# CHEMICAL ENGINEERING DESIGN

## *Problem-Solving Strategy*

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A significant fraction of our undergraduates accept industrial employment that requires dealing with problems associated with an operating system (production). These responsibilities depend on an ability to both predict problems *before* they occur and to diagnose problems *after* they occur, in addition to designing and developing new processes. Problems must be solved under the constraints imposed by physical equipment and the existing processes. Neither course work nor the typical capstone design course makes a conscious effort to develop such abilities in the student.

To address this problem, the chemical engineering department at West Virginia University has initiated a process in the senior design course that focuses on the development of the necessary skills for solving problems which production engineers may expect to confront.[1,2,3] The program introduces a series of comprehensive problems, extracted from a single process flowsheet, into the two senior design courses. The problems are worked out individually under the same rules that apply in the AIChE student-contest problem wherein the student presents a written report and a one-hour oral report on each problem. The student is "escorted" through the transition from a detailed consideration of a single unit operation to management problems that can include several interrelated unit operations. This is accomplished by providing intensive individual and group feedback after each assignment.

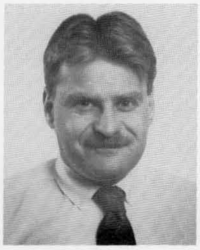

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**TABLE 1**
**Unit Function: Intellectual vs. Industrial**

| UNIT | INTELLECTUAL CONCEPT | INDUSTRIAL APPLICATION |
|---|---|---|
| 1 | Visualization plus Analysis | Trouble Shooting |
| 2 | Analysis plus Synthesis | Retrofit |
| 3 | Synthesis plus Optimization | New Process Design |

Major adjustments in student attitudes are sometimes necessary. It is difficult for the student to go from solving narrow, focused, single-answer problems that involve no creativity to global, multi-answer problems that require considerable creativity. They find that the well-entrenched strategies for problem solving that worked for them in the past are no longer effective.

## DISCUSSION

The general content of the comprehensive problems are summarized in Table 1. It shows the skills that are necessary for solving the problem and the area of its industrial application. The order of the problems is significant. The skills required in a previous problem must be mastered in order to solve each new problem. Each problem develops a single skill while introducing a new skill that is the basis for the following problem. For example, the first problem develops an ability to visualize—and introduces analysis. The second problem assumes the ability to visualize, develops an ability to analyze—and introduces synthesis. In terms of industrial application, the three problems will cover trouble-shooting, retrofit operations, and new process design.

The problems are introduced to the student through industrial "role-playing." The student (a novice engineer) joins a company and is assigned to a plant site where three assignments are given that cover the areas shown in Table 1. The student is given a packet of materials that includes a process flowsheet and flow table, a description of changes that have been made to the process, thermodynamic data, and various other items of information describing the process and the company that may be useful.

The process flowsheet is special. It represents a poor process design (it was built many years ago) under current conditions and includes several poor design areas that could be improved. Some defects have been distorted (like big ears and long noses) to make them stand out and be easy to detect. The special flowsheet represents a "caricature flowsheet" and is an aid to the early development of visualization skills. In addition to poor design, several process modifications (operating conditions) have been made in response to changes in constraints and availability of new technology.

In the process of solving problems, students 1) will identify all of the "caricature problems" and offer solutions, 2) will identify many other problems, not highlighted for identification, and offer solutions, and 3) will create new processes that improve the original process and eliminate the poor engineering of the original system. All solutions must be justified by economic considerations.

All three projects are associated with the production of the same chemical commodity. Since each successive problem requires mastery of the previous problem, it has been necessary to provide extensive individual and group feedback during the oral and after each project.

***The assignments and experiences of our 1988 class are used here as an example of how the comprehensive problems, along with the "caricature flowsheet," are used to introduce and develop skills.***

## STUDENT ASSIGNMENTS

The assignments and experiences of our 1988 class are used here as an example of how the comprehensive problems, along with the "caricature flowsheet," are used to introduce and develop skills. Figure 1 is a "caricature" flowsheet for the production of acrylic acid. It was created from a 1986 AIChE student contest problem on the production of acrylic acid via partial oxidation of propylene.

A packet of material (about twenty pages) was provided that contained information concerning the instability of the acrylic acid with temperature (even with the addition of an inhibitor, it will rapidly polymerize at above 90°C when present in large concentrations). Some additional information on current operations is also given.

EQUIPMENT LIST
AB-1 Quench Tower
AB-2 Off Gas Absorber
C-1 Inlet Air Blower
E-1 Reactor Coolant Exchanger
E-2 Absorber Product Cooler
E-3 Solvent Separator Condenser
E-4 Solvent Separator Reboiler
E-5 Waste Water Separator Condenser
E-6 Waste Water Separator Reboiler
E-7 Product Separator Condenser
E-8 Product Separator Reboiler
E-9 Incinerator Waste Heat Boiler
H-1 Off Gas Incinerator
M-1 Solvent-Product Mixer
S-1 Solvent-Product Liquid Separator
T-1 Solvent Separator
T-2 Waste Water Separator
T-3 Product Separator

UTILITY LIST
BFW Boiler Feed Water
CW Cooling Water
CWR Cooling Water Return
CR Condensate Return
DI Deionized Water
NG Natural Gas
STM Steam

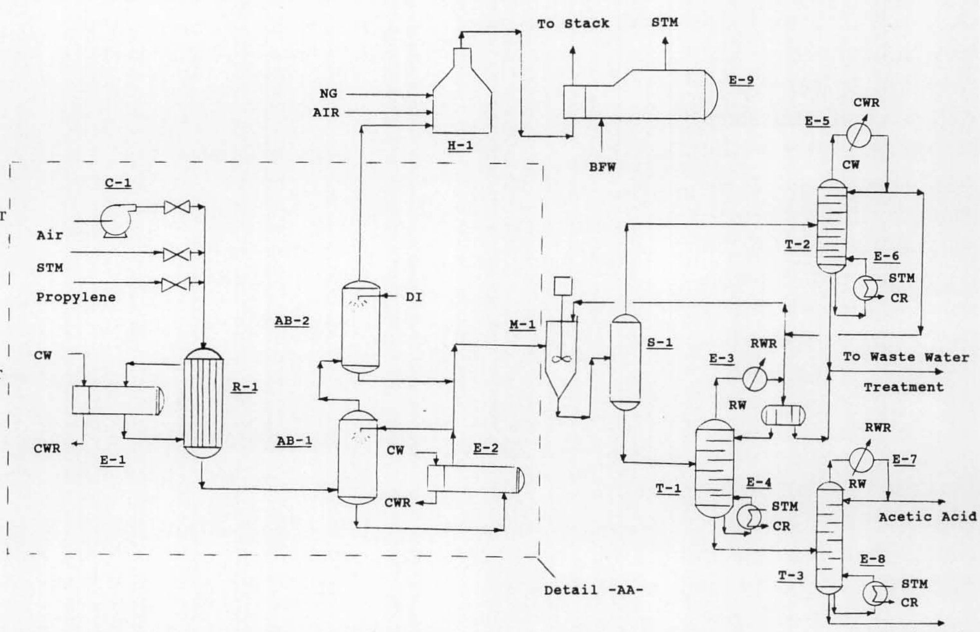


***Figure 1.*** *Acrylic Acid Process Flowsheet*

### ASSIGNMENT 1

The plant faces a serious problem. Our largest customer cancelled its order. We shipped off-spec material (a slight discoloration in the normally clear acrylic acid). It damaged their process and their product was worthless (colored). The potential loss to our company is in excess of $500,000/day, and this is the economic incentive that calls for an immediate resolution. The assignment, to be completed in one week, is 1) to identify the cause of the off-spec material, 2) to recommend action to be taken to correct the situation, 3) to present a written report, and 4) to make an oral presentation to the company president.

There are several potential explanations for the "off-spec" material. There is evidence to support some of the explanations, while others are no more than speculation. Table 2 gives a partial list of some of the explanations. They can be separated into three groups: 1) global, 2) numerical, and 3) research. An example from each group follows and possible solutions are included in Table 2.

Global problems require that the student consider items outside of the process unit for an explanation. For example, the off-spec material may have resulted from low-quality feed. There is evidence in the material packet given to the student that supports this explanation: the amount of feed has increased (feed may not be pure propylene); the amount of steam generated in the waste heat boiler increased (the non-propylene material in the feed may not react in the reactor and burns in the afterburner); the non-propylene material was colored.

This problem was intentionally set up for the student to discover. Poor feed is, in fact, the most common cause of an off-spec product. We shipped our customer tainted feed and ruined their product. This could be the same problem we have. We could have *received* tainted feed material. We have evidence to support this explanation. Students not only fail to make a connection between these two situations but they also are not ready to accept the explanation.

A limited number of explanations can be verified numerically (the purpose of this problem was to limit the number of necessary calculations). The refrigerated water (at 10°C) to E-7 (Figure 1) was replaced with cooling water (at 30°C). Many of the students noted this and suggested that it might have caused the temperature of the acrylic acid to reach +90°C, causing polymerization. When asked to determine this temperature, many of the students had a vague idea of how to approach the solution, but only one in twenty was able to fully analyze the problem and calculate the temperature. The level of analysis required to solve the problem is similar to that used by a plant engineer. We expect our students to understand and be able to employ such an analysis.

Figure 2 gives the temperature-duty profile for the design case (all this information was available to the student). The temperature of the cooling water is known and is plotted on the same figure. For the same recycle ratio, the condenser duty is constant.

**TABLE 2**
**Possible Explanations for Off-Spec Product**

| *Possible Cause* | *Evidence* | *Solution* |
|---|---|---|
| PRE-PROCESS | | |
| Feed is not pure | 1. Increased feed rate to maintain output<br>2. Increased steam production in waste heat boiler<br>3. New supplier<br>4. Temperature and pressure of storage vessel has changed | Check feed for impurities and return to the supplier |
| PROCESS | | |
| Reactor system | 1. Increase in feed rate and lower conversion<br>2. Lower selectivity | Replace spent catalyst |
| Separation systems | | |
| 1. High temperature in purification columns | Change from refrigerated to cooling water in condenser E-7 | Return to refrigerated water |
| 2. Absorber malfunction | Increase in feed rate and steam production in waste heat boiler. | Increase the flow of water to absorbers. |
| POST PROCESS | | |
| Product storage | Inhibitor not added to product in storage | Check inhibitor and injection system |
| Product transportation | Dirty tank cars or product exposed to air and sunlight | Check transportation company |
| Customer error | Mishandling of material by customer | ? |
| OTHER | | |
| Product not discolored | Check analytical equipment, testing procedures, and records | Rerun samples in our lab |

To achieve a constant duty, $Q = U^*A^*T_{ln}$. Where A is constant and U is assumed constant, the value of $T_{ln}$ must be constant. If the curves for the refrigerated water coolant are shifted upward until the low temperature line corresponds to cooling water, the process temperature at the top becomes 46°C. This is the equilibrium temperature for the exiting acetic acid.

Figure 3 provides the vapor pressure curve for the distillate and the bottoms that were obtained from the vapor pressures of the pure components (and Raoult's law). From Figure 3, for a temperature of 46°C the condenser pressure is 6.2 kPa. The pressure drop in the column is largely the result of the liquid level on each plate and the number of plates. Since this remains constant (at 15.9 kPa), the bottom pressure is 22.1 kPa. From Figure 3 this corresponds to a temperature of 95°C. This is well over the 90°C limit for polymerization.

Some students elected to look for information outside of the material packet that was provided and came across the information that iron enhances polymerization. Iron may have come in with the feed and been the cause of the off-spec material.

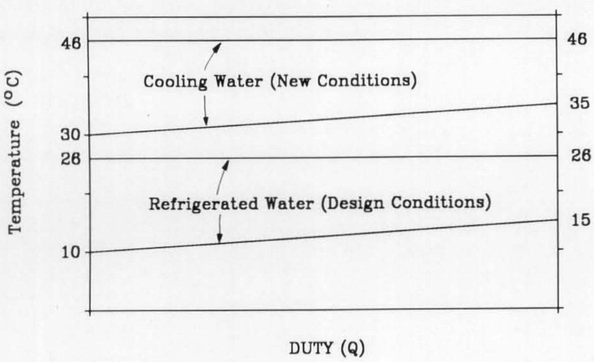


***Figure 2.*** *Temperature vs duty diagram for product overhead condenser*

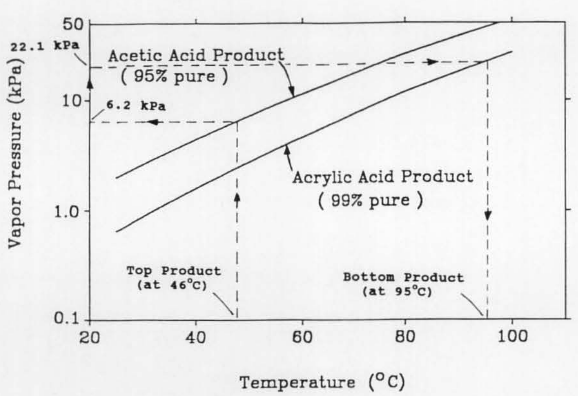


***Figure 3.*** *Vapor pressure curves for acrylic and acetic acid product streams.*

Student performance on this assignment was poor. Unfortunately, once a single explanation was identified, most students ended their search. No consideration was given to the economic loss of $500,000/ day when they made their recommendations. Recommended changes were sequential, and no thought was given to making simultaneous changes to save time and money.

### *Assignment 2*

The plant was returned to the original feed material, refrigerated water was returned to condenser E-7, and the catalyst was replaced. The high product quality returned and the immediate problem was solved.

The next assignment was to improve the plant profitability. There are recent changes in the value of steam and credit for excess steam will no longer be given.

The first step was to identify the major costs under the current conditions or base case. Figure 4 shows the costs of feed materials and utilities that were calculated from information provided. It identifies the major costs and shows that the overwhelming cost is propylene. There was no information on the catalyst that had been replaced. A recommendation that serious consideration be given to the development of a new catalyst with higher conversion and selectivity is appropriate.

The next largest cost is steam. If large savings are to be realized, the purchase of steam must be curtailed. Two methods of reducing the steam costs could be reducing the use of steam or generating steam in the process. The acrylic acid reaction is exothermic, and the heat generated is removed with cooling water in E-1 (another example of the caricature nature of the problem). Replacing E-1 with a steam boiler eliminates the need to purchase steam.

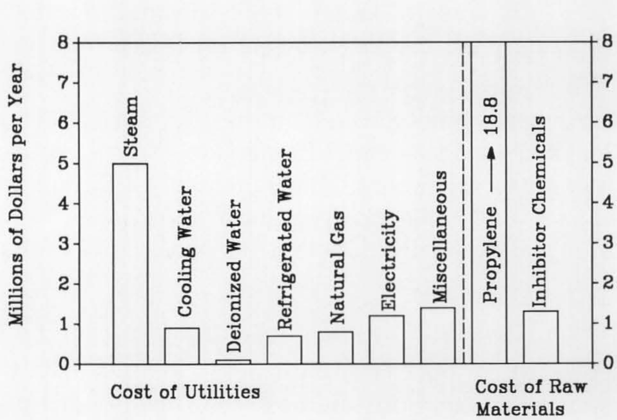


***Figure 4.*** *Operating costs for the design case.*

Table 3 lists some of the options for using the steam produced to reduce the costs of utilities shown in Figure 4.

Student performance on this assignment improved dramatically from the first assignment. While the assignment was more difficult and the changes were subtle, the students uncovered and corrected many process changes that improved profitability. The changes were ranked by incremental return on investment.

### *Assignment 3*

This assignment requires the design of a new plant based on new technology. The students are free to be as innovative as possible under the given structure. There are new catalysts that provide very high selectivity at low conversion; they are temperature sensitive and ideal for a fluid bed. The single reactor system is replaced by a two-reactor system that can operate at different temperatures and pressures. The students are provided with detailed kinetics along with a computer program that considers both the kinetics and a fluid-bed model. This program allows computation of the reactor size (given the conversion and operating conditions). It is clear that the new catalysts provide increased selectivity and, with a recycle stream, the possibility of high overall conversion.

Even though the students are provided with the computer program, they will likely fail if they proceed to obtain the optimum design by a random approach. Using the kinetic expressions or performing a few well-chosen simulations will provide a feel for the effects of operating variables. Solely from the reaction kinetics point-of-view, astounding savings are possible by increasing the recycle. However, once the cost of compressing the recycle gas is considered, the advantages rapidly diminish and a sharp optimum is reached. In the old plant without recycle, large amounts of steam were introduced into the reactor. With the recycle stream this is not necessary.

The students did well on this assignment. Figure 5 is a typical flowsheet for section -AA- of Figure 1, using new technology. It is noticeably different from the old flow diagram. The plant costs are estimated along with the predicted return on the investment.

## CONCLUSIONS

Teaching the student about acrylic acid is not the objective of this course. It is only a vehicle to demonstrate how to approach a complex open-ended problem. While it is true that every process is different, it is equally true that the methodology of visualizing, analyzing, and synthesizing are universal and transferrable to other processes.

The goal of these problems is modest. The student is not expected to master the strategies needed to be effective in working problems of the type outlined. We only hope to introduce the student to these types of problems and to move them to the breakpoint on the learning curve where the rise becomes rapid with a little more experience. We feel that if we have accomplished this, the process has been successful. The final conclusion deals with student motivation. Motivation provides both a high driving force and a low resistance to learning, enabling the student to learn more rapidly. One student's view of the sequence of problems is as follows:

> *On September 15th, 1988, we were presented with our first in a series of design projects. It was apparent that our experience in the classroom had to be challenged by the real-world situation. Instead of performing a "cookbook"*

**TABLE 3**
**Possible Uses for Excess Steam in the Acrylic Acid Plant**

1. Place a trim cooler in series with the waste heat boiler and produce just enough steam for the process.
2. Use any excess steam in a turbine to power the feed air compressor and reduce the overall power consumption in the plant.
3. Place a preheater on the feed or air streams into the incinerator and use excess steam to reduce the consumption of natural gas.
4. Use incinerator effluent to preheat incinerator feed streams and a trim waste-heat boiler to make steam balance within the plant.

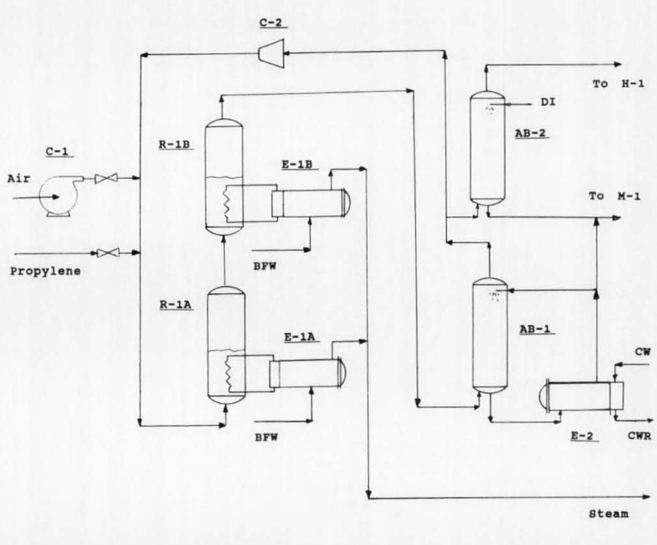


***Figure 5.*** *Modified section (detail -AA-) from Figure 1.*

*type problem, we were supplied with a minimal amount of information. Assumptions, answers , and suggestions for rather vague situations had to be made. The time to test our knowledge in a real world situation was suddenly upon us.*

*As the semester progressed, many hours of sleep were lost, many times tempers became short, and often the most docile student exhibited impatient behavior. The effort put forward was not wasted though; the increase in knowledge greatly outweighed the amount of time put forth towards the projects.*

*It is for the above reasons that I am pleased to present this final in a series of three design projects. The knowledge which has accumulated over the past two semesters will be of great importance in the years to come.*

An expanded version of this paper and copies of the original problems are available from the authors.


## ACKNOWLEDGEMENTS

The authors would like to acknowledge that the concept of these individual projects or "majors" has been in existence at WVU for almost twenty years and that many faculty have contributed to its success. Most recently, we would like to recognize the contributions of A.F. Galli and W.B. Whiting.


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# REVIEW: Chemical Kinetics

*Continued from page 33.*

Chapter 5 with catalysis. The former is conventional in its coverage, while the latter introduces autocatalysis and oscillating reactions (a subject of much current interest in chemical engineering) in addition to homogeneous catalysis, heterogeneous catalysis, and enzyme reactions. These first five chapters, two hundred pages in length, comprise nearly half the book.

Chapter 6, a brief discussion of the transition from the macroscopic to the microscopic level, sets the stage for the remainder of the text. It introduces the description of reactive collisions in terms of collision cross sections and relates the cross section to the rate coefficient. Also introduced at this point are the quantum state description of reactions (state-to-state kinetics), microscopic reversibility and detailed balance, and a short discussion of the relationship between macroscopic and microscopic kinetics.

Chapter 7 discusses the role of the potential energy surface in governing the outcome of reactive events. Succeeding chapters take the microscopic approach to kinetics, covering the kinetics of elementary reactions, and chemical dynamics. A treatment of bimolecular collision dynamics and molecular beam scattering is followed by another chapter on experimental methods, this time for state-to-state kinetics. Chapters on transition-state theory (including variational transition-state theory) and unimolecular reactions are followed by one on dynamics in solution and at interfaces. Chapters 13 and 14 cover the advanced topics of the information-theoretic approach to dynamics, including surprisal analysis and the master equation. The book concludes with a chapter on applications: atmospheric chemistry, and hydrogen and methane combustion.

This book has been used for the past two years in a one-quarter course given to chemical engineering graduate students at the University of Minnesota. In the ten weeks of lectures it has not been possible to cover the entire book. The chapters on reactions in solution and dynamics in solution, catalysis (which is covered in another course), information theory, and the master equation have been omitted, and supplementary material on bimolecular collision dynamics, chain reactions, and the kinetics of combustion reactions has been incorporated. It has proved to be a satisfactory text, treating the subject at a level suitable for graduate students and giving more comprehensive coverage (particularly of modern developments) than many other texts.

For undergraduates, portions of the book could be employed as the basis for a series of lectures on kinetics that would introduce students to material of interest to engineers in a more modern vein than most chemical engineering kinetics texts. For example, at Minnesota juniors are given approximately six weeks of lectures on kinetics during the spring quarter. The first five chapters of this book, plus some selected material on rate theory from the chapters on collision dynamics, transition state theory, and unimolecular reactions (and perhaps atmospheric chemistry and combustion reactions), would provide good reading material to accompany the lectures. Students mastering this material would have an excellent foundation for future work in kinetics and reaction engineering.

Chemical kinetics in an enormously broad area. It is difficult to find a text that gives good treatment of the fundamentals of the subject, as well as coverage of subjects of interest to chemical engineers. This book is one that succeeds and can be recommended. ❐