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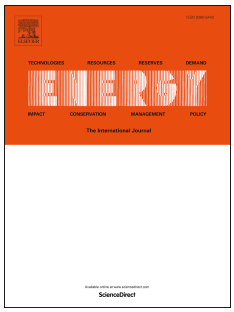

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Maciej Z. Lukawski, Ronald DiPippo, Jefferson W. Tester

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Molecular property methods for assessing efficiency of organic Rankine cycles

Maciej Z. Lukawski[a,*], Ronald DiPippo[b], Jefferson W. Tester[c]

[a,*] M.Z. Lukawski, Cornell Energy Institute and School of Chemical and Biomolecular Engineering, Cornell University, Ithaca, NY 14853, USA, mzl8@cornell.edu (*corresponding author)

[b] R. DiPippo, Chancellor Professor Emeritus of Mechanical Engineering, University of Massachusetts Dartmouth, Dartmouth, MA 02748, USA, rondipippo@comcast.net

[c] J.W. Tester, Cornell Energy Institute, School of Chemical and Biomolecular Engineering, and Atkinson Center for a Sustainable Future, Cornell University, Ithaca, NY 14853, USA, jwt54@cornell.edu

Keywords: Organic Rankine cycle (ORC); working fluid screening; molecular structure; low global warming potential (GWP); molecular group contribution method, computer aided molecular design (CAMD).

Abstract

This paper presents a robust method for assessing the efficiency of organic Rankine cycle (ORC) plants based on the molecular structures of the working fluids employed. The developed methodology uses molecular group contribution methods and does not require equations of state or extensive experimental data. The maximum utilization efficiency η_u* of an ORC plant was correlated with two thermodynamic properties of the working fluid, namely, its critical temperature T_c and reduced ideal gas heat capacity C_p^0/R. The developed correlations predict η_u* with an average error of 0.9 to 1.5 percentage points. The optimum ORC heat source temperature T_{hs}* can be predicted with an average error of 3.5 °C to 6.6°C. The developed methodology was validated using a numerical model of an optimized ORC. It was then used to estimate η_u* and T_{hs}* of 92 working fluids with low global warming potentials (GWP_{100} < 150) and low flammability values (LFL > 0.1 kg/m^3). Lastly, best candidate next-generation, low-GWP working fluids were selected for a more detailed examination.

1. Introduction

1.1. Motivation and scope

Organic Rankine cycle (ORC) technology is commonly used for converting low temperature heat into electricity. ORC systems are typically used for the generation of electricity from waste heat or renewable resources including geothermal, biomass, and solar energy. By employing a low-boiling point working fluid in a Rankine cycle, ORCs can efficiently produce electricity from low-temperature heat (typically at 100-150°C), which would be insufficient for conventional steam cycle to achieve efficient operation.

In addition to desirable thermodynamic characteristics, working fluids used in ORC plants should have low toxicity, flammability, and corrosiveness along with minimal environmental impacts, and sufficient