Available online at www.sciencedirect.com

ScienceDirect

Energy Procedia 129 (2017) 152–159

Energy Procedia

www.elsevier.com/locate/procedia

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

Integrated computer-aided working-fluid design and thermoeconomic ORC system optimisation

M. T. White[a], O. A. Oyewunmi[a], M. A. Chatzopoulou[a], A. M. Pantaleo[a,b], A. J. Haslam[a], C. N. Markides[a,*]

[a]*Clean Energy Processes (CEP) Laboratory, Department of Chemical Engienering, Imperial College London, South Kensington Campus, London, SW7 2AZ, UK*
[b]*Department of Agro-environmental Sciences, University of Bari, Via Amendola 165/A 70125, Bari, Italy*

Abstract

The successful commercialisation of organic Rankine cycle (ORC) systems across a range of power outputs and heat-source temperatures demands step-changes in both improved thermodynamic performance and reduced investment costs. The former can be achieved through high-performance components and optimised system architectures operating with novel working-fluids, whilst the latter requires careful component-technology selection, economies of scale, learning curves and a proper selection of materials and cycle configurations. In this context, thermoeconomic optimisation of the whole power-system should be completed aimed at maximising profitability. This paper couples the computer-aided molecular design (CAMD) of the working-fluid with ORC thermodynamic models, including recuperated and other alternative (e.g., partial evaporation or trilateral) cycles, and a thermoeconomic system assessment. The developed CAMD-ORC framework integrates an advanced molecular-based group-contribution equation of state, SAFT-γ Mie, with a thermodynamic description of the system, and is capable of simultaneously optimising the working-fluid structure, and the thermodynamic system. The advantage of the proposed CAMD-ORC methodology is that it removes subjective and pre-emptive screening criteria that would otherwise exist in conventional working-fluid selection studies. The framework is used to optimise hydrocarbon working-fluids for three different heat sources (150, 250 and 350 °C, each with $\dot{m}c_p$ = 4.2 kW/K). In each case, the optimal combination of working-fluid and ORC system architecture is identified, and system investment costs are evaluated through component sizing models. It is observed that optimal working fluids that minimise the specific investment cost (SIC) are not the same as those that maximise power output. For the three heat sources the optimal working-fluids that minimise the SIC are isobutane, 2-pentene and 2-heptene, with SICs of 4.03, 2.22 and 1.84 £/W respectively.

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

Keywords: organic Rankine cycle; ORC; computer-aided molecular-design; CAMD; group contribution; SAFT-γ Mie; technoeconomic optimisation.

1. Introduction

The working fluid used within an organic Rankine cycle (ORC) can affect performance, component design, size, cost and operational procedures. However, with increasing concerns over global warming and air pollution, certain

* Corresponding author. Tel.: +44 (0)20 759 41601.
E-mail address: c.markides@imperial.ac.uk

1876-6102
Peer-review under responsibility of the scientific committee of the IV International Seminar on ORC Power Systems.
10.1016/j.egypro.2017.09.095

Nomenclature

A_c, A_h	condenser/evaporator area, m^2
C_n	number of Carbon atoms
c_p	specific heat capacity, J/(kg K)
C_p^0	component cost, £
F	material factor
P_2	evaporation pressure, Pa
P_{cr}	critical pressure, Pa
P_r	reduced pressure
PP_c, PP_h	condenser and evaporator pinch points, K
SIC	specific investment cost, £/W
T_1	condensation temperature, K
$T_{3'}$	temperature at end of evaporation, K
T_{hi}, T_{ci}	heat-source and heat-sink inlet temperatures, K
Z	cost coefficient
X	sizing attribute
η_p, η_e	pump and expander isentropic efficiencies
$\dot{m}$	mass flow rate, kg/s
$\dot{W}_p, \dot{W}_e, \dot{W}_n$	pump, expander and net power output, W
ΔT_{sh}	amount of superheating, K

fluids such as CFCs have already been phased out, whilst fluids such as HCFCs and HFCs are set to be phased out in the coming years. From the perspective of an end-user, technical solutions are required that are not constrained by such legislation, in addition to being economically feasible. This demands the identification of both novel working fluids that meet all legislated requirements, and ORC systems that are optimised in terms of performance indicators such as the net-present value or the levelised cost of energy.

Compared to conventional working-fluid selection studies, in which a group of fluids are screened based on predefined criteria after which parametric optimisation studies are performed, computer-aided molecular design (CAMD) can be used to simultaneously optimise the working fluid and the ORC system. CAMD-ORC models have the potential to identify novel working-fluids which may otherwise be overlooked, whilst removing preemptive and subjective screening criteria. Papadopoulos et al. [1] used CAMD to identify potential working-fluid candidates before completing a more conventional ORC process simulation, and later applied CAMD to the optimal design of working-fluid mixtures [2]. Brignoli and Brown [3] used group-contribution methods to investigate the effect of a working-fluid's critical point on the thermodynamic performance of the ORC, whilst Palma-Flores et al. [4] demonstrated the potential of CAMD to identify new fluids with higher thermal efficiencies and better safety characteristics. Furthermore, Su and Deng [5] developed a thermodynamic ORC model, intended for future application within a CAMD-ORC framework. However, these previous studies have relied on empirical group-contribution methods. More advanced group-contribution equations of state have also been applied within a CAMD-ORC framework. For example, Lampe et al. [6,7] optimised ORC systems for a geothermal application. The CAMD-ORC optimisation was split into two stages. In the first stage an optimal, but hypothetical, working fluid was identified, and in the second stage real working fluids with similar performance were identified. More recently, Schilling et al. [8] reduced the problem to a single stage optimisation in which the working-fluid structure and ORC system are simultaneously optimised.

The major limitation of previous CAMD-ORC models is a focus on optimising the thermodynamic cycle; however, achieving the successful commercialisation of ORC systems across a range of applications requires a consideration thermoeconomic performance. Quoilin et al. [9] evaluated the specific-investment cost (SIC) of small-scale waste-heat driven ORC units, whilst Lecompte et al. [10] optimised the design of ORC units for large-scale CHP plants and waste-heat recovery. Multi-objective optimisation studies can be also found in the literature [11–13], where the authors considered the trade-off between maximising power output whilst minimising the SIC. However, all of these previous thermoeconomic studies consider only predefined working fluids, and conduct a separate optimisation for each specific fluid. On the contrary, thermoeconomic methods have not been previously applied to CAMD-ORC