

Effect of VLE Uncertainties on the Design of Separation Sequences by Distillation

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It is widely recognized by experts that the computer-based design of chemical processes depends strongly on the correlated thermodynamic and transport properties, and that the effect of overall property uncertainties should be incorporated into the design. The most significant source of property uncertainties on process design is from the correlations of phase equilibrium. Many approaches have been proposed, but uncertainty analysis is not a routine element of today's industrial practice, mainly because education and awareness are lacking, and the proposed methods are difficult to apply. In order to help rectify the situation, Mathias [1] developed an intuitive and easy-to-apply method based upon treating the mixture, for the purpose of perturbation, as a set of pseudobinaries described by the Margules equation. Mathias applied his method to two examples – (1) a propylene-propane superfractionator for which small changes in correlated relative volatilities have a large effect on the design of the distillation column; and (2) a dehexanizer column that separates a mixture containing many close-boiling components – and demonstrated that the proposed methodology provides quantitative insight into the effect of property uncertainties and helps to quantify the safety factors that need to be imposed upon the design. In this presentation the Margules perturbation method is applied to the “textbook” separation of an acetone-chloroform-benzene mixture; this example was proposed by Westerberg and Wahnschafft [2], and was previously studied by Parodi and Campanella [3]. The approach of Parodi and Campanella uses different levels of data fitting to quantify uncertainties, while Mathias' methodology is to obtain the best fit of the data, and then apply uncertainties based upon experimental uncertainties and any model inadequacies. Comparison between the two uncertainty-analysis methods enables better understanding of the use of uncertainty analysis in the industrial practice of process engineering.

References

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- [3] Parodi, C. A.; Campanella, E. A. “Effect of Vapor-Liquid Equilibrium on the design of separation Sequences by Distillation,” *Latin American Applied Research*, 2009, 39, 33-40.