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Simultaneous molecular and process design for waste heat recovery

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ABSTRACT

Processing streams featuring low temperatures are common in industrial systems. Because of low temperatures it turns out to be a challenge to use these type of streams for energy recovery. This is especially true if water is used as the main fluid for energy recovery since large amounts of energy are required for water vaporization. To cope with this energy problem different types of organic fluids used in Rankine-like thermodynamic cycles have been proposed. However, high cost and sustainability issues (i.e. large toxicity) related to organic fluids call for the design of a new type of working fluids suitable for low-temperature energy recovery. This generation of new working fluids should feature target properties such as high vapor pressure and low flammability and toxicity values. Moreover, the performance of these new working fluids also depends on the operating conditions of the thermodynamic cycle where such working fluids will be used. In this work we address the simultaneous product and process design problem of working fluids for energy recovery from low-temperature energy sources in Rankine-like cycles to obtain improved optimal solutions. We compare the energy recovery performance of both the new family of working fluids and processing conditions against similar energy performance obtained using organic fluids previously used for the same aim. By using a system of coupled cycles, work production was increased. Moreover, the new working fluids feature improved safety margins. The results indicate the benefits of the simultaneous product and process design approach and permit us to identify a family of working fluids with better sustainability characteristics.

1. Introduction

Nowadays, efficient use of energy represents a subject of wide range of social and research interest. The imminent depletion of fossil fuels is an issue due to the increasing demand for energy around the world. Present works referring to energy use and production have been focused in renewable energies as sustainable alternatives. Today, one of the major challenges in energy research lies in proposing new energy alternatives that are green, economical and efficient. In particular, there is a kind of energy source which is not considered in the normal industry operation for energy recovery. This energy source is related to low-temperature processing streams which are normally below 200° C. Commonly, this kind of low-temperature streams can be found in processing plants, geothermal and solar energy sources. In most cases, typical Rankine cycles are used for energy recovery from these kinds of energy sources. However, the reason why energy recovery is inefficient when these systems are deployed has to do with the fact that water is the fluid used for energy recovery. Therefore, there is a good opportunity for enhancing energy recovery from low-temperature energy sources if novel low-boiling components are used for this aim. Moreover, if the optimal design of the Rankine cycle and the design of such novel compounds are tackled simultaneously, the natural interactions between the design of both systems can be taken into account leading to improved optimal solutions.

In this work we address the efficient heat recovery issue from low-temperature heat sources. As stated before, the use of conventional systems such as the Rankine cycle, with water as working fluid, becomes inefficient for power generation purposes. Therefore, to improve the efficiency of the Rankine cycle for energy recovery from low-temperature heat sources it is necessary to employ working fluids with lower boiling point, with respect to the water boiling point. At low temperatures the operation of the Rankine cycle in most of the cases is carry out by organic fluids. When an organic fluid is used as working fluid in the Rankine cycle such a system is named an ORC (organic Rankine cycle). We propose the implementation of CAMD (computer-aided molecular

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design) techniques to synthesize a set of new compounds that can be used as working fluids in the organic Rankine cycle process with the aim to improve the cycle efficiency for waste heat recovery at low-temperature processing conditions. In a previous work [1] a methodology was established for waste heat recovery through the implementation of the CAMD approach for the synthesis of new compounds with optimal properties to be used as working fluids in the organic Rankine cycle process (Fig. 1). In the sequential methodology used in a previous [1] work a series of new compounds were synthesized through the optimization of the physical and thermodynamic properties that were considered as key properties for the suitable performance of the compounds as working fluids in the ORC process. Then the performance of the novel organic compounds was tested in a conventional Rankine cycle. The results reported in Ref. [1] were comparable to results obtained when common organic fluids are employed. However, it has been well known for a while that strong interactions exist between the design of products and the equipment were such compounds will be used [2–4]. Taking advantage of such interactions would lead to obtain better and efficient optimal solutions in comparison to traditional sequential design methods. Therefore, in this work we propose the simultaneous optimization of the ORC operating conditions and the synthesis of the working fluid with the aim to improve the recovery of waste energy from low temperature sources that we will assume are available at 200° C [5–7].

In summary, the contributions of this work can be stated as follows. We will extend the results presented in Ref. [1] to approach the efficient energy recovery from low-temperature energy sources. In Ref. [1] we have shown that energy recovery efficiency increase when proper organic working fluids are designed. However, efficient energy recovery also depends upon the processing conditions. Therefore, by tackling simultaneously both the optimal design of the organic working and the optimal design of the Rankine cycle improved optimal solutions can be obtained. We use two case studies to illustrate this point.

2. Problem definition

We propose to employ the CAMD approach with group contributions methods, for the estimation of the physical and thermodynamic properties, for the synthesis of new compounds to be employed as working fluids in the organic Rankine cycle. For this implementation we propose a basis set of functional groups, where these groups can be combined in different ways to synthesize new compounds with properties that can be adapted for the optimal process operation for waste heat recovery at low-temperature conditions.

Then, the statement of the research problem to be addressed in this work goes as follows: “Given a low temperature heat source and a basis set of functional groups, the problem consist of the simultaneous optimal design of both the working fluid and the ORC process (i.e.; operating temperatures and pressures, working fluid mass flow, output work of the turbine, evaporator and condenser operating heat duties, heat transfer areas and the ORC process configuration) with the aim to improve the recovery of waste energy from low-temperature energy sources”. The modeling constraints and structural assumptions are thoroughly discussed in Ref. [1]. For the heat source, we have assumed a processing stream available at 200° C. While the aim is to compute new molecules, the physical and thermodynamic properties will be estimated by group contribution methods.

3. Formulation and methodology

In this section we present the methodology for the optimal design of the working fluids and the power cycle operating conditions for waste heat recovery from a low-temperature heat source. In a first case study we consider the simultaneous design of the power cycle and the working fluid, where the aim is to improve the cycle first law efficiency. While, in a second case study we propose to increase the net work output which can be generated by the heat recovery from the low-temperature heat source. In this case study we propose a system of coupled ORC processes, where the condenser of a first ORC process can play the role of the evaporator of a second ORC process. The aim is to increase the energy that can be recovered from a heat source with specific conditions of availability. Employing CAMD (computer-aided molecular design) techniques, a family of new working fluids for the ORC system can be synthesized.

In this work we will employ the ORC process configurations proposed by Saleh et al. [8] and Desai & Bandyopadhyay [9]. Saleh et al. [8] have suggested the inclusion of an IHE (internal heat exchanger), this configuration is shown in Fig. 2, whereas Desai & Bandyopadhyay [9] proposed the addition of a DCH (direct contact heater) and a turbine bleeding system shown in Fig. 3. These configurations were established with the aim to improve the ORC

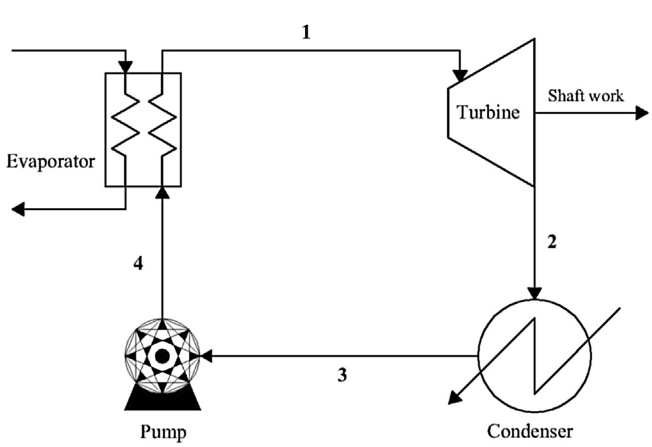

Fig. 1. Typical Rankine Cycle (configuration A) using water as working fluid. If the working fluid turns out to be an organic fluid the process is called and ORC (organic Rankine cycle).

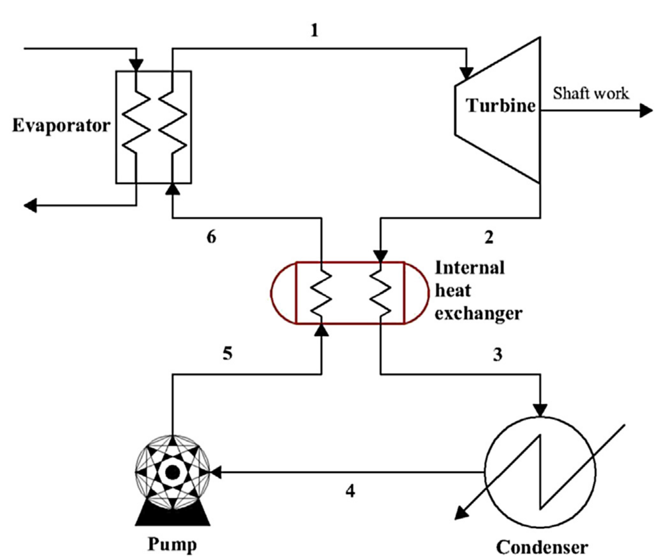

Fig. 2. ORC process with internal heat exchanger (configuration B).