



## Efficient and Effective Instruction in Process Simulation Across the Chemical Engineering Curriculum

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# Efficient and Effective Instruction in Process Simulation across the Chemical Engineering Curriculum

## Abstract

One challenge to incorporating process simulation instructional activities into the chemical engineering curriculum is the placement of said activities. Placed too early in the curriculum, one might worry that students become overly reliant on the software, failing to truly understand the fundamentals of mass and energy balance calculations and of equipment rating/sizing calculations. Placed too late in the curriculum, one might worry that students don't have extensive experience with the software to effectively use it as a tool in the senior design courses. Inclusion of process simulation only in the senior design courses also results in a lost opportunity for students to connect calculations/results from process simulators directly to the underlying fundamentals. This paper focuses on activities readily integrated into the chemical engineering thermodynamics, separations and reactor design courses. How does one integrate process simulation exercises into these courses, without sacrificing current instructional content? What avenues of approach allow the students to gain confidence and experience with the process simulation software in these courses, so that they are well versed in its use when they begin the senior design sequence? Approaches and activities are presented so that others can readily adapt them to the process simulation program in use at their institutions.

## Introduction

Over the past two decades, process simulation has gained significant ground in the educational arena. In 1990, the first simulators with graphical user interfaces were introduced: Aspen/SP with its SPEXPRT system (JSD Simulations, Inc.), Aspen Plus (Aspen Technology), and ProSim/ProVision (Simulation Sciences, Inc.). As these tools became available to those in the academic community, the question arose as to how best to educate students in the use of these very powerful tools. Various approaches of incorporating the design experience across the curriculum have been reported in the literature.<sup>1,2,3</sup> Many of these articles address the need for introducing design at earlier stages in the curriculum and describe how to best integrate these experiences across the curriculum. The use of process simulators in select courses to demonstrate concepts and reinforce fundamental principles is also discussed in the literature.<sup>4</sup>

After two decades, this question of how best to educate students still remains unanswered, although the majority of chemical engineering programs now do have some form of process simulation instruction in place. From an educational standpoint, the need still existed, and exists to this day, for students to understand the underlying theory as well as assumptions/approximations made to design and rate various unit operations/processes. As professors, it is titillating the opportunity that this wonderful tool (process simulation) presents for students to explore and pose 'What if' type queries and glean understanding of how process variable A affects process performance variable B; all these wonderful educational outcomes without students having to spend sleepless nights in the campus computer room, or isolated in the corner with their calculator, spewing numbers out. The contents of this paper were developed over many years of teaching a variety of chemical engineering courses where use of

process simulation facilitates the incorporation of real world design experiences into the classroom.

### **Background of Process Simulation at Mississippi State University**

At Mississippi State University (MSU), a discussion of the curriculum in the early 90's focused on numerical analysis tools and how best to educate students in their use. At that time, the curriculum contained a 2 credit hour course in which students learned Basic and FORTRAN, and also contained a numerical analysis course taught in the Mathematics Department. Elimination of the numerical analysis course from the curriculum allowed the inclusion of additional design-focused courses, but it was quickly realized that these numerical tools were needed by students to solve the complex problems encountered in chemical engineering. Thus, a scant 4 years later, a 3 credit course, Analysis and Simulation, was added back into the curriculum, but the focus was primarily numerical analysis with little exposure to process simulation. In 2003, the course was restructured and split into two separate courses: CHE Analysis – a 2 credit hour course with emphasis on numerical analysis and numerical methods and a 1 credit hour laboratory added to the existing Process Design course where process simulation would be explored. However, this approach resulted in a disconnect between the calculations/concepts learned in earlier courses and learning how they are implemented in the process simulation software. Within the process simulation laboratory, there was not sufficient time to review the calculations/concepts learned earlier as well as provide instruction regarding use of process simulator for design-oriented activities.

### **Approach to Incorporating Process Simulation Activities into a Curriculum**

The structure of process simulation software lends itself to a distributed instructional approach. Since each chemical process/equipment item is represented through a 'unit operation block' that performs the relevant mass and energy balance calculations, it is straight forward to partition these blocks into small groups, each group related to a particular chemical engineering course. Thus, for the first thermodynamics course, the group including blocks associated with simple heat exchange, stoichiometric reactor, turbine, pump and compressor. In the second thermodynamics course, the group includes blocks where phase equilibria and chemical equilibria are important, such as the two-phase flash, three-phase flash and equilibrium reactor blocks. In the separations course, the group includes the shortcut column block, as well as the rigorous column blocks, which can be used for simulation of distillation in all its various forms as well as for simulation of absorbers/strippers.

The approach used to introduce the process simulation package into each of the courses where it was employed was to devote one lecture period (or an optional instructional session) to a hands-on activity where process simulation and the associated software were introduced. A tutorial (developed for each course, but essentially containing the same basic information, with only the examples employed tailored to the particular course) was provided to students. All of the students were required to have the process simulation program installed on their laptop, and licensed for use. At MSU, the Chemcad process simulation program (Chemstations, Inc.) is used, primarily due to its low annual license cost and to the ease with which it can be distributed

to students and faculty for use. Chemcad is a sequential modular processing process simulation program, and is similar to Aspen and ProVision.

During the introductory lecture, students completed the necessary steps in building a simulation for the example problem along with the instructor. Similar steps are required to build the simulation, regardless of the actual program employed, and include:

- specification of components
- selection of engineering units
- selection of appropriate thermodynamic model
- drawing of the flowsheet, including selection of unit operation block(s), and connection of the blocks with streams
- definition of each feed stream (including 2 independent properties selected from temperature, pressure, quality, and enthalpy) and its composition and flowrate.
- definition of each unit operation block (specification of how the particular device will operate)

Rather than assume that students will know what to choose/specify and why, the specific details for the example problem are provided along with an explanation of why a particular choice was made. For example, in defining a stream, one must choose two properties from among the four (temperature, pressure, quality, and enthalpy). While completing the example, the instructor points out that of the four choices, really only three can be used readily (specifying enthalpy would require knowledge of the reference point employed by the simulation program), and of the remaining three, temperature and pressure are the combination appropriate for most streams, excepting those streams that are known to be at conditions of saturated liquid ( $x = 0$ ), saturated vapor ( $x = 1$ ) or a mixture of saturated liquid and vapor. Chemcad actually uses the term vapor fraction rather than quality, and thus, this clarification ensures that the student doesn't inadvertently select a vapor fraction of 1 along with either T or P to represent a fluid in the ideal gas state.

Once the example has been successfully simulated, the remainder of the introductory lecture focuses on generation of the simulation report, learning about each section of the simulation report and what information is included therein (as well as how the information/format can be altered). These reports can be quite lengthy, depending on the particular output information selected and/or automatically generated for a particular unit operation block. Thus, electronic submission of generated reports for each assignment was accomplished using the MyCourses classroom management program. This allowed the instructor to download each student's submitted report and grade it, and upload the graded report, without a single printout of the report having to be generated.

The hands-on learning approach led by the instructor was quite effective in acclimating students to the process simulation program. In courses where there is insufficient time to include such an activity in-class, the use of the presentation as an out-of-class activity for students can also be employed, although this platform does not allow for the immediate addressing of questions students might have as they work through the examples/exercises.

## CHE Thermodynamics

In many CHE curriculums, thermodynamics is taught as a two course sequence. The emphasis in the first course on the first and second laws of thermodynamics, use of steam tables, ideal gas calculations, heat effects associated with reaction, isentropic efficiencies/performance of turbines, pumps and compressors, power cycles and refrigeration cycles and introduction to equations of state and compressibility,. In the second course, the emphasis is on non-ideal effects of pressure on thermodynamic properties, phase change behavior, solution thermodynamics, phase equilibria and chemical equilibria. These two courses offer a wealth of opportunities for incorporation of process simulation activities. For all activities, a two-step assignment was employed. Students were assigned a homework problem to complete using the traditional approach (first step: solution by hand, use of Excel or Polymath for finding a root, etc.). A subsequent Chemcad assignment (second step) required them to complete the same homework problem using the process simulator, and answer questions/compare answers/explain differences. The Chemcad assignment was very explicit in terms of providing information regarding selection of thermodynamic model, and specifications for the unit operation block(s). The focus here is not for the student to figure out what information should be provided to the process simulator, but to successfully run the simulation and compare the obtained solution to that obtained via the traditional approach. The connection between the calculation performed by hand and the calculation performed by the process simulation is established through the two-step assignment. This just-in-time introduction of process simulation allows students to better connect the operations the simulation program performs with the calculations that they themselves carry out to solve a particular problem.

### *Use of Heater Block (Simple Heat Exchanger)*

**Example 1: Heating of Ideal Gas – Determination of Heat Duty.** Taken from Smith et al. (Problem 4.2),<sup>5</sup> the heating of an ideal gas at approximately atmospheric pressure requires the determination of the energy addition needed to achieve a given temperature increase.

**Example 2: Heating of Ideal Gas – Determination of Outlet Temperature.** Also taken from Smith et al. (Problem 4.4), the addition of energy to an ideal gas at approximately atmospheric pressure requires the determination of the outlet temperature. If a temperature dependent heat capacity is employed, then this results in a polynomial that must be solved for temperature.

Both examples are similar in that the traditional solution requires integration of the temperature dependent heat capacity expression. For Example 1, the heat duty calculation is a simple plug and chug calculation; for Example 2, the unknown is the outlet temperature, so the root must be determined either analytically or numerically. Using the process simulator, both calculations are of the same degree of difficulty; the only difference is in the information supplied to the heater block in each example. Hints are provided along with the problem statements to aid the student in successfully setting up the simulation with the appropriate options.

**Example 3: Evaluation of Latent Heat of Vaporization of Pure Substance.** Also in Chapter 4 of Smith et al., students learn to estimate the latent heat of vaporization using the Watson correlation. This estimation can also be carried out using the Cranium<sup>6</sup> program (Molecular

Knowledge Systems, Inc.) using the Joback group contribution methods. Using the heater block, one can evaluate the latent heat of vaporization. 1 kg/s of pure material is fed to the unit at approximately atmospheric pressure and in the saturated liquid state (vapor fraction = 0). Specifying that the heater block operates with no pressure drop and yields a saturated vapor (vapor fraction = 1) results in the heat duty for the block being equivalent to the latent heat of vaporization for the material (power unit set to kW = kJ/s). One can select a variety of species including normal hydrocarbons as well as polar substances such as ethanol and ammonia and have students carry out the specified computations (Watson correlation, group contribution method as implemented in Cranium, and Chemcad) and compare the results of the estimation techniques. The comparison should allow students to conclude that some estimation techniques may be better-suited and more reliable for particular classes of materials.

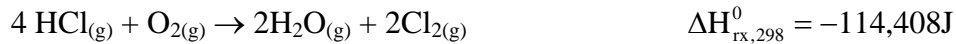
The key to all of these activities is for the student to correctly simulate the given problem, so that they: 1) can answer questions posed by the instructor comparing the simulation solution to the traditional calculation, and; 2) do not get frustrated trying to get information properly entered into the simulation program or have to guess what information to enter. Minimizing these frustrations will help the students better relate what happens in the process simulator to the computations that they have learned to perform by hand and will establish a better connection between the simulation and traditional calculations. This is one advantage of introducing process simulation across the chemical engineering curriculum, rather than exclusively in the senior design courses.

### *Use of Stoichiometric Reactor to Assess Heat Effects of Reactions*

In Chapter 4 of Smith et al., heat effects associated with chemical reaction are extensively covered. Students are exposed to the evaluation of the standard heat of reaction, as well as the evaluation of the temperature dependence of the heat of reaction. These calculations can be quite involved, particularly if temperature dependent heat capacities are employed. The evaluation of adiabatic flame temperature is also included in this chapter, with variations of the problem arising from the use of excess oxygen/air and inclusion of diluents. These calculations can be examined readily using the stoichiometric reactor unit operation block. This block performs the mass and energy balances for a single reaction occurring in a single phase. The input information required is minimal; reaction stoichiometry must be specified along with the key component and fractional conversion based on that component; thermal mode (isothermal, adiabatic, with heat exchange) must also be specified. For all of the simulations involving chemical reactions from Chapter 4 of Smith et al., ideal gas behavior is assumed. Thus, the appropriate K-value and Enthalpy models to be used in simulation of these examples are the 'Ideal Vapor Pressure' for K-value and 'Latent Heat' for Enthalpy. These examples can be easily adapted to the Chapter 4 end of chapter problems in Smith et al. involving these concepts and varied from semester to semester.

**Example 1. Evaluation of Standard Heat of Reaction.** The feed stream to the stoichiometric reactor is specified using stoichiometric mixture of the various reactants, with temperature and pressure specified as 25 °C and 101.325 kPa, respectively. In the stoichiometric reactor module, the thermal mode is selected to be 'isothermal' with a reaction temperature of 25 °C. The key component is specified as HCl with a fractional conversion of 1. Reaction stoichiometry is

defined on the menu also. The standard heat of reaction (J/gmol) is reported for the chemical reaction in the equipment summary; multiplying by 4 gives the standard heat of reaction for this reaction as written. Example 4.5 in Smith et al. examines the reaction:



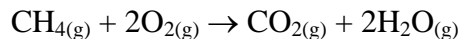
The feed is specified as  $T = 25 \text{ }^\circ\text{C}$ ,  $P = 101.325 \text{ kPa}$ , with flowrate of 5 gmol/s (4 gmol/s HCl, 1 gmol/s  $\text{O}_2$ ). The standard heat of reaction reported in the equipment summary is  $-28.608 \text{ J/gmol}$ , resulting in  $\Delta H_{\text{rx},298}^0 = -114,432\text{J}$ .

**Example 2. Evaluation of Heat of Reaction at Elevated Temperature.** Example 4.6 in Smith et al. examines the heat required to produce methanol from synthesis gas. The methanol reaction is:



To simulate this reaction process, a stoichiometric synthesis gas mixture is fed at 800 K, 101.325 kPa to the reactor. Within the stoichiometric reactor menu, the basis component is specified as CO, with a fractional conversion of 1; the thermal mode is ‘isothermal’ at 800 K; no pressure drop and stoichiometric coefficients specified as given in the reaction above. The required heat duty is calculated by Chemcad to be  $-103,622 \text{ J}$ .

**Example 3. Adiabatic Flame Temperature and Associated Calculations.** Example 4.7 of Smith et al. examines the combustion of methane achieved adiabatically with air as the source of oxygen. Complete combustion is ensured through use of excess air. With the stoichiometric reactor, it is possible to use two feed streams (one for methane, one for air). It is then possible to use some of the advanced features within Chemcad (Sensitivity) to vary the % excess air and examine the impact on the adiabatic flame temperature. Also interesting is to have students examine the use of enriched air ( $> 21 \text{ } \%$   $\text{O}_2$ ) and its impact on the adiabatic flame temperature. For Example 4.7, the chemical reaction is:



Two feed streams, each entering at  $25 \text{ }^\circ\text{C}$ ,  $101.325 \text{ kPa}$ , are specified. For the methane stream, a flowrate of 1 gmol/s is specified. For the air stream, a flow rate of  $2[1 + (\% \text{ excess}/100)] \text{ gmol/s}$  is specified with 79%  $\text{N}_2$ , 21 %  $\text{O}_2$ . Within the stoichiometric reactor menu, the basis component is specified as  $\text{CH}_4$ , with a fractional conversion of 1. The thermal mode is specified as ‘adiabatic’, pressure drop specified as zero, and stoichiometric coefficients specified. In the text example, the adiabatic flame temperature is calculated as  $1793 \text{ }^\circ\text{C}$ . In Chemcad, the temperature of the reactor effluent is the adiabatic flame temperature and is calculated to be  $1795 \text{ }^\circ\text{C}$ .

With all three of these examples, it is appropriate to discuss why the simulation results may differ from the answers given in the example problems. Differences in critical properties and ideal gas heat capacities among other data contained in the thermodynamic database accompanying the process simulation can be examined for their contribution to these differences in results.

### *Throttling Process – Non-ideal Effects Due to Pressure*

Throttling of carbon dioxide from high pressure to approximately atmospheric pressure is an isenthalpic process. In Chemcad, this process can be simulated using the VALV block or using the heater block. When using the VALV block, one must just supply the pressure drop across the valve (or the outlet pressure). When using the Heater block, one has to specify both the pressure drop across the unit (or the outlet pressure), as well as specifying that the process operates adiabatically. With high pressure, it is appropriate to use an equation of state to calculate the residual properties (enthalpy, entropy). During lectures, students are exposed to estimation/calculation of residual properties using both generalized correlations and equations of state. For simplicity, the homework assignment usually requires evaluation of these non-ideal contributions due to pressure using the Redlich-Kwong or Peng Robinson equation of state. In Chemcad, students evaluate the same process using the Peng-Robinson equation and the ideal gas law (ideal vapor pressure/latent heat K-value/enthalpy option). Students can compare results of the three different approaches through examination of the outlet temperature and power output. They should conclude that including the non-ideal effects due to pressure is important for systems when high pressure is present.

### *Use of Turbine (Isentropic Efficiency)*

**Example 1:** Many of the problems at the end of Chapters 6 of Smith et al. involve flow of a fluid through a turbine or compressor. Turbine operation is typically isentropic while compression is carried out either isentropically or isothermally. All of these scenarios are readily evaluated by hand using generalized correlations or an equation of state to evaluate the residual properties and via process simulation using an equation of state. A typical assignment would be Problem 6.62 from Smith et al.: “A stream of ethane gas at 220 °C and 3000 kPa with flowrate of 1 kmol/s expands isentropically in a turbine to 260 kPa. Determine the temperature of the expanded gas and the work produced by the turbine. Use the Peng-Robinson equation of state for K-Value and for Enthalpy Model. The turbine block is actually called an ‘Expander’ in Chemcad. Isentropic expansion means adiabatic and reversible. To specify adiabatic expansion, one must specify the outlet pressure and the efficiency. The efficiency as specified in Chemcad is actually the ‘isentropic efficiency’ discussed in the text. An efficiency of 1.0 means the turbine operates reversibly (Chemcad automatically assumes that all turbines are well-insulated and thus, adiabatic).”

**Example 2:** In Chapter 7 of Smith et al., the concept of isentropic efficiency is introduced for turbines, compressors and pumps operating with steam as the working fluid. With Chemcad, when water is the only component in the simulation, all properties are evaluated using the steam tables. The determination of the outlet state from a real turbine when the isentropic efficiency is less than 1 requires that the isentropic power output first be determined. The efficiency is then used to evaluate the actual power output. The outlet state from the real turbine is defined by the outlet pressure and the enthalpy.

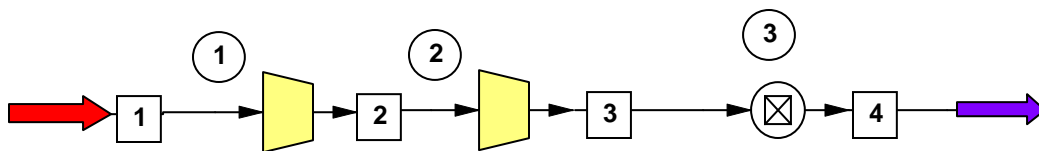


## Two Turbines with Matched Power Output

In this example, two turbines are connected in series. Steam enters the first turbine (flowrate of 1 kg/s) at 650 °C, 7000 kPa. The exhaust pressure from the second turbine is 20 kPa. Both turbines operate with an isentropic efficiency of 78 %. At what pressure should the first turbine discharge so that the power output from the two turbines is the same?

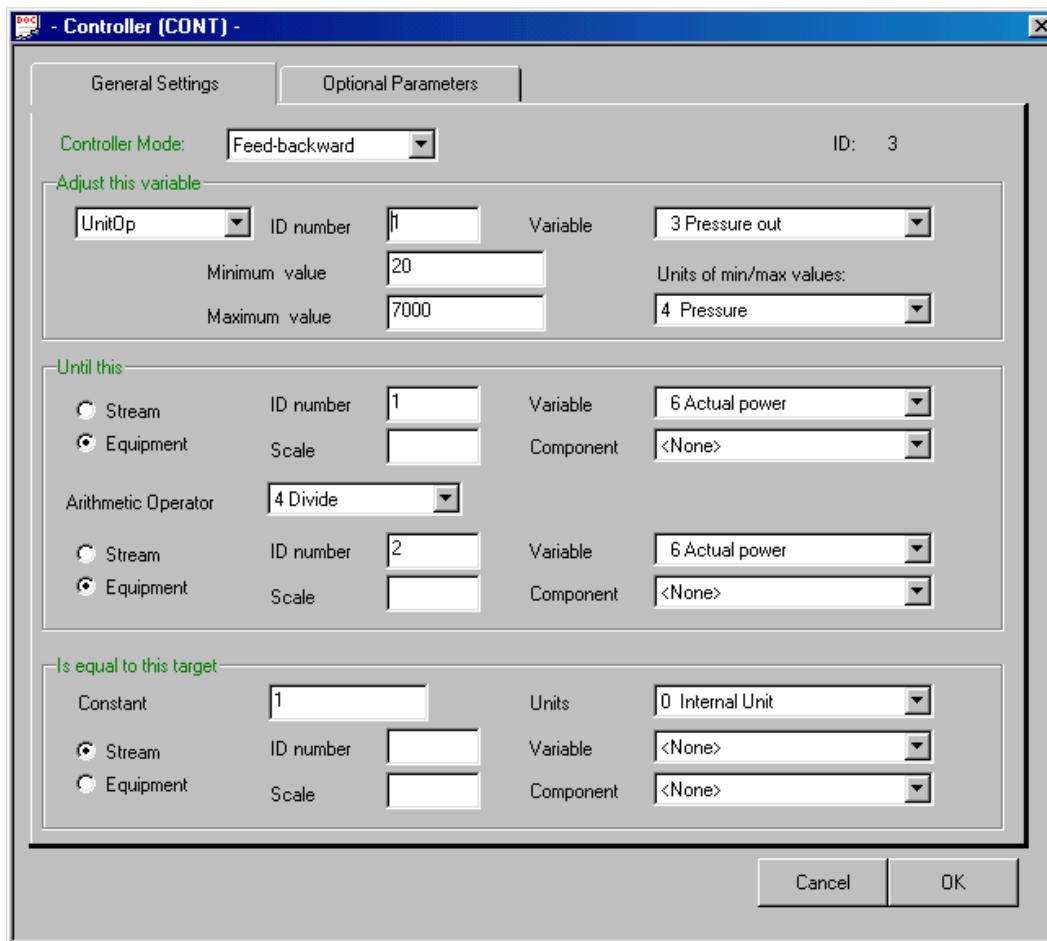
This is a pretty involved calculation to perform by hand. One must assume a discharge pressure from the first turbine, evaluate the isentropic power output, calculate the actual power output using the efficiency, and determine the enthalpy of the steam exiting the first turbine (along with entropy of this stream). The same calculations must then be carried out for the second turbine. If the actual power outputs of the two turbines are not equal, the assumed discharge pressure from the first turbine is changed and the entire calculation repeated. In practice, this problem is usually an example using during lecture with at least one iteration of the calculation process demonstrated, as well as discussion as to whether the assumed pressure should be adjusted upwards or downwards for the second iteration.

Simulation of this process can be carried out with the student adjusting the discharge pressure from the first turbine by hand until he/she achieves matched power outputs from the two turbines. However, this process offers the opportunity to introduce a very useful tool in the Chemcad simulation package – the Controller block. The controller block is a unit operation block that can be used to adjust a stream parameter or an equipment parameter to achieve a particular outcome. Operating in feedback mode, the controller block must be placed downstream of all quantities that must be sampled in order to carry out the comparison. Figure 1 shows the flowsheet for this simulation. Units 1 and 2 are the turbines, while unit 3 is the controller.



**Figure 1. Flowsheet for Two Turbines with Matched Power Output**

Specifications for the first turbine are an assumed discharge pressure (somewhere between 20 kPa and 7000 kPa) and an isentropic efficiency of 0.78. For the second turbine, discharge pressure is 20 kPa and isentropic efficiency is 0.78. The controller specifications are shown in Figure 2. The discharge pressure for UnitOp 1 is adjusted (the first turbine) between the values of 20 kPa and 7000 kPa until the ratio of actual power for turbine 1 divided by actual power for turbine 2 is equal to 1. There are actually a number of ways that this constraint could be specified. One could simply subtract the two power outputs and adjust the pressure until this difference is 0. Using the ratio is preferable, as the ratio is independent of the magnitude of the individual power outputs. The ratio should always be close to a magnitude of 1, so the convergence tolerance of 0.001 can be readily achieved in a reasonable number of iterations. With a discharge pressure of 766.77 kPa, the power output from each turbine is -0.567887 MJ/s, resulting in a ratio of 1.000007.

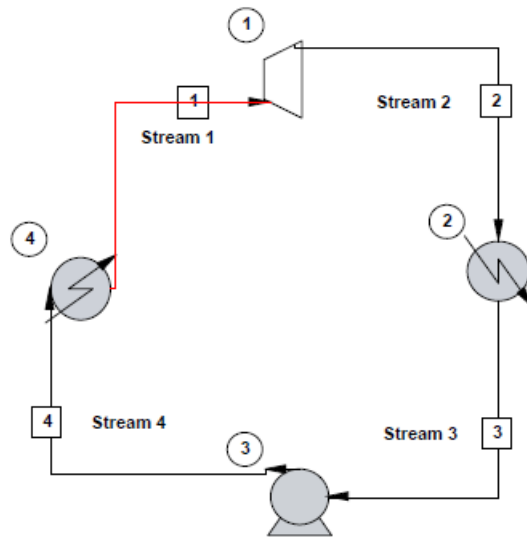


**Figure 2. Specifications for Controller Block**

### *Rankine Power Cycle*

Power cycles are covered in the first thermodynamics course at MSU. The Rankine cycle can be readily simulated using Chemcad. This simulation offers the opportunity to introduce a second feature of Chemcad to the students. When there is a cycle or recycle nature to the process being simulated, Chemcad automatically identifies a ‘Cut Stream’, where the flowsheet is artificially segmented. This ‘Cut Stream’ actually consists of two streams connected by a ‘Convergence’ block. Not all choices of cut streams are equivalent, and sometimes it is better to have two cut streams, rather than a single cut stream in a flowsheet. The placement of the cut stream is very important. In simulating a Rankine cycle, it is best if the cut stream is the stream that we know the most about (i.e., in a typical Rankine cycle, this will be the stream entering the high pressure turbine). Figure 3 shows the flowsheet as constructed in Chemcad. Note the red stream indicates the ‘Cut Stream’ for this flowsheet.

Example problems such as found in Chapter 8 of Smith et al. (specifically 8.3, 8.4, and 8.5) can be readily employed. Note that these problems have the steam rate as a unknown (power output from turbine is given), so that students could also use the controller block to adjust the mass flowrate of steam into the turbine until the turbine power output is the specified 80000 kW.



**Figure 3. Rankine Cycle Flowsheet**

### ***Flash Unit – Two Phase and Three Phase***

Activities for examining the behavior of flash tanks/drums can be included in the thermodynamics course or in the separations course. Lecture content in either course typically involves the construction of Pxy/Txy diagrams and their use to graphically solve two phase flash problems. A typical assignment to help students develop their knowledge base with regards to flowrates as well as liquid and vapor compositions and how these change as a function of the fraction vaporized in the flash tank is shown in Figure 4. Students then answer the following questions, based on their results:

- What trends do you see in: 1) the toluene liquid phase mole fraction? 2) the toluene vapor phase mole fraction? 3) the temperature of the flash tank?
- Provide a general conclusion regarding the effect of V/F on the operation of the flash tank – what does selection of V/F primarily impact in your results?

A similar table (also shown in Figure 4) is provided for students to examine the impact of feed composition on the vapor and liquid flowrates and stream compositions for an isothermal/isobaric flash (P-T flash).

Chemcad is also equipped with a Three Phase Flash (LLV) block. In Chapter 14 of Smith et al., a number of problems are provided where an organic solvent and water (14.24, 14.25) are equilibrated or an organic mixture and water are equilibrated. In the two component systems (organic solvent and water), it is often assumed that the two species are completely immiscible.

#### Understanding Operation of Flash Tank

To build the simulation: set units (Format – Engineering Units – to SI, change pressure units to kPa; temperature units to °C). Choose components (Toluene, Ethylbenzene). Select K-Value model as “Ideal Vapor Pressure”, Enthalpy Model as “Latent Heat”. This combination gives Raoult’s Law. In Edit Flowsheet mode: Choose ‘Flash’, 1 feed point, 2 product points. Connect the feed and product arrows to the flash unit.

Effect of V/F on  $T$ ,  $x_1$ ,  $y_1$ : Feed stream:  $T = 25^\circ\text{C}$ ,  $P = 101.325\text{ kPa}$ , 50/50 mixture of Toluene/Ethylbenzene, total flowrate of 1 kmol/hr. In Flash Block, choose option 1: Specify V/F and P; Calculate T and Heat. Complete the following table:

Fraction of Feed Leaving as Vapor V/F	Temperature T (°C)	Mole Fraction Toluene in Liquid $x_1$	Mole Fraction Toluene in Vapor $y_1$
0.0			
0.0001			
0.2			
0.4			
0.6			
0.8			
0.9999			
1			

Effect of Feed Composition on Liquid/Vapor Compositions: Feed stream:  $T = 25^\circ\text{C}$ ,  $P = 101.325\text{ kPa}$ , variable mixture of toluene/ethylbenzene, total flowrate of 1 kmol/hr. In Flash Block, choose option 2: Specify T and P; Calculate V/F and Heat. Specify temperature as  $120^\circ\text{C}$ , pressure as 101.325 kPa. Complete the following table:

Mole Fraction Toluene in Feed $z_1$	Fraction of Feed Leaving as Liquid L	Fraction of Feed Leaving as Vapor V	Mole Fraction Toluene in Liquid $x_1$	Mole Fraction Toluene in Vapor $y_1$
0.0				
0.2				
0.4				
0.55				
0.56				
0.60				
0.65				
0.71				
0.72				
0.8				
1				

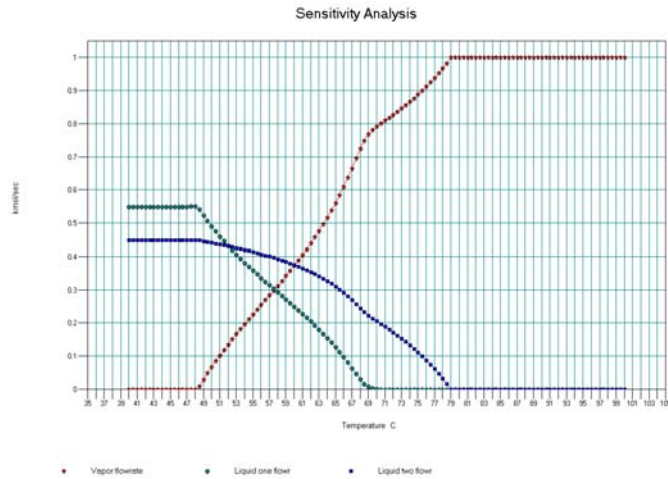
**Figure 4 – Flash Tank Simulation**

Depending on the overall composition of the mixture, one pure component will condense from a vapor mixture, leaving the vapor richer in the other pure component. The demarcation point for identifying which pure component condenses is denoted by  $T^*$ ,  $y_1^*$  in the text. If the overall composition,  $z_1$ , is less than  $y_1^*$ , then pure component 2 condenses from the vapor, with the vapor composition increasing in component 1 and the temperature at which condensation occurs dropping as the condensation proceeds. If the overall composition,  $z_1$ , is greater than  $y_1^*$ , then pure component 1 condenses from the vapor, and the vapor becomes richer in component 2, with the temperature at which condensation occurs dropping as the condensation proceeds. This is not a process that students can readily grasp, even with a phase diagram (although the phase diagram helps!). The condensation process can also be examined using the three phase flash unit in Chemcad.

A more complicated system, water(1)/n-pentane(2)/n-heptane(3), is the focus of Problem 14.27. Given an overall composition of the vapor phase at 101.33 kPa and  $100^\circ\text{C}$ , the mixture is cooled at constant pressure until completely condensed. Water and the organic phase (n-pentane/n-heptane) are assumed immiscible, the organic mixture obeys Raoult’s law and the vapor phase is assumed ideal. Posed are questions regarding dew point temperature and composition of first condensate; temperature at which second liquid phase appears and the bubble point temperature and composition of the last vapor bubble. These are actually quite involved calculations, but can be examined using the Sensitivity tool in Chemcad.

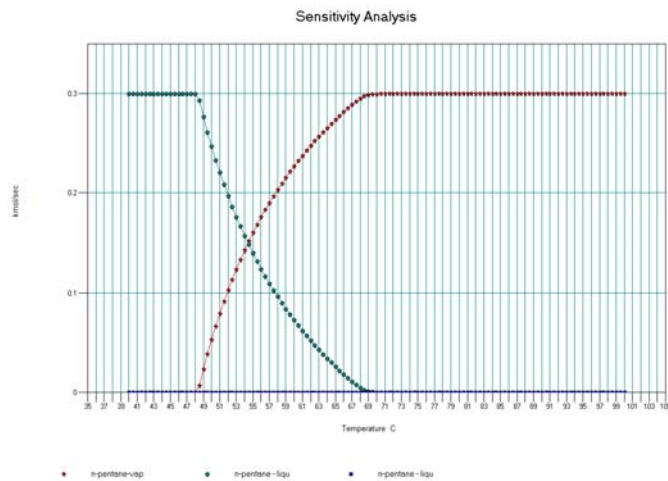
The Sensitivity tool in Chemcad allows one to determine how a process reacts to variation of key operating and/or design variables. One or more of the flowsheet input variables can be varied to examine the effect on other calculated flowsheet variables. The simulation is constructed with the single feed stream entering the three phase flash unit, and three exiting streams are defined (vapor, organic liquid and aqueous liquid). The feed stream is defined by its flowrate, composition ( $z_{\text{water}} = 0.45$ ,  $z_{\text{n-pentane}} = 0.30$ ,  $z_{\text{n-heptane}} = 0.25$ ), temperature and pressure. One key element of this simulation is that a phase equilibria model (K-value model) must be chosen that allows for the existence of two liquid phases. The three phase flash unit is set to operate in P-T flash mode ( $P = 101.33$ ,  $T = 100^\circ\text{C}$  initially). Operation of the simulation with these conditions

would yield only one effluent stream, the vapor, with the given overall composition. Use of the sensitivity tool, where the temperature of the flash unit is varied between 40 °C and 100 °C, provides output information on the flowrates of the three effluent streams (vapor, liquid 1 and liquid 2), and their compositions as a function of flash temperature. These data can then be plotted. Shown in Figure 5 is the variation of flowrates as a function of temperature.

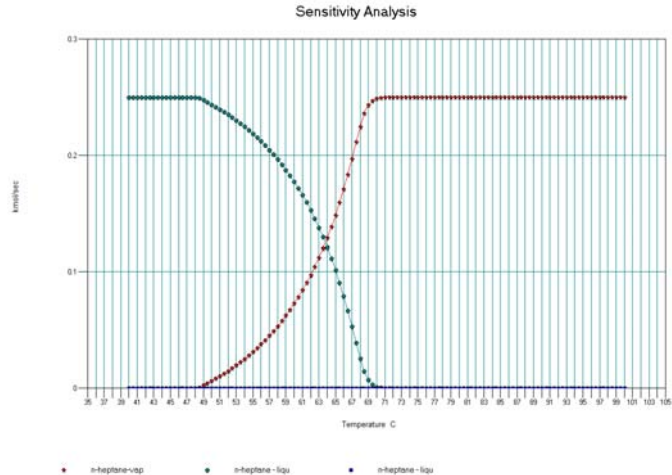


**Figure 5 – Flowrates Exiting Three Phase Flash Unit**

Liquid one is the organic phase, while liquid two is the water phase. The onset of condensation occurs just below 79 °C, with pure water condensing from the vapor. The second liquid phase appears at approximately 69 °C. Condensation is complete at approximate 48.5 °C. Similar plots can be prepared for the compositions/flowrates of the various components. The plots for n-pentane and for n-heptane are shown in Figures 7 and 8. From these data, the composition of the organic phase when first condensing can be evaluated as  $x_{n\text{-pentane}} = 0.147$ ,  $x_{n\text{-heptane}} = 0.850$ ,  $x_{\text{water}} = 0.003$ . The bubble point is evaluated as 48.5 °C, and the composition of the first bubble of vapor is  $y_{\text{water}}^* = 0.113$ ,  $y_{n\text{-pentane}}^* = 0.807$ , and  $y_{n\text{-heptane}}^* = 0.079$ .



**Figure 7 – Flowrates of n-pentane from Three Phase Flash**



**Figure 8 – Flowrates of n-heptane from Three Phase Flash**

## CHE Separations

### *Generation of Pxy/Txy Diagrams*

This activity can be carried out in either the thermodynamics course on phase equilibria or in the separations course. One of the biggest issues with simulation of chemical processes is the selection of the appropriate thermodynamic models for evaluation of phase equilibria and thermal properties. Thus, it is beneficial to include an exercise where students are given (or select) a chemical system from the literature (typically within the constraints of low to moderate pressure – i.e., less than 2 bar total pressure; and a binary system that does not exhibit phase splitting). Much of the VLE data published in the *Journal of Chemical and Engineering Data* satisfy these criteria and exhibit non-ideal behavior of some type (deviations from Raoult’s law, either mild or extreme). Students can generate Pxy or Txy data/diagrams for the given chemical system using variety of K-value/enthalpy models (ideal vapor pressure/latent heat for Raoult’s law; other activity coefficient models for the liquid phase, or an equation of state for both liquid and vapor phases). Comparison of the Chemcad generated data with the experimental data will lead the students to the conclusion that not all K-value models are the same, and that certain behaviors (i.e., azeotropes) cannot be represented using Raoult’s law.

### *Two Phase Flash with Purity Constraint*

When a flash tank is employed for a rough separation between components of very different volatilities, there is a constraint on how much of the high boiler can be lost to the vapor (or the low boiler entrained in the liquid) leaving the flash unit, usually driven by economics. The simulation of this process is fairly straightforward, with specification of the feed stream/composition/temperature and pressure as well as how the flash tank operates (P-T – isothermal flash; or P-H – adiabatic flash). The question posed might be ‘at what pressure should the flash tank operate if the vapor can contain no more than 0.02 mole fraction of the high boiler?’ One could set up the simulation and manually adjust the flash tank pressure until the desired mole fraction of high boiler in the vapor is achieved. An alternative would be to employ the Controller block, and adjust the flash tank pressure until the constraint (desired mole fraction

of high boiler in the vapor phase) is achieved. This would require sampling of the molar flowrate of the high boiler in the vapor stream as well as the molar flowrate of the vapor streams, with division of these quantities yielding the target mole fraction. A number of the end-of-chapter problems in Separation Process Engineering: includes Mass Transfer Analysis by Wankat<sup>7</sup> can be used as the basis for assignments. In this newest edition of his text, Wankat also includes additional problems targeting the use of commercial process simulation software.

### ***Binary Distillation – Shortcut Method***

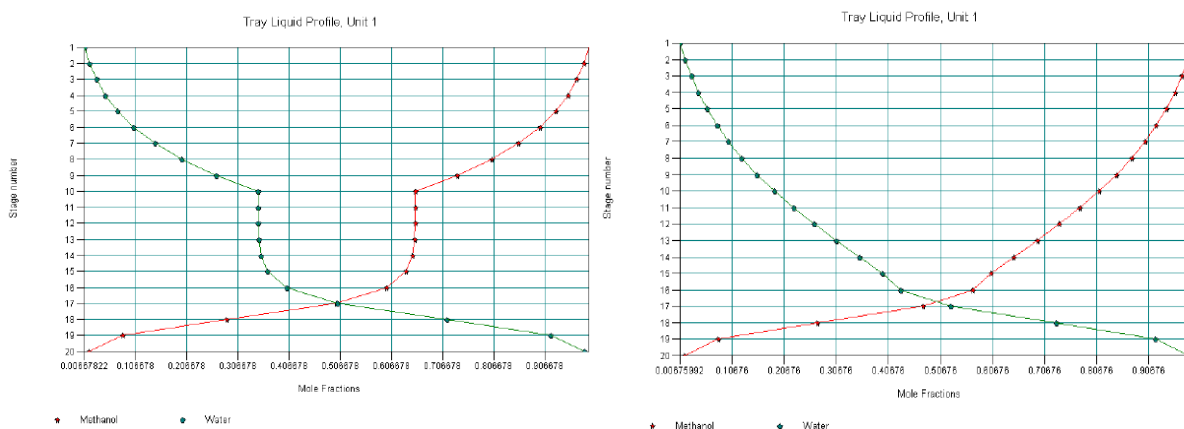
One of the most challenging processes to simulate is a distillation tower. While most industrial distillation processes involve more than two components, providing instruction on simulation of these processes using a simple binary system is invaluable. The McCabe Thiele graphical analysis of binary distillation is typically covered early in the separations course at MSU. When the shortcut method (Fenske-Underwood-Gilliland method) is introduced, the first example used in class is for a binary system. This is beneficial to the student because: 1) there are only two components, with one identified as the low boiler and one as the high boiler; and 2) it is easy to relate to the graphical method that they have already seen. The example used is the separation of methanol and water. This system is one used widely in the early chapters of Wankat. The developed tutorial leads the students through the various options available in the shortcut method as implemented in Chemcad (rating case, design with Fenske feed, design with Kirkbride feed). The identification of the light key and heavy key and evaluation of their recoveries are discussed as is specification of other required input (for design, this is typically  $R/R_{\min}$ ). Output for a design case includes minimum reflux ratio, minimum number of stages, optimum feed location as well as condenser and reboiler duties. Through the example, students see that they obtain the same results that they would calculate by hand (for  $R_{\min}$  as well as the number of stages and the location of the feed stage). One of the most important uses of the shortcut method is to provide input information for the more rigorous simulation models for distillation in the process simulator.

### ***Binary Distillation – Rigorous Simulation***

In the rigorous simulation models of Chemcad, the user must provide information obtained from the Shortcut simulation, including number of stages, feed stage and reflux ratio. There are three rigorous models (TOWR, TPLUS, and SCDS); input to each of these models is similar. Options include specifying pressure drop across the condenser and the column, but default values are zero. Additional specifications must also be provided, including constraints for the condenser and the reboiler. Specifying the condenser and reboiler modes is critical to a successful simulation. One safe option is to specify fractional recovery of the light key in the distillate for the condenser mode and to specify fraction recovery of the heavy key in the bottoms for the reboiler. Other options may give rise to convergence difficulties (for example, a particular mole fraction of a component in the distillate stream may prove impossible to achieve with the other operating conditions selected for the column). Estimates for the distillate flowrate/temperature and for the reflux rate can be provided, but no estimates are better than bad estimates, so can often be omitted.

The output from the rigorous model includes tray compositions, tray properties, refined condenser and reboiler duties, refined reflux ratio estimate, as well as temperature, pressure and flowrate profiles through the column. What is very interesting is to have students examine the assumption constant molal overflow through use of the flowrate profiles.

With the Shortcut column, both the number of stages and the placement of the feed stage are calculated. With the rigorous models, it is often useful to demonstrate that the location of the feed tray can be adjusted, sometimes resulting in improvements in the separation achieved on each tray. The liquid mole fractions of methanol and water are shown in Figure 9. On the left, the profiles shown are for the input information taken from the Shortcut model; on the right, the same input information is used to generate the profiles shown, except that the feed tray has been adjusted from Stage 12 to Stage 16. Note that the stages between Stage 12 and Stage 16 actually contribute to the desired separation in the profiles on the right.



**Figure 9. Liquid Mole Fraction Profiles obtained for the Methanol/Water Separation**

### *Column Sizing (Generation of Column Profiles)*

Generation of column profiles (compositions, properties, temperature, pressure and flowrates) is advantageous when one is interested in sizing the distillation column. As part of a multi-part/multi-day homework activity, students work through the simulation of a distillation tower separating n-hexane and n-heptane or another separation problem where they have used the FUG method for hand calculations. The basis of the n-hexane/n-heptane separation is the example in Wankat's text in Chapter 10 where column sizing is discussed. The shortcut method must be used in Chemcad along with the rigorous model, TOWER, to generate the necessary flowrate, composition and property profiles. These results are uploaded using the available course management software. Students also must develop a spreadsheet where column diameter is determined at four different points in the column (tray below the condenser, tray above the reboiler, trays adjacent to the feed tray). This spreadsheet, if correct, is then available for them to use when sizing columns for their semester design project. The necessary data (flowrates, surface tension, vapor and liquid density) required for the diameter calculation are obtained from their generated column profiles.



## ***Comprehensive Design Project***

During the latter portion of the semester, a multicomponent separation process forms the basis of a design project. Designed as an open-ended project, the objective is to recover two or more of the chemicals from the mixture to produce at least two streams meeting required purities while maximizing recovery of the chemicals. Very little information is given other than the composition/flowrate of the feed, the temperature/pressure at which the feed is stored and the desired product streams with specified purity. Heuristics governing the design of separation processes (taken from Wankat and from Turton et al.<sup>8</sup> are discussed in class prior to the assignment of the project.

## ***Gas Absorption/Stripping***

The evaluation of gas absorbers/strippers is also covered in the Separations course. Lectures covering single component absorption and stripping as well as multi-solute absorption and stripping have been presented during class. It is interesting for the students to realize that the same rigorous models that were used for distillation are also used for simulation of absorption and stripping processes. One key element in the simulation of these processes is selection of the appropriate thermodynamic model (students encouraged to use K-value wizard for selection). The rigorous model, SCDS, is used for modeling absorbers and strippers. Required input includes operating pressure, number of stages, feed stage for liquid inlet, and feed stage for gas inlet. Typically known are the operating temperature and pressure for the unit, feed stream compositions (gas and liquid inlet streams). Also known is the degree of removal required for a particular contaminant, but the number of stages is generally not known. One approach is to set up an absorber in Chemcad with 2 stages – liquid inlet set at stage 1, gas inlet at stage 2 – then run the simulation. The outlet conditions (for stripper, contaminant concentration in liquid effluent; for absorber, contaminant concentration is gas effluent). If required degree of removal has not been met, the number of stages is increased until desired contaminant concentration is achieved. Students work through a multi-component stripping example where groundwater (1500 GPM, 60 °F, 1 atm) is contaminated with 1,2-dichloroethane (85 ppmw, Henry's constant = 60), trichloroethylene (120 ppmw, Henry's constant = 650) and 1,1,1-trichloroethane (145 ppmw, Henry's constant = 275) was to be stripped with air (60 °F, 1 atm). Preliminary calculations by hand indicated a minimum gas flowrate of 208.2 lb<sub>m</sub>/min, with operation at twice the minimum gas flowrate yielding  $G = 416.5$  lb<sub>m</sub>/min. In multi-solute absorption or stripping, the assumption of dilute solutions was made, and it was necessary to identify the most problematic of the contaminants (most difficult to remove or has the largest required fractional recovery – for example, to meet existing emissions limits).

From given information, 1,2-dichloroethane was identified as the target solute, based on its Henry's constant ( $m_i = 60$ ), and its required removal (inlet = 85 ppmw; outlet = 0.005 ppmw). Simulation input for SCDS was established using the suggested approach (start with absorber of 2 stages, increase number of stages until necessary removal is achieved – 13 were required for this example). Sample output for the SCDS block is shown in Figure 10.

The last column in Figure 10 is an estimate of the partition coefficient between the phases, essentially an estimate of Henry's constant on that stage. Comparing these values with those

used in the preliminary hand calculation, the values for 1,2-dichloroethane (60 versus 48.7) and 1,1,1-trichloroethane (275 versus 284.5) are similar, but that used for trichloroethylene is significant different (675 versus 1.1). So perhaps some investigation into the thermodynamic model is warranted or a review of the literature to identify a more reliable Henry's constant for trichloroethylene is warranted. In this case, if the Chemcad estimate of the Henry's constant is valid, then the stripping problem should be revisited with trichloroethylene as the solute on which the separation is designed.

Unit type : SCDS    Unit name:    Eqp # 1				
Stage #	1	59.98 F	1.00 atm	
		Vap lb/min	Liq lb/min	Y/X
Water		4.61688	12490.62793	0.01749
Air		416.20578	0.26244	75026.89063
1,2-DiCl-Ethane		0.99987	0.97131	48.69969
TriCl-Ethylene		0.03467	1.49940	1.09387
111-TriCl-Ethane		1.81177	0.30126	284.51270
Total lb/min		423.6690	12493.6615	
Stage #	2	59.98 F	1.00 atm	
		Vap lb/min	Liq lb/min	Y/X
Water		4.61839	12490.62793	0.01750
Air		416.46826	0.26267	75023.11719
1,2-DiCl-Ethane		0.90910	0.88412	48.65557
TriCl-Ethylene		0.03467	1.49940	1.09423
111-TriCl-Ethane		0.30126	0.05012	284.42596
Total lb/min		422.3317	12493.3240	

**Figure 10. Partial Output from SCDS for Multi-Solute Stripping Example**

## CHE Reactor Design

At MSU, students complete the reactor design course during the fall of the senior year, along with the first course in the capstone design sequence. In the tutorial for reactor design, all of the reactor unit operation blocks are presented. In Chemcad, there are four such blocks, three of which are strictly used for mass and energy balance calculations, while the fourth block, KREA, can be used for sizing calculations also. The tutorial example is an example from Fogler<sup>9,10</sup> where the reactor volume required to produce 300 million pounds of ethylene annually via the cracking of ethane. The rate law is provided along with the required conversion, as well as the operating temperature and pressure for the reactor. This tutorial has been used as both an out-of-class activity as well as a hands-on, in-class activity. All four reactor modules are examined, and the required input for each is developed. For the equilibrium reactor (EREA), one must provide information regarding the equilibrium constant as a function of temperature (in the form of the van t'Hoff equation,  $\ln(K) = A + B/T$ ). The development and calculation of the constants, A and B, is carried out in the tutorial. For the kinetic reactor, KREA, the key element to successful simulation is specification of the units for the rate law. Students work through the provided examples to gain experience with the process simulation of chemical reactors. As part of the course requirements, students complete a design project where the objective is to maximize production of a desired species, while minimizing production of undesirable byproducts. In this project, students were provided with a variety of variables to explore including:

- PFR versus CSTR. For a PFR, assume that necessary reactor volume is achieved using 4.03 inch ID, 4.50 inch OD pipes, length of 15 feet. If CSTR is used, feed stream might need to be partitioned into parallel CSTR's. Need to justify that your choice of reactor (PFR or CSTR) is superior to the alternative (CSTR or PFR).
- Feed condition (if feed is preheated or cooled, estimation of heat duty is required).

- Operating temperature and pressure. May assume that the reactor(s) operate(s) isobarically. Should investigate isothermal, adiabatic and non-adiabatic/non-isothermal modes of operation. For non-adiabatic/non-isothermal operation, may assume an overall heat transfer coefficient of 9 BTU/(hr-ft<sup>2</sup>-°F) and that sufficient utilities are available (cooling water at 30 °C, LPS, MPS, HPS, flue gas at 1600 °F). An examination of the selectivity of the desired product to the undesired product may help identify appropriate temperature and/or pressure ranges. Ranges of typical operation are temperature between 350 and 650 °C, and pressures between 1 and 5 bar.
- Inlet temperature - typical inlet temperatures are between 350 and 650 °C.
- Addition of inerts such as steam to the feed mixture. The presence of inerts in the feed may not only serve as a diluent to help mitigate the drop in temperature realized due to the endothermic reaction, but may also influence the reaction progress in terms of selectivity and yield. The inclusion of inerts will also significantly increase the required volume of the reactor, thus, their use should be well justified.

Use of Chemcad allowed the students to readily examine different operating modes/conditions as generate plots of pertinent data that could be used to justify their design decisions. A variety of examples/end of chapter problems from Fogler have been successfully simulated using the Chemcad software; these are available from the authors upon request.

### **Student Perceptions**

During this spring semester, perceptions of students regarding their process simulation activities/experience in the two course thermodynamic sequence and in the separations course were gathered. Perceptions were evaluated using a 5-point scale (1 – strongly disagree to 5 – strongly agree). Shown in Table I are the questions for each of the surveys (Thermo I, Thermo II, Separations).

Compiled survey results are shown in Figures 11 to 13. The first question on each survey asked about the adequacy of instruction; all instruction was in the form of a hands-on instructional lecture with students working through the simulation with the instructor. This mode of instruction was positively received by the students (> 50 % of responses either strongly agreed or agreed). The last question on each survey asked about the connection between the underlying calculations performed by hand and the use of the process simulation software to perform the calculations; again, the majority of students were able to see the connection between the two activities (> 50 % of responses either strongly agreed or agreed). An additional question on the separations survey queried prior exposure to Chemcad in a course (yes/no response). Coverage in the Separation Processes course occurred later in the semester compared to the thermodynamics courses; approximately 2/3 of the respondents had used Chemcad in a previous course (48 out of 65 students). Question 6 on the separations survey queried student confidence in refining a separation (i.e., using the column composition profiles by adjusting a model input parameter such as the feed tray); students were less confident in their ability to perform this refinement. However, it is the experience of the instructor (RT) that such confidence will grow with continued use of the rigorous models to examine performance with industrial separation problems, such as the students would see in a ‘real-world’ design project.

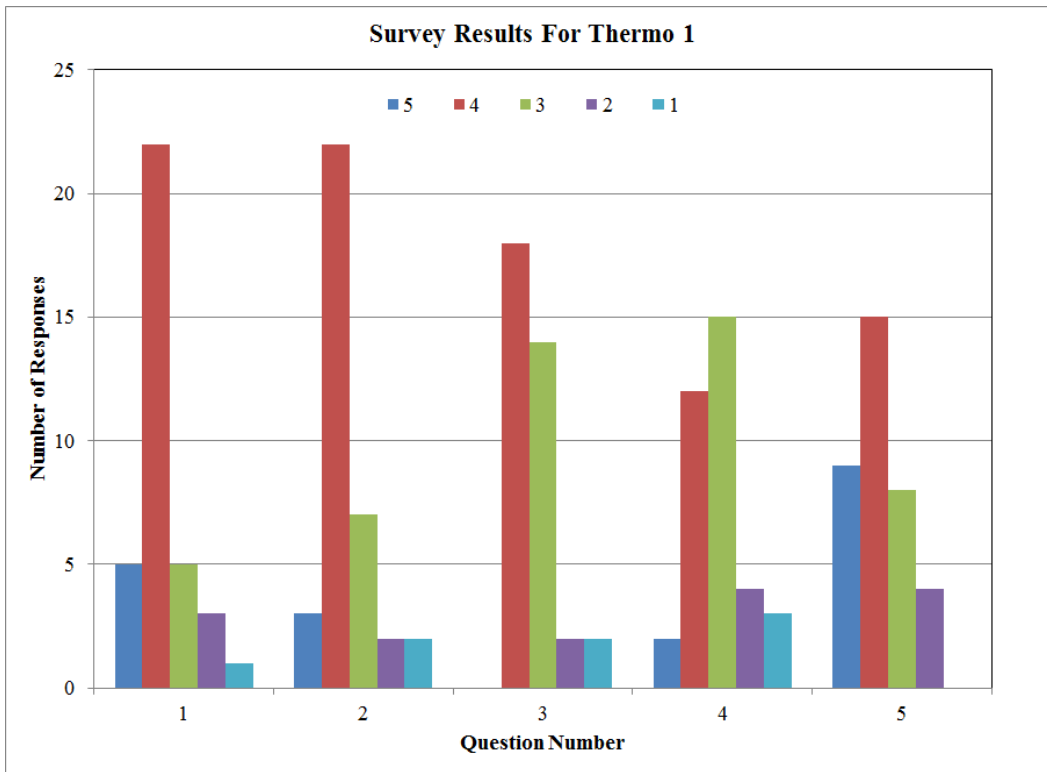
As an anecdote, students in the Thermo 2 course took part in the hands-on lecture during a Wednesday evening lecture session. Homework due the following Friday examined a problem where a stream was partially condensed, given a known amount of energy removed from the system. One group of students came into class that Friday and told the instructor that they had used Chemcad to check their hand calculation! This is exactly the outcome the authors were trying to foster in their students with the inclusion of these simulation activities in their classes.

### **Summary**

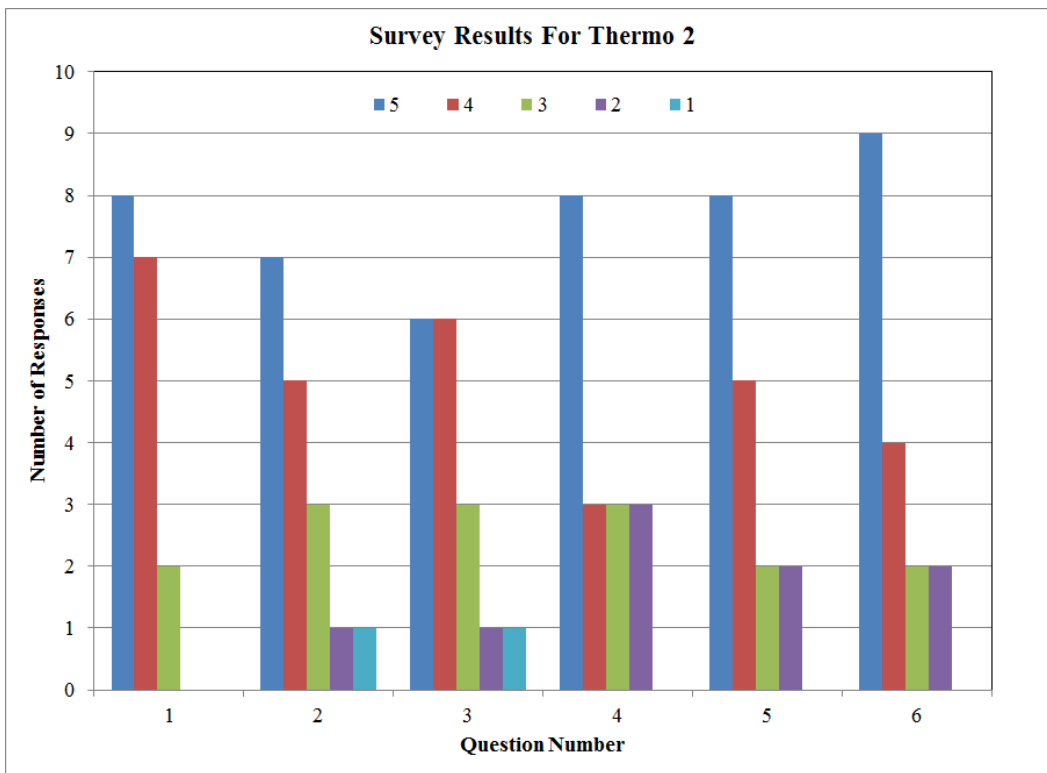
A variety of activities have been presented that can be used to introduce chemical engineering undergraduates to process simulation concurrently with pertinent topics in their core courses. These activities have been designed to aid in the connection of the underlying fundamentals learned in a particular course to how that process may be successfully simulated. By providing step-by-step instructions and explaining the significance of key input parameters as well as providing values for these parameters, students can focus on the output from the simulation to develop their understanding of a process. Key to this effort is making the use of the process simulation program as painless as possible, so that the opportunity to learn and understand is not lost to frustration.

**Table I. Survey Questions**

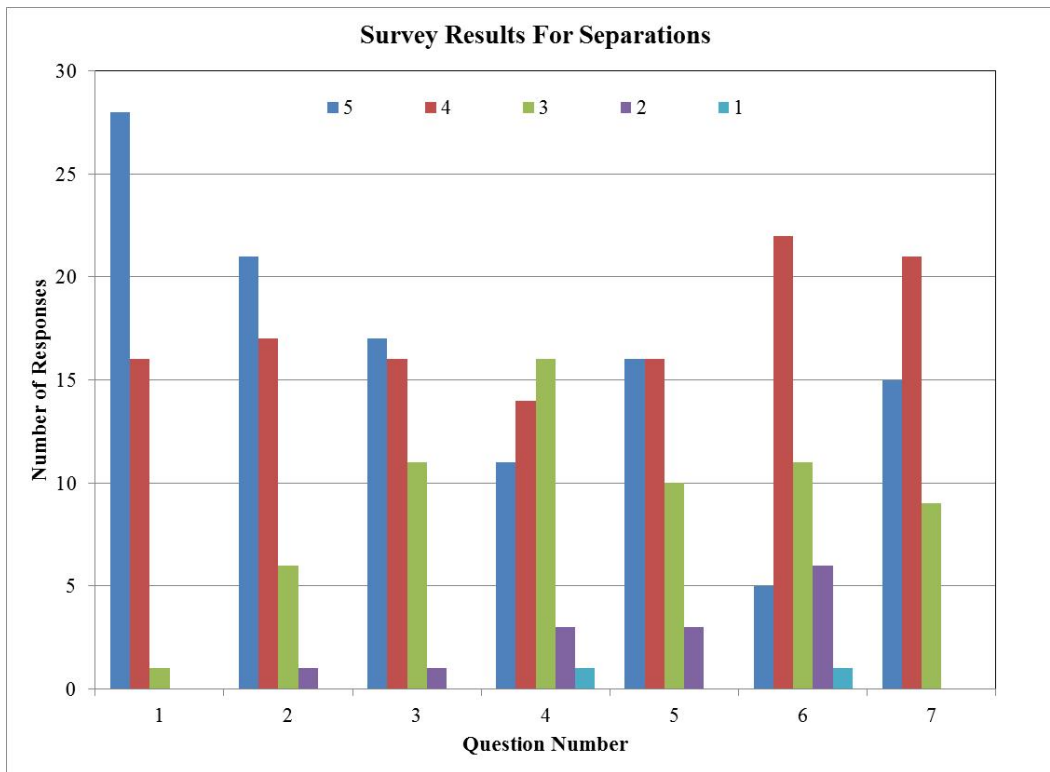
<b>CHE Thermodynamics I Questions</b>	
1. _____	Instruction regarding use of process simulation for simulation of stoichiometric reactor was adequate.
2. _____	I feel confident in my abilities to use the reactor model to simulate a reaction at 25 °C and calculate the standard heat of reaction.
3. _____	I feel confident in my abilities to use the reactor model to simulate a reaction at elevated temperature and calculate the heat of reaction at elevated temperature.
4. _____	I feel confident in my abilities to use the reactor model to evaluate the adiabatic flame temperature for a reaction.
5. _____	I was able to see the connection between the calculation methods learned in class and how they are used in the process simulation program.
<b>CHE Thermodynamics II Questions</b>	
1. _____	Instruction regarding use of process simulation for simulation of heater block was adequate.
2. _____	I feel confident in my abilities to use the heater block to evaluate the heat duty required when an ideal gas is heated from $T_1$ to $T_2$ .
3. _____	I feel confident in my abilities to use the heater block to evaluate the final temperature when an ideal gas at $T_1$ has a known amount of energy added to it.
4. _____	I feel confident in my abilities to use the heater block to evaluate the heating of one stream by cooling of a second stream.
5. _____	I feel confident in my abilities to use the heater block to evaluate the latent heat of vaporization for a pure substance.
6. _____	I was able to see the connection between the calculation methods learned in class and how they are used in the process simulation program.
<b>Separation Processes Questions</b>	
1. _____	Instruction regarding use of process simulation for simulation of shortcut model was adequate.
2. _____	Instruction regarding use of process simulator for simulation of rigorous distillation model was adequate.
3. _____	I feel confident in my abilities to use the shortcut model to model a multi-component separation process.
4. _____	I feel confident in my abilities to use the rigorous distillation model to model a multi-component separation process.
5. _____	I feel confident in my abilities to use the process simulator to generate necessary tower profiles, tray composition profiles and tray properties profiles.
6. _____	I feel confident in my abilities to examine the composition profiles for a column and adjust input parameters for the rigorous model to improve desired separation and fully utilize each tray for separation.
7. _____	I was able to see the connection between the calculation methods learned in class and how they are used in the process simulation program.
8. Yes	No I had previously used the Chemcad program in another class.



**Figure 11. Survey Results for CHE Thermodynamics I Course**



**Figure 12. Survey Results for CHE Thermodynamics II Course**



**Figure 13. Survey Results for Separation Processes Course**

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