The object of this column is to enhance our readers' collections of interesting and novel problems in chemical engineering. We request problems that can be used to motivate student learning by presenting a particular principle in a new light, can be assigned as novel home problems, are suited for a collaborative learning environment, or demonstrate a cutting-edge application or principle. Manuscripts should not exceed 14 double-spaced pages and should be accompanied by the originals of any figures or photographs. Please submit them to Dr. Daina Briedis (e-mail: briedis@egr.msu.edu), Department of Chemical Engineering and Materials Science, Michigan State University, East Lansing, MI 48824-1226.

OPTIMIZATION PROBLEMS

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Optimization is often considered to be an advanced, highly mathematical, and sometimes a somewhat obscure discipline. While it is true that many advanced optimization techniques exist, optimization problems can be developed that are suitable for undergraduates at all levels. Two of these problems will be described in this paper, and many others are available on the web.[1] A pedagogy is described that requires students to identify the trends of the components of the objective function and to understand how trade-offs between these components lead to the existence of the optimum.

The ability to solve "routine" optimization problems has been simplified by advances in computing power over the last generation. Earlier editions of current design textbooks[2] presented a sequence of optimization techniques aimed at minimizing the number of cases that had to be considered to close in on the optimum. Now, it is possible to perform optimization calculations involving numerous cases with a few clicks of a mouse, and an entire chemical process can be simulated and results exported to a spreadsheet in a matter of minutes.

Several optimization examples are routinely discussed in undergraduate textbooks; however, the objective function does not usually involve economics. These examples include optimum interstage compressor pressure,[3] optimum insulation thickness,[4] and identifying conditions for the optimum selectivity.[5] Qualitative representations of the economic optimum pipe diameter[6] and reflux ratio[7] are also available. Other examples of optimization problems are available, but these do not involve an economic objective function.[8-10] The problems presented here all involve an economic objective function.

TYPES OF PROBLEMS

Three types of optimization problems are available, and they are summarized in Table 1. The ones highlighted in italics are discussed in this paper, and the others are available on the web.[1] The numbers in parenthesis indicate the number of different versions available for each problem. All of these have been used successfully in a freshman class designed to develop computing skills appropriate for an undergraduate chemical engineering student. Most of these problems would also be suitable for assignments or projects in unit operations

TABLE 1
Available Optimization Problems

Single Variable	Multi-variable	Projects
Pipe diameter (2)	Absorber	Generic chemical process (2)
Reactor/ preheater (2)	*Batch reactor/preheater*	Geothermal energy (2)
Reflux ratio	Staged compressors	Fuel production from biomass (4)

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classes or as problem assignments for the portion of a design class where optimization is taught.

Problem 1: Bioreactor

Background

A liquid-phase, biological reaction is used to produce an intermediate chemical for use in the pharmaceutical industry. The reaction occurs in a large, well-stirred, isothermal bioreactor, such that the reactor temperature is identical to the inlet temperature. Because this chemical is temperature sensitive, the maximum operating temperature in the reactor is limited to 65 ˚C by using a heating medium available at this maximum temperature. The feed material is fed to the reactor through a heat exchanger that can increase the temperature of the reactants (contents of the reactor), which in turn increases the rate of the reaction. This is illustrated in Figure 1. The time spent in the bioreactor (known as the space time) must be adjusted to obtain the desired conversion of reactant. As the temperature in the reactor increases so does the reaction rate, thereby decreasing the size (and cost) of the reactor required to give the desired conversion. The problem to be solved is to determine the optimal value for the single independent variable; namely, the temperature ($T_{c,2}$) at which to maintain the reactor (preheat the feed). The costs to be considered are the purchase costs of the reactor and heat exchanger and the operating cost for the energy to heat the feed.

Problem Statement

It is desired to optimize the preheat temperature for a reactant feed flow of 5,000 gal/h. The feed has the properties of water (ρ = 1,000 kg/m³, C_p = 4.18 kJ/kg ˚C) and enters the heat exchanger at a temperature of 20 ˚C. The reactor feed is to be heated with a heating medium that is available at a temperature of 65 ˚C and must leave the heat exchanger at 30 ˚C. Therefore, the desired reactor inlet temperature is adjusted by changing the flowrate of the heating medium. The physical properties of the heating medium are ρ = 920 kg/m³, C_p = 2.2 kJ/kg ˚C.

The reaction rate for this reaction, $-r_A$, is given in terms of the concentration of reactant A (C_A) by the following equation:

$$-r_A = kC_A \tag{1}$$

where

$$k\left[s^{-1}\right] = 2.5\exp\left[-\frac{3{,}500}{T\left[K\right]}\right] \tag{2}$$

The design equation for the reactor is given by:

$$V = \frac{v_o X_A}{k\left(1 - X_A\right)} \tag{3}$$

where V is the reactor volume (m³), v_o is the volumetric flowrate of fluid into the reactor (m³/s), and X_A is the conversion (assumed to be 80% or 0.8 for this reaction).

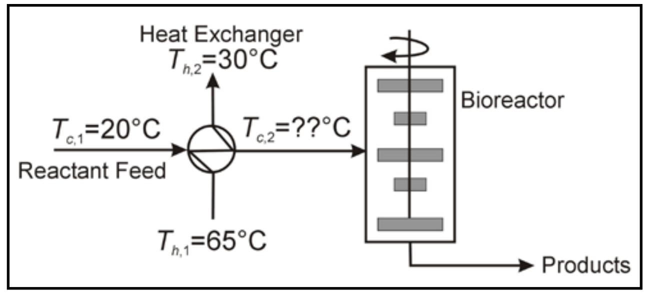

Figure 1. *Process flow diagram of the feed preheater and bioreactor.*

The design equation for the heat exchanger is given by:

$$Q = M_c C_{p,c}\left(T_{c,2} - T_{c,1}\right) = M_h C_{p,h}\left(T_{h,1} - T_{h,2}\right) = UAF\Delta T_{lm} \tag{4}$$

where

$$\Delta T_{lm} = \frac{\left(T_{h,2} - T_{c,1}\right) - \left(T_{h,1} - T_{c,2}\right)}{\ln\dfrac{\left(T_{h,2} - T_{c,1}\right)}{\left(T_{h,1} - T_{c,2}\right)}} \tag{5}$$

and

F = log-mean temperature correction factor = 0.8 (assume that this is constant for all cases)

U = overall heat transfer coefficient = 400 W/m²K

The optimum reactor inlet temperature is the one that minimizes the equivalent annual operating cost (EAOC). The EAOC is given by

$$EAOC\left[\$/y\right] = \sum_{i=1}^{2} PC_i\left[\$\right]\left(A/P, i, n\right)\left[1/y\right] + UC\left[\$/y\right] \tag{6}$$

where PC_i are the purchase equipment costs for the heat exchanger and reactor, UC is the operating (utility) cost for the heating medium, and (A/P, i, n) is the capital recovery factor given by

$$\left(A/P, i, n\right) = \frac{i\left(1+i\right)^n}{\left(1+i\right)^n - 1} \tag{7}$$

For this problem, use i = 7% and n = 12 years.

The purchase cost of the reactor is given by:

$$PC_{reactor} = \$17{,}000V^{0.85} \tag{8}$$

where V is the volume of the reactor in m³. The cost of the heat exchanger is:

$$PC_{exchanger} = \$12{,}000\left\{A\left[m^2\right]\right\}^{0.57} \tag{9}$$

where A is the area of the heat exchanger in m². The cost of the heating medium is:

$$UC\left[\$/h\right] = \$5\times10^6 Q\left[kJ/h\right] \tag{10}$$

The results should be presented as two plots. The first should show how each term in Eq. (6) changes with $T_{c,2}$, and the second plot should show the EAOC (y-axis) as a function of $T_{c,2}$ (x-axis). The report should contain a physical explanation of the reason for the trends on these plots.

Problem 2: Batch Bioreactor

Background

A liquid-phase, biological reaction is used to produce an intermediate chemical for use in the biotech industry. The reaction occurs in a large, well-stirred, isothermal bioreactor, such that the reactor temperature is identical to the inlet temperature. Because this chemical is temperature sensitive, the maximum operating temperature in the reactor is set to 55 ˚C. The feed material is fed to the reactor through a heat exchanger that increases the temperature of the reactants (contents of the reactor), which in turn increases the rate of the reaction. This is illustrated in Figure 2.

The reactor runs as a batch operation in which the contents remain in the equipment for a given period of time. The time spent in the bioreactor must be adjusted to obtain the optimal conversion of reactant. Because of the fear of contamination by pathogens and parasitic fungi, the reactor must be cleaned thoroughly between batch operations. The cleaning time per batch (t_{clean}) and the cost of cleaning both vary based on the size of the reactor used.

As the time spent in the reactor increases, the amount of product also increases but at a decreasing rate. The problem to be solved is to determine the optimum values of the two independent variables; namely, the time for the products to spend in the reactor, or the batch time, and the reactor size.

For this problem, it is assumed that only standard size vessels are available (1,000, 5,000, or 10,000 gallons), and that the costs of the feed are fixed. Therefore, the costs that vary are the revenues from sales, the reactor cost, and the cost for cleaning.

Problem Statement

It is desired to optimize the production of product from the reactor. The feed has the properties of water (ρ = 1,000 kg/m^3, Cp = 4.18 kJ/kg ˚C) and enters the heat exchanger at a temperature of 20 ˚C. The reactor feed is to be heated with a heating medium that is available at a temperature of 65 ˚C and must leave the heat exchanger at 30 ˚C. The desired reactor inlet temperature is fixed at 55 ˚C. The physical properties of the heating medium are ρ = 920 kg/m^3, C_p = 2.2 kJ/kg ˚C.

The reaction rate for this reaction, $-r_A$, is given in terms of the concentration of reactant A (C_A) by the following equation:

$$-r_A = kC_A \tag{11}$$

where

$$k\left[s^{-1}\right] = 2.5\exp\left[-\frac{3{,}500}{T\left[K\right]}\right] \tag{12}$$

The design equation for the reactor is given by:

$$t\left[s\right] = \frac{1}{k\left[s^{-1}\right]}\ln\frac{1}{1-X_A} \tag{13}$$

where t is the time spent in the reactor and X_A is the fractional conversion of reactants to products. The amount of product formed in time t is given as NX_A, where N is the number of moles of reactant fed to the reactor.

The energy balance equation for the heat exchanger is given by:

$$Q = M_c C_{p,c}\left(T_{c,2} - T_{c,1}\right) = M_h C_{p,h}\left(T_{h,1} - T_{h,2}\right) \tag{14}$$

where

M is the mass of fluid to be heated or cooled (kg)

C_p is the specific heat capacity of the fluid (kJ/kg ˚C)

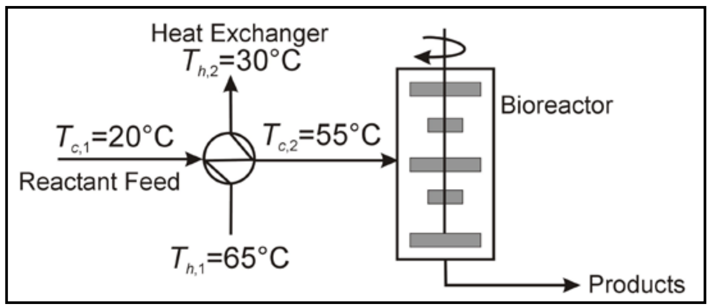

Figure 2. *Process flow diagram of feed preheater and bioreactor.*

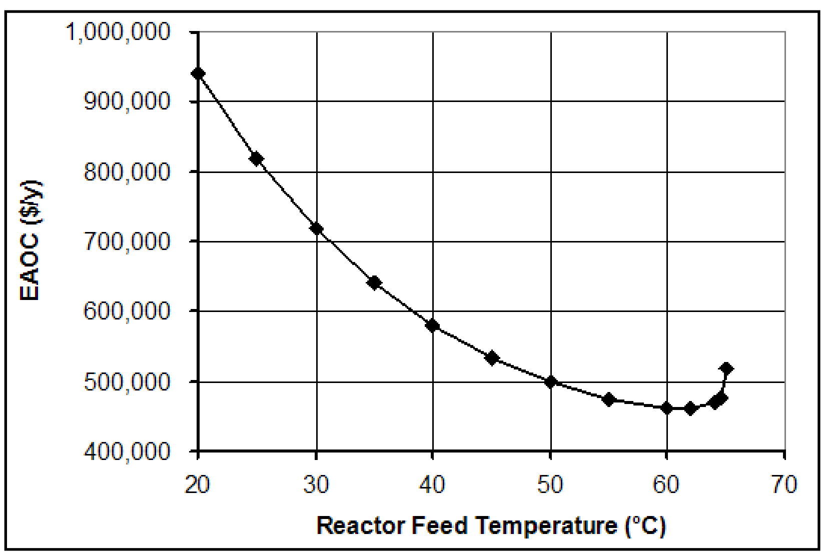

Figure 3. *Optimization plot for Example 1.*

T is the temperature (˚C)
1 and 2 refer to inlet and outlet conditions, respectively.
h and c refer to the hot and cold stream, respectively.

The optimal reactor configuration is the one that minimizes the equivalent annual operating cost (EAOC). The EAOC is given by:

$$EAOC[\$/y]=\sum_{i=1}^{2}PC_i[\$](A/P,i,n)[1/y]+\sum_{i=1}^{3}UC_i[\$/y]-R[\$/y] \qquad (15)$$

where PC_i are the purchase equipment costs for the heat exchanger and reactor; UC_i are the operating (utility) costs for the heating medium, the cost of the feed stream, and the cost of cleaning; and R is the revenue from sales of the product. For this problem, use i = 0.07 and n = 12 years.

The purchase cost of the reactor is given by

$$PC_{reactor}=\$17{,}000V^{0.85} \qquad (16)$$

where V is the volume of the reactor in m^3. The cost of the heat exchanger may be taken to be equal to 20% of the cost of the reactor from Eq. (16).

The cost of the heating medium is given by:

$$UC_{heating}[\$/h]=5\times10^{-6}Q[kJ/h] \qquad (17)$$

where Q is the heat duty obtained from Eq. (14).

The price of the feed is $2/mol, the value of the product is $10/mol, and the molar density (concentration) of both feed and product is 100 mol/m^3. The cost of cleaning the reactor is given by

$$UC_{clean}[\$/cleaning]=1{,}000[\$/cleaning]\left(1+0.5\frac{V_{reactor}[gal]}{1{,}000[gal]}\right) \qquad (18)$$

and the time to clean a reactor is

$$t_{clean}[h]=4[h]\left(1+0.5\frac{V_{reactor}[gal]}{1{,}000[gal]}\right) \qquad (19)$$

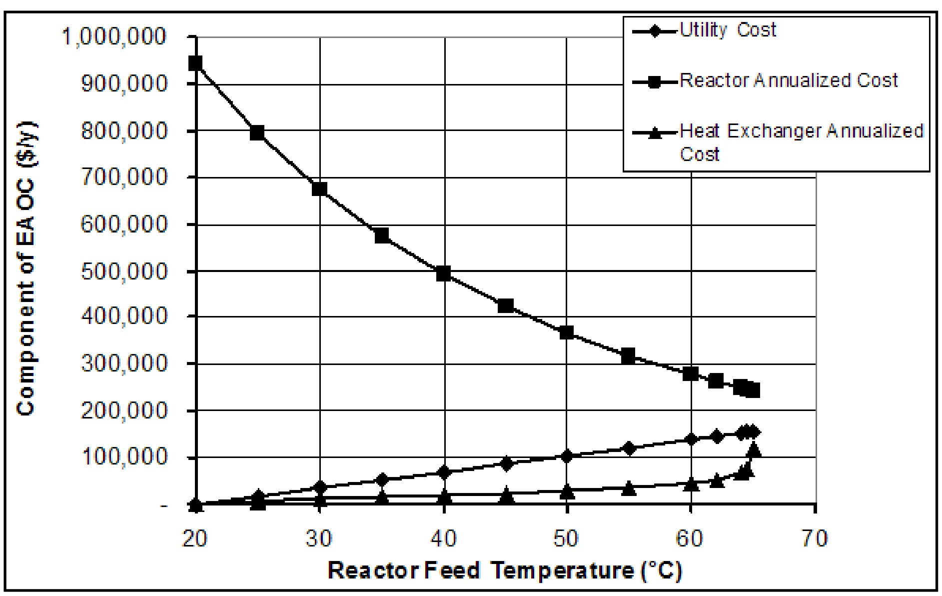

Figure 4. *Component optimization trends in Problem 1.*

The ability to solve "routine" optimization problems has been simplified by advances in computing power over the last generation.

The final results should be presented as two plots. The first plot should show how each term in Eq. (15) changes with the batch time, t, and the second plot should show the EAOC (y- axis) as a function of t (x-axis). The report should contain a physical explanation of the reason for the trends on these plots.

OPTIMIZATION PROBLEMS

In Problem 1, the optimum reactor feed temperature is to be determined. There is a trade-off, which is necessary to obtain an absolute maximum or minimum in the objective function (EAOC) as the decision variable (reactor feed temperature) varies. In this case, at higher temperatures, it costs more to heat the reactor feed, but, since the reaction rate increases with temperature, the reactor cost is lower because a smaller reactor is needed. Additionally, at higher reactor feed temperatures, a larger heat exchanger is needed. Students can develop a spreadsheet that varies the reactor inlet temperature and plot the EAOC vs. the reactor inlet temperature. This plot is illustrated in Figure 3. They can also plot EAOC vs. reactor cost, heating medium cost, and heat exchanger cost to see the trends. This is illustrated in Figure 4. The trend for the heat exchanger clearly illustrates how the heat exchanger cost goes to infinity as the reactor feed temperature approaches the heating medium inlet temperature, causing the log-mean temperature driving force to go to zero and the heat exchanger area to become infinite. This is an example of why it is important for students to analyze a series of data and understand the trends. It is possible to solve this entire problem on Excel using the Solver tool; however, much of the understanding/synthesis

Since these problems have been used successfully in a freshman class for several years, we believe they can be used anywhere in the curriculum.

of the problem is lost. We believe that optimization is more than finding an answer. An understanding of the underlying trends is essential.

It is also possible to illustrate how changes in operating conditions change the optimum. In a problem similar to Problem 1,[11] if the reaction kinetics are increased (pre-exponential factor increased to 7.0 and the activation energy reduced to 3300), the optimum temperature shifts down to about 35 ˚C. Many different versions of this and other problems can be created by changing some parameters or by changing the economics. We use different versions of these for different groups in the same class. During oral presentations, we ask them to explain why the optima differ.

In Problem 2, there are two decision variables (bivariate optimization) due to the batch processing. Therefore, this problem in slightly more complex than Problem 1, and it illustrates that there may be more than one decision variable. One decision variable is the reactor volume, which in this case is limited to three standard sizes (an arbitrary number), and the other decision variable is the processing time. The trade-off is that for longer processing times, more product is made, but fewer batches can be made per year. For a larger reactor, more product can be made per batch, but fewer batches can be made per year due to the longer cleaning time. Although this problem does not include it, the reactor feed temperature could also be varied, as in Problem 1, to create a three-variable optimization. In this problem, it turns out that the optimum is the 10,000 L reactor with a reaction time of 9.1 h, at about 97% conversion, as is illustrated in Figure 5. For higher conversions, the additional processing time is long enough to make the annual product revenue drop. This problem also illustrates some of the issues associated with batch processing to students who might be very used to continuous processes. Figure 5 also illustrates a bivariate optimization plot, with the x-axis containing one decision variable with several curves indicating the second decision variable.

DISCUSSION

We believe that an important part of the pedagogy of optimization is for students to understand the trends of the components of the objective function and to understand how trade-offs between these components lead to the existence of the optimum. That is why methods, such as using the Excel Solver, are not emphasized, and making plots to investigate trends *is* emphasized. Once the trends are understood, Excel Solver can be used to obtain a more exact value of the optimum.

We have used these problems as part of a freshman class taken by students who know that they are interested in chemical engineering. Other students take a college-wide programming class. In our class, students are taught computer skills applicable to chemical engineering, mostly using the advanced features of Excel in addition to some elementary programming techniques and algorithms. All assignments are based on industrially relevant chemical engineering problems. Some of these problems also appear in the optimization chapter of our textbook.[11] Since these problems have been used successfully in a freshman class for several years, we believe they can be used anywhere in the curriculum.

Since all students in chemical engineering do not take the class in which these problems are assigned, assessment of their long-term impact is difficult. The freshmen do a good job on these problems, and they seem to appreciate the actual chemical engineering application compared to their peers in the programming class.

Additional optimization problems are available on the web.[1] It is observed that virtually an infinite source of these problems could be obtained by manipulating some of the values given in these problems.

CONCLUSION

Two example optimization problems that are believed to be suitable for all levels of chemical engineering students have been presented. These problems do not require advanced mathematical techniques; they can be solved using typical software used by students and practitioners, such as Excel. These problems involve an economic objective function with

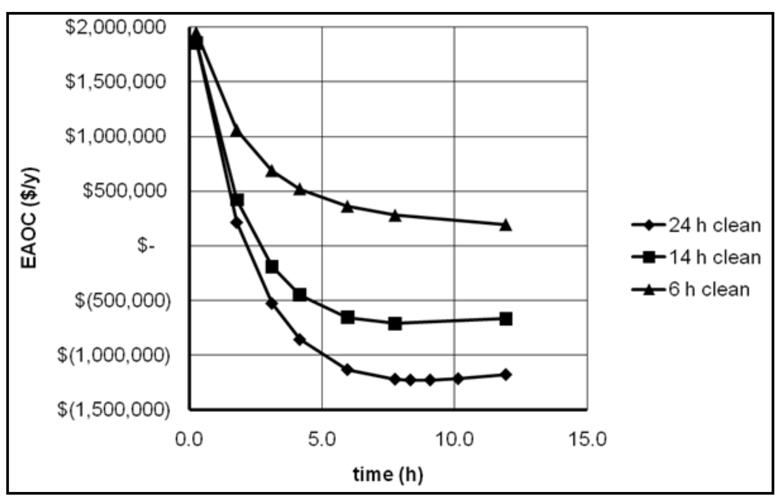

Figure 5. *Optimization plot for Example 2.*

component capital and operating cost terms. An important part of the pedagogy of these problems is an understanding of how the trends of the components terms in the objective function contribute to the trade-off involved in most optimization problems.

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