THE TECHNICALLY FEASIBLE DESIGN

TW FRASER RUSSELL AND N. ORBEY
University of Delaware
Newark, DE 19716

Introductory Note

It is frustrating to attempt to capture effective classroom experiences in an article, but I am tempted to try again to do so because this past year I had the very rewarding experience of supervising a DuPont Teaching Fellow (Ms. Linda Broadbelt) while team teaching a junior level chemical engineering course in reaction and reactor design with Dr. N. Orbey, a visiting professor at the University of Delaware from Middle East Technical University (Turkey). Their enthusiasm for the "technically feasible design" approach has prompted this paper. It is my hope that it will encourage classroom experimentation and help educate students about design problems.*

TW Fraser Russell

Chemical engineers design, build, operate, and modify process equipment, or carry out the research necessary to do so more creatively and more efficiently. Not all chemical engineers are directly involved in the art and science of design, but all chemical engineers are exposed more or less effectively to various aspects of design in the educational programs in our universities. Indeed, it is part of our profession's criteria for accreditation, as shown by Section IV.C3(a) of "Criteria for Accrediting Programs in Engineering in the United States":

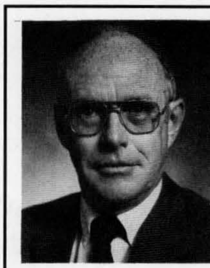
> (IV.C.3(a)) Engineering Design
>
> (a) Engineering design is the process of devising a system, component, or process to meet desired needs. It is a decision-making process (often iterative), in which the basic sciences, mathematics, and engineering sciences are applied to convert resources optimally to meet a stated objective.

and by the "Program Criteria for Chemical and Similarly Named Engineering Programs":

> Engineering Design. (Amplified criteria section IV.C.2.d(3))
>
> The various elements of the curriculum must be brought together in one or more capstone engineering design courses built around comprehensive, open-ended problems having a variety of acceptable solutions and requiring some economic analysis.

These legal sounding criteria, which attempt to define design content, do not give us any insight into the value of design as a tool for making courses more intellectually challenging or more interesting. In fact, the "Chemical Engineering Criteria" which calls for a "capstone" design course has been interpreted by some educators as allowing them to ignore design until the final year of a four-year program in chemical engineering.

We tend to educate in the early years of the curriculum by using ideal technical problems in our courses. The ideal technical problem is one in which all the information is given and for which a single correct answer is most frequently obtained by solving an equation or sets of equations. Much effort is expended, both by professors in class and by students doing homework, on mathematical manipulation. While this serves a purpose in that it helps teach problem-solving methodology, it tends to pro-



TW Fraser Russell *is the Allan P. Colburn Professor of Chemical Engineering and Director of the Institute of Energy Conversion, a laboratory at the University of Delaware devoted to thin-film photovoltaic research. He received his BSc and MSc degrees from the University of Alberta and his PhD from the University of Delaware, all in chemical engineering. He is the author of over seventy technical publications and is coauthor of two texts.*

Nese Orbey *received her BS and MS in chemical engineering from Middle East Technical University (METU), Turkey, where she is currently an associate professor, and her PhD from McGill University, Canada. She served as Visiting Associate Professor at the University of Delaware from 1990 to 1992. Her research interests are in the area of polymer rheology.*

* *The E.I. duPont de Nemours and Company's DuPont Teaching Fellows Program is designed to encourage graduate students to become interested in university-level teaching.*

duce students who do not understand that engineering problem solving and/or the creation of engineering opportunity must go beyond routine mathematical manipulation.

This serious difficulty can be avoided and students can be introduced to the art of engineering earlier in the curriculum if faculty would require that the students produce a "technically feasible design" rather than a single-answer solution to a problem.

TECHNICALLY FEASIBLE DESIGN

A technically feasible design is one which defines the size of a piece of process equipment to meet a stated goal, and in so doing initiates an analysis of the factors affecting optimal design. It could be specification of the volume for a reactor, the total area for an exchanger, or the height and diameter of a separation unit. The use of a technically feasible design can be illustrated for chemical engineering students by considering a simple problem in chemical reaction engineering.

Chemical engineers frequently become involved in a reactor-process design problem at an early stage, *i.e.,*

> How can our firm safely make a product ("D") for which there appears to be a good market at a fair profit?

While this is the type of problem that we would like a chemical engineer to be able to solve, it is too open-ended for students in their first few years of study. It is time-consuming and difficult even for many faculty to do. It also disrupts the logical flow of subject matter to introduce the issues of market development, competitive market-share pricing, and capital and operating cost estimating which are necessary to solve the problem.

The following is a simple, technically feasible design problem that can be presented to the student:

> Our firm has determined that we can sell 1260 metric tons/year of product "D," a raw material for the manufacture of an important fiber. "D" has a molecular weight of 50 and the reactor is assumed to operate 24 hours a day, 350 days a year.
>
> Our laboratory has studied the homogeneous liquid phase reaction which produces "D"
>
> $$A + B \rightarrow D$$
>
> This reaction can be carried out isothermally in an excess of B with the kinetics determined as follows:
>
> $$r_{A-} = kc_A$$
> $$k = 0.005 \text{ min}^{-1}$$

The simplest possible technically feasible design can be completed if the student is told at this point to assume that the reactor will be a continuous flow stirred tank (CFSTR) with a feed stream concentration of A, $C_{AF} = 0.2$ g-moles/liter.

We tend to educate . . .by using ideal technical problems in our courses . . .in which all the information is given and for which a single correct answer is most frequently obtained by solving an equation or sets of equations.

We have tested this problem with chemical engineering students in courses such as "Introduction to Chemical Engineering Analysis" and "Chemical Engineering Kinetics" and with a great many non-chemical engineers (mostly chemists and other engineers) in professional society-sponsored courses throughout the Delaware Valley. So far, over two thousand students have been asked to carry out this technically feasible design in class.

At the stage in any course when we introduce this exercise, the students are capable of deriving the required mass balances:

$$\text{species A} \qquad 0 = qC_{AF} - qC_A - kC_AV \tag{1}$$

$$\text{species D} \qquad 0 = 0 - qC_D + kC_AV \tag{2}$$

The technically feasible design is required for

- $C_{AF} = 0.2$ g-moles/liter
- $k = 0.005 \text{ min}^{-1}$
- total production of 1260 metric tons/year ($qC_D = 50$ g-moles/min, or 2.52×10^7 g-moles/year)

We ask students to carry out this exercise during class so we can observe their thought processes and can thus generate more effective discussion. When the exercise is introduced, the students are told that the design will be considered complete when the reactor volume, V, has been determined.

In order to maximize the educational gain for both the instructor and the students, the class should work unaided on the design for about thirty minutes, with each student attempting to obtain the reactor volume, V. We have found that students rarely obtain the reactor volume on their own without additional class discussion. A walk around the classroom, observing how the students attempt to carry out this very simple design, is most instructive. They will manipulate and remanipulate Eqs. (1) and (2) in an effort to obtain V. It has never been clear to us why almost all students do this, since counting unknowns and equations clearly shows that one variable in addition to those given must be specified. (Students should have done enough algebraic manipulations by this time in their academic lives to be thoroughly familiar with solutions of such a simple system of equations.)

Students are often reluctant to complete the technically feasible design by selecting values for the variables, q or C_A, probably because they have been taught to solve problems in which they had to derive and manipulate equations to obtain a solution. A very simple design decision (*i.e.,* select a value for C_A, the exit concentration of raw material A, and determine reactor size V) turns out to be foreign to the student's whole experience in problem solving.

To achieve a technically feasible design by assuming a value for q or for C_A, it is convenient to rearrange Eqs. (1) and (2). The most effective way to compute a reactor volume, V, is with Eq. (2):

$$V = \frac{qC_D}{kC_A} \tag{3}$$

$$V = \frac{50}{0.005\,C_A}$$

Since C_A can only vary between $C_{AF} = 0.2$ g-moles/liter and 0, the student can quickly obtain a technically feasible design. For example, if $C_A = 0.1$ g-moles/liter, then V = 100,000 liters.

If the students are encouraged to experiment with the set of equations, about a third of them will eventually derive Eq. (3). Others will assume a value for q, calculate C_D from $qC_D = 50$ g-moles/min, obtain C_A from $C_{AF} - C_A = C_D$ (the addition of Eqs. 1 and 2), and then solve for V using either Eq. (1) or Eq. (2). This more involved approach has the disadvantage that limits on the value of q are not as obvious as limits on the value of C_A. For instance, if q is assumed to be 200 liters/min

$$C_D = 50/200 \quad \text{and} \quad C_A = 0.2 - 0.25 = -0.05$$

Obviously, C_A cannot be negative, so q must be greater than 250 liters/minute for a technically feasible design (q qC_D/C_{AF}).

The problem is discussed in more detail in *Introduction to Chemical Engineering Analysis,*[1] and the role of the technically feasible design in initiating an analysis of the factors affecting optimal design is illustrated in Table 1.

It is very important to again stress that almost all the educational impact of the technically feasible design concept is lost if students do not have an opportunity to work on the problem by themselves in a classroom setting, with an instructor who is willing and capable of initiating discussion. Table 1 shows that the optimal size of a reactor cannot be considered without also considering how unreacted A is separated from product D. It also shows students how the reactor analysis affects the downstream process design. A large reactor with a small concentration of A in the effluent (high conversion) costs more than a small reactor with a large concentration of A in the effluent (low conversion). If a customer can use D with a small amount of A present, then it might be possible to eliminate an A-D separation unit which requires an expensive reactor. To reduce reactor costs one must pay for the capital and operating costs of the separation unit.

TABLE 1

q (liters/min)	C_D (g-moles/liter)	C_A (g-moles/liter)	V (liters)	θ=V/q (mins)
250	0.200	0	∞	∞
300	0.167	0.033	303,000	1000
400	0.125	0.075	133,000	333
500	0.100	0.100	100,000	200
800	0.0625	0.1375	72,600	90.7
1000	0.0500	0.1500	66,600	65
2000	0.0250	0.1750	58,100	27
4000	0.0125	0.1875	53,200	13.3

TABLE 2

C_A(g-moles/liter)	C_D(g-moles/liter)	t(min)	batches/year	V(liters)
0.01	0.19	599	700	190000
0.05	0.15	277	1269	133000
0.10	0.10	139	1945	130000
0.15	0.05	57.5	2839	178000

An "optimal" design is discussed in *Introduction to Chemical Engineering Analysis.* Also, a process design game that has been widely used and which very effectively illustrates the economics and introduces the concept of competition is described in a paper titled "Teaching the Basic Element of Process Design with a Business Game."[2]

The CFSTR technically feasible design problem can be used with students at any level in the curriculum (when providing Eqs. 1 and 2, we have even used it with high school seniors and first-semester freshmen). We expect University of Delaware chemical engineering majors to be able to derive Eqs. (1) and (2) after their sophomore year.

The design problem is used throughout the junior-level chemical engineering kinetics course, and we require that the students carry out a commercial-scale technically feasible design for the following reactor design situations:

- CFSTR (isothermal single reaction)
- batch reactor (isothermal single reaction)
- semi-batch reactor (isothermal single reaction)
- tubular reactor (isothermal single reaction)
- CFSTR and tubular reactor (isothermal series-parallel reactions)
- CFSTR (non-isothermal)

EXAMPLE: BATCH REACTOR

The technically feasible design for the batch reactor requires significantly different thinking, even though the same problem is addressed. The students are expected to derive the pertinent material balances

$$\frac{dC_A}{dt} = -kC_A \tag{4}$$

$$\frac{dC_D}{dt} = kC_A \tag{5}$$

and solve the differential equations

$$\ell n\left(\frac{C_A}{C_{Ao}}\right) = -kt \tag{6}$$

$$C_D = C_{Ao} - C_A \tag{7}$$

At this stage the problem differs from the CFSTR example in that the volume V for a technically feasible design cannot be directly obtained since the material balance equations for the batch reactor do not contain a volume term. Reaction time, t, must be obtained from Eq. (6) and then used to obtain the reactor volume.

Again, students need to work on their own in a classroom setting and must be given an opportunity to discuss the design with the instructor. Most students have difficulty obtaining the reaction time despite having encountered a similar situation with the CFSTR design. Equation (6) has two unknowns: C_A and t. The value of t can only be solved as a function of C_A, and any pair of t-C_A is one solution leading to a technically feasible design. Students must assume a value for C_A just as they did in the CFSTR example. For example, if $C_A = 0.1$ g-moles/liter

$$t = 138.6 \text{ min and } C_D = 0.1 \text{ g-moles/liter}$$

Students must also make additional judgments to obtain a technically feasible design. The total yearly production is known and the volume of the reactor is related to the reaction time.

$$2.52 \times 10^7 = (VC_D)\,(\text{Batches/year}) \tag{8}$$

Both C_D and the number of batches per year that can be processed depend on the reaction time (Eqs. 6 and 7).

$$C_D = C_{Ao}(1 - e^{-kt}) \tag{9}$$

To find the total time in hours to process a batch, time for charging raw materials, removing product, and cleanup must be considered in addition to the reaction time. We can then obtain V from Eq. (8) by assuming there are 350 x 24 hours in a year. The results of some sample calculations for technically feasible values of V are given in Table 2, assuming that the time for charging raw materials, removing product, and cleanup is two hours.

Table 2 also provides information for a discussion of the important factors in any optimal design. The optimal size of the reactor depends on downstream processing. In the case of a CFSTR, volume decreases monotonically as conversion decreases (see Table 1). Batch processing is a labor-intensive process. At very low conversions ($C_A = 0.15$) with low reaction time, the time required for charge and cleanup (two hours) is almost twice that of the reaction time. The reactor volume is thus greater than for $C_A = 0.10$.

In the CFSTR, low conversions had the advantage of low reactor capital cost and the disadvantage of high separation costs. In the batch process, low conversion leads to the double disadvantage of high reactor capital cost and high separation costs.

In Table 2, batches/year are given, but in classroom discussions either batches/day or batches/shift can be computed to promote discussion on the issues of labor requirements and costs.

CONCLUSIONS

The importance of design in chemical engineering education has been effectively taught to both chemical engineers and chemists by requiring students to complete simple, technically feasible designs in class.

ACKNOWLEDGMENTS

The authors would like to thank the Department of Chemical Engineering for supporting Dr. N. Orbey and for encouraging experiment in chemical engineering education. Ms. L. Broadbelt was a valued teaching colleague, and the E.I. duPont de Nemours and Company is acknowledged and thanked for the creation and sponsorship of the E.I. duPont Teaching Fellows Program that provided her support.

NOMENCLATURE

- C species concentration, g-moles/liter
- k specific reaction rate constant, $\min^{-1}$
- q volumetric flow rate, liters/min
- r_A rate of reaction, g-moles/liter, min
- t time, minutes
- V reactor volume, liters

Subscripts

- A,D chemical species
- F feed condition
- o initial condition

REFERENCES

1. Russell, T.W.F., and M.M. Denn, *Introduction to Chemical Engineering Analysis,* John Wiley & Sons (1972)
2. Russell, T.W.F., and D.S. Frankel, "Teaching the Basic Element of Process Design with a Business Game," *Chem. Eng. Ed.,* **12**, 18 (1978) ❒