Abstract

To exploit the full thermo-economic potential of an Organic Rankine Cycle (ORC), the process, equipment and working fluid have to be optimized simultaneously. Today, working fluid selection and thermo-economic process optimization are commonly separated. This separation leads to suboptimal solutions if the prior working fluid selection fails. In this work, we present an approach for the integrated thermo-economic design of ORC process, equipment and working fluid using consistent thermodynamic modeling. The approach is based on the Continuous-Molecular Targeting–Computer-aided Molecular Design (CoMT-CAMD) approach. In CoMT-CAMD, the properties of the working fluid are modeled by the physically-based Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT) equation of state. A CAMD formulation allows the design of novel working fluids during the process optimization. So far, CoMT-CAMD was limited to equilibrium thermodynamics. Some of the authors recently developed models for the transport properties viscosity and thermal conductivity based on entropy scaling and PC-SAFT. The integration of these models allows designing the equipment within the CoMT-CAMD approach. In particular, the heat exchanger of the ORC can be designed using detailed correlations for single phase, evaporation and condensation heat transfer. Based on the equipment sizing, a thermo-economic objective function can be considered in the resulting mixed-integer nonlinear optimization problem. Thereby, the thermo-economically optimal working fluid is identified in a single optimization problem jointly with the corresponding optimal process and equipment. The resulting approach is illustrated for the design of a subcritical ORC for waste heat recovery. We show that the predicted specific purchased-equipment costs are in good accordance with real ORC applications.

Keywords: CoMT-CAMD, integrated design, fluid selection, economics, transport properties

1. Introduction

Organic Rankine Cycles (ORC) generate electrical power from low temperature heat [1]. Low temperature heat can be obtained from renewable heat sources or waste heat. To ensure an economically efficient process, the ORC has to be tailored to its specific application. For this purpose, process, equipment and working fluid have to be optimized simultaneously.
Today, however, working fluid selection and thermo-economic process optimization are usually carried out separately following a two-stage approach [2]: In a first stage, working fluid candidates are preselected using heuristic guidelines. In a second stage, the preselected working fluids are assessed by individual thermo-economic process optimizations. However, if the preselection in the first stage fails, the two-stage approach leads to suboptimal solutions. Thus, several authors recommended to integrate the working fluid selection directly into the process optimization [2,3]. The resulting integrated design of process and working fluid leads to a challenging mixed-integer nonlinear program (MINLP) optimization problem [4], since discrete degrees of freedom are added to the process optimization. Systematic solution approaches based on equilibrium thermodynamics have been developed as recently reviewed by Linke et al. [5]. A two-stage design approach has been proposed for pure working fluids based on Computer-aided Molecular Design (CAMD) and a cubic equation of state (EoS) by Palma-Flores et al. [6]. In a first stage, a set of working fluid candidates is obtained based on a deterministic optimization before different process configurations are investigated for the working fluid candidates in a second stage. An approach for the integrated design of ORC process and mixture based on a process-level objective function and CAMD is presented by Papadopoulos et al. [7]. Mavrou et al. [8] showed a better process performance for mixtures identified using an integrated design approach.

Bardow et al. [9] proposed an optimization-based targeting approach for the integrated design of processes and solvents using PC-SAFT [10], the so-called Continuous-Molecular Targeting (CoMT). Subsequently, the CoMT approach was applied for the design of ORC processes and working fluids [11] and extended by a CAMD formulation [12] to so-called CoMT-CAMD. In the so-called CoMT stage, the discrete pure component parameters describing a working fluid in PC-SAFT are relaxed to continuous variables transforming the MINLP into a nonlinear program (NLP). The result of the NLP is a hypothetical optimal working fluid, the so-called target. In a second stage, a second-degree Taylor-approximation around the target is used to estimate the objective function value of real working fluids generated by CAMD. Recently, the CAMD formulation was directly linked to the process model and PC-SAFT allowing the authors to solve the integrated design problem in solely one stage [13]. The resulting 1-stage CoMT-CAMD approach solves the MINLP using outer-approximation extended by a relaxation strategy. Since an equilibrium fluid model is used, 1-stage CoMT-CAMD was limited to a thermodynamic objective function. However, the thermodynamic optimum may differ from a thermo-economic optimum [14]. To perform a thermo-economic design, equipment sizing has to be integrated into the design of process and working fluid to quantify the investment costs. Sizing the equipment requires not only an equilibrium fluid model but also a model for transport properties to capture transport-related trade-offs. Previously, integrated thermo-economic design was mainly addressed in process engineering. Pereira et al. [15,16] proposed an approach for thermo-economic design of solvent and process for CO₂ absorption based on the fluid model SAFT-VR. The approach is limited to the design of linear alkanes and heuristic equipment sizing, but shows the advantages of a thermo-economic design approach. The presented approach is extended by Burger et al. [17] for the design of linear alkyl ethers using a hierarchical method with shortcut models of the process and SAFT-γ Mie. Herein, the viscosity is calculated using a group contribution (GC) approach. A thermo-economic design approach has also recently been proposed by the same group combining an outer-approximation formulation with a physical-domain reduction [18]. A hybrid stochastic-deterministic design approach is presented by Zhou et al. [19] for thermo-economic design of solvents for Diels-alder reaction. Since no models for transport properties are considered, the equipment sizing is performed based on heuristics.

This brief review shows that a lack of a model for transport properties enforces equipment sizing based on heuristic design correlations. In this work, we extend the 1-stage CoMT-CAMD approach for the thermo-economic design of ORC process, equipment and working fluid. For this propose, we integrate newly proposed models for the transport properties viscosity and thermal conductivity based on PC-SAFT [20,21] yielding a consistent model for both equilibrium and transport properties. Thereby, the equipment design of the heat exchanger can be performed based on detailed heat transfer correlations. The paper is structured as follows: In section 2, the framework of the extended 1-stage CoMT-CAMD approach is presented. The approach is applied for a thermo-economic design of an Organic Rankine Cycle in section 3. Conclusions are drawn in section 4.

2. 1-stage CoMT-CAMD for integrated thermo-economic design

To allow for a thermo-economic design using the 1-stage CoMT-CAMD approach, the approach has to be extended by models for equipment design and cost correlations. For this purpose, a model for transport properties is required beside the equilibrium fluid model. In section 2.1, the problem formulation of extended 1-stage CoMT-CAMD for
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