ChE classroom

# ACETONE PRODUCTION FROM ISOPROPYL ALCOHOL

An Example Debottlenecking Problem and Outcomes Assessment Tool

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hemical engineering educators are searching for outcomes assessment measures to incorporate as assessment-plan components in order to satisfy the requirements of ABET EC 2000. Student and alumni questionnaires are always a staple, but an assessment plan should not rely too heavily on these self-assessment instruments. Faculty evaluation instruments are also necessary.

All chemical engineering programs have capstone experiences such as the unit operations lab and chemical process design. In these courses, students are expected to apply knowledge learned earlier in the curriculum to solve complex problems. The capstone design experience presents an excellent opportunity for outcomes assessment since it requires that material from several classes be synthesized and applied. It can provide detailed information on what seniors have learned in their earlier classes. In this case, student assessment of the capstone design experience is being used as a program-assessment measure. In particular, the technical content of the capstone design experience can provide

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data on EC 2000, Criterion 3, outcomes a, c, and e (ability to apply knowledge of mathematics, science and engineering; ability to design a system, etc.; ability to identify, formulate, and solve engineering problems).<sup>[1]</sup>

One key to using the capstone design experience for outcomes assessment is the measurement method. For over twenty-five years, seniors in chemical engineering at West Virginia University have been required to do a series of projects in the two-semester senior design course, to submit a written report, and to defend their results to an audience of at least two faculty. A typical defense lasts one hour, with a fifteen- to twenty-minute presentation followed by a question-and-answer session. Students do these projects and defend them individually, which is a unique feature of our curriculum. The question-and-answer period is tantamount to an individual tutorial. Students get immediate feedback on their work and faculty can determine in great detail the level of each student's understanding of and ability to apply fundamental principles. Historically, students were not permitted to ask questions of anyone while doing this assignment, but in recent years, they have been permitted to buy consulting from faculty for a minor grade deduction. This system ensures that students ask only well-formulated questions and that they do not try to "nickel and dime" a solution from faculty.

Oral examinations like this have advantages and disadvantages as an outcomes assessment measure.<sup>[2]</sup> The advantages include an ability to measure student learning in great detail through follow-up questions. Faculty can learn how and why students obtain their results and develop an understanding of students' thought patterns. This makes it easier to determine if a reasonable result was obtained by accident from a series of unreasonable procedures. Additionally, the immediate student feedback is an excellent learning experience. Oral and written communication skills are also developed. The major disadvantages to this method are the faculty time required and the potential for student intimidation.

In this paper, the production of acetone from isopropyl alcohol (IPA) is used as an example. The assignments are described, followed by a brief summary of the issues involved in the problem's solution. Then, a typical series of questions asked of students and how learning is assessed through the responses to these questions is discussed.

# THE PROBLEM

Figure 1 is a process flow diagram for the production of 15,000 tonne/y acetone from IPA. Most of the world's supply of acetone is produced as a by-product of reacting cumene to phenol via the cumene hydroperoxide process. Acetone used for pharmaceutical applications, however, is sometimes produced from IPA due to the requirement of zero aromatic impurities. The problem assigned is one of debottlenecking. As will be discussed later, the ability to use this process for assessment purposes is independent of whether a traditional process design, debottlenecking, or troubleshooting is involved in the assignment.

The assignment scenario is that a company has designed this process to produce 15,000 tonne/y of acetone and equipment has already been ordered. The process was designed assuming an 8,000-hour year, but it has now been learned that the process is to produce the desired yearly amount of acetone in 6,000 hours, allowing the equipment to be used to produce another product for the remainder of the year. Therefore, a method to scale the process up by 33% must be found at minimum equipment cost, particularly for special-ordered equipment that cannot be returned to the vendor for replacement.

This problem was assigned in two parts. The first part was to analyze the process up to T-401, the acetone scrubber, and the second assignment was to implement heat integration between the reactor effluent and the reactor feed (more details later) and to analyze the second distillation column, T-403. Students were given equipment specifications, some design calculations, and stream and utility flow tables. Much of this information is available elsewhere,<sup>[3,4]</sup> and interested faculty can contact either of the authors for additional information. It should be noted that prior to these assignments, our students receive significant instruction on analysis of performance problems, *i.e.*, problems in which the equipment and input is specified and where the outlet conditions must be determined.<sup>[5]</sup>

#### THE DEBOTTLENECKING PROBLEM

A brief summary of the debottlenecking problem is presented here. This information in incomplete and descriptive in nature. It is presented to provide background for the discussion on assessment.

**System Pressure Drop** The details of the problem statement make it clear that the ideal scale-up situation is for the input to the separation vessel, V-402, to be at the same temperature and composition as in the original design, just at a higher flowrate. This fixes the pressure entering the vessel. It is stated that pressure drop in the pipes is negligible;



Figure 1. Process flow diagram for acetone production from isopropyl alcohol. Stream numbers refer to Stream Table in Reference 3.

therefore, at the increased flowrate (assuming incompressible flow) the pressure drop through certain pieces of equipment increases by a factor of 1.33<sup>2</sup>. For gas flows, the effect of pressure on density and its effect on the pressure drop can also be included, but a trial-and-error solution is required. At the specified scale-up, the pressure drop in the fluidized bed reactor is constant. The result is that the front end of the process is pressurized relative to the original design. Each piece of equipment has a maximum allowable working pressure that must be checked at the scaled-up design.

Feed Pump A pump curve and a curve showing the net positive suction head required by the pump (NPSH<sub>R</sub>) curve are provided for P-401 A/B. The system curve must be plotted with the pump curve to determine if the maximum allowable flowrate has been exceeded. If so, remedies such as running both pumps in parallel (and ordering another spare) or attempting to exchange these pumps for ones generating more head are possible. If the former solution is chosen, it must be determined if there is sufficient NPSH available for the new suction-side flow.

Heat Exchanger E-401 The effluent from this heat exchanger is saturated vapor. The steam temperature, and hence the steam pressure, must be increased to accommodate the increased flow. Since the outlet pressure increases, the outlet temperature also increases.

**Reactor** The reaction is endothermic. In the reactor, energy is supplied by molten salt heated in the fired heater. The fired heater only has 10% additional capacity. The simple solution is to purchase an additional fired heater. A more elegant solution is to use the reactor effluent at 350°C to preheat the reactor feed, which can lower the heat duty on the fired heater, even at scaled-up conditions. The fluidized bed has about 50% inert filler, so the fraction of active catalyst can be increased to handle the increased throughput. But the amount of additional active catalyst required is much less than 33% since the space velocity decreases at the increased reactor pressure.

Molten Salt Loop The performance of the molten salt loop must be analyzed correctly to determine the molten salt temperatures entering and leaving the reactor at scaled-up conditions. Both the energy balance and the design equation for the reactor heat exchanger must be solved simultaneously. The two temperatures plus the flowrate of molten salt are unknown. One may be set to solve for the other two. In practice, the flowrate would be controlled and the temperatures would respond to changes in flowrate.

Heat Exchangers E-402, E-403, and E-408 At the new inlet conditions, the outlet conditions must be determined for these three heat exchangers. There is a restriction that cooling water and refrigerated water flowrates can only be increased by 20% due to velocity considerations.

*Tower*, *T*-401 The original specification is 1-in ceramic Raschig rings. The tower will flood at 33% increased throughput of both gas and liquid. One solution is to change the packing to 1.5-in ceramic Raschig rings, 1-in Berl Saddles, or 1-in Intalox Saddles. All of these have lower packing factors, and the saddles have similar interfacial areas per unit packing. which would presumably lead to similar mass transfer rates.

Tower T-403 and Peripheral Equipment The tower will flood at 33% scale-up. There are three possible solutions. Because this tower has a small diameter, the trays have been designed as a module to drop into the vessel's shell, so the number of trays can be easily increased if the tray spacing is decreased. This permits the reflux ratio to be decreased and avoids flooding, which is an example of the trade-off between the number of stages and the reflux ratio. But the effect of decreased tray spacing on tray efficiency should be considered. The pressure of the column can be increased if a pump is added after T-402. Increasing the pressure increases the vapor densities, decreasing the vapor velocity and avoiding flooding. Some combination of increased pressure and decreased reflux ratio provides a satisfactory solution.

Perhaps the best solution is just to decrease the reflux ratio. The distillate is a near azeotropic mixture of IPA and water. The original design, as illustrated in a McCabe-Thiele diagram given to students, has more travs than necessary in an attempt to get closer than necessary to the azeotrope. Decreasing the reflux ratio to avoid flooding only reduces the top IPA mole fraction from 0.65 to 0.64! Once the reflux ratio is determined, the reboiler and condenser performance must be analyzed to determine the new outlet conditions. Also, the reflux pump must be analyzed. For cases involving an increase in overhead liquid flow, there may be insufficient NPSH for pump P-405 A/B, but the original design uses very small diameter (0.5 in) suction and discharge lines. Increasing the diameter of these lines to 0.75 or 1 inch easily lowers the friction since the pressure drop is inversely proportional to d<sup>5</sup>.

It should be noted that all aspects of basic chemical engineering are included in this project. This is desirable when a process such as this is used for program assessment.

## ASSESSMENT

Three scenarios of faculty-student interaction during questioning are presented as examples of how projects such as this one can be used for outcomes assessment. All of these scenarios are paraphrased actual responses from several students. The reader should observe how the student receives immediate feedback on results presented.

The first example is the absorber, T-301. The student has presented the solution of increasing the water rate by 33% to handle the same increased rate of gas to be scrubbed. The student also suggests changing the packing from 1-in ceramic Raschig rings to 1.5-in ceramic Raschig rings because the decrease in packing factor allows the column to remain below flooding. Consider the following exchange between student and professor.

- Professor Why did you increase the water flowrate by 33%?
- Student To maintain the same liquid-to-gas ratio so I could get the same separation.

Professor Why did you go to 1.5-in Raschig rings?

- Student Because the packing factor is smaller. This lowers the y-position (ordinate) on the flooding graph enough so the column will not flood at the increased gas flowrate.
- Professor What about the interfacial area of the new packing?
- Student I really did not think about that.
- Professor Well, let's think about it now. What happens to the interfacial area?
- Student (stumbles around for an answer)
- Professor What has a smaller surface area per unit volume a bed packed with sand or a bed packed with marbles?
- Student Marbles. So, I guess the surface area decreases with larger Raschig rings.
- Professor *Will this have any effect on the absorber?* Student *Yes, it will have an effect.*
- Professor *OK*. *Will it help or hurt the separation?*
- Student It will probably decrease the separation.
- Professor Correct. So, what would you now have to do to maintain the desired separation?
- Student Well, I would increase the water rate more.
- Professor Would this cause the column to flood?
- Student I'm not sure since I did not do this calculation.
- Professor Well, what is the trend?
- Student Increasing the liquid rate would increase the xposition (abscissa) on the flooding graph, which moves the column toward flooding.
- Professor OK. Let's assume that flooding again becomes a problem. What else could you do to maintain the desired separation without increasing the water rate?
- Student (stumbles around for an answer)
- Professor Let me ask the question differently. What else can you change to make the separation easier? What will increase the affinity of the acetone for the water?
- Student *Oh. The pressure and temperature could be changed.*
- Professor In what direction?
  - Student Let's see. Lower temperature and higher pressure favor the liquid phase.

Clearly, this student understands most everything one would expect a student to understand about absorbers, but the presentation of the student's solution alone does not reveal this fact. It only becomes clear as a result of the question-andanswer session. When this problem was assigned, increasing the size of the Raschig rings was the most common solution. Very few students proposed using larger Berl or Intalox *Summer 1999*  saddles, which have similar interfacial areas to small Raschig rings. Upon questioning, the better students immediately understood the problem and responded as illustrated above. When students have trouble answering a question, as in the case above on packing area and other ways to maintain the desired separation, the question is always rephrased in such a way as to provide a hint for the student.

This type of faculty-student dialog can reveal situations in which a student arrives at a good solution without fully understanding the reasons why it is a good solution. The following is an example from a solution to scale up T-403.

Student (proposes lowering the reflux ratio in T-403)

- Professor How did you arrive at the solution of only lowering the reflux ratio?
- Student I did the simulation on Chemcad and found that I could lower the reflux ratio without really affecting the distillate or bottom mole fractions.
- Professor Based on what you learned in separations, does this make sense?
- Student I didn't think about it. I assumed the simulation results were correct.
- Professor They may well be correct, but we need to understand why. So, does it make sense that lowering the reflux ratio with the same feed and the same number of trays does not affect the outlet concentrations?
- Student No, I would expect the separation to be worse.
- Professor So, what is special about this case that allows the separation to be maintained at the lower reflux ratio?

The discussion now continues as the student is shown the McCabe-Thiele diagram, which was provided with the assignment but apparently ignored. This reveals that the original column was overdesigned. There are several stages approaching the azeotrope that provide very little incremental separation. Therefore, fewer stages at the top or lowering the reflux ratio do not appreciably affect the distillate concentration.

Once again, only the question-and-answer session reveals that a correct solution was presented without in-depth analysis, perhaps without a detailed understanding of the reason why the solution was correct. Both situations illustrated above are examples of how student learning can be assessed while students are simultaneously provided with individual feedback on their work. It is a win-win situation.

The following is an example of dialog when an incorrect solution is presented. In this case, the student has attempted to draw the system curve on the pump curve graph (which is provided) for the reflux pump, P-405 A/B, to determine if the pump has sufficient head to handle the increased overhead liquid flowrate for a solution that involves replacing the existing trays while maintaining the same reflux ratio.

Student (Presents Figure 2; claims that doubling the diameter of the suction and discharge lines is not

sufficient to operate at the scaled-up conditions and suggests purchasing a new pump with a more favorable pump curve or running both pumps in parallel and purchasing another spare.)

Professor I do not understand your pump and system curve analysis. Please explain it to me.

Student The pump curve was supplied. I plotted the system curve. Since the desired flowrate is larger than the point at which the two curves intersect, the existing pump does not supply sufficient head at the desired flowrate.

Professor From what we did in class, does it make sense that there is so little effect of pipe diameter?

Student I didn't think about that. I did the calculation just like we did it in class, and this is what I got.

Professor Let's try to analyze this in more detail. What relationship does the system curve represent?

Student (stumbles around, cannot generate the desired relationship)

Professor The system curve has an intercept. What does this represent physically?

- Student Oh. Isn't that the static pressure difference?
- Professor For this case, yes. Now, what else causes pressure drop?
- Student Friction.

Professor And, what part of the curve represents the frictional pressure drop?

Student (stumbles around for an answer)

Professor What is frictional pressure drop most significantly dependent upon?

Student Velocity.

Professor Where is velocity represented on the graph?

Student Ummm. Oh. It is in the flowrate on the x-axis.

Professor OK. So how is frictional pressure drop related to flowrate or velocity?

Student It goes with velocity squared.

Professor OK. So how is this shown on the graph?

Student It is in the parabolic shape of the graph.

Professor OK. So we now know that the intercept of the graph is the static pressure change, and the curvature of the graph is related to the frictional loss. So, let's look at the frictional pressure drop. Let's pick the point on the original (0.5-in) system curve for your scaled-up flowrate. What happens to this point if the diameter of the suction and discharge lines are doubled?

Student It should be lower on the y-axis.

Professor Which you show on this graph. However, how much lower should it be?

Student Well, this is what I got.

Professor If you increase the pipe diameters, what does that do to the friction?

Student (stumbles around for an answer)

Professor What is the relationship for frictional pressure drop? Do you remember it?

Student (Writes the equation  $\Delta P = 2\rho f L_{eq} v^2 / d$  on the

board, perhaps with some assistance. Most students know the square relationship on velocity and the inverse relationship on d, but not all can remember all of the other terms.)

- Professor So, what happens to the frictional pressure drop if the diameter is, for example, doubled?
- Student It is half the original value. This is what my graph shows.
- Professor Yes, that is what your graph shows, but are you sure that you have the correct relationship? Does anything else in that equation change if the diameter is doubled?
  - Student Oh. The velocity decreases. I guess I forgot to consider that.
- Professor By how much does it decrease:

Student (Figures out from  $\dot{m} = \rho A v$  that velocity is inversely proportional to d<sup>4</sup>, so that the frictional pressure drop is inversely proportional to d<sup>5</sup>. Assistance and coaching may be required.)

- Professor So, if the diameter is doubled, by how much does the frictional pressure drop decrease?
- Student Let's see. By a factor of two to the fifth. That's 32.
- Professor So, if the frictional pressure drop decreases by a factor of 32, how does this affect the graph?
- Student The y-axis value decreases by a factor of 32.

Professor Are you sure? Remember the intercept.

- Student *Oh. The difference between the intercept and the y*value decreases by a factor of 32.
- Professor So, what does that do to the system curve? Student It will be almost flat. So I guess the existing pumps will work after all if the pipe diameters are doubled.

This exchange is an example of the tutorial nature of the interaction. An erroneous result is analyzed, via careful questioning, to lead the student to a correct result. Through questioning and coaching, the student "independently" discovers the error made and determines the correct result.



Figure 2. Sketches of pump and system curves for P-405. Solid curves are student result; dashed curve is correct calculation for larger pipe diameter.

**Chemical Engineering Education** 

### USING ASSESSMENT RESULTS—CLOSING THE LOOP

Assessment results from this exercise are used in several different ways, all of which "close the loop" on the assessment process. The one-hour presentation and question period provide students with immediate feedback. After all of the presentations have been completed, class time is devoted to project review. One or two of the best projects are presented. Faculty review the problem, noting areas where better solutions could have been presented. Follow-up problems are usually assigned. Sometimes these are assigned only to individuals, *i.e.*, to students who did not do them correctly on the project. In the case of this acetone problem, the heat integration option was ignored by most student on the first project. Therefore, it was assigned specifically on the second project.

An assessment report following each project is also prepared and circulated to all faculty. It describes the project, what types of solutions were expected and what types were actually submitted. Areas where a significant number of students did well are pointed out. For example, if a majority of students responded to questions about T-401 as the student in the example did, this would be specifically stated. Areas where a significant number of students were found to be deficient are also pointed out-if a number of students did not think about the meaning of process simulator results, simply accepting the results on faith, or if a significant number made the error regarding frictional losses, this would be specifically cited. In these cases, remedies to ensure that future students are not deficient in the same area are suggested. Faculty are expected to respond to the suggestions. Do they? In general, our faculty do because of our culture supporting these projects and due to the pressure we all feel not to have material we taught show up as being deficient on these projects.

## IMPLEMENTATION SUGGESTIONS

Outcomes assessment using oral presentations of capstone projects can be implemented by making only minor changes in how typical design classes are run. First of all, it is not necessary to use a performance (debottlenecking or troubleshooting) problem such as the one described here, although such problems lend themselves to this type of assessment process. Since our students enter the senior year having already completed a process design during their sophomore and junior years,<sup>[6]</sup> they are prepared for this type of assignment. Asking probing questions in a typical capstone design project can yield the same type of assessment information. The best questions to ask are "why" and "what if." For example, ask why the column was designed for a specific reflux ratio. Was it chosen ad hoc, or was it based on an optimization of the trade-off between number of stages and reflux ratio? What if scale-up is required in the future? Similarly, why were the reactor temperature, pressure, and/ or conversion chosen at the specified values? Were they merely convenient values? Or, was the selectivity analyzed Summer 1999

to determine conditions that maximize profit?

It is also not necessary for students to do projects individually for the presentations to be used for assessment purposes. To implement this in a group of 3-5 students, interim progress reports (which can be informal) are suggested. Students can make a brief presentation to either a professor or a TA (who would need some training in what to look for and how to ask questions), and the students would then be expected to respond to questions. Questions should be directed to individual group members to avoid domination by one person. The assumption should be that any student is prepared to respond to any question, not just to the material presented by that student. If a student is unable to respond, then another student can be chosen or the question could be answered by a volunteer. Assessment information would be gathered and students would get feedback on their project while it is in progress, which would probably improve the final product.

A project review is also desirable to close the assessment loop. This should be done after all presentations have been completed, preferably after all project reports have been graded.

#### CONCLUSION

Performance problems such as the debottlenecking problem illustrated here are a rich opportunity for outcomes assessment, as are process design problems. Asking "why" and "what if" type questions probes students' understanding of fundamental principles. The oral presentation format provides students with immediate feedback, closing one feedback loop. Another way to close the assessment loop is by project assignment review in class and/or follow-up assignments. Feedback to faculty regarding students' ability to apply the principles they are expected to understand closes another feedback loop. The only real disadvantage is the investment in faculty time for the oral presentations. If it is believed that outcomes assessment and EC 2000 will result in increased faculty time devoted to the undergraduate curriculum, a key choice is how to invest this time. Questioning students in oral presentations of capstone projects is one potentially beneficial way to invest that time.

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