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ScienceDirect

Energy Procedia 129 (2017) 97–104

Energy Procedia

www.elsevier.com/locate/procedia

IV International Seminar on ORC Power Systems, ORC2017
13-15 September 2017, Milano, Italy

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

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Abstract

Organic Rankine Cycles (ORC) use low-temperature heat to generate electrical power. To use the full potential of a heat source, the ORC has to be tailored to the specific application. Tailoring a cycle means an integrated design of both process and working fluid. This integrated design leads to complex mixed-integer nonlinear program (MINLP) optimization problems. To avoid this complexity, working fluid candidates are commonly preselected using heuristic guidelines; subsequently, the process is optimized for the set of preselected working fluids. However, the preselection can fail, leading to suboptimal solutions.
An approach for integrated design of ORC process and working fluid is the Continuous-Molecular Targeting–Computer-aided Molecular Design (CoMT-CAMD) approach. CoMT-CAMD employs the physically-based Perturbed-chain Statistical Associating Fluid Theory (PC-SAFT) equation of state as thermodynamic model of the working fluid. In PC-SAFT, each working fluid is described by a set of pure component parameters. In a first step, the so-called CoMT step, the discrete pure component parameters are relaxed resulting in a hypothetical optimal working fluid and the corresponding optimal process. In a second step, real working fluids with similar properties are identified using Computer-aided Molecular Design and a second-order Taylor approximation of the objective function around the hypothetical optimum. So far, the process models in CoMT-CAMD were implemented in a procedural programming language, which hinders the reusability, the use for more complex processes and dynamic simulations.
In this work, we integrate CoMT-CAMD into the object-oriented modelling language Modelica. For this purpose, Modelica is directly linked to PC-SAFT. Thereby, already existing model libraries for Modelica can be used to model the ORC process. The resulting design approach is applied to the integrated design of an ORC process and working fluid for a geothermal power station.

Peer-review under responsibility of the scientific committee of the IV International Seminar on ORC Power Systems.

Keywords: Modelica; PC-SAFT; fluid design; Computer-aided Molecular Design; optimization

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1876-6102
Peer-review under responsibility of the scientific committee of the IV International Seminar on ORC Power Systems.
10.1016/j.egypro.2017.09.169

1. Introduction

Organic Rankine Cycles (ORC) generate electrical power from low temperature heat [1]. Low temperature heat sources can be, e.g., waste heat, solar heat or geothermal heat. To use the full potential of a heat source, the ORC has to be tailored to the specific application. For tailoring a cycle, both process and working fluid have to be optimized simultaneously. Today, the fluid selection and process optimization are usually performed in 2 steps [2]: In a first step, a preselection of potential working fluids is carried out based on heuristic guidelines and experience. Subsequently, the preselected working fluids are assessed in individual process optimizations. However, the preselection relies on heuristic guidelines. If the heuristics fail, the 2-step approach leads to suboptimal solutions.

Therefore, the fluid selection has to be integrated into the process optimization to obtain overall optimal solutions [2]. However, such an integrated design leads to a challenging mixed-integer nonlinear programming (MINLP) optimization problem [3]. Thus, systematic solution approaches for the integrated design of ORC process and working fluid have been developed as recently reviewed by Linke et al. [2]: Papadopoulos et al. presented an approach for the integrated design of ORC process and working fluid mixtures based on a process-level objective function and Computer-aided Molecular Design (CAMD) [4]. A CAMD-based design approach for pure working fluids is proposed by Palma-Flores et al. [5]. Here, working fluid candidates are selected using multi-objective optimization and subsequently assessed in three ORC flowsheet configurations. Integrated design approaches for fluids and processes are also addressed for further engineering problems such as solvent design in chemical engineering. An approach for the integrated design of process and solvent has been presented by Pereira et al. for the absorption of CO_2 [6]. Herein, the search space is limited to linear alkanes, but this approach shows the advantages of an integrated design of processes and solvents. Recently, the same group extended their work by Burger et al. to a hierarchical approach for the integrated design of solvent and process using simplified shortcut models [7].

Our group proposed the so-called Continuous-Molecular Targeting–Computer-aided Molecular Design (CoMT-CAMD) approach for the integrated design of process and solvents for CO_2 absorption [8]. This approach has also been successfully applied for the integrated design of ORC processes and working fluids [9]. In CoMT-CAMD, the physically-based Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT) [10] equation of state is used to model the working fluid. In PC-SAFT, a working fluid is represented by a set of pure component parameters. In a first step, the so-called CoMT step, the pure component parameters of PC-SAFT are relaxed during the integrated design of process and working fluid transforming the MINLP into a nonlinear program (NLP). The result of the CoMT step is a hypothetical optimal working fluid, the so-called target, and the corresponding optimal process conditions. In the second step, the so-called structure-mapping, real working fluids with similar properties as the target are identified. For this purpose, the objective function values of real working fluids are estimated using a second-order Taylor approximation of the objective function around the target. A CAMD formulation allows designing promising working fluids by solving the resulting mixed-integer quadratic program (MIQP) [11].

Previously, CoMT-CAMD was implemented in a procedural programming language which hinders the reusability of the equipment models, fast development and easy adaptation of processes, as well as the consideration for more complex systems and dynamic simulations. These shortcomings can be overcome by using a programming language suited for object-oriented and equation-based modeling like Modelica [12].

In this work, we present the CoMT-CAMD approach for the integrated design of ORC process and working fluid based on Modelica process models. The object-oriented and equation-based modeling with Modelica enables the reusability of models as well as using existing model libraries (see reference [13] for a dynamic ORC library from Casella et al.), easy drag-and-drop flowsheeting and modeling of complex processes within CoMT-CAMD.

In section 2, the general framework of CoMT-CAMD is presented. The integration of CoMT-CAMD in Modelica is shown in section 3. In section 4, the resulting design approach is applied for the design of a geothermal ORC application, while conclusions are drawn in section 5.

2. CoMT-CAMD approach for integrated design of ORC process and working fluid

The Continuous-Molecular Targeting−Computer-Aided Molecular Design (CoMT-CAMD) approach for integrated design of process and working fluid was originally proposed by Bardow et al. (2010). In CoMT-CAMD,