

## Low Pressure Vapor-Liquid Equilibria Measurements of Detergent Range Alkanes and Alcohols

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Currently, azeotropic distillation is employed to achieve the post-production separation of detergent range alkanes and alcohols, however safety concerns are evident. Supercritical fluid fractionation (SFF) has recently been shown to be a viable alternative. Several studies have attempted to further understand, classify, characterize and model the complex interactions occurring in the mixtures encountered in the SFF process, to aid in developing, optimizing and modelling the SFF of detergent range alkanes and alcohols. Previous studies have shown a lack of low pressure vapor-liquid equilibrium (LPVLE) data for 1-alcohol + n-alkane systems. This data will aid in understanding the underlying molecular interactions between the alkanes and alcohols. Previously LPVLE data were measured for 1-alcohol + n-alkane systems where the alkane has 4 more carbon atoms than the alcohol. However, further measurements are still required. This study presents experimentally measured binary LPVLE data for n-alkane + 1-alcohol systems at 40 kPa with the 1-alcohol between C5 – C10 and n-alkane between C8 – C13. These data will further the understanding of the complex azeotropic phase behavior observed and allow the assessment of thermodynamic model predictions for these systems. The data were generated utilizing a dynamic recirculating modified Gillespie still (PiloDist VLE100 D). The equilibrium samples were analyzed with an Agilent 7890B gas chromatograph equipped with an Agilent DB-FFAP column and flame ionization detector. The thermodynamic consistency of the data were confirmed using the L-W Wisniak and the McDermott-Ellis tests. The experimental data generated shows how the phase behavior, particularly the azeotrope, changes as the molecular mass of the components change. Furthermore, the measured data allows for future thermodynamic modeling with the predictive Soave-Redlich-Kwong group contribution equation of state and the non-random two-liquid activity coefficient model as implemented in Aspen Plus, amongst others, to ultimately contribute towards a fully predictive model for n-alkane + 1-alcohol systems.