145d An Application of Aspen Software in Undergraduate Thermodynamics

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In order to increase a chemical engineering student's familiarity with process simulation software, all opportunities in the core courses should be explored. In the undergraduate thermodynamics course, one opportunity is with the topic of vapor-liquid equilibrium in solution thermodynamics. If the Smith, Van Ness, and Abbott textbook is used, solution thermodynamics is covered in Chapter 12. The software can be introduced to solve Problem 12.1, which gives experimental VLE data (pressure versus liquid and vapor composition) for the simple binary methanol/water system at 333.15 K (constant temperature). The Aspen assignment is given in two parts: Part 1 involves the students building a flash model on Aspen of the methanol/water system, and calculating compositions versus pressure using Raoult's law (ideal liquid/ideal gas); Part 2 involves the students taking the flash model built in Part 1, and investigating other thermodynamic property models introduced in Chapter 12. For liquid data, the Wilson, NRTL, UNIQUAC, and Van Laar property models are investigated, and for gases, the Redlich-Kwong or ideal property models are used. Each student is given a unique combination of property models to use for the liquid and gas (which is possible with our small class size), e.g., Wilson/Redlich-Kwong, so each student has to develop their simulation independently. The students are asked to compare the experimental data with the data calculated from the property models by plotting all the data on one graph, and calculating residuals between the ideal and experimental data, and again for other property model combination assigned. This assignment reinforces the limitation of modeling (the ideal model fit worse than other models) as well as providing another opportunity for student exposure to process simulation software.