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#### ACCEPTED MANUSCRIPT

Computer-aided working-fluid design, thermodynamic optimisation and technoeconomic assessment of ORC systems for waste-heat recovery

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#### Abstract

The wider adoption of organic Rankine cycle (ORC) technology can be facilitated by improved thermodynamic performance and reduced costs. In this context the power system should be evaluated based on a thermeconomic assessment with the aim of improving economic viability. This paper couples the computer-aided molecular design (CAMD) of the working-fluid with thermodynamic modelling and optimisation, in addition to heat-exchanger sizing models, component cost correlations, and a thermoeconomic assessment. The proposed CAMD-ORC framework, based on the SAFT-γ Mie equation of state, allows the thermodynamic optimisation of the cycle and working-fluid in a single stage, thus removing subjective and pre-emptive screening criteria that would otherwise exist in conventional studies. Following validation, the framework is used to identify optimal working-fluids for three different heat sources (150, 250 and 350 °C), corresponding to small- to medium-scale applications. In each case, the optimal combination of working-fluid and ORC system is identified, and investment costs are evaluated. It is observed that fluids with low specific-investment costs (SIC) are different to those that maximise power output. The fluids with the lowest SIC are isoheptane, 2-pentene and 2-heptene, with SICs of 5,620, 2,760 and 2,070 /kW respectively, and corresponding power outputs of 32.9, 136.6 and 213.9 kW.

Keywords: organic Rankine cycle; ORC; computer-aided molecular-design; CAMD; group contribution; SAFT- $\gamma$  Mie; technoeconomic.

#### 1. Introduction

- 2 Despite growing interest in improving energy-efficiency to reduce fossil fuel consumption and our impact
- 3 on the environment, there remains a significant amount of waste heat that is currently rejected to the
- atmosphere. Of the technologies that can be considered for waste-heat recovery, the organic Rankine cycle

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