A Robust Setup for Efficient Characterization of Multicomponent Vapor-Liquid Equilibria Using Raman Spectroscopy

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Vapor-liquid equilibrium (VLE) is a crucial thermodynamic property with significant implications for various industrial processes, such as separation processes and gas absorption [1]. However, challenges in obtaining accurate VLE data, including large sample volumes, lengthy measurements, and complex apparatus handling, have impeded progress [1,2]. Recent studies have highlighted the utility of Raman spectroscopy in determining VLE for binary molecular systems at high pressure [3]. An alternative method involves employing a static VLE cell with Raman spectroscopy at lower pressure. There are now various options for applying Raman spectroscopy through a static VLE cell.

Liebergesell et al. demonstrated the efficacy of a static equilibrium cell in quaternary mixtures at lower pressures [4], but faced challenges in optical setup alignment by using a beampath in a 90° arrangement for collecting the scattered light and a very laborious experimental implementation. To enhance the practicality of this method, two additional approaches based on backscattering have been developed based on Liebergesell et al.'s findings. At the Energy and Process Systems Engineering laboratory of ETH Zurich, in collaboration with our group, a plan facilitating spectroscopic examination of an equilibrium cell has been devised. This involves illuminating an equilibrium cell with a horizontal arranged Raman probe and recording Raman light. In our contribution, we introduce a novel measurement setup utilizing Raman spectroscopy in the vertical direction for rapid, precise, and user-friendly multicomponent VLE characterization. The highly compact isothermal equilibrium cell ensures fast and reliable VLE control with a minimal sample consumption of less than 2 mL for multiple data points. Combining this cell with a highly confocal fiber-coupled Raman probe and a compact high-throughput spectrometer results in an efficient measurement setup for VLE data. Emphasizing user-friendliness during development, the system incorporates the Indirect Hard Modeling approach, simplifying measurement and evaluation. This approach allows even non-specialized users to operate the system. Demonstrating applicability for binary, ternary, and other multicomponent molecular systems, the use of small sample volumes, rapid measurements with Raman spectroscopy, and user-friendly operation all meet crucial industry requirements, paving the way for this efficient technology to enter industrial application.

References

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