An Introduction To Process Simulation For The Capstone Design Course

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Introduction

The use of process simulators during the capstone process design course has become an expected part of most chemical engineering curricula. Unfortunately, the mechanisms to teach students how to use these tools have often been ad hoc or completely lacking. Ideally, students would gain familiarity with process simulation throughout the curriculum so that when starting senior design, they have a good understanding of the benefits, limitations, and general functionality of the process simulator. In practice, most students arrive in their senior design classes without knowing how to use a simulator to help solve open-ended problems. In general, their experience has been with small, well-defined problems. To help alleviate this problem, a short-term design project has been developed to teach the basics of process simulation within the context of analyzing an existing plant and suggesting process improvements. Specific goals of this project include (1) learn how to simulate a wide variety of unit operations, (2) learn benefits and limitations of different thermodynamic models, and (3) understand system-wide effects of changing process variables (as part of the process improvement aspect).

The project, based on the synthesis of maleic anhydride from n-butane, involves several important unit operations that will often be encountered in the capstone project. The students are given a set of equipment specifications and process data from which they are supposed to develop a simulation of the process as it currently exists. Strategies for simulating the process are discussed in detail and the course instructor is available in the student computing laboratory to help with issues as they arise.

The project includes a reactor (PFR) with kinetic models, absorption column, vacuum distillation column with vent, atmospheric distillation, and recycle (of absorber oil). The students can start with the simple distillation column, and proceed to add more complicated pieces of equipment. This incremental approach allows them to quickly achieve some success to build confidence before confronting them with the difficulties of catalytic reactions in a PFR. Some additional complications in the simulation help to stress that the simulation is just a model and that some aspects of the model are best dealt with outside of the simulation program. For example, the maleic anhydride will continually react with residual water throughout the process (i.e., in pipes, columns, condensers, reboilers, etc.) to form maleic acid.

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After completion of the simulation, the students then seek out non-capital process improvement opportunities. They approach this issue by varying process parameters and understanding the system-wide effects of the changes. For most students, this is the first opportunity they have had to see how different unit operations interact within the context of the overall system. Thus, although increasing the absorber oil flowrate may increase the recovery of the product, it has the undesired effects of increasing the utility requirements to separate and recover the products from the absorber oil.

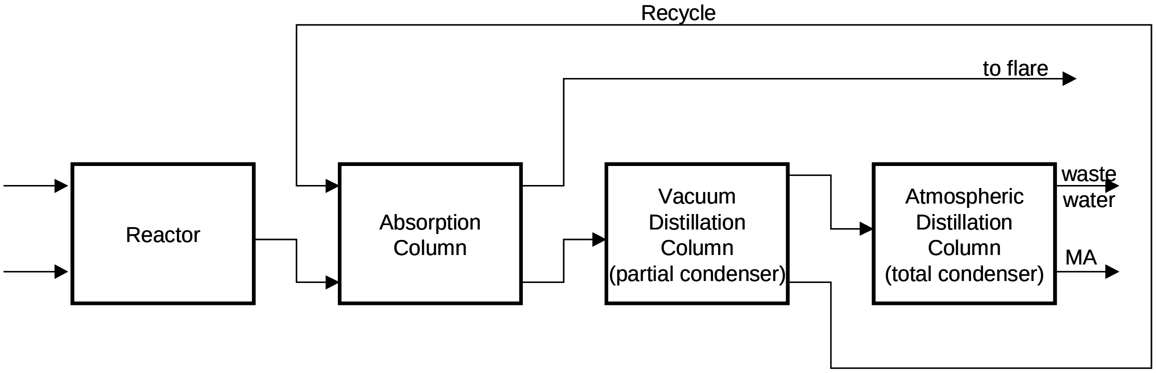
The following sections describe the maleic anhydride introduction to process simulation and process improvement project in detail and our recent experience with it at Michigan Tech.

Design Assignment

The project was initially assigned with a memo asking the students to examine the current operation of the Tapiola Maleic Anhydride Plant to identify potential process improvement opportunities by conducting the project in two phases:

- Phase 1: Simulation and Sensitivity Study
- Phase 2: Process Optimization

The students were told to proceed with Phase 1 by developing a suitable model of current plant operations that could then be used to predict the probable performance of the plant as key operating variables were changed. The students were given a process flowsheet, a stream summary table, a set of simplified reaction rate equations and a set of equipment specifications. This simplification of the kinetics was required because reactor design was a spring semester, senior class under our quarter-based curriculum. A simple block flow diagram is given below to give an overview of the process.



On the day of the initial assignment, we began with an introductory tutorial on getting started with the process simulator. Our students were running Hysys; however, our approach should be equally suitable to any other simulator. In this introduction, we demonstrated how to start building a simulation, emphasizing that the first step needs to be selection of a fluid package, or thermodynamic property package. At the time, we brought up the importance of understanding the limitations of whatever package they picked and reminded them about the importance of interaction parameters. Later on, we realized that although the students had successfully completed the thermodynamics course, they were not prepared to understand how to go about choosing an appropriate thermo package. In the following section, we give a general description of our approach for introducing important thermodynamic concepts as they relate to process simulation.

Following the basics on how to start the simulator and enter components, we start by describing how to develop a distillation column model. The following describes how to develop a model in Hysys. First, we tell the students not to use the "input expert". We have found that this confuses the students and the simulator. Since the simulator is just a tool, we should be able to model any parts of the plant of interest to us, without necessarily simulating the entire plant. Many students have trouble grasping this idea, but it is key to building this simulation. In the MA plant, it is best to start with the third column, a simple atmospheric distillation. This is a relatively easy column to get to work and should give the student confidence to continue to the more challenging operations. We discuss the elements of simulating simple columns, reviewing degrees of freedom and addressing some of the common pitfalls, such as specifying variables that are mutually exclusive or do not adequately define the boundaries. From there, we move on to partial condensers (required for them to simulate the second column, a vacuum distillation column). As part of this initial tutorial session, we also introduce some advanced concepts regarding how to save information about various process runs in the databook. Finally, we remind the students that as with any software, they should save their work often to avoid the frustration of having to repeat their work.

The second major tutorial session centered on the reactor. Because the students had not yet had a reactor course, considerable time was spent describing some basics about reactors. After introducing the major theoretical types of reactors (PFR & CSTR), we discussed the different ways of simulating reactions, using either simple conversion or actual kinetics. Examples of both approaches were demonstrated along with a discussion of the advantages and disadvantages of both approaches. An emphasis was placed on kinetic models for PFR's. As part of this lecture, the use of adjust blocks were introduced. They provide a way of adjusting internal unit parameters (such as reactor volume) so that other outputs attain a specified value. We use this to adjust the apparent volume of the reactor so that a conversion and selectivity that approximately matches the real plant data are obtained.

The final major tutorial discussed simulation with recycle. In general, recycle loops should be connected last, since they add considerable complexity to the simulator's iterative solution strategy. The effect of recycle can be approximated, by having an inlet and outlet stream labeled recycle, but not yet connected. Once the different units are simulating correctly and are close to their desired states, then the recycle can be connected. Trying to connect a recycle too soon could cause a wide variety of streams and parameters to be set to erroneous values that can cause the simulation to be unable to converge.

As the students work on the simulation, there are several issues that they should discover. These are purposely placed in their “real” plant data to help them remember that a simulation is just a model. For example, MA can react with water to form maleic acid. This will be continually occurring during the process, but there is no simple means for simulating those reactions in pipes and columns. Although Hysys theoretically supports reactive distillation models, they are quite limited in their ability, only supporting certain reaction types under a limited set of solvers. Of fifty student groups, only one group was able to successfully simulate the degradation reactions directly in the column. An alternative, adequate solution would be to add conversion reactors after columns to adjust the stream composition to account for reactions that occurred inside the column.

Process Thermodynamics

As described above, we found that we needed to provide additional direction to the students regarding how to choose an appropriate thermodynamics package. It is often advisable to begin a design project, such as the one described in this paper, not by attempting to solve the real problem, but rather by constructing an idealized model which can be rigorously solved, then extrapolating based on assumptions and sensitivity analysis, to an estimation of the real solution. For example, a preliminary simulation of a distillation column using the Raoult’s law (ideal liquid solution) assumption eliminates the composition dependence of the vapor-liquid K-factors, thereby making the simulation easier to converge. Once this idealized simulation is working, its mass and energy flows are then initial estimates for further simulations based on more rigorous liquid-phase thermodynamics.

An overview of basic mathematical techniques for property data correlation is presented to students in MTU’s capstone design course, together with a road map for their use. (Two excellent references on thermodynamics and property estimation within process simulators is found in the online documentation for HYSYS® and in the ChemCAD® printed manual. For property estimation methods, see also Lyman et al., 1982; DIPPR® Data Prediction Manual, 1986; Reid et al., 1987.) Methods are presented in the course for the correlation of observed experimental data to physical properties such as critical properties, normal boiling point, molar volume, vapor pressure, heats of vaporization and fusion, heat capacity, surface tension, viscosity, thermal conductivity, acentric factor, flammability limits, enthalpy of formation, Gibbs energy, entropy, activity coefficients, Henry’s constant, octanol-water partition coefficients, diffusion coefficients, virial coefficients, chemical reactivity, and toxicological parameters. Correlation methods discussed include basic mathematical and numerical techniques, and approaches based on reference substances, empirical equations, nomographs, group contributions, linear solvation energy relationships, molecular connectivity indexes, and graph theory. Chemical data correlation foundations in classical, molecular, and statistical thermodynamics are also introduced in the course.

For chemical engineering students, a key concept to learn in a design course is how simulators perform phase equilibrium calculations, both vapor-liquid and liquid-liquid. Two choices are possible for vapor-liquid equilibrium: Type I K-factors calculated from the ratio of the liquid and vapor fugacity coefficients, (Φ_i^l/Φ_i^v); and (2) Type II K-factors calculated from $(\gamma_i \cdot P_i^o/(\Phi_i^v \cdot P_T))$, using a liquid-phase activity coefficient model. When a physical property package in the simulator contains only an equation of state (EOS), it is used by the simulator to calculate vapor-phase and liquid-phase fugacity coefficients (for Type I K-factors) as well as enthalpy and entropy residual (departure) functions that account for deviations from ideal gas behavior. Property packages containing an EOS and a liquid-phase activity coefficient for Type II K-factors are included in recognition that an EOS often cannot represent vapor and liquid phases simultaneously; therefore, the activity coefficient model represents liquid-phase PVT behavior where the EOS representation is characteristically poor. Although new mixing rules are being added to simulator property packages to enhance EOS capabilities in the liquid region, Type II K-factors are generally more accurate and require fewer empirical parameters.

To calculate vapor-liquid and liquid-liquid equilibria for most chemical systems, it is necessary to construct activity coefficient models which, by necessity, are only approximations containing parameters that must be obtained empirically. All of the popular activity coefficient models are based on excess molar Gibbs free energy change of mixing, g^E, functions of various forms including the Non-Random Two-Liquid (NRTL) equation, the modified three-parameter Wilson equation (Wilson and Deal, 1962), the two-parameter UNIQUAC equation (Abrams and Prausnitz, 1975). The UNIQUAC Functional-group Activity Coefficient (UNIFAC) equation is a group contribution extension of the UNIQUAC equation can be used in situations where system-specific, binary chemical interaction parameters are not available for UNIQUAC or NRTL. UNIFAC has a prominent position in the chemical engineering literature (Abrams, 1975; Fredenslund et al., 1975; Skjold-Jorgensen et al., 1979; Kikic, 1980; Gmehling et al., 1982; Macedo et al., 1983; Tiegs and Gmehling, 1987; Hansen et al., 1991) and is widely used in process simulation. It has several clear advantages over most other semiempirical methods: (1) it has an explicit temperature dependence; (2) it has a large library of functional groups from which thousands of chemicals can be built; and (3) it can be updated and expanded as more experimental data become available. We review these methods as they apply to process simulation and discuss benefits and limitations in detail.

Process Diagnostics

In Phase 2 of this project, the students are asked to perform a process optimization. We have found that the evaluation and optimization of an existing process is an area that is not well covered in current undergraduate design texts. In addition, the ability to identify key opportunities for optimization often requires experience that students do not possess. To overcome these difficulties, we have developed a formalized series of evaluation tables, called process diagnostic summaries (PDS) that we require students to prepare and apply to all process optimizations. A simple Pareto analysis can then be used to guide their optimization efforts. The minimum PDS that they must prepare are:

- Mass/molar Input/output
- Energy Input Output
- Manufacturing Profit and Loss

- Utility Annual Expenses
- Utility Incremental Costs
- Theoretical Maximum Revenue

There are two other PDS that can sometimes yield significant insight on processes that are primarily involved with separation sequences:

- Contribution of Feeds to Profit and Loss
- Contribution of Equipment to Profit and Loss

The mass or molar input/output table shows the component flows of all feed and product streams. The format is designed to provide a summary of the material flows, product distribution, yields, etc. In addition to illustrating opportunities for process improvement related to material flow, this PDS feed information to several other PDS.

The energy input/output PDS summarizes inflows and outflows of energy to the process. A datum or reference temperature must be selected to permit calculation of stream enthalpy flows. This PDS shows major sources and sinks and helps to identify and rank conservation, integration or recovery opportunities. It also feeds data to several other PDS.

The manufacturing profit and loss PDS translates process information into the common denominator of annual economics. There are several practical and pedagogical advantages to using profit and loss for the economic tool at this stage. For one thing students at all levels including freshman can readily grasp the concept even if they have not yet encountered capital cost estimation or cash flow techniques. Since we are working with an existing process, the capital costs are sunk costs so the use of profit and loss will yield rigorous answers that will remain consistent with cash flow evaluations that may be applied later. Also the techniques will be consistent with material the students may have encountered in business classes or elsewhere. Finally we note that the profit and loss PDS can be readily applied to a cost center or portion of a larger plant if we introduce the concept of transfer pricing. This also sets the stage for the later introduction of incremental analysis.

We use the term “manufacturing” to distinguish the profit and loss PDS from the more comprehensive profit and loss statement that would include depreciation, taxes and sales and distribution expenses. Here again the process optimization is no less rigorous without these items since they will cancel out in any incremental analysis. We do however require the students to estimate and include labor in the analysis whether or not labor expense is likely to be affected by the optimization. We feel that it is important for them to consider this component whether or not it is part of the scope of work.

The review of the manufacturing profit and loss PDS will generally determine where optimization efforts should be concentrated. A Pareto analysis will identify which costs are most important but we also require the students to temper this analysis with some judgment about which items are under their control. For example, if the raw material rate and price are fixed, then the fact that raw materials are a major component of manufacturing expenses may not be significant to our optimization efforts.

Utilities are almost always under the control of the process engineer in an evaluation. Thus we anticipate that utility costs will be part of an optimization effort unless the profit and loss analysis shows that they are trivial. The utility annual expense PDS is thus designed to provide much more detail on this component of the profit and loss statement. It summarizes, for each utility, both consumption rate and annual expense associated with each piece of equipment. A Pareto analysis of this PDS often allows us to identify and rank those items of equipment that are worthy of optimization effort. Both here and in the profit and loss PDS the student is forced to recognize that material and energy flows are generally reported on a stream hour basis and economics on a calendar year basis.

The utility incremental cost PDS translates the unit costs for all utility options into an equivalent unit cost on a common basis such as $/MM Btu. In addition we add a column for efficiency and then generate a unit cost as actually delivered to the process. This tool can be very useful in helping to identify utility swap incentives. In some cases it has directly identified less than optimal equipment selections such as direct fired heaters or air cooled condensers.

The PDS titled Maximum Theoretical Revenue addresses the issue of how much potential revenue is being lost to waste or byproduct, etc. The calculation is performed by assuming that all of the raw materials can be converted to the highest valued products at 100 percent yield and can be perfectly separated so as to just meet minimum specifications. This PDS identifies how much revenue is "left on the table" and helps to spot separation and yield opportunities.

The two optional PDS, Contribution of Feeds and Contribution of Equipment to Profit and Loss, attempt to allocate the Profit and Loss results to each feed in the first case or to each piece of equipment in the latter case. In the case of multiple, discretionary feed streams, we have found it useful to use composition information to track revenues and costs associated with the processing of each stream. In some cases this has identified significant optimization opportunities with something as simple as shutting off a particular feed. In the case of processes that consist primarily of separation sequences, we have found it similarly desirable to allocate the Profit and Loss results to the incremental contribution of each piece of equipment. In a recent refinery case study, for example, this PDS allowed the students to address the issue of whether the C3 recovery column should continue to be operated to reclaim propane stocks from fuel gas stocks or whether an i-C4/n-C4 separation was incrementally justified. Such incremental analyses are common in the conceptual design stage but tend to be overlooked in the optimization of an existing plant where the capital cost for the equipment is a "sunk cost". The results can be very enlightening in plants that have evolved over extended periods.

In the optimization of the MA plant we encountered substantial computer network difficulties associated with recent changes to our system. In an effort to relieve some of the load on the computer system, we reduced the scope of the optimization effort by providing sensitivity studies on a selected list of variables that, we informed the students, had been generated by plant personnel in previous optimization attempts. In effect we were prejudging the diagnostic results by providing the following sensitivity studies:

- Reactor discharge temperature
- Feed rate of air
- Absorber oil flow rate
- Reflux ratio for the C-103 column

Because of time constraints, we further limited the scope of the PDS assignment as follows:

- Conduct input/output mass and energy analyses of current operations.
- Use these analyses to help identify key performance or cost components in the process and to recommend variables that should be analyzed in sensitivity studies.
- Use the existing sensitivity studies to perform a preliminary analysis of how we might improve performance of the plant.

We intend to repeat this assignment next year with expanded time allocation and scope of work.

Conclusions

In conclusion, we have described a short-term design project has been developed to teach the basics of process simulation within the context of analyzing an existing plant and suggesting process improvements. Specific goals of this project include (1) learn how to simulate a wide variety of unit operations, (2) learn benefits and limitations of different thermodynamic models, and (3) understand system-wide effects of changing process variables (as part of the process improvement aspect). We found that the students responded favorably to the more formalized introduction to process simulation. As with any new topic some students approached the project with great vigor while others tried to get by with minimal effort. We also found that the use of Process Diagnostic Summaries significantly enhanced the ability of the students to identify and rank process improvement opportunities. Their lack of experience continues to be an impediment to capitalizing on all of the opportunities but the PDS approach provides a basis for teaching new material.

We intend to use this approach again next year with the following changes. First, we will spend more time formally describing how and when to use the various thermodynamic packages available in the simulator package. Second, we will provide more economic information so that the students can better make use of the process diagnostics to gage the desirability of different process improvement possibilities.

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