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Integrated working fluid-thermodynamic cycle design of organic Rankine cycle power systems for waste heat recovery

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HIGHLIGHTS

- A new simultaneous approach is presented for integrated pure working fluid and process design.
- A 37 MW marine diesel engine's exhaust gas waste heat is recovered.
- The design solution is a 1.2 MW organic Rankine cycle unit with recuperator.
- A UA-optimization study designed a 1.25 MW cycle and a HCFO fluid.
- The new method provided a global optimal design with 5.04 CPU seconds.

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ABSTRACT

Today, some established working fluids are being phased out due to new international regulations on the use of environmentally harmful substances. With an ever-increasing cost to resources, industry wants to converge on improved sustainability through resource recovery, and in particular waste heat recovery. In this paper, an organic Rankine cycle process and its pure working fluid are designed simultaneously for waste heat recovery of the exhaust gas from a marine diesel engine. This approach can overcome design issues caused by the high sensitivity between the fluid and cycle design variables and otherwise high resource demands, which through conventional methods cannot be addressed. The global optimal design was a 1.2 MW cycle with 2,2,3,3,4,4,5,5-octafluorohexane as the new fluid. The fluid has no ozone depletion potential and a global warming potential under the regulatory limit. By using the simultaneous design approach the optimum solution was found in 5.04 s, while a decomposed approach found the same solution in 5.77 h. However, the decomposed approach provided insights on the correlation between the fluid and cycle design variables by analyzing all possible solutions. It was shown that the high sensitivity between the fluid and cycle design variables was overcome by using the simultaneous approach. Correlation between net power output and the product of the overall heat transfer coefficient and the heat transfer area could further be addressed by employing a new solution strategy including maximum constraints for this product. The use of such constraints resulted in the design of a new fluid (5-chloro-4,5,5-trifluoro-2,3-dimethylpent-2-ene) with a 1.25 MW net power output. Finally, a comparison with conventional fluids was shown where 2,2,3,3,4,4,5,5-octafluorohexane offered an improvement on net power output and economic and environmental metrics.

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1. Introduction

Recovering waste heat from processes requires significant effort in the design and optimization of the working fluid as well as the thermodynamic cycle. Environmental regulations have been a driving force for the industry to seek novel working fluids since many conventional fluids are being phased out. This follows the Kyoto Protocol in 1997 and more recently new EU regulations from 2014 [1,2], which restrict the use of some working fluids currently in use [3]. However, design of a new working fluid poses a challenge and finding an optimum solution for a given application often results in a trade-off between cycle performance, and environmental and safety criteria. Furthermore, low-temperature (low-grade) waste heat sources pose additional challenges to make the recovery technically and economically feasible [4–6]. Amongst

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Nomenclature

Symbol

A	heat transfer area (m^2)
$C_{p,A}$	ideal gas heat capacity parameter
$C_{p,B}$	ideal gas heat capacity parameter
$C_{p,C}$	ideal gas heat capacity parameter
$C_{p,D}$	ideal gas heat capacity parameter
$C_{p,ig}$	ideal gas heat capacity (J/mol/K)
F_r	flow rate working fluid (mol/s)
GWP	global warming potential (CO2 eq)
h	enthalpy (J/mol)
n	number of group
ODP	ozone depletion potential (R11 eq)
P	pressure (bar)
P_c	critical pressure (bar)
q	molecular structure type
s	entropy (J/mol/K)
T	temperature (K)
T_c	critical temperature (K)
U	overall heat transfer coefficient ($W/m^2/K$)
v	valency
$\dot{W}_{net}$	net power output (W)
Z	compressibility
φ	fugacity coefficient
Ψ, Ω	equation of state parameter
ω	acentric factor

Superscript

U	upper bound
L	lower bound

Subscript

g	exhaust gas
i_1	group set
LMTD	logarithmic mean temperature difference
ph	phase set
s	isentropic process
st	stream/stage set
w	cooling sea water

others, hydrofluoroolefins (HFOs) have been suggested as a potential future class of low global warming potential working fluids. However, data for such fluids is scarce in conventional databases [7–10]. These issues have led to the development of several methods and tools for designing new working fluids and organic Rankine cycle (ORC) power systems.

Most of these methods are based on computer-aided molecular design techniques (CAMD) to design alternative or novel working fluids [11]. Papadopoulos et al. [12–14] proposed a systematic design approach for working fluid generation for ORC units. Here, a weighted objective function based on scaled pure properties was proposed and used. As reported in their work, ten pure fluid properties are influential in the cycle performance and in the feasibility of the solution. Specifically, three of these process metrics are important to optimize. Initially [12], the authors used the weighted objective function employing all of the important pure fluid properties. Subsequently, the problem was reformulated into a multi-objective optimization problem considering only five of the pure fluid properties [13]. Finally, the cycle performance was evaluated for one or more solutions. Palma-Flores et al. [15] also proposed a method for choosing the optimal pure working fluid for an ORC unit using a CAMD approach. The objective function here was based on temperature dependent pure fluid properties.

Other authors have taken approaches which avoid CAMD method and start either with a set of chosen fluids or apply a reverse engineering approach. For example, Andreasen et al. [16] proposed a methodology for working fluid selection for an ORC unit for use of low-temperature heat. Thirty pure and mixed working fluids were selected through optimization of the ORC unit. The fluids were ranked according to the objective function, which was the cycle net power output. Likewise a reversed engineering approach can be employed, where the optimal fluid properties are found through an optimization problem without regard to chemical feasibility or stability of the molecule. Molecules that then match these properties are found in a subsequent step. Such methods have been reported in several works and frequently such a solution approach has been found necessary due to the complexity of the thermodynamic model employed [17–19]. These methods are usually termed a continuous-molecular targeting approach (CoMT-CAMD). The works presented tend to optimize all the fluid properties, which is a difficult task, given the correlation between properties that may make the result in local optima [5,20]. The issue of correlated properties also holds true when considering the detailed design of certain components in the ORC unit that cannot solely be based on primary fluid properties [21].

The current state-of-the-art offers methods for designing fluids for organic Rankine cycle units from a sequential (or decomposed) approach, where the working fluid design and process optimization are carried out in separate steps. This results in sub-optimal solutions on account of high correlation between fluid and process variables. In this way, the methods are not able to obtain a global optimal design of working fluid and process.

In contrast, in the work we report here, for the first time, a simultaneous approach is proposed for integrated pure working fluid and process design for organic Rankine cycle power systems. We reasoned that such an approach would have the benefit of: (i) a pre-screening step to avoid a sub-optimal starting point, (ii) the design of alternative or new fluids that are environmentally friendly and have similar or improved cycle performance compared to conventional fluids, (iii) a rapid search for the global optimum. The approach is based on the use of CAMD, property prediction and mathematical programming techniques to define the fluid-process targets and models, which are combined and solved simultaneously. Additionally we have included for the first time the design of bicyclic and branched cyclic molecules using CAMD.

This paper will first present the problem description, followed by the approach used and the models needed. Subsequently, the results for the simultaneous design strategy are presented and compared to a decomposed design strategy. The discussion section focusses on the sensitivity of the design variables, the advantage of the simultaneous approach, and on whether the global optimum is found. Finally, the novel fluid resulting from the optimization is compared to conventional fluids.

2. Methods

The integrated method employed in this work is summarized in the workflow shown in Fig. 1. Several methods were used to simultaneously design alternative or novel working fluids for the organic Rankine cycle process. CAMD was used to enable a model-based

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