

11g Evaluation of the Integrate and the Combined Methods in Mixture Phase Equilibrium Calculations Using Equations of State

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Phase equilibrium calculations play a vital role in the design, simulation, and optimization of chemical processes. The simulation and design work in engineering is performed on computers with calculations of necessary thermodynamic properties in that work consuming 60 to 80 % of the computer time. The development of faster, more efficient and more reliable computational algorithms for thermodynamic calculations is therefore a high priority task in designing and simulating chemical and petroleum engineering processes. By keeping the above objective in mind, we have developed a novel technique known as the Integrate method that involves a differential form of the equilibrium constraints followed by numerical integration. This method has been applied to binary mixtures involving both cubic and complex equations of state that exhibit vapor liquid equilibrium (VLE) and liquid-liquid equilibrium (LLE). In general, we found that the Integrate method provides a computational speedup over a conventional root-finding algorithm for several systems examined. We also found that a Combined method that uses the Integrate method as a predictor step and a root-finding method as a corrector step merges the best of both the techniques.