Phase Behavior of CO_2 with High Molecular Mass *n*-Alkanes and/or 1-Alcohols

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Supercritical CO_2 fractionation is an alternative technique for the separation of detergent range alkanes and alcohols (10 to 16 carbon atoms). While the technique has been demonstrated on pilot plant scale, further process development is hampered by the inability to describe the underlying phase behavior. The aim of this presentation is to evaluate the phase behavior of the CO_2 + n-alkane and CO_2 + 1-alcohol homologous series as well as available CO_2 + n-alkane + 1-alcohol systems for n-alkanes and 1-alcohols with 10 to 16 carbon atoms. The CO_2 + n-alkane homologous series has significantly different phase behavior from that of the CO_2 + 1-alcohol homologous series. The 1-alcohols undergo hydrogen bonding to form dimers and multimers, changing the molecular structure of the mixture and increasing the pressure for complete miscibility with CO_2. The presence of these dimers and multimers result in interesting phase behavior phenomena, such as temperature inversions, and may even contribute to the formation liquid-liquid-vapor regions and a barotropic inversion. Conversely, n-alkanes do not form hydrogen bonds and therefore such phenomena are not prominent for the CO_2 + n-alkane homologous series for the n-alkanes considered here. Considering the difference in CO_2 + n-alkane and CO_2 + 1-alcohol phase behavior, the phase behavior of CO_2 + 1-alcohol + n-alkane systems is also of interest. From the limited data available, co-solvency is noted at high n-alkane concentrations and temperature inversions and other phenomena usually observed for the CO_2 + 1-alcohol system are observed for high 1-alcohol concentrations. It is envisioned that in the future the insights obtained from studying the phase behavior can aid in the thermodynamic modelling of these systems and ultimately contribute towards improved process modelling for the supercritical CO_2 fractionation of detergent range alkanes and alcohols.