

Preliminary selection of polymeric entrainers for the azeotropic distillation of MTBE/methanol and ethanol/water mixtures using the UNIFAC group-contribution calculations method.

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Abstract

The UNIFAC group-contribution calcns. method was used to det. relative volatility in the presence of selected polymeric entrainers at different wt. fractions in ethanol/water and MTBE/methanol systems. To quantify the effect of the added polymers, the ratio of relative volatility with and without the polymer was calcd. The purpose of these calcns. was to identify the systems that have ratios of relative volatility distinct from unity because they may indicate polymers with the ability to break the azeotrope. This information should guide the initial selection of potential polymers capable of breaking the azeotrope and thus save time and effort. The results of these calcns. are reported. Because these polymers must be sol. in the system, soly. tests were performed and the results are reported. Comparison of these predictions with previously published exptl. vapor-liq. equil. data for the same systems gave conflicting results: some predictions were confirmed and others were not. Thus, the UNIFAC group-contribution calcns. were not always reliable in predicting relative volatility. More accurate group-contribution methods would make the polymer design more reliable.