



Are Your Students Getting the Most out of the Process Simulator?

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Introduction

Process simulators allow students to perform in-depth analyses of chemical process designs, including economic optimization, due to the ability to run multiple case studies rapidly. The ability to simulate alternative process configurations and to vary design parameters rapidly allows them to make decisions and move towards an optimum process based on an objective function, often a profitability criterion. However, students often use simulators carelessly and treat the results superficially, *i.e.*, they treat the simulator like a game rather than a tool to help them solve a complicated problem.

The importance of validating software¹ and being certain that plant data match simulation results have been discussed.^{2,3} That students can use simulators carelessly should come as no surprise to most instructors. It has been observed how students can use simulators to construct models without a full understanding of the process.⁴ It is also apparent that students often resort to simulators when they are not needed, and the results are often not evaluated critically.⁵ Moreover, students often do not understand the underlying physical phenomena in a simulation⁶ and how simulation results can differ from reality.⁷

In this paper, specific, observed examples of careless use of simulators will be presented. One of the key points of emphasis is the difference between a simulated unit and the reality of actual pieces of equipment. For example, a simulation block or unit does not always correspond to a single piece of equipment. Other examples involve students not looking at the available information to guide their design. There are also cases in which the simulator defaults should not be used. An example might be simulating the reboiler and condenser separately from a distillation column. Additional examples include certain types of performance problems, such as scale-up, debottlenecking, and troubleshooting, which might be more appropriately solved outside the simulation environment. These are discussed elsewhere.⁸

Fluid Mechanics

In all simulators, if streams of different pressures are mixed, the lower pressure is taken as the mixing-point outlet pressure, which is physically incorrect. If a process was designed to specifications such that two streams with different pressures were mixed, in actual operation, the mixing-point inlet pressures would be the same, and the flowrates would change accordingly. This phenomenon is correctly modeled in a pressure-driven dynamic simulation but not in steady-state simulators. Therefore, the process would not operate as designed. Since valves would be needed for the pressures to be equal at a mixing point, they should be included in the simulation. Students should recognize that simulations should represent reality. Perhaps an underlying issue is that students do not really understand the pressure-reducing/control role of valves in a chemical process. This can be taught in fluid mechanics class, control class, or design class. It has been found useful to emphasize multiple times to students that valves are about the only thing that can be adjusted in a chemical process, and that adjustments in temperature, pressure, and composition, for example, all occur by turning a valve.

Heat Exchangers

Zoned Analysis Required. In many organic chemical processes, a subcooled liquid stream must be vaporized and superheated for a vapor-phase, catalytic reaction. A typical heat source is steam condensing at constant temperature from saturated vapor to saturated liquid. An approximate T - Q diagram is shown in Figure 1. The solid lines represent the actual situation. The dashed line represents the situation often observed in student simulations. With the dashed line, the different zones are not considered, and when sizing the heat exchanger, the different heat transfer coefficients in each zone are not considered. A typical simulation menu only requires one heat transfer coefficient be entered. The correct method for simulating this type of heat exchanger is to simulate a separate heat exchanger for each zone with a different heat transfer coefficient for each zone. A similar situation may occur when condensing a reactor effluent prior to separation. It has been observed over many years that students may know about a zoned analysis when it is taught in heat transfer, but while using a simulator, they tend to overlook the correct analysis.

Heat Integration. If an economic objective function is involved in optimization, or if heat integration is emphasized in design class, students will often try to heat cold streams with hot streams. If these involve phase changes, a careless analysis can lead to an infeasible result. Consider the T - Q diagram in Figure 2. The solid lines represent vaporizing a stream, like the feed stream discussed previously, using a hot stream as the heat source. If the zones are ignored, the situation shown by the dashed lines can occur, which involves a temperature cross. All simulators generate these “heat curves.” So, students should be strongly encouraged to look at the heat curves to ensure the feasibility of their design.

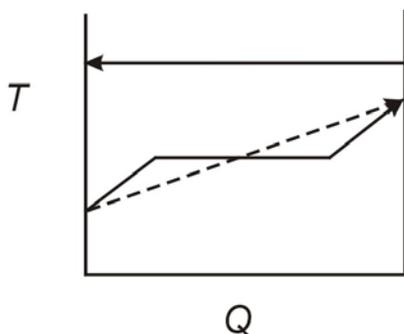


Figure 1: T - Q diagram for zoned analysis

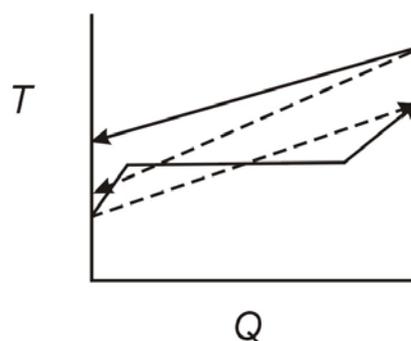


Figure 2: T - Q diagram with possible temperature cross

LMTD Correction Factor. For heat exchangers without phase change, as illustrated in Figure 3, it is possible for there to be a close approach temperature. This can occur when matching streams based on a minimum utility, minimum number of exchangers (MUMNE) heat integration analysis⁹, because the minimum utility requirement occurs when matching streams with close approach temperatures. If it is assumed that the base heat exchanger configuration is a 1-2 exchanger, the close approach temperature makes the Log Mean Temperature Difference (LMTD) correction factor very small, possibly undefined. More shell (and tube) passes are

needed to raise the LMTD correction factor. Once again, this is a situation that students often forget when doing simulations.

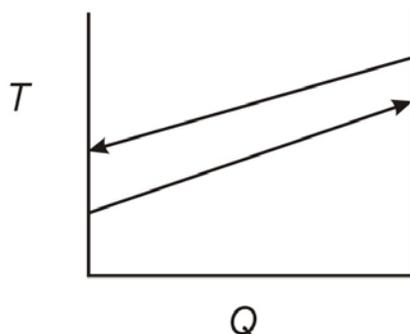
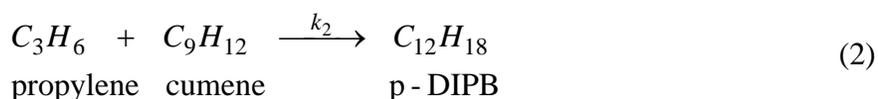
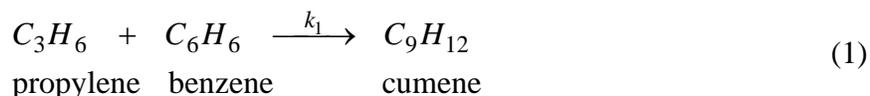


Figure 3: T - Q diagram with close approach requiring multiple shell passes

Reactors

As with heat exchangers, plug flow reactor profiles can be obtained from the simulation. This includes component mole flowrates, mole fractions, and temperatures. The temperature profile is useful for checking the magnitude of a hot spot or for determining whether a runaway reaction is imminent. However, it is often observed that students stop when they get a reactor that works. This can result in an oversized reactor or a reactor that is large enough for the desired product to continue to react to an undesired product, reducing selectivity. Figure 4 shows an example of an oversized reactor for the production of cumene from benzene and propylene. More details about this project can be found on the Web.¹⁰ The reactions are shown here for clarity.



Equation 1 is the desired reaction, and Equation 2 is an undesired reaction. As illustrated in Figure 4, the propylene is all reacted in the first 1.2 m of the reactor. The maximum selectivity for cumene relative to p-diisopropyl benzene occurs at the reactor entrance; however, a practical/economic optimum is probably in the region of 0.6-0.8 m from the reactor inlet, based on the ratio of the cumene and p-diisopropyl benzene curves. This is another example where students should be encouraged to take advantage of the information in the simulator beyond the stream and equipment information.

Distillation Columns

Real vs. Actual Trays. A typical simulation interface for a distillation column requires entering the number of equilibrium stages. However, typical tray efficiencies are on the order of 50% for distillation and lower for absorption/stripping. Students often forget to include the tray

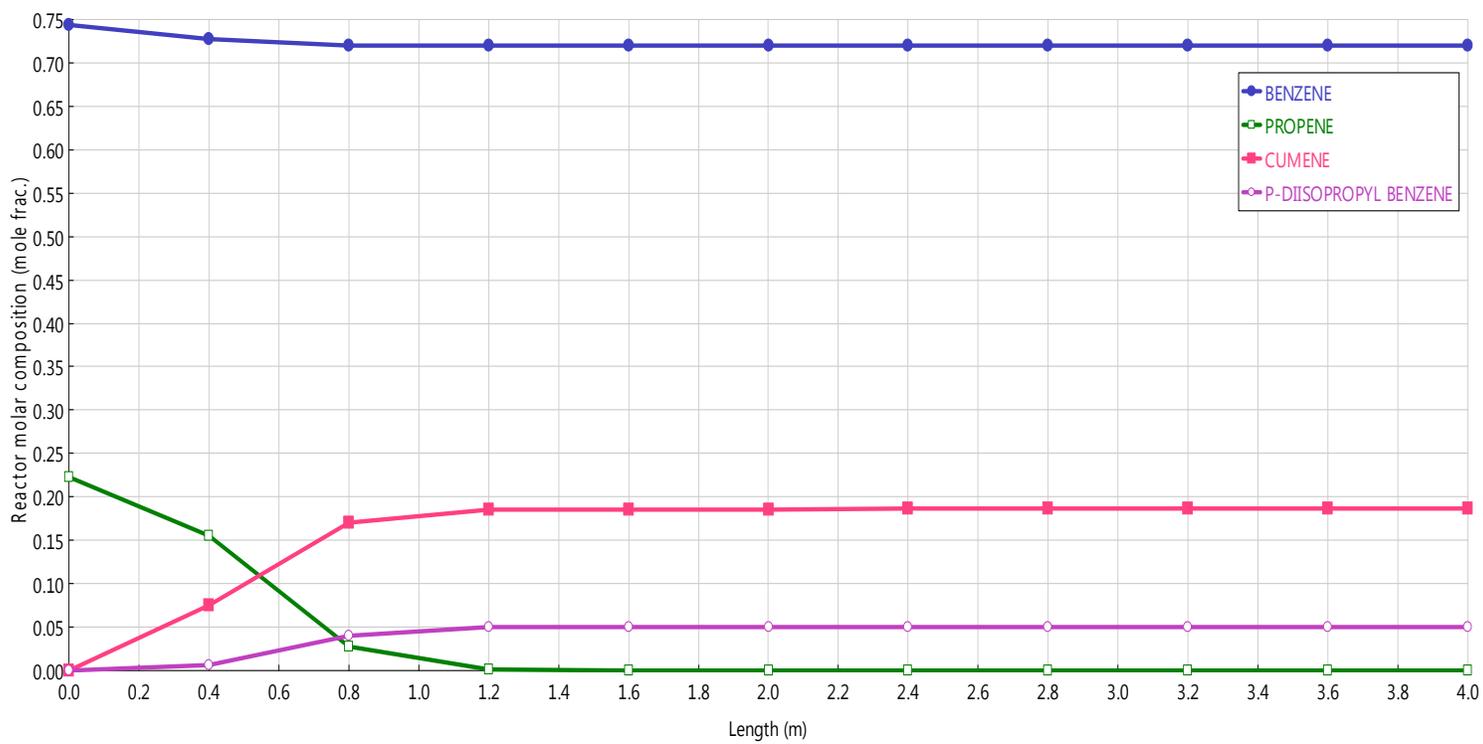


Figure 4: Reactor Profiles Illustrating an Oversized Reactor

efficiency. It can be added when sizing the column, *i.e.*, adding trays when determining the column cost; however, the issue with column pressure drop discussed later is not addressed by using this method. Once a base simulation is completed, students should be encouraged to calculate or to estimate tray efficiencies and then simulate the process again with the actual number of trays and the efficiency included in the simulation or at least to account for the additional pressure drop per tray that is caused by having more actual trays than theoretical ones.

Column Pressure Drop. If a distillation column is to be simulated realistically, it must include a pressure drop. However, the pressure drop cannot be estimated until the number of trays is known. Here, it is assumed that the pressure drop per tray can be estimated based on the head of liquid on each tray, which is approximated by the weir height. A reasonable compromise for students is to calculate the weir height that corresponds to the pressure drop in the simulation. If the weir height is larger than one-half of the tray spacing, which is a typical limit, a lower pressure drop is needed in the simulation. If the weir height is less than 2 inches, the pressure drop in the simulation is probably too small. This is a good example of requiring student simulations to correspond to equipment realities. This situation becomes even more important when considering vacuum columns, where the gas phase densities are low and column pressure drop may cause the absolute pressure in the column to change by a large factor. The use of theoretical vs. actual trays in determining the column pressure drop will have a large effect on the required diameter needed to avoid flooding for these vacuum systems.

Flash Separations

All simulators have a unit called “flash.” This unit performs the thermodynamic calculations of partial vaporization or partial condensation. It is possible to specify this unit at a different temperature and pressure from the feed. However, there is no single piece of equipment that accomplishes the “flash” process. Either a heat exchanger or a valve is required to bring the feed stream into the two-phase region, and then a drum is needed to allow the vapor and liquid to disengage. The “flash” unit, which is actually a knockout drum, can then be simulated such that the outlet streams are at the same temperature and pressure as the feed stream. When evaluating the economics, both the heat exchanger and the drum costs are needed plus the utility cost in the heat exchanger. This is a situation where the simulator performs a calculation that does not correspond to actual equipment. Once again, students should be encouraged to have their simulations correspond to actual equipment.

Discussion

What can be done to alleviate this problem? Experience provides some suggestions. It is probably unrealistic to expect students to understand equipment details before the design class unless that is a point of emphasis in lower level classes. In many programs, the introductory transport classes focus more on theory than on equipment. Even in a separation class, the stage calculations often dominate the coverage of tray sizing and performance. One approach would be to integrate equipment details throughout the curriculum; however, this might be unrealistic in large programs with different instructors for the same course in different semesters. So, if students do not know the equipment details, the correspondence between simulation and reality should be taught along with teaching the simulator, with an emphasis on making the simulator

mimic actual equipment. Similarly, the information available within the simulation results should be demonstrated to students, and they should be expected to use that information during the design. If students have weekly meetings with the instructor or teaching assistant while completing the design, all of the items discussed in this paper could be emphasized during those meetings. Ultimately, there is no single solution; the best solution for a given instructor will be dependent on curriculum and department specifics.

Conclusion

Students should learn to use process simulators, and process simulators give students the ability to investigate chemical process designs in detail and to optimize these processes. However, experience suggests that students often use process simulators superficially and incorrectly, with simulations that do not correspond to actual equipment. The most logical location for students to learn to make simulations correspond to actual equipment is while learning the simulator. Students do not always make use of the information available within the simulation results. One good way to force them to use that information is to ask them questions during the design process that require them to find that information in the simulation results.

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