Efficient Characterization of Multicomponent Vapor-Liquid Equilibria Using Raman Spectroscopy

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A novel setup is presented for the efficient characterization of multicomponent vapor-liquid equilibria (VLE) using Raman spectroscopy. VLE data are at the fundamental core of thermal separation processes such as distillation. Large databases of VLE data already exist in literature. Still, VLE data are hardly available for novel compounds and their mixtures. The experimental characterization of multicomponent VLE is usually time consuming and costly. Furthermore, conventional experimental methods require rather large amounts of substance, while novel compounds are often very expensive or only available in small amounts. In addition, handling procedures are often complex: Static isothermal methods require thoroughly degassed substances to be added to a fully evacuated equilibrium chamber. Most analytical methods rely on sampling from the equilibrium chamber, which is challenging and known as an error source in the analytical chain. Subsequently to every analysis, the equilibrium chamber is cleaned and evacuated again, before a new experiment can be started. As a result, these procedures are time consuming and material intensive. In this work, we present a novel VLE setup overcoming these issues. We avoid potential disturbances to the phase equilibrium due to sampling by employing non-invasive Raman spectroscopy for the characterization of phase compositions. Spectroscopic analysis is very fast, taking only several seconds. We characterize several VLE data sets based on a single filling of the equilibrium cell (<3 ml). Handling is simplified by degassing directly in the equilibrium chamber. The systems' small dimensions lead to fast heat and mass transfer. Consequently, equilibration is typically achieved within several minutes. The setup is validated by reproduction of binary VLE data from literature. Additionally, we present new phase equilibrium data of a quaternary system and its binary subsystems. The novel data demonstrates the potential of the novel setup for efficient and accurate VLE measurements in multicomponent mixtures.