37k Computational Tools to Understand Liquid-Vapor Equilibrium for Undergraduate Students

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The study of liquid-vapor equilibrium of binary and multicomponent mixtures is the primary focus during the stage of equipment design for the separation and purification processes of a chemical plant. During the study of this subject, the Chemical Engineering student faces the challenge of learning many abstract concepts (activity, fugacity coefficient, excess Gibbs free energy) and algorithms, while the professor deals with the explanation of mathematical procedures and expressions to provide the student the elements needed to accomplish this task. A computer program that helps to compare the predictions using different equilibrium coefficient expressions is presented in this work. It is important to have a graphical output of the results obtained from liquid-vapor equilibrium calculations. Convergence information and equilibrium binary diagrams let the students make analysis and comparisons with different equilibrium coefficient expressions (K value) to be used on liquid-vapor equilibrium calculations. In order to achieve this goal, a computer program was developed taking advantage of the graphical capabilities of Microsoft Excel and the Visual Basic for Applications programming language. The developed application, named TermAXL, performs binary interaction parameters fittings from experimental data using four excess Gibbs free-energy models and two cubic equations of state with two mixing rules each one. The optimization procedure is executed automatically minimizing one of several objective functions using Solver®, the non linear programming tool built-in Excel®. The parameters obtained can be used later to make liquid-vapor equilibrium calculations by means of one of five available equilibrium coefficient expressions and one of seven programmed algorithms in a friendly and practical fashion. In addition to the displayed diagrams, the undergraduate student may also access a generated report showing the internal iterations performed to reach the final results. It is important to mention that other excess Gibbs free energy models, equations of state and mixing rules could be added to the programming code allowing therefore the growth of this program under the same structure.