INTEGRATED WORKING-FLUID DESIGN AND ORC SYSTEM OPTIMISATION FOR WASTE-HEAT RECOVERY USING CAMD AND THE SAFT-γ MIE EQUATION OF STATE

M. T. White, O. A. Oyewunmi, A. J. Haslam and C. N. Markides

Clean Energy Processes (CEP) Laboratory, Department of Chemical Engineering,
Imperial College London, South Kensington Campus, London SW7 2AZ, UK
e-mail: c.markides@imperial.ac.uk Tel. +44 (0)20 759 41601
Web page: www.imperial.ac.uk/clean-energy-processes

Highlights: The integration of CAMD with ORC modelling facilitates the simultaneous optimisation of the working fluid and thermodynamic cycle. This work investigates this in the context of waste heat recovery by benchmarking a CAMD-ORC model against a conventional ORC model that uses REFPROP, and by presenting a full MINLP optimisation framework.

Key words: Computer aided molecular design (CAMD), SAFT-γ Mie, working fluid design

EXTENDED ABSTRACT

Introduction

The selection of an optimal working fluid for an organic Rankine cycle (ORC) remains a critical aspect of the power system design. Furthermore, as the interest in engine waste heat recovery grows, so does the interest in siloxane and hydrocarbon working fluids, which are forecasted to replace the more conventional refrigerants used in low-temperature ORC applications. In working-fluid selection studies, a large group of working fluids are typically screened based on predefined criteria, before a parametric study is carried out whereby the ORC system (with each pre-screened working fluid) is optimised for a specified heat source. However, this method can lead to sub-optimal system designs since optimal fluids could be excluded based on the subjective screening criteria.

Group contribution equations of state (EoS), in which thermodynamic properties are calculated based on the properties of the chemical groups that make up the molecule, have been around for decades [1]. However, the recent advancements in advanced group contribution EoS (such as SAFT-γ Mie), and increasing computing power, presents an opportunity for the full integration of computer aided molecular design (CAMD) with ORC system and component models. This removes the need for fluid pre-screening and presents an opportunity to integrate the working-fluid design into the power system optimisation process, leading not only to the selection of the optimal working fluid, but also the opportunity to develop new and novel working fluids.

Methods, approach and results

Statistical associating fluid theory (SAFT) EoS are based within statistical mechanics, which gives them a predictive capability not seen in other equations of state that rely on experimental data. This capability makes them ideal candidates for CAMD where optimal working fluids could lie outside the range where experimental data is available. SAFT-γ Mie is a group contribution EoS based on SAFT that uses a Mie potential to describe the interaction between two molecular groups. Currently, SAFT-γ Mie parameters are available for various molecular groups [2], including the $–CH_3$, $–CH_2$ and –CH groups. This means SAFT-γ Mie can be used as an effective tool for the calculation of the thermodynamic properties of aromatic hydrocarbon working fluids, such as toluene and benzene, and

high-boiling alkanes, which are suitable working fluids for engine waste-heat recovery applications [3]. In this work, the working-fluid properties obtained using SAFT-γ Mie are compared and validated against available experimental data from NIST, obtained from the REFPROP program.

Furthermore, a non-linear programming (NLP) ORC optimisation problem is formulated for a case study concerning waste-heat recovery from a stationary internal combustion engine fired with biogas, with 230 kW_{th} of thermal energy available. This problem is formulated using both SAFT-γ Mie and REFPROP in parallel, and the effect of the working-fluid property package on the resulting optimal cycle is compared. Finally, the mixed integer non-linear programming optimisation problem (MINLP) that allows the optimisation of both the working fluid and the thermodynamic cycle in a single design space is posed (Figure 1).

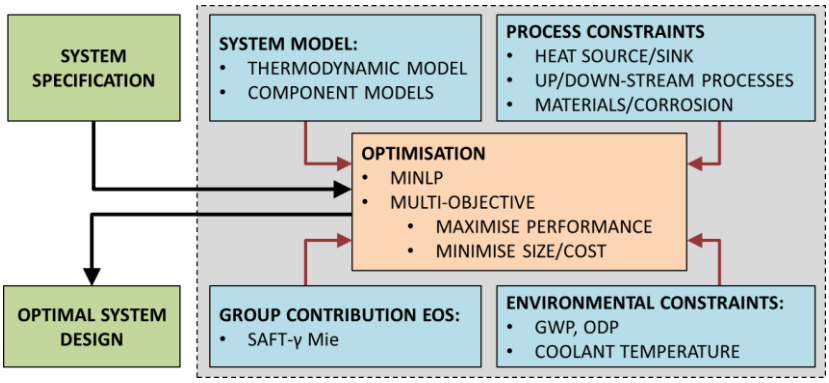


Fig. 1. Schematic of the CAMD-ORC MINLP optimisation framework.

Conclusions

The use of the SAFT γ Mie equation of state is proven for the prediction of the thermodynamic properties of hydrocarbon working fluids suitable for WHR applications, and a framework for the optimisation of the working fluid and thermodynamic cycle has been presented. Future efforts should now apply this optimisation to a WHR application, and develop the group parameters required to model alternative working fluids such as siloxanes.

References

[1] K. G. Joback & R. C. Reid, Estimation of pure-component properties from group-contributions, Chemical engineering communications 57 (1987) 233-243.

[2] S. Dufal, V. Papaioannou, M. Sadeqzadeh, T. Pogiatzis, A. Chremos, C. S. Adjiman, A. Galindo, Prediction of thermodynamic properties and phase behavior of fluids and mixtures with the SAFT-γ Mie group-contribution equation of state, J. Chem. Eng. Data 59 (2014) 3272-3288.

[3] G., Shu, X. Li, H. Tian, X. Liang, H. Wie, and X. Wang, Alkanes as working fluids for high-temperature exhaust heat recovery of diesel engine using organic Rankine cycle, Applied Energy 119 (2014) 204-217.

Background of the research and development team

The mission of the Clean Energy Process Laboratory, led by Dr Christos Markides, is to conduct significant research in applied thermodynamics, heat and mass transfer, and energy efficiency in power generation, heat and/or cooling provision. Alongside the development of small-scale reciprocating expanders for waste heat recovery, the CEP group is involved in both the European Up-THERM project aimed at providing affordable alternatives to conventional heat engines for CHP applications, and the UNIHEAT project focused on improving energy efficiency in power generation.