145i Teaching Thermodynamics through Software Development

R. Chavela-Guerra, A. Alarcón-García, and L.G. Ríos-Casas

Over the last years, great efforts have been made to integrate computer-based simulation throughout the Chemical Engineering curriculum. In most cases, this approach is accomplished by the assistance of both academic (from textbooks or web-based) and commercial process simulators (Aspen Plus, CHEMCAD or HYSYS). However, their use requires a reasonable understanding of the concepts and procedures involved in the numerical solutions; otherwise, these software packages become a black-box and could represent a drawback. In order to fulfill this possible shortcoming, freshmen and sophomore students are faced to develop their own software, before the gradual exposure to the simulators. As part of the overall teaching tools, this methodology has been applied effectively in Thermodynamics. For example, for Phase Equilibria and Chemical Thermodynamics courses, students should work on a set of programs, which are a key tool to complete successfully coursework, exams and projects. These programs deal with the solution of linear and nonlinear algebraic equations (i.e. mass and energy balances, vapor-liquid equilibrium calculation, solution of cubic equations of state). Thus, students should integrate some of their previous knowledge (algebra, numerical methods, programming), further more the only comprehension of thermodynamic concepts. Throughout several years, this methodology has evolved and undergraduates have developed different programs to satisfy the courses requirements. At the beginning, FORTRAN, PASCAL and BASIC were used as programming languages. Recently, spreadsheets, like Microsoft Excel, have gained great popularity because their widespread availability. Moreover, they provide an excellent way to display and manipulate data. In consequence, they have been adopted as the tool of choice. The success of this approach has been assessed over the last decade. It helps students to expand and enrich the theoretical and practical understanding of classical Thermodynamics. Following this methodology, students become aware of what information is needed and how can be obtained. By this way, they also develop a healthy skepticism toward any numerical result from a process simulator, making a competent and critical use of them.