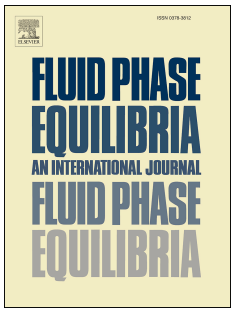

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PII: S0378-3812(16)30435-6

DOI: 10.1016/j.fluid.2016.09.001

Reference: FLUID 11249

To appear in: *Fluid Phase Equilibria*

Received Date: 14 July 2016

Revised Date: 30 August 2016

Accepted Date: 1 September 2016

Please cite this article as: Z. Wang, J.L. Kern, B.B. Laird, The phase equilibrium, transport and local liquid structure of the methanol/water/ethylene ternary system: A molecular simulation study, *Fluid Phase Equilibria* (2016), doi: 10.1016/j.fluid.2016.09.001.

The Phase Equilibrium, Transport and Local Liquid Structure of the Methanol/Water/Ethylene Ternary System: a Molecular Simulation Study

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Abstract

Gas-expanded liquids have received significant interest as catalytic reaction media. While most GXL studies involve CO_2 as the expansion gas, there is growing interest in non-CO_2 based GXLs, especially when the expansion gas is also a reactant. In this work, we focus on ethylene as an expansion gas, motivated by recent experimental studies on the catalytic epoxidation of ethylene using ethylene-expanded methanol/H_2O_2/water mixtures within metal doped silica mesopores. Reported simulation studies on GXLs, even for bulk properties, have been primarily limited to single-component or binary systems. Here we extend the use of simulation to the study of a bulk ternary GXL system - namely, ethylene-expanded mixtures of methanol and water mixtures. We investigate the phase behavior and transport properties in the liquid phase with respect to temperature, pressure and water content. The model force fields are validated by comparing compositions and transport properties to existing experiments. In addition, we study local liquid solvation structure as a function of composition.

Keywords: Vapor-liquid equilibrium, Ternary phase diagrams, Methanol, Ethylene, Water, Monte Carlo simulation, Molecular-dynamics simulation

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