

OPTIMAL MIXTURES FOR ORGANIC RANKINE CYCLES: INTEGRATED DESIGN OF PROCESS AND MIXTURE USING PC-SAFT

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ABSTRACT

Organic Rankine Cycles (ORC) generate electrical power from low-temperature heat. To exploit the full potential of ORCs, an integrated design of ORC process and working fluid is required. Today, methods for an integrated design are commonly limited to the design of pure working fluids [1]. However, mixtures can improve the ORC efficiency significantly due to favourable thermodynamic properties [2].

In this work, we present a method for the integrated design of ORC process and working fluid mixtures based on the 1-stage Continuous-Molecular Targeting – Computer-Aided Molecular Design (1-stage CoMT-CAMD) method [3]. In 1-stage CoMT-CAMD, the thermodynamic properties are modelled using the physically-based PC-SAFT equation of state. A computer-aided molecular design (CAMD) formulation enables us to consider the molecular structure as degree of freedom during process optimization. Detailed models for equipment sizing allow the optimization of an economic objective. The resulting mixed-integer nonlinear program (MINLP) optimization problem identifies the optimal working fluid jointly with the optimal process conditions and equipment. However, so far, 1-stage CoMT-CAMD was limited to the design of pure working fluids. In this work, we extend the CAMD formulation, the process model as well as the models for equipment sizing to consider a working fluid mixture as degree of freedom of the MINLP. Thereby, the optimal working fluid mixture is identified in a single optimization problem jointly with the corresponding optimal process and equipment.

The resulting approach is applied for the design of an ORC for waste heat recovery. The integrated design of ORC process and working fluid mixture is performed considering thermodynamic as well as thermo-economic objective functions. The presented method allows us to systematically exploit the potential of working fluid mixtures for ORCs.

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- [1] Angelino, G., Colonna, P. (1998). Multicomponent Working Fluids for Organic Rankine Cycles (ORCs). *Energy*, 23(6), 449–463.
- [2] Papadopoulos, A. I., Tsivintzelis, I., Linke, P., Seferlis, P. (2018). Computer-Aided Molecular Design: Fundamentals, Methods, and Applications. Reference Module in Chemistry, Molecular Sciences and Chemical Engineering, Elsevier. <https://doi.org/10.1016/B978-0-12-409547-2.14342-2.0>
- [3] Schilling, J., Tillmanns, D., Lampe, M., Hopp, M., Gross, J., Bardow, A. (2017). From molecules to dollars: integrating molecular design into thermo-economic process design using consistent thermodynamic modeling. *Mol. Sys. Des. Eng.*, 2(3), 301-320.