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Integrated design of ORC process and working fluid using process flowsheeting software and PC-SAFT

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Abstract

Organic Rankine Cycles (ORC) transform low-temperature heat into electrical power. To make best use of a heat source, ORC process and working fluid have to be optimized simultaneously. Thus, integrated design approaches of fluids and processes have been developed. However, integrated design approaches are usually complex and based on specific software tools which prevents fast and easy development of the ORC models. In this work, we have integrated the so-called 1-stage CoMT-CAMD approach into the process flowsheeting software gPROMS ProcessBuilder allowing for integrated design of process and working fluid. In 1-stage CoMT-CAMD, thermodynamic properties are modeled by the Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT) equation of state, which we use directly from the gSAFT physical property package. To introduce the molecular structure of the working fluid as an additional degree of freedom within the process optimization, we implemented the homosegmented group contribution approach of PC-SAFT and the Computer-aided Molecular Design (CAMD) formulation of 1-stage CoMT-CAMD in ProcessBuilder. Existing model libraries of ProcessBuilder were adapted to employ the Variable Molecular Structure Compound feature (VMSC) of gSAFT during process optimization. The resulting mixed integer nonlinear program (MINLP) optimization problem is solved by the standard MINLP solver integrated in ProcessBuilder. Thereby, the optimal working fluid and the corresponding optimal process are identified in one single optimization. The resulting tool enables the easy definition of integrated design problems based on the drag-and-drop feature of a process flowsheeting software for ORCs and beyond.

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Keywords: CoMT-CAMD, integrated design, fluid selection, gPROMS, flowsheeting

1. Introduction

Organic Rankine Cycles (ORCs) generate electrical power from low-temperature heat [1]. Low temperature heat can be obtained from renewable heat sources (e.g., solar or geothermal heat) and waste heat (e.g., from industry or automotive applications). To exploit the full potential of the heat source, the cycle needs to be tailored to the specific application. For tailoring a cycle, both process and working fluid have to be optimized simultaneously.
Today, however, the working fluid selection and process optimization are usually carried out separately: In a first stage, working fluid candidates are preselected based on heuristic guidelines defining favorable properties of a working fluid.

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In a second stage, the preselected working fluids are obtained by individual process optimizations. To select from existing databases of candidates, high-throughput screening approaches are developed combining a physical domain reduction and subsequent process simulations [2]. However, the success of the preselection relies on the heuristic criteria employed. In literature, a variety of different, partially conflicting heuristic criteria has been proposed. If these heuristic criteria for working fluid selection fail, a separation of working fluid selection and process optimization leads to suboptimal solutions.

To capture the interaction between process and working fluid, the working fluid selection has to be integrated into the process design [3,4]. Thereby, an assessment criterion on process level (e.g., efficiency) can be considered for the fluid selection. However, a direct integration of the fluid design into the process design leads to a challenging mixed-integer nonlinear program (MINLP) optimization problem [5]. To solve this challenging problem, systematic solution approaches have been developed for the integrated design of ORCs and working fluid, as recently reviewed by Linke et al. [6]. Papadopoulos et al. [7] use multi-objective optimization and Computer-aided Molecular Design (CAMD) to identify promising pure working fluid candidates, which are assessed in a subsequent process optimization. The approach is extended for mixture design [8] and the proposed designed mixtures are compared to conventionally selected mixtures, whereby a better performance of the designed mixtures is shown [9]. A CAMD-based design approach for pure components is also proposed by Palma-Flores et al. [10]. Here, the working fluid candidates are designed using multi-objective optimization and subsequently assessed for different ORC flowsheet configurations.

Integrated design approaches are also addressed for solvent design in the field of chemical engineering. A pioneering approach for the design of process and solvent has been presented by Pereira et al. [11,12] for CO_2 absorption. Herein, the Statistical Associating Fluid Theory for Variable Attractive Range (SAFT-VR) is used to predict the fluid properties. Recently, the method was extended to a hierarchical approach for integrated solvent and process design by Burger et al. [13] using simplified shortcut models and SAFT-γMie as fluid model.

Our group proposed the so-called Continuous-molecular Targeting (CoMT) approach for the integrated design of process and solvent for CO_2 absorption [14]. Herein, the Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT) [15] is used as thermodynamic model of the solvent. The approach was also successfully applied for the design of ORCs and working fluids [16] and extended by a CAMD formulation to so-called CoMT-CAMD allowing for the in silico design of novel working fluids [17]. In the CoMT stage, the pure component parameters describing a working fluid in PC-SAFT are relaxed transforming the MINLP into a nonlinear program (NLP). The result of the NLP is a hypothetical optimal working fluid, the so-called target, and the corresponding optimal process. The target provides an upper bound of the objective function. In a second stage, a CAMD formulation is used to design promising real working fluids. To design real working fluids with performance close to the hypothetical target, the CAMD method uses a second-order Taylor-approximation around the target as objective function leading to a mixed-integer quadratic program (MIQP). Recently, the CAMD formulation was directly integrated in the process model by the present authors [18] allowing us to solve the resulting MINLP in one stage. For this purpose, an outer-approximation algorithm extended by a relaxation strategy is employed in the so-called 1-stage CoMT-CAMD approach.

However, integrated design approaches are usually complex and based on specific software and tools, which prevent fast and easy development and reusability of the ORC models. In this work, we integrate the 1-stage CoMT-CAMD approach into the process flowsheeting software ProcessBuilder [19]. Thereby, the ORC flowsheet can easily be developed and adapted using the equation-based equipment model libraries of ProcessBuilder. The MINLP can be directly defined and solved in ProcessBuilder allowing for an integrated design with solely one user-friendly tool.

The paper is structured as follows: In section 2, the general framework of 1-stage CoMT-CAMD is presented. The implementation of 1-stage CoMT-CAMD in ProcessBuilder is described in section 3. In section 4, 1-stage CoMT-CAMD with ProcessBuilder is applied for the design of a solar thermal ORC. Conclusions are drawn in section 5.

2. Framework of 1-stage CoMT-CAMD

The 1-stage CoMT-CAMD approach allows for the integrated design of ORC process and working fluid based on a process-level objective function. For this purpose, a model of the process is directly coupled to a model of the working fluid, the thermodynamically consistent PC-SAFT equation of state [15]. The design of the working fluid is enabled by a CAMD formulation, which is is linked to the process and fluid model using the group contribution (GC) approach of PC-SAFT [20]. In section 2.1, the problem formulation of 1-stage-CoMT-CAMD is presented. A detailed description can be found in Schilling et al. [18]. The PC-SAFT equation of state is introduced in section 2.2.