Phase Equilibrium Engineering: Chapter 12. Phase Equilibrium Engineering in Conceptual Process Design (Supercritical Fluid Science and Technology)

Esteban Brignole, Selva Pereda

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The application of the principles of phase equilibrium engineering to the development of two innovative technologies for the production of biofuels is discussed in this chapter. The first technology is the production of biodiesel by transesterification of vegetable oils with supercritical methanol; the second, the extraction and dehydration of alcohols by near-critical dual effect solvents that exhibit good solvent power to extract alcohols and water entrainment effect to dehydrate the extracted alcohol. In the first case, the complexity of the reacting system, the large size asymmetry, and strong molecular interactions of the mixture components: methanol, vegetable oils, fatty esters, and glycerin precluded the design and analysis of the process conditions based on thermodynamic model predictions. Therefore, in this case, a systematic approach based on experimental studies was used to unveil the phase scenario and the physical properties required for the design and optimization of this technology. The conceptual design of extraction and dehydration of alcohols by near-critical solvents followed a different path. The process development was initially based on very limited experimental information. In this case, an equation of state for highly nonideal systems was the main tool for exploration of the process conditions over a wide range of pressures, temperatures, and compositions. This equation of state was based on a group contribution approach (GC-EOS) that allowed extrapolating the scarce experimental information available not only in pressure, temperature, and composition but also in molecular structure. The basic conceptual design was later confirmed by experimental information and pilot plant studies. In this case, the design of the experimental studies was guided by the process conceptual design. The experimental results provided key information for the upgrading of the thermodynamic model.

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