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The potential of mixtures of pure fluids in ORC-based power units fed by exhaust gases in Internal Combustion Engines

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Abstract

ORC represents an effective challenge in the waste heat recovery from ICEs. In spite of technological aspects, its thermodynamic design still deserves attention. Mixtures of pure fluids show interesting properties able to improve exergetic efficiency of the Rankine cycle, thanks to the positive slope of the phase changing. They can reduce also ODP and GWP, helping the replacement trends of working fluids. The paper optimizes cycle exergetic efficiency considering mixtures of pure fluids. The use of hydrocarbons in mixtures is particularly suitable and when used in limited fractions with other organic fluids they loses the limits related to the flammability. R245fa is a fluid that obtains a large net power increase when used in mixtures with hydrocarbons, compared to pure fluid an optimized R245fa/benzene mixture, for instance, attains an 11% net power increase.

Keywords: Organic Rankine Cycle (ORC), Internal combustion engine (ICE), Waste heat recovery, Refrigerant mixtures, efficiency

1. Introduction

The internal combustion engines (ICEs) are the most used powertrains for road transport applications. Concerning the energy balance, up to 60-65 % of the fuel energy of ICEs is lost to the environment ([1,2]). The major part of this energy is lost in the exhaust gases (typical value of the loss is around 30-35 % of the fuel energy) and can be used for energy recovery. The recovery of the heat on the exhaust gas and its conversion into mechanical energy is under

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a wide investigation [3] as a way to improve overall efficiency. The most considered technology is the recovery via ORC. Organic fluids have lower critical temperatures (with respect to water) and allow their evaporation at low and medium temperatures making possible the recovery from low and medium grade heat sources (like exhaust gases). ORC technology is quite conventional for high power ranges and high and medium temperature sources. It shows good results, in particular for steady or quasi-steady applications. On the other hand, for low thermal sources a proven technology is not commercially ready, in spite of the very wide potential applications (solar power, geothermal, conventional streams, medium and low temperature sources, etc.) [4]. More critical are the on-board units vehicles, because of the variable conditions characterizing the hot and cold sources, often transients. Further studies are needed in order to increase efficiency and net power recoverable as well as control strategies.

The problem of the fluid choice in the ORC-based units is one of the oldest issues found in literature [5,6]. It has a great importance on the efficiency of the system, size and design of the components [7]. Safety, flammability, GWP, ODP, oil miscibility, corrosion with metals and rubbers are important parameters but the temperature difference between fluid critical temperature and inlet temperature of the heat source plays a key role in limiting the performance of the thermodynamic cycle [8]. One of the most promising fluids is R245fa [9], as it has no ODP, it is not flammable and nearly non-toxic. Furthermore, for ICEs heat recovery, it shows best performances for its ability to work at higher temperature [10]. Other studies show that working fluids with high boiling temperature (pure hydrocarbons) yielded better thermodynamic performance [11], but they are flammable.

The interest in mixtures of organic working fluids concerns thermodynamic efficiency [12, 13], components optimization [14] and economic performance [15]. Mixtures, in fact, have variable temperature during changing phase and this will make condensation and vaporization conditions closer to the heat sources during heat transfer, improving exergetic efficiency and, definitively, net useful work [16]. Moreover, high GWP and flammability fluids, which are banned as pure fluids, can be used in small fraction in blends with other fluids. When mixtures are used, an important degree of freedom is gained being possible to choose the number of fluids of the mixtures and the mass-ratios among pure fluids. This makes the prediction of thermal power recoverable, cycle efficiency and net power much more complex. A real important issue not fully exploited in literature for on board recovery units, in fact, is the design criterion of the power unit itself which still calls for a deeper thermodynamic analysis. In absence of other constraints (cold source availability), the optimization criterion is the maximization of the net mechanical power produced by the unit: this means that the product of the working fluid flow rate (produced at the evaporator) and the cycle work must reach its maximum value.

Starting from these considerations, in this paper the Authors developed a comprehensive thermodynamic model of the ORC plant, considering both hot and cold source available on board vehicle. The model provides an ORC optimization analysis where both pure fluids and mixtures are considered as possible working fluids, aiming to maximize the net ORC power output. The best candidates are evaluated based on: thermodynamic performance, pressure levels, fluid hazard levels and GWP, critical temperature and the temperature glide. The reference made to pure fluid mixtures opens also the way to non-conventional cycles whose thermodynamic performances have not been exploited in literature. In this regard, the use of fluid mixtures can increase the degree of cycle regeneration and strongly reduce the thermal power to be exchanged towards the cold source, with great benefit in on-board application. Therefore, a wide comparison between pure fluids and mixtures has been done, detecting the principle sources of irreversibility and individuating the benefits related to the use of hydrocarbon mixtures.

2. Description of the mathematical model

The analysis of the power recoverable from the exhaust gases of an ICE has been conducted with a thermodynamic model, which is able evaluate the behavior of fluid mixtures in comparison with pure fluids. For each working fluid (or mixture) considered, the model finds the highest mechanical power recovered optimizing condensation and evaporation pressure as well as maximum cycle temperature.

2.1. The mathematical model

Energy and exergy mathematical models are based on preliminary assumptions: a) the cycle runs under steady working conditions; b) there are no heat losses and pressure drops in heat exchangers and pipes; c) heat exchangers are counter-flow type; d) zeotropic mixture behaviour is based on Lemmon – Jacobsen model [17]; e) for sake of simplicity, volumetric and mechanical efficiencies of pump and expander have been considered equal to 1. Making reference to the sketch represented in Figure 1, each component of the ORC can be represented with specific equations. The maximal uncertainties of the equation of state are 0.2% in density for the liquid, 0.4% for the vapour, and 0.4% in vapour pressure concerning all the examined organic working fluids.

2.2. Evaporator

First, the working fluid mass flow rate can be written as in eq. 1, according a thermal balance in the evaporator.

$$m_{WF} = \frac{Q_{ev}}{h_3 - h_2} = \frac{m_{hs}(h_{hs,in} - h_{hs,out})}{h_3 - h_2} \tag{1}$$

Considering an adiabatic system, the irreversibility of the evaporator can be written as in eq. 2:

$$I_{ev} = T_{ref}\left[m_{WF}(s_3 - s_2) - m_{hs}(s_{hs,in} - s_{hs,out})\right] \tag{2}$$

2.3. Pump

Pump power is expressed as in eq. 3, irreversibility are in eq.4:

$$P_p = m_{WF}(h_2 - h_1) = \frac{m_{WF}(h_{2,ad,is} - h_1)}{\eta_{ad,is,p}} \tag{3}$$

$$I_p = P_p - m_{hs}\left[h_2 - h_1 - T_{ref}(s_2 - s_1)\right] \tag{4}$$

2.4. Expander

The power delivered by the expander (which represents its exergy) and expander irreversibility are written according to equations 5:

$$\begin{gathered} P_{\exp} = m_{WF}(h_3 - h_4) = m_{WF}\eta_{\exp,ad,is}(h_3 - h_{4,ad,is}) \\ I_{\exp} = m_{WF}[(h_3 - h_4) - T_{ref}(s_3 - s_4)] - P_{\exp} \end{gathered} \tag{5}$$

2.5. Condenser

The thermal power exchanged in the condenser is calculated according to eq. 6, irreversibility according to eq. 7:

$$Q_{cond} = m_{WF}(h_4 - h_1) \tag{6}$$

$$I_{cond} = m_{wf}\left[(h_4 - h_1) - T_{ref}(s_4 - s_1)\right] \tag{7}$$

2.6. Overall ORC performance

The useful power P_u of the system is calculated as the difference between expander and pump power (eq. 8).

$$P_u = P_{\exp} - P_p \tag{8}$$

Next equations show the thermodynamic and exergetic efficiencies.

$$\eta_{th} = \frac{P_u}{Q_{ev}} \tag{9}$$

$$\eta_{ex} = 1 - \frac{I_{ev} + I_{\exp} + I_{cond} + I_p}{m_{hs}\left[h_{hs,in} - h_{hs.out} - T_{ref}(s_{hs,in} - s_{hs.out})\right]} \tag{10}$$

2.7. Model integration and optimization procedure

The model aims to maximize power recovery, which may be defined as the product of flow rate and cycle net work. The optimization procedure is summarized in the flow chart of Figure 2, where the free variables can be identified: condensing and evaporating pressures and superheating value.

Firstly, fixed input parameters are defined: among these the hot source fluid, its pressure, evaporator inlet and outlet temperatures and flow rates, cold source fluid, pressure and inlet temperature in heat exchanger. Then, thermodynamic cycle can be evaluated: for each working fluid (or mixture) considered, the optimal tern of values composed by condensing temperature, evaporating pressure and superheating degree is searched (Figure 2). The software changes possible evaporation temperature combining for each of them several superheating steps. Adopting zeotropic mixture as working fluid, the model refers to liquid saturation point 3' (Figure 3). Then, the model strategy increases maximum temperature till hot source inlet temperature in the heat exchanger decreased of the difference of temperature specified for the pinch point. The results are energy and exergy analysis of thermodynamic cycle characterized by highest power recovered among possible ones.

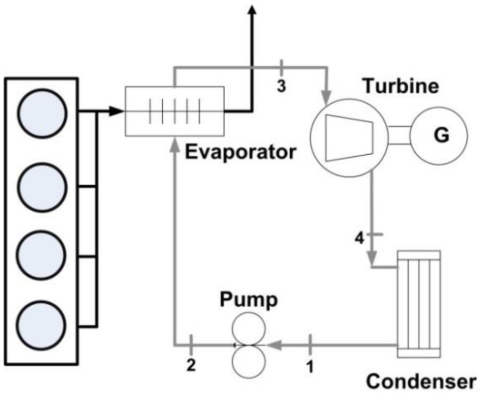

Figure 1: ORC bottoming ICE sketch

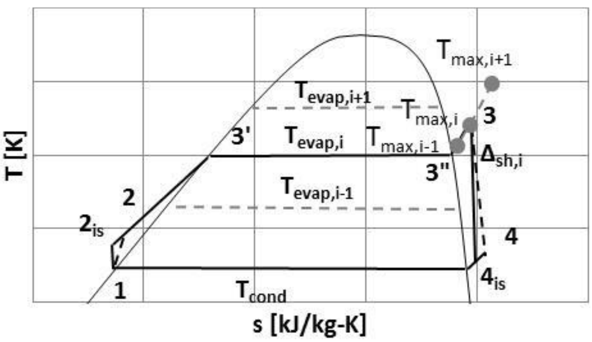

Figure 3: optimal evaporation temperature and pressure evaluation

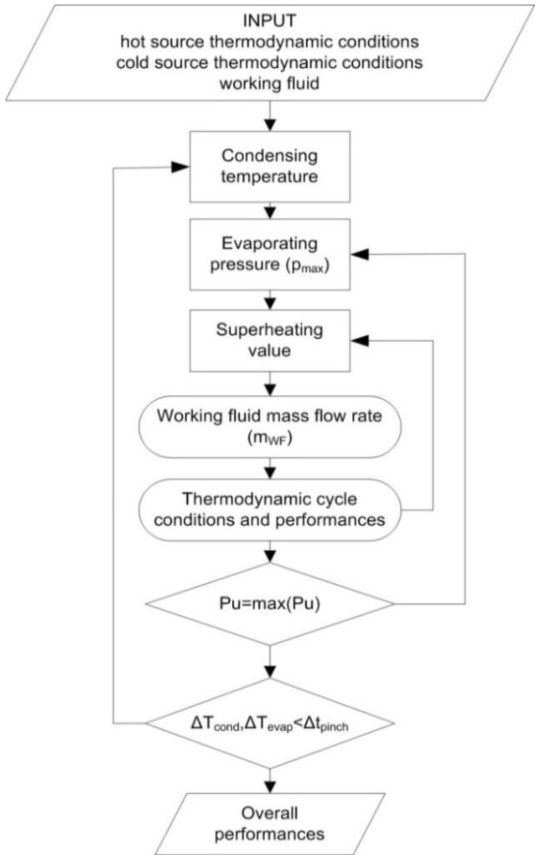

Figure 2: flow chart

3. Definition of the case study

The model described previous has been applied on a case study representing a waste heat recovery from ICE. The following characteristics have been considered:

a) concerning ORC machines, pump efficiency was set at 0.8, while expander adiabatic-isentropic one is 0.75 [19]. When volumetric and mechanical efficiencies are taken into account the overall expander efficiency decreases. The two effects are very complex to be estimated especially for rotary vane machines. Considering that the overall expander efficiency is in the range of 0.5-0.55 [20], the product of volumetric and mechanical efficiency is in the range of 0.70-0.75;

b) some assumptions have been made on cold source available on board: it has been represented by environmental air at 35°C having a mass flow rate of about 1 kg/s: considering the condenser as an air cooled radiator, this is an average value of the air flow that cross the front end of a passenger car [21, 22]. With such heat exchanger technology, the pinch point temperature can be set at 5 K;

c) expander technology considered is the sliding vane rotary one, which is suitable for its flexibility and easy to manage different kind of fluids in several thermodynamic conditions. For technological and economic reasons (components safety and sealing) maximum working fluid pressure has been limited to 20 bar and maximum temperature to 130°C. Expansion ratio can not be higher than 7;

d) the hot source is represented by the exhaust gases of an internal combustion engine propelling a light duty vehicle. The engine considered is an IVECO F1C 3.0L, whose exhaust temperature and mass flow rate have already been known from previous experimental activity (Figure 4, [20, 23]). A typical working point characteristic of this engine has been chosen (130 Nm@2250 RPM) where exhaust mass flow rate is 0.07 kg/s and temperature is 330°C (magenta star in Figure 4). Considering a discharge temperature of 100°C, the available thermal power is about 17 kW. At current stage the model does not consider the off design conditions in the optimization procedure;

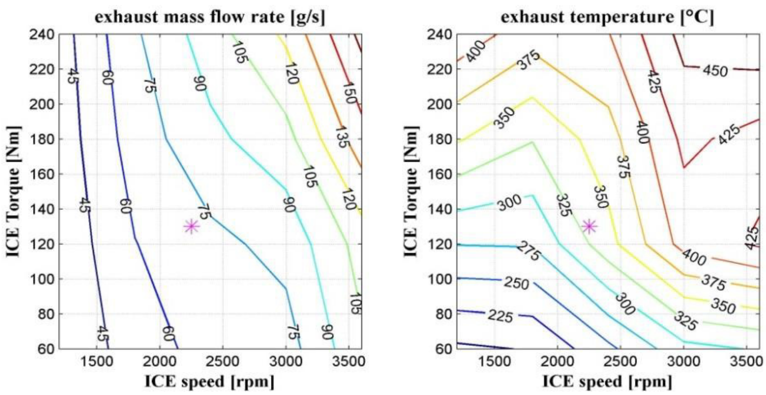

Figure 4: exhaust gas characterization of the ICE

e) the working fluid selection takes in consideration safety information and environmental issue related to fluorinated gases regulations. Some fluids have good thermodynamic properties but at the same time have undesirable environmental and safety constraints. Safety criteria includes the flammability level and safety classification. Environmental and safety criteria consider ODP and GWP which are nowadays phasing out many fluids [18]. Therefore, fluids having GWP < 1500, low toxicity and low flammability (≤A2L) have been selected. Pure hydrocarbons have been considered, in spite of their flammability, because of their high critical temperature which can lead to a thermodynamic cycle closer to the hot thermal source. In fact, they can be suitable for mixtures with HFCs: when they are present in small fractions in mixture, the flammability can be neglected, critical temperature is higher and GWP is lower than the pure HFC.

Zeotropic mixtures have been considered to better follow external sources glide during evaporation and condensation, so reducing irreversibility and enhancing exergy efficiency of the ORC. An important parameter for zeotropic mixtures is, therefore, the temperature glide in phase changing. In this work, only binary zeotropic mixture have been considered. Several mixtures have been considered, the most promising ones have been individuated among those of R245fa and hydrocarbons.

4. Analyses and results

Firstly, the pure fluids were considered. The mathematical model described in section 2 has been used for each single fluid to find the thermodynamic cycle which give the higher value of useful power (product between mass flow rate and cycle work). As shown in Figure 5 and Figure 6, pure hydrocarbons shows very good performances, overcoming the value of 2 kW recovered. These cases, however, have two critical aspects: flammability and high expansion ratio, that is not actually realizable with conventional machines and with a 0.75 efficiency. They have been considered for mixtures. Among the other fluids, the best ones are R245fa and R1233zdE: the first one has 1.7 kW of mechanical power recoverable, thermodynamic efficiency of about 10%, exergy efficiency of about 28% and expansion ratio is 5; the second one has a slightly higher power recovered, but also higher expansion ratio (not suitable for being mixed with hydrocarbons). Then, with these similar performances, R245fa has been chosen for its market availability and higher affordability and it has been taken as the reference fluid for new proposed mixtures.

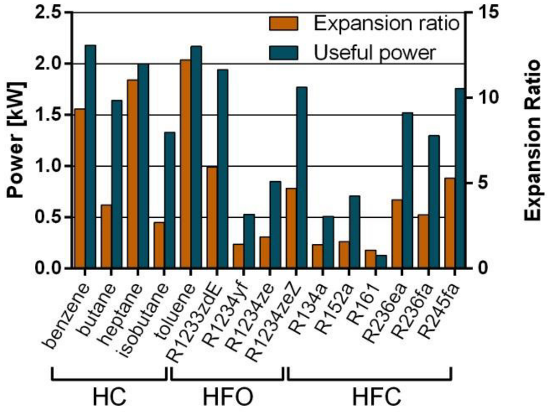

Figure 5: useful power and expansion ratio for pure fluids

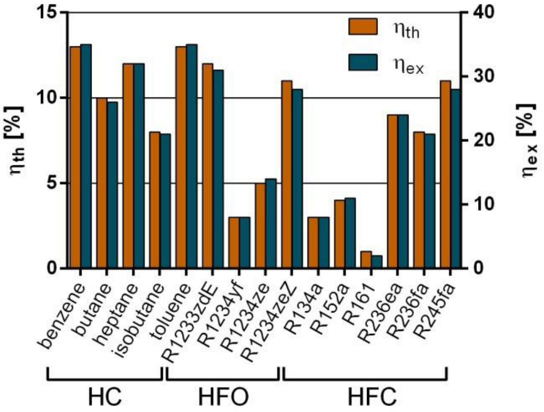

Figure 6: thermodynamic and exergy efficiency for pure fluids

In Figure 7-10 several mixtures of R245fa with hydrocarbons in different mass fractions have been investigated. Hydrocarbons considered were toluene, benzene, heptane, hexane, isohexane, octane. Useful power reaches values very close to 2 kW with small fractions of hydrocarbons (<10%) with a thermodynamic efficiency over 11% (Figure 9). The expansion ratio is slightly increased but still manageable by the expander. The best case is the mixture R245fa-benzene 0.95/0.05 with P_u=1.9 kW, η_{th}=11.5%, η_{ex}=31%.

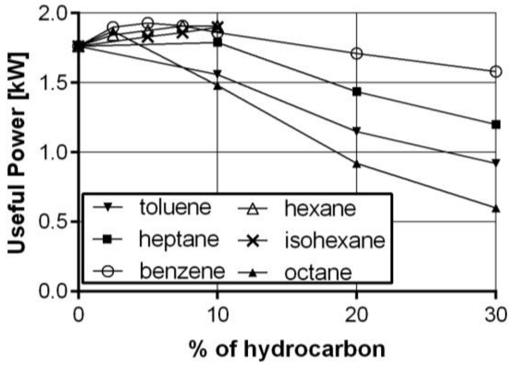

Figure 7: useful recoverable power for R245fa mixtures

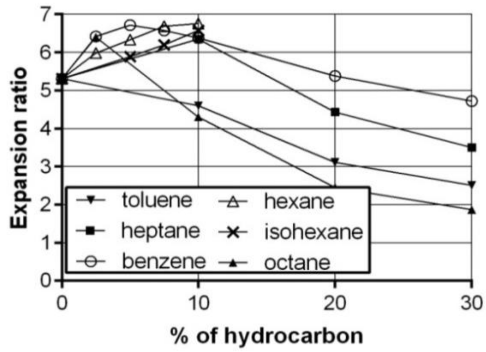

Figure 8: expansion ratio for R245fa mixtures

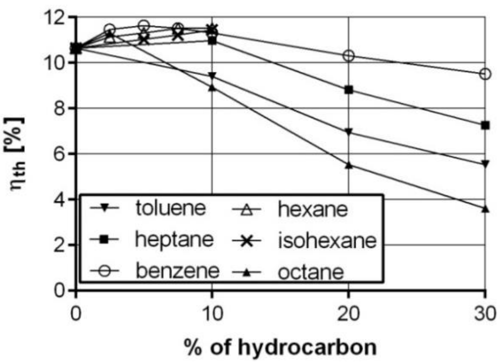

Figure 9: thermodynamic cycle efficiency for R245fa mixtures

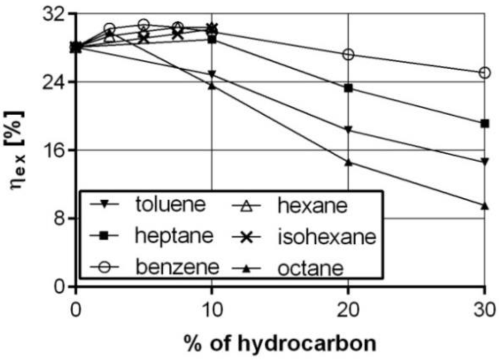

Figure 10: exergy efficiency for R245fa mixtures

In Figure 11 and 12, finally, the T-s diagrams of the pure fluid (R245fa) and that of the best mixture (5% of benzene in R245fa) are shown. The distance between the hot source and the vaporization curve are evident. This is due to the imposed choice of maximum pressure and temperature. Removing these constraints, the cycle could be transcritical and it is possible to increase the performances, but the plant could not be realizable with actual components. The improvement reached with the mixture is 10-12% of mechanical power recovered. Comparing the two cycles, the most relevant improvement seems to be the closeness during the condensation phase obtained through the glide effect of the zeotropic mixture.

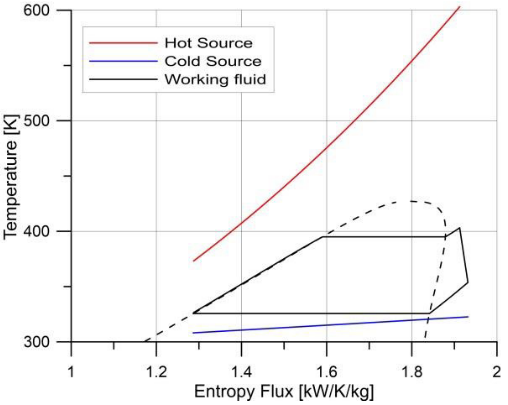

Figure 11: thermodynamic cycle for R245fa

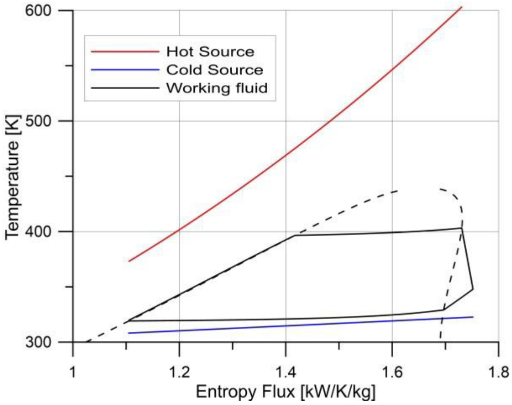

Figure 12: thermodynamic cycle for R245fa/benzene 0.95/0.05

5. Conclusion

In this work, a mathematical model and a procedure of optimization has been presented for ORC bottoming ICEs, under technological constraints of actual proven and reliable components. The model has been used in a case study regarding a hot source of 17 kW at 330°C. Technological constraints are 20 bar as maximum pressure, 130°C as maximum temperature and expansion ratio not higher than 7. The cooling of the condenser is realized in an air cooled radiator. Under these constraints, R245fa is proved to be the optimal fluid leading to a recovered power of 1.7 kW with an overall thermodynamic and exergetic efficiency of 10% and 30%. Using this as reference fluid, many possible mixtures have been investigated: the optimal one is the R245fa-benzene 0.95/0.05 leading to a net power output of 1.9, η_{th}=11.5%, η_{ex}=31%.

The procedure proposed is of a general purpose and can be used in several cases, varying hot source fluid and cooling technologies. A further model extension will regard the cycle performance in off-design conditions which constitute a common working conditions in ICEs for propulsive applications. Results shown are, however, a good reference for the ORC sizing bottoming ICE, especially for quasi-steady state applications.

References

[1] D. Di Battista, M. Mauriello, R. Cipollone, Waste heat recovery of an ORC-based power unit in a turbocharged diesel engine propelling a light duty vehicle, Applied Energy, Volume 152, 15 August 2015, Pages 109-120, ISSN 0306-2619

[2] Cipollone, R., Di Battista, D., Perosino, A., and Bettoja, F., "Waste Heat Recovery by an Organic Rankine Cycle for Heavy Duty Vehicles," SAE Technical Paper 2016-01-0234, 2016, doi:10.4271/2016-01-0234.

[3] Huijuan Chen, D. Yogi Goswami, Elias K. Stefanakos, A review of thermodynamic cycles and working fluids for the conversion of low-grade heat, Renewable and Sustainable Energy Reviews, Volume 14, Issue 9, December 2010, Pages 3059-3067, ISSN 1364-0321

[4] Roberto Cipollone, Giuseppe Bianchi, Davide Di Battista, Giulio Contaldi, Stefano Murgia, Mechanical Energy Recovery from Low Grade Thermal Energy Sources, Energy Procedia, Volume 45, 2014, Pages 121-130, ISSN 1876-6102

[5] Gianfranco Angelino, Costante Invernizzi, Experimental investigation on the thermal stability of some new zero ODP refrigerants, International Journal of Refrigeration, Volume 26, Issue 1, January 2003, Pages 51-58, ISSN 0140-7007

[6] V. Maizza, A. Maizza, Unconventional working fluids in organic Rankine-cycles for waste energy recovery systems, Applied Thermal Engineering, Volume 21, Issue 3, 1 February 2001, Pages 381-390, ISSN 1359-4311, http://dx.doi.org/10.1016/S1359-4311(00)00044-2.

[7] Yongqiang Feng, TzuChen Hung, Kowalski Greg, Yaning Zhang, Bingxi Li, Jinfu Yang, Thermoeconomic comparison between pure and mixture working fluids of organic Rankine cycles (ORCs) for low temperature waste heat recovery, Energy Conversion and Management, Volume 106, December 2015, Pages 859-872, ISSN 0196-8904, http://dx.doi.org/10.1016/j.enconman.2015.09.042.

[8] J. Vivian, G. Manente, A. Lazzaretto, A general framework to select working fluid and configuration of ORCs for low-to-medium temperature heat sources, Applied Energy, Volume 156, 15 October 2015, Pages 727-746, ISSN 0306-2619

[9] S. Amicabile, J. Lee, D. Kum, A comprehensive design methodology of organic Rankine cycles for the waste heat recovery of automotive heavy-duty diesel engines, Appl. Therm. Eng. 87 (2015) 574–585.

[10] C. Sprouse III, C. Depick, Review of organic Rankine cycles for internal combustion engine exhaust waste heat recovery, Appl. Therm. Eng. 51 (2013) 711–722.

[11] Saleh B, Koglbauer G, Wendland M, Fischer J. Working fluids for low temperature organic Rankine cycles. Energy 2007;32:1210–21

[12] B. Kolsch, J. Radulovic, Utilisation of diesel engine waste heat by organic Rankine cycle, Appl. Therm. Eng. 78 (2015) 437–448.

[13] Gholamreza Bamorovat Abadi, Eunkoo Yun, Kyung Chun Kim, Experimental study of a 1 kW organic Rankine cycle with a zeotropic mixture of R245fa/R134a, Energy, Volume 93, Part 2, 15 December 2015, Pages 2363-2373, ISSN 0360-5442

[14] Liu Q, Duan Y, Yang Z. Effect of condensation temperature glide on the performance of organic Rankine cycles with zeotropic mixture working fluids. Appl Energy 2014;115:394–404.

[15] Le VL, Kheiri A, Feidt M, Pelloux-Prayer S. Thermodynamic and economic optimizations of a waste heat to power plant driven by a subcritical ORC (Organic Rankine Cycle) using pure or zeotropic working fluid. Energy 2014;78:622–38.

[16] B. Dai, M. Li, Y. Ma, Thermodynamic analysis of carbon dioxide blends with low GWP (global warming potential) working fluids-based transcritical Rankine cycles for low-grade heat energy recovery, Energy, Volume 64, 1 January 2014, Pages 942-952, ISSN 0360-5442

[17] E. W. Lemmon, R. T Jacobsen - A Generalized Model for the Thermodynamic Properties of Mixtures - International Journal of Thermophysics May 1999, Volume 20, Issue 3, pp 825-835 – Nist Refprop user's manual

[18] Regulation (Eu) No 517/2014 Of The European Parliament And Of The Council of 16 April 2014 - on fluorinated greenhouse gases and repealing Regulation (EC) No 842/2006

[19] Cipollone R, Bianchi G, Murgia S, Contaldi G. Energy recovery using sliding vane rotary expanders. In: Proceedings of the 8th International Conference on Compressors and their Systems at London. ISBN 978-1-78242-169-6; 2013, p. 183 - 194.

[20] R. Cipollone, G. Bianchi, A. Gualtieri, D. Di Battista, M. Mauriello, F. Fatigati - Development of an Organic Rankine Cycle system for exhaust energy recovery in internal combustion engines - 33rd UIT Heat Transfer Conference, L'Aquila, June 22-24, 2015 - Journal of Physics: Conference Series, Volume 655, conference 1

[21] Cipollone, R. and Di Battista, D., "Performances and Opportunities of an Engine Cooling System with a Double Circuit at Two Temperature Levels," SAE Technical Paper 2012-01-0638, 2012

[22] Cipollone, R., Di Battista, D., Gualtieri, A. - A novel engine cooling system with two circuits operating at different temperatures (2013) Energy Conversion and Management, 75, pp. 581-592

[23] Di Battista D, Mauriello M, Cipollone R. Effects of an ORC based heat recovery system on the performances of a diesel engine. SAE technical paper 2015-01-1608; 2015

Nomenclature

h	specific enthalpy [kJ.kg^{-1}]
I	irreversibility [kW]
m	mass flow rate [kg.s^{-1}]
P	power [kW]
Q	thermal power recovered from hot source [kW]
s	specific entropy [kJ.kg^{-}1.K^{-1}]
S	entropy [kJ.K^{-1}]
T	temperature [K]
ΔT	temperature difference [T]
η	efficiency [%]

Subscripts

1,2,3,4	cycle point
ad,is	adiabatic-isentropic
cond	condenser
ev	evaporator
ex	exergy
exp	expander
hs,in	hot source inlet
hs,out	hot source outlet
P	pump
ref	reference state
th	thermodynamic
u	useful
wf	working fluid

Abbreviations

GWP	global warming potential
HC	hydrocarbon
HFC	hydrofluorocarbon
HFO	hydrofluoroolefin
ICE	internal combustion engine
ODP	ozone depletion potential
OEM	Original Equipment Manufacturer
ORC	Organic Rankine Cycle