

Development of a Helmholtz Energy Based Empirical Model for Thermodynamic Properties of Ethanol-Oil Mixtures

Theresa Eckermann^{C, S} and Roland Span
Lehrstuhl für Thermodynamik, Ruhr-Universität Bochum, Bochum, Germany
t.eckermann@thermo.rub.de

Eric W. Lemmon
Applied Chemicals and Materials Division, NIST, Boulder, CO, U.S.A.

The knowledge of thermodynamic properties of fluids and fluid mixtures is necessary for the development of technical ORC processes. Nevertheless it is a common standard to design ORC processes using only the working fluid equations, whereas in many applications there is a relevant amount of oil involved. This approach is caused by a lack of knowledge for describing such complex mixtures. The presented preliminary model makes it possible to consistently model mixtures of ethanol and a poly-alpha-olefin (PAO). In order to describe the PAO as a pure fluid, a Helmholtz equation has been fitted using the functional form developed by Alexandrov *et al.* [1]. This generalized form was fitted to many short and long chained hydrocarbons and leaves only the critical temperature and density as well as the acentric factor as parameters that can be specified. This approach was chosen since only very limited data are available for the oil. In order to model the binary mixture, the reference equation for ethanol by Schroeder *et al.* [2] has been used. The new empirical mixture model was formulated in terms of the Helmholtz energy. Only limited phase equilibria data are available in a temperature range from 413 K to 453 K. The model qualitatively reproduces the vapor-liquid equilibria of this complex mixture. Furthermore, it seems feasible to also qualitatively represent mixtures of R134a or CO₂ and the PAO with this approach, although there is no accurate data available for the validation of these systems.

References

- [1] I. Alexandrov, A. Gerasimov, B. Grigor'ev: Generalized Fundamental Equation of State for the Normal Alkanes (C5–C50). *Int. J. Thermophys.*, 34, 1865-1905 (2013).
- [2] J.A. Schroeder: A New Fundamental Equation for Ethanol, Master's Thesis, University of Idaho (2011).