

Thermodynamic modeling for phase equilibrium and surface tension of multicomponent polymer solutions

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The liquid-liquid equilibrium (LLE) and surface behavior of polymer solutions were investigated. Systems of poly vinyl methyl ether (PVME)/water and polystyrene (PS)/cyclohexane were chosen as model systems because they show different types of LLE and surface behavior. Ternary polymer solutions of PVME/water/alcohol and PS/cyclohexane/alcohol were also studied. The cloud points of given systems were determined by thermo-optical analysis (TOA) method. For surface tension measurements at the air/polymer solution interface, the well-known plate method was utilized. The modified double lattice model with chain length dependence (MDL-CL) is used for description of the phase equilibrium. To improve the interpretation of the surface behavior of the polymer solution, we developed a new thermodynamic frame work based on density gradient theory (DGT). The surface energy difference and interchange energy had an important role in the driving force of the surface behavior. Utilizing the predetermined model parameters from the phase equilibrium calculation, the proposed model provides satisfactory agreement with measured surface tension data.