Estimation of Physical Property on Simulation of Packed Column Distillation with a Rate-Based Model

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In order to meet increasing demands on rigorous simulation for distillation, a rate-based model has been developed by considering heat and mass transfer between vapor and liquid phases. In order to conduct properly the rate-based simulation of distillation, we need a number of estimation models for physico-chemical properties. The thermodynamic factor models do not affect largely the simulation results in the distillation simulation where the mass transfer resistance of the vapor phase film is dominant. The liquid excess molar volumes of the ternary mixture of Methanol, Ethanol, and Water shows at most 3% deviations from the averaged molar volumes. It affects the simulation results markedly where the composition of the liquid mixture passes through the region of the large excess molar volume. A proper estimation of the liquid mixture molar volume is required in the distillation simulation when the liquid composition varies with the time such as a batch operation.