}	kW	1.8	1.8	1.8
$\dot{W}_{backpressure}$	kW	1.6	1.6	1.6
η_{system}	%	5.6	6.6	6.1
₩ _{system}	kW	13.5	17	15.7

795 Table 4 Screening methodology overview for the water-organic blend study

Number	Property	Value		
1	Blend classification	Homogeneous positive azeotrope		
2	Water mass fraction	25-50%		
3	T _{organicfreezing}	≤ –75°C		
4	Number of atoms (organic)	10-20		
5	Ozone depletion potential (organic)	0		
6	Global warming potential (organic)	≤150		
7	NFPA instability/reactivity rating (organic)	0 (minimal hazard)		
8	Similarity to the engine coolant (blend)	High		
9	Compatibility with engine materials (blend)	High		
10	T _{blend} boiling	Lowest for a approximately similar water mass fraction		

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820 Table 5 Fluid properties for the chosen organic constituents

Formula	Name	$T_{critical}$ °C	P _{critical} bar	$T_{boiling}$ °C	M_{wt} g/mol	$ ho_{liquid}~{ m kg/m^3}$	$T_{freezing}$ °C	NFPA Health
C ₅ H ₁₂ O	3-Methyl-1-Butanol	304	39.3	131	88.1	812	-117	1
C ₃ H ₈ O	1-Propanol	264	51.7	97	60.1	806	-126	1
	Pormula C ₅ H ₁₂ O C ₃ H ₈ O	Pormula Name C ₅ H ₁₂ O 3-Methyl-1-Butanol C ₃ H ₈ O 1-Propanol	romula Name Teritical C C ₅ H ₁₂ O 3-Methyl-1-Butanol 304 C ₃ H ₈ O 1-Propanol 264	romula vame <u>reritical C Peritical Dar</u> C ₃ H ₂ O 3-Methyl-1-Butanol 304 39.3 C ₃ H ₈ O 1-Propanol 264 51.7	Pormula Name Territori C Peritori Diffing *C C3H12O 3-Methyl-1-Butanol 304 39.3 131 C3 C3	Portulat Name Territori C Peritori District District <thdistrit< th=""> Distrit <thdistrit<< th=""><th>romua viane <u>remea 2 remea 3 i 3 autor 0 μega 8000</u> CgH₂O 3-Methyl-F-Buland 204 51.7 97 80.1 806</th><th><u>reimia vane</u> <u>Lenizer</u> <u>C</u> <u>Pereira</u> <u>00</u> <u>Pagua RJm</u>, <u>Pagua RJm</u>, <u>Previn</u> <u>Cyll₂</u> <u>0</u> <u>1</u> <u>Propanol</u> <u>284</u> <u>517</u> <u>97</u> <u>601</u> <u>806</u> <u>-126</u></th></thdistrit<<></thdistrit<>	romua viane <u>remea 2 remea 3 i 3 autor 0 μega 8000</u> CgH ₂ O 3-Methyl-F-Buland 204 51.7 97 80.1 806	<u>reimia vane</u> <u>Lenizer</u> <u>C</u> <u>Pereira</u> <u>00</u> <u>Pagua RJm</u> , <u>Pagua RJm</u> , <u>Previn</u> <u>Cyll₂</u> <u>0</u> <u>1</u> <u>Propanol</u> <u>284</u> <u>517</u> <u>97</u> <u>601</u> <u>806</u> <u>-126</u>

Table 6 Relative comparison of the key fluid properties for potential replacement of engine coolant at 90°C

	Engine coolant	W28	W47	R245fa	Water
Molecular weight, M _{wt}	1	1.30	1.12	4.80	0.65
Liquid density, ρ_{liquid}	1	0.80	0.85	1.14	0.97
Specific heat, c _p	1	1.05	1.06	0.46	1.31
Heat of vaporisation, Hvap	1	0.61	0.79	0.08	1.31
Surface tension, γ	1	0.75	0.93	0.20	0.50
Thermal conductivity, λ_{liquid}	1	0.48	0.51	0.18	1.96
Viscosity, $\mu_{dynamic}$	1	0.79	0.74	0.39	0.63