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Fluid selection and thermodynamic optimization of organic Rankine cycles for waste heat recovery applications

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Abstract

Organic Rankine cycles are effective to convert waste heat to power. One of the advantages and challenges of these cycles is that the most suitable working fluid and cycle configuration have to be selected for every application. Numerous fluids can be used in organic Rankine cycles, including hydrocarbons, HCFCs, HFCs, siloxanes, alcohols, or even mixtures of fluids. The selection of the working fluid can be based on many different criteria including the thermodynamic match with the heat source and sink, chemical stability, environmental concerns, safety, or cost and it is not possible to find a single best fluid for a given application. For this reason, the fluid selection and cycle optimization is usually a compromise between different factors. In this work, an organic Rankine cycle is proposed for a waste heat recovery application where the heat source is a 10 kg/s mass flow rate of air at 250 °C (with a low temperature limit of 100 °C) and the heat sink is liquid water at 10 °C. 80 pure working fluids from the REFPROP library were considered and several screening criteria were used to preselect 27 of these fluids. A robust, steady-state solver for cycles with and without recuperation was developed in MATLAB. The REFPROP libraries were linked to the solver to compute the thermodynamic properties of the working fluids. In order to select the most suitable fluids, a single objective, thermodynamic optimization was performed using a genetic algorithm with the second law efficiency as objective function and the expander performance of the optimal solutions was analyzed. The second law efficiency of the recuperated cycles was higher than that of simple cycles for most cases. In addition, the results show that the second law efficiency of simple cycles has a strong dependence with the choice of working fluid while it is relatively independent for recuperated cycles. The results of the optimization were presented in terms of a reduced temperature parameter to define some criteria for the selection of the optimal working fluids and cycle configurations. It was found that the transcritical-recuperated cycle configuration using *dry* or *isentropic* substances was optimal when the critical temperature of the working fluid is slightly lower than the temperature of the heat source. Conversely, no general trend was discovered for the optimal cycle configuration when critical temperature of the working fluid is higher than the temperature of the heat source.

Keywords: heat-to-power; ORC; fluid screening; process modeling and simulation; genetic algorithm; transcritical; exergy;

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1. Introduction

A solid scientific consensus indicates that global warming is unequivocal and that it is caused by the increased concentration of greenhouse gases in the atmosphere. In addition, there is an agreement that the increased concentration of these gases is caused mainly by human activities and natural causes only represent a minor effect [1]. The recovery of waste heat from industrial processes is an effective manner to increase energy efficiency and reduce CO_2 emissions. Thermal energy from an industrial process can be regarded as waste heat when it cannot be used in direct applications, such as district heating. In this case, the heat can be potentially converted into power. The works by Quoilin et al. [2] and Colonna et. al [3] review applications where waste heat recovery is possible.

The conventional gas Brayton cycle and steam Rankine cycle are not well suited for heat sources of low to medium temperatures[1] because of thermodynamic and technical reasons, respectively [5]. The adoption of Rankine cycles using *dry* organic fluids with high molecular mass rules out many of the problems of using water as working fluid. These cycles are usually know as organic Rankine cycles (ORC) and the selection of the optimal working fluid and cycle configuration is one of the main challenges. This is usually investigated using an enumerative approach, in which every fluid candidate is simulated and optimized to find the best choice of working fluid and cycle layout.

In the last years, there have been several works on the fluid selection and *thermodynamic optimization* of Rankine cycles for waste heat recovery applications. Dai et al. [6] analyzed waste heat recovery from a source of 16 kg/s at 145 °C. They used a *genetic algorithm* to optimize the second law efficiency of Rankine cycles for 10 different working fluids. Wang et al. [7] presented a working fluid selection and multiobjective optimization using a *simulated annealing* algorithm. In that work, they analyzed 13 working fluids for heat sources from 100 to 220 °C. Larsen et al. [8] studied Rankine cycles for waste heat recovery in marine applications (180–360 °C). They considered 109 working fluids and used a *genetic algorithm* with the first law efficiency as objective function for the optimization. These works found the optima solutions for different case studies and provided qualitative guidelines for the selection of working fluid and cycle configuration. However, they did not provide any quantitative criterion.

Astolfi et al. [9,10] analyzed ORC for the exploitation of geothermal brines from 120 °C to 180 °C in a two-part paper where they perform both a thermodynamic optimization [9] and a techno-economic optimization [10]. They used an *active set* algorithm with the second law efficiency as the objective function for the thermodynamic optimization. 54 working fluid were studied considering both simple and recuperated cycles in subcritical and transcritical configurations. These works are highlighted because it was the first time (to the authors' knowledge) when a simple quantitative criterion was presented to select the optimum working fluid and cycle configuration for a given heat source. They found that the optimal plant efficiencies are obtained for transcritical, recuperated configurations when ratio of the critical temperature of the working fluid to the inlet temperature of the heat source is between 0.88–0.92.

Other authors have also proposed quantitative criteria relating the critical temperature of the working fluid and the inlet temperature of the hot source. Zhai et al. [11] analyzed heat sources in the 150–350 °C range and proposed an indicator to select the optimum working fluid as a function of the critical and boiling temperatures. Yang et al. [12] analyzed heat sources in the 150–300 °C range and proposed a correlation for the critical temperature of the working fluid as a function of the heat source inlet temperature. Despite both works cover a wide range of temperature and give a quantitative criterion for the selection of the optimum working fluid, they are limited to simple, subcritical cycles.

The aim of the present study is to: 1) find the optimal working fluid and cycle configuration for a waste heat source of hot air at 250 °C in order to extend the results from [9] to other temperature ranges, 2) discuss if superheating should always be as low as possible, and 3) analyze the expander performance of the optima solutions. Different cycle configurations (subcritical-transcritical, saturated-superheated, simple-recuperated) and 80 pure working fluids were considered in this work. The fluid screening methodology used to reduce the number of fluid candidates, the details of the cycle simulation and optimization, and the expander analysis are described in Section 2. After this, the results of the fluid screening, thermodynamic optimization, and expander performance are presented and discussed in Section 3. Finally, Section 4 contains the main conclusions drawn from the results obtained in this work.

[1] Several authors, including [3] and [4] classify waste heat sources according to their temperature level as: low-temperature ($T < 230$ °C), medium-temperature (230 °C $< T <$ 650 °C), and high-temperature ($T >$ 650 °C).