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Multi-criteria evaluation of several million working fluids for waste heat recovery by means of Organic Rankine Cycle in passenger cars and heavy-duty trucks

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HIGHLIGHTS

- 72 million working fluids are screened for their use in mobile ORC systems.
- Realistic boundary conditions from series engines of different manufacturers are used.
- A multi-criteria approach evaluates thermodynamic, constructional and regulatory aspects.
- An objective scoring systems to find optimal working fluids is developed.
- So far unknown ORC working fluids can be identified by the large-scale screening.

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ABSTRACT

Automotive industry is driven by economic and legislative constraints to increase fuel efficiency and reduce CO_2-emissions to a certain extend. To reach the required threshold values, manufacturers consider waste heat recovery by means of Organic Rankine Cycle (ORC) in passenger cars and heavy-duty trucks. This work deals with the crucial issue of identifying an optimal working fluid which is flexible in terms of application and condensing temperature and which is applicable in real systems. For this purpose, a large-scale screening based on computational chemistry and thermodynamic process simulation is coupled with a multi-criteria evaluation. In total, about 72 million chemical substances provided by the PubChem database are screened and more than 3000 promising candidates are evaluated considering COSMO-RS based thermodynamic data as well as constructional, regulatory and security aspects. Five promising working fluids are identified and it is shown that these fluids outperform widely discussed candidates like synthetic refrigerants. Even more remarkably is the fact that within the TOP 100 working fluids only twelve have already been reported in ORC literature. However, the optimal set of working varies as it depends on configuration (with and without mass flow splitting) and condensing temperature. In general, the study demonstrates that a large-scale screening of the complete chemical space can reveal unconventional working fluids for thermodynamic cycles.

1. Introduction

Transport system is driven by economic and legislative constraints to increase fuel efficiency and reduce CO_2-emissions. Manufacturers of passenger cars and trucks consider waste heat recovery by means of Organic Rankine Cycle (ORC) to reach these goals [1,2]. The main differences between the reported systems include the following aspects (Table 1 gives a comprehensive overview about main research work carried out in the last decade without claim of completeness):

- *Application:* Waste heat recovery by means of ORC is relevant for light and heavy duty trucks as well as for automotive applications.
- *Heat sources:* Depending on the application, exhaust gas can be used within the exhaust gas recirculation (EGR) and after the exhaust gas aftertreatment (EGA). Further heat sources are the compressed air charger (CAC) and the cooling loop. If more than one heat source is

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Nomenclature

Ar	argon
CO_2	carbon dioxide
$\dot{m}$	mass flow rate (kg/s)
N_2	nitrogen
O_2	oxygen
P	electric power (kW)
p	pressure (bar, kPa)
$\dot{Q}$	heat flux (kW)
s	specific entropy (kJ/kg K)
T	temperature (°C, K)

Abbreviations

AIT	autoignition temperature
ASHRAE	American Society of Heating, Refrigerating and Air-Conditioning Engineers
CAMD	Computer Aided Molecular Design
ECHA	European Chemical Agency
EGA	exhaust gas aftertreatment
EGR	exhaust gas recirculation
GWP	Global Warming Potential
ODP	Ozone Depletion Potential
OP	Operational Point
ORC	Organic Rankine Cycle
R	refrigerant
REG	regulatory
TD	thermodynamic

Greek letters

Δh	specific enthalpy difference (kJ/kg)

Subscripts

cond	condenser
net	net power output
ORC	Organic Rankine Cycle

utilized, split circuits are often used as ORC configuration.

- *Condensation:* Condensation can be realized by ambient air but also by the available cooling water circuit.

Main objectives of available simulative and experimental analyses are first and second law efficiency and in some publications also technical aspects of the system. The selection of an appropriate working fluid is hardly investigated for mobile applications. The publications given in Table 1 select working fluids based on main publications from stationary applications, which might be inappropriate due to different boundary conditions in mobile compared to stationary applications. Few research groups investigate working fluid selection with special concern to mobile applications. Glover et al. [3,4] carried out a working fluid selection based on process simulation of sub- and supercritical mode of operation. They screened 95 pure fluids and 10 azeotropic blends from the RefProp database regarding critical temperature and pressure, toxicity and flammability. They identified 18 possible working fluids without defining an optimal one. Lang et al. [5] suggested 3 working fluids (hexamethylcyclotrisiloxane D3, octamethycyclotetrasiloxane D4, water) out of 32 candidates. They included melting temperature, thermal stability, pressure levels, environmental impact, toxicity, flammability, availability, costs, material compatibility, and lubrication properties into account during the screening and evaluation process. Shu et al. [6] considered off-design behavior of seven different working fluids for harvesting of marine engine's exhaust waste heat, Girgin and Ezgi [7] emphasized for the same application how important it is to include safety aspects into the working fluid selection as even in the shipping industry benzene as efficient but carcinogenic working fluid would be a problem. A large-scale screening is carried out by Panesar et al. [8,9]. They investigated water/alcohol-mixtures as working fluid for a novel system whereas a large database of possible second constituents of water blends has been screened. The exact number of screened constituents is not given. Wang et al. [10] investigated nine working fluids from the RefProp database and took safety aspects, environmental impact and performance into account. R245fa and R245ca seem to be promising based on their results. Yang et al. [11–13] investigated ethanol, zeotropic mixture R416A and R245fa/R152a-mixtures. Furthermore, they evaluated eight fluid mixtures based on performance, heat transfer, physical and chemical properties, intersolubility with lubrication oil, security aspects, environmental aspects, electrical isolation capability, and economic aspects. Further studies include fully dynamic ORC simulations for ethanol in heavy duty trucks [14,15], investigation of hot-spots for dynamic operation [16], cascade systems with two expansion units [17] and dynamic response characters for 14 working fluids in engine waste heat recovery [18].

Based on the available studies, the following shortcomings in the available literature are identified:

- It has not been investigated if split cycles with two heat sources (mostly used in trucks) and basic cycles with one heat source (mostly used in automotive industry) require different working fluids or if one working fluid is efficient for both applications.
- It has not been investigated if working fluid selection is influenced by the choice of the condensation temperature.
- The number of investigated working fluids is rather small and depends on the available database.
- A multi-criteria evaluation of working fluids including thermodynamic, constructional, safety, regulatory and environmental aspects has not been carried out.

This leads to the research question, which is addressed in our contribution:

> Is it possible to identify an optimal working fluid, which is suitable for split and basic ORCs at different condensation temperatures in real mobile applications?

To answer this question, we screened about 72 million chemical structures given in the PubChem database by application of the COSMO-RS methodology [19] and evaluated them for two different ORC configurations and three different cooling concepts to get a multi-criteria ranking based on ten different criteria. Our work aims to increase the number of screened working fluids and their chemical classes tremendously compared to group contribution methods (e.g. screening of hydrofluorocarbons [20,21]) or available thermodynamic databases. Furthermore, we intend to increase the number of different evaluation parameters especially concerning construction issues compared to other publications [22]. As the evaluation criteria are discussed and selected together with an industrial advisory board, the study aims for a highly practical approach. To summarize, it is our goal to give a contribution to ORC application in real mobile systems by identifying more elaborate working fluids which are able to fill the gap to profitability of such systems reported recently by Pili et al. [23].