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A stochastic optimization approach for the design of organic fluid mixtures for low-temperature heat recovery

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HIGHLIGHTS

- A stochastic optimization approach is proposed to design organic heat transfer fluids.
- Risk metrics are used to design fluids that withstand strong variability in system conditions.
- Non-intuitive mixture compositions are identified.

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ABSTRACT

Over 50% of the heat generated in industry is in the form of low-grade heat (with operating temperatures below 370 °C). Recovering heat from these sources with standard Rankine cycles (using water as working fluid) is inefficient and expensive. Organic working fluids have become an attractive alternative to mitigate these inefficiencies. In this work, we address the problem of designing flexible multi-component organic fluids capable of withstanding variability in heat source temperatures and efficiencies of individual cycle equipment units. The design problem is cast as a nonlinear stochastic optimization problem and we incorporate risk metrics to handle extreme variability. We show that a stochastic optimization framework allows us to systematically trade-off performance of the working fluid under a variety of scenarios (e.g., inlet source temperatures and equipment efficiencies). With this, it is possible to design working fluids that remain robust in a wide range of operational conditions. We also find that significant flexibility of the working fluid can be obtained by using optimal concentrations as opposed to using single component mixtures. We also find that state-of-the-art nonlinear optimization solvers can handle highly complex stochastic optimization problems that incorporate detailed physical representations of the system.

1. Introduction

Low-grade heat is a low-temperature (below 370 °C) heat source that is deemed too inefficient/expensive to recover [1,2]. Over 50% of the total heat generated in industry is in the form of low-grade heat [3]. In the cement industry, for instance, 40% of the heat available for recovery is lost to the environment via flue gases (at temperatures in the range 215–315 °C) [4]. According to the US Department of Energy, 33% of the energy used in the manufacturing sector is waste heat and approximately 60% of this waste heat is at temperatures below 230° [2]. Power generation is an important source of waste heat, which include: liquid streams (50–300 °C), stack losses (150–180 °C), steam losses (100–250 °C), and processing gases and vapors (80–300 °C). Low-grade heat is also found in emerging sustainable power generation technologies that include concentrated solar (below 300 °C), biomass-based (150–320 °C), and geothermal power generation (60–200 °C) [5,1,6]:

The conventional Rankine cycle (steam power cycle) has long been the workhorse in power generation. These systems use water as working fluid which makes the recovering of low-grade waste heat inefficient and expensive [7]. This is because water, while inexpensive and scalable, has limited thermodynamic flexibility. The Organic Rankine Cycle (ORC) provides a more attractive avenue to recover low-grade heat. In this cycle, an organic heat transfer fluid with low-boiling point and high vaporization enthalpy is used to drive the cycle [8,7,9–12]. An organic multiple component

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mixture can also be used to target thermodynamic properties that maximize cycle efficiency and flexibility [13]. ORCs are currently being used in diverse sustainable power generation systems [14,15], as shown in Fig. 1.

Recent reports have shown that, compared to the use of single organic fluids, multicomponent mixtures can significantly enhance the power efficiency of low-temperature heat recovery Rankine cycles [16,17]. In this context, an important related problem consists in determining the optimal blending of organic fluids. Diverse studies exist in the literature on the evaluation, selection, and design of multicomponent organic fluid mixtures and on the optimization of ORC operations. In particular, Papadopoulos and co-workers presented a computer-aided molecular design method for the synthesis and selection of binary working fluid mixtures used in ORCs [18]. Yin and co-workers investigated mixtures of SF_6-CO_2 as working fluids for geothermal power plants [19]. Shu and co-workers studied mixtures based on blending of hydrocarbon with refrigerant retardants used in ORC [20]. Andreasen and co-workers presented a methodology for ORC optimization based on multicomponent mixtures [21]. The use of zeotropic mixtures in ORC is explored in [22–29]. More recently, Molina-Thierry and co-workers used a simultaneous optimal design approach for organic mixtures and ORC operation [9]. Liu and co-workers optimized and analyzed a geothermal organic Rankine using mixtures of R600a and R601a [30]. Fen and co-workers used multi-objective optimization for performance of low-grade ORC using R245fa and pentane [31,32]. Habka and co-workers evaluated the performance of organic mixtures in ORC using geothermal water as heat source [33]. Sadeghi and co-workers presented a thermodynamic analysis and used multi-objective optimization techniques to design zeotropic mixtures [28]. Papadopoulos et al. presented a sensitivity analysis on the effect of different system and fluid parameters on the performance of ORCs [18,34,35]. Recently, Frutiger et al. [36] used a Monte Carlo simulation procedure to evaluate the performance of fluid mixtures in the face of system uncertainties. High-throughput screening of working fluids using detailed thermodynamic and process simulations is reported in [37]. Additional applications of ORCs in industry have also been addressed [38–40].

In this work, we address the problem of designing multicomponent organic fluid mixtures capable of achieving optimal performance in the face of uncertainty in heat source temperatures and efficiencies of individual components of the ORC. The design problem is cast as a stochastic optimization problem and we use risk metrics to trade-off flexibility and average performance. We show that the methodology can identify new and non-intuitive heat transfer fluid mixtures that withstand extreme variability in system conditions while maintaining close-to-optimal performance. To the best of our knowledge, our work is the first to propose the combine advanced stochastic optimization techniques and first-principles modeling to design multi-component heat transfer fluids. We highlight that the stochastic optimization approach finds a single optimal design for a fluid mixture that behaves optimally under a range of uncertainties. Monte Carlo and sensitivity techniques reported in the literature, on the other hand, evaluate performance of different fluids under multiple scenarios but cannot systematically identify a single fluid that works best in all scenarios. We also highlight that our proposed approach simultaneously identifies an optimal composition for the fluid mixture and optimal operating conditions for the ORC. This simultaneous approach is necessary to capture dependencies between the physical properties of the heat transfer fluid and the operating conditions of the system.

The paper is structured as follows. In Section 2 we describe ORCs. In Section A we present an optimization formulation that seeks to maximize the overall cycle efficiency by determining an optimal composition of the mixture and operating conditions for the ORC units while satisfying thermodynamic equilibrium conditions, conservation equations, and constraints. In Section 3 we discuss how to extend this formulation to account for uncertainty (variability) in operational factors affecting the performance of the cycle. Case studies are presented in Section 4.

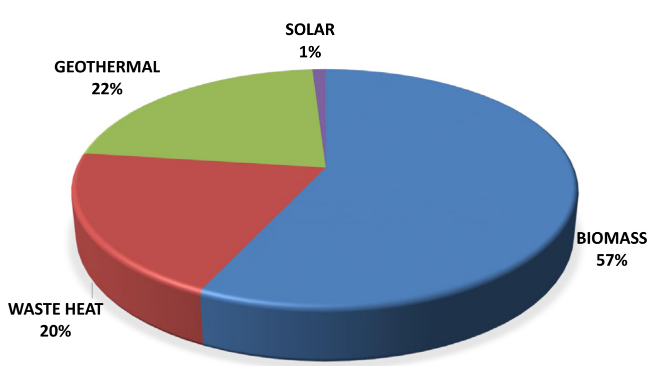

Fig. 1. Current applications of ORC in industry [1].

2. Organic Rankine cycles

An ORC converts low-grade heat to electricity by using an organic working fluid instead of water. Organic working fluids have lower boiling points than water and thus can be used to recover heat at lower temperatures [10,7]. The ORC (see Fig. 2) uses the same equipment as a conventional Rankine cycle. It consists of an evaporator (heating area), a turbine, a condenser (cooling area), and a pump [5,9]. As shown in Fig. 2, the ORC is composed of the following steps:

1. Constant pressure heating of the working fluid to a superheated vapor state.
2. Expansion of the vapor to a low pressure level.
3. Constant pressure cooling of gas until condensation conditions are reached.
4. Compression at high pressure level.

The cycle performance strongly depends on the thermodynamic properties of the working fluid [41,35]. When a multicomponent mixture is used as working fluid, operational efficiency can be increased [42,9,18,34]. In particular, by altering its composition, we can implicitly manipulate: (i) Temperature gradients at phase equilibria, (ii) pressure ratios, and (iii) the superheating degree. Thermodynamic cycle analysis shows that, for a pure component under a constant-pressure phase change, the temperature remains constant (see Fig. 3). In the two-phase region, the process starts and ends at the saturation temperature ($T_{Be} = T_{De}$). For a multicomponent mixture, on the other hand, the phase change occurs at a range of temperatures and compositions (i.e., $T_{Be} \neq T_{De}$) [9]. This nonisothermal phase change of the mixture allows for a much better match between the temperature profiles of the working fluid and of the heat source [43]. In Fig. 4 we illustrate this behavior. In particular, we show five points: three internal points ($N_\Psi = 3$) that represent the vaporization fraction Ψ_f and the bubble and dew points; P_{Low} and P_{High} are pressure levels as well as the isentropic points subcoolS (subS) and overheatS(overS) that correspond to compression and expansion points, respectively.