Two-phase equilibrium calculation at given moles, volume and temperature based on quasi-Newton optimization

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Solving of phase equilibrium at given moles, volume and temperature is required by various applications including control volume hydrodynamic simulations of multiphase flows and transport coefficient models based on density. We present an approach for solving the problem based on [1, 2]. The problem is divided into testing of stability of a single-phase state and, in case of unstable state, splitting of the phases. In contrast to [1] we pose the stability problem as optimization of Helmholtz free energy, rather than a system for necessary conditions for the equilibrium. Using optimization formulation for both phase stability and phase split means that both problems can be solved using the same optimization method, the difference being only in the objective functions. We present simulation results of equilibrium properties for mixtures containing up to four components. In addition, we tested performances of Newton's optimizer used in [2] and a quasi-Newton optimizer for the phase split. Our results shows a significant better performance of quasi-Newton optimizer for mixtures up to 25 components.
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[1] Mikyška J and Firoozabadi A 2012 *Fluid Phase Equilibria* **321** 1–9
[2] Jindrová T and Mikyška J 2013 *Fluid Phase Equilibria* **353** 101–114