Prediction of the fluid phase behavior of the quaternary system ethylene oxide + air by molecular simulation

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Motivation

According to the vision of the Industrial Fluid Property Simulation Collective (IFPSC), "molecular simulation will become a breakthrough technology that is widely accepted in the chemical industry and applied (...) to meet the industry's evolving fluid property data needs" [1]. This is of particular interest for hazardous fluids which are economically vital, but often little explored experimentally. In 2007, The IFPSC has therefore challenged the development of new molecular models for such a substance, i.e. ethylene oxide (EO) [2]. The response of the community has shown that state-of-the-art molecular models are indeed capable of quantitatively covering a wide range of thermodynamic properties in a predictive manner. The present contribution is built upon the EO model developed in our group [3], which was the first entry of the challenge. It agrees almost throughout with the available reference data, taking the combined error bars into account.

In this work, the molecular model for EO [3] is combined with a ternary model for air [4]. Two of the three unlike interactions affecting EO (with nitrogen and with argon) were calibrated to experimental Henry's law data, altering the dispersion energy by less than 4% from the Lennard-Jones rule. On the basis of this model, the vapor-liquid equilibrium was predicted for the quaternary system and all its binary and ternary subsystems for a broad range of temperatures and pressures. Furthermore, compressed liquid densities are predicted as well. In order to facilitate the use of these data for subsequent work, cubic equations of state were parameterized to the whole model. In total, this case study aims to present a straightforward route to include molecular simulation into industrial applications.

Molecular models

Available experimental data on phase coexistence

Pure ethylene oxide

Henry's law constant

Binary VLE

Quaternary VLE

Binary bubble density and enthalpy of Nitrogen + Oxygen

Ternary VLE

Literature

[1] https://www.ifp-scientific.org