AC 2011-127: OPTIMIZATION PROBLEMS FOR ALL LEVELS

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Optimization Problems for all Levels

Introduction

Optimization is often considered to be an advanced, highly mathematical, and a somewhat obscure discipline not suited for undergraduates. While it is true that many advanced optimization techniques exist, optimization problems can be developed that are suitable for undergraduates at all levels, from freshman through seniors. Two of these problems will be described in this paper, two have been described elsewhere,[1] and many others are available on the web.[2] Sophisticated mathematical techniques are not involved; instead 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[3] 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.

Some optimization examples are routinely discussed in undergraduate textbooks; however, the objective function does not usually involve economics. These examples include optimum interstage compressor pressure[4], optimum insulation thickness[5], and identifying conditions for the optimum selectivity.[6] Qualitative representations of the economic optimum pipe diameter[7] and reflux ratio[8] are also available. The optimum interstage compressor pressure minimizes the work done. The optimum insulation thickness minimizes the heat transfer rate. The optimum selectivity maximizes production of the desired product. However, these are not necessarily economic optima. The problems presented here all involve an economic objective function.

Types of Problems

Three levels of optimization problems are available, and they are summarized in Table 1. Those highlighted in italics are discussed in this paper, and the others are available on the web.[2] 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 classes or as problem assignments for the portion of a design class where optimization is taught.

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)

Problem 1: Staged Compression

Problem Statement

Background

Compressors are used to increase the pressure of a gas. Pumps are used to increase the pressure of a liquid. In general, it is less expensive to pump a liquid than to compress a gas; therefore, in chemical plants, it is generally less expensive to change phase to a liquid or maintain the liquid phase before increasing the pressure. However, there are times when compressors cannot be avoided. For example, when using air as a source of oxygen in oxidation reactions, air must be compressed if the reaction requires high pressures.

When a gas is compressed, its density increases, but the temperature rises, lowering the density of the gas somewhat. You will learn later that the least expensive gas to compress is gas that is already compressed, a definite conundrum, because as gas pressure increases the gas density increases.

One method to reduce compression cost is to "stage" the compressors. This is illustrated in Figure 1. If multiple, "staged" compressors are used with intercooling, the temperature increase can be reduced, which keeps the gas density high and lowers the compression cost. The disadvantage is the extra equipment cost.

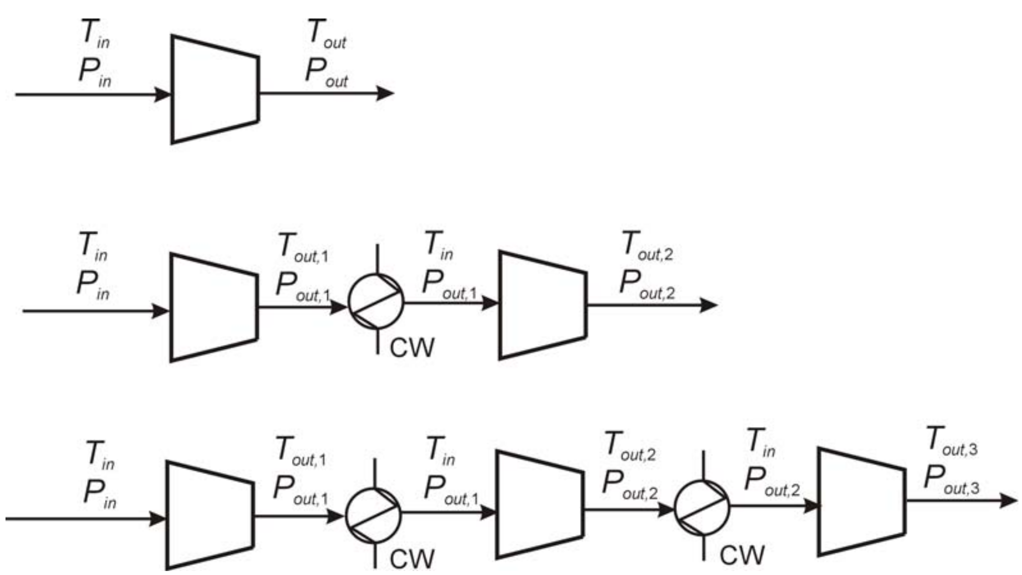

Figure 1: Single- and Multi-stage Compressor Systems

There are many types of compressors. One commonly used compressor is a centrifugal compressor. An equipment limitation of a centrifugal compressor is that the pressure ratio cannot usually exceed five.

Project Details

When designing a staged compression system, it is necessary to minimize the cost of the system. This cost is termed the Equivalent Annual Operating Cost (*EAOC*), and it is given as Equation (1). This cost includes one-time purchase costs for the compressor(s) and heat exchanger(s), the continuous operating (utility) costs (UC_i) for the cooling water used in the heat exchangers and for the electricity to run the compressors. The terms in [ ] show the units for the calculation.

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

The term ($A/P,i,n$) is the factor to convert the one-time purchase cost of equipment into an equivalent annuity. You should assume that the effective annual interest rate, i, is 7% p.a., and that the length of the project, n, is 10 years. The equation for ($A/P,i,n$) is:

$$(A/P,i,n) = \frac{i(1+i)^n}{(1+i)^n - 1} \tag{2}$$

Assignment

You are to optimize a compression system by determining the optimum number of stages. A stage consists of one compressor and one intercooler, with no cooler for a single-stage compressor or after the last compressor. Therefore, for n stages of compression, there are $n - 1$ coolers. The feed to the first compressor is air at 25°C. The goal is to compress 4000 kg/h air (C_p = 1.0 J/g K) from atmospheric pressure (assume to be 1 bar = 100 kPa) to 30 bar. As a general rule, the compression ratios (P_{out}/P_{in}) for all staged compressor are equal. Cooling water (C_p = 4.184 J/g K) is used in the heat exchangers to cool the air, and the cooling water enters at 30°C and is returned at 40°C. For the first optimization, assume that the compressed air exiting any intercooler is at 50°C, and determine the optimum number of compressor stages. Then, continue the optimization to determine both the optimum number of compressor stages and the optimum air temperature exiting each intercooler (assume all are the same).

The power required to run a compressor is

$$\dot{W}[\text{W}] = 3600\dot{m}[\text{kg/s}]\left(T_{out} - T_{in}\right) \tag{3}$$

where $\dot{m}$ is the mass flowrate of air, the temperatures are in Kelvin, and

$$T_{out} = T_{in}\left(\frac{P_{out}}{P_{in}}\right)^{0.286} \tag{4}$$

The cost of electricity to run the compressors (UC_{elec}[\$/y]) can be calculated from the power in Equation 3 and the cost of electricity, which is 0.07/kWh. A year is assumed to be 8000 h, which allows for about one month of plant shut down for maintenance.

The purchased cost of each compressor is given by:

$$PC_{comp}[\$] = \$15.9\left(\dot{W}[\mathrm{W}]\right)^{0.8} \tag{5}$$

The design equation for the heat exchanger is given by:

$$\begin{aligned} &Q[\mathrm{W}] = \dot{m}_{air}[\mathrm{kg/s}]C_{p,air}[\mathrm{J/kg\ K}]\left(T_{air,in} - T_{air,out}\right) = \\ &\dot{m}_{cw}[\mathrm{kg/s}]C_{p,cw}[\mathrm{J/kg\ K}]\left(T_{cw,out} - T_{cw,in}\right) = U[\mathrm{W/m^2K}]A[\mathrm{m}^2]F\Delta T_{lm} \end{aligned} \tag{6}$$

where

$$\Delta T_{lm} = \frac{\left(T_{air,in} - T_{cw,out}\right) - \left(T_{air,out} - T_{cw,in}\right)}{\ln \dfrac{\left(T_{air,in} - T_{cw,out}\right)}{\left(T_{air,out} - T_{cw,in}\right)}} \tag{7}$$

and

$F = 0.8$ (assume that this is constant for all cases)

U = overall heat transfer coefficient = 100 W/m^{2}K

The cost of the heat exchanger is based on its area, which can be calculated by solving for A in Equation 6. The cost equation is

$$PC_{hx}[\$] = \$12{,}000\left(A[\mathrm{m}^2]\right)^{0.57} \tag{8}$$

The cost of cooling water is given by:

$$UC_{cw}[\$/\mathrm{h}] = 2.5\dot{m}_{cw}[\mathrm{kg/s}] \tag{9}$$

You should present your final results as three plots. The first should show how each term in Equation 1 changes with the number of stages, and the second should show the optimization for a constant compressor stage inlet temperature of 50°C after the first compressor. The third should show the two-variable optimization for number of compressor stages and compressor stage inlet temperature. Your report should contain a physical explanation of the reason for the trends on these plots.

Discussion of Problem 1

In Problem 1, the optimum compressor configuration is to be determined. There are two decision variables, the number of compressors and the temperature to which the stream is to be cooled between stages. Since cooling water at 30°C is used as the heat sink, the temperature to which the stream can be cooled is limited. There is a trade-off, which is necessary to obtain an absolute maximum or minimum in the objective function (EAOC) as the number of compressors varies. Figure 2 shows how the components of the objective function change with the number of stages. As the number of compressors increases, the compressor cost stays roughly constant, since, while more compressors are needed, they are smaller. The electricity cost decreases slightly, since it is always less expensive to compress a colder (more dense) stream. With more interstage heat exchangers, the cooling water cost and the heat exchanger purchased cost both increase. The optimization plot for an interstage temperature of 50°C is not shown here, but the optimum number of stages is either 3 or 4, because the EAOCs are almost identical. Figure 3 shows the bivariate optimization plot. The lowest temperature shown is the optimum, based on the electricity cost, and four compressor stages is optimum. Although it is not shown on this optimization plot, as the interstage temperature decreases below 34°C, the relative cost of the heat exchangers is small enough that the EAOC continues to decrease until the interstage temperature is below 30.5°C. This is an artifact of keeping the log-mean temperature correction factor (*F*) constant, because, in reality, as the interstage temperature decreases, additional shell passes would be needed, which increase the cost of the heat exchangers. By changing the heat exchanger cost or by including the effect of the close temperature approach, this optimum could be moved. Hence, there are many variations possible for a single optimization problem.

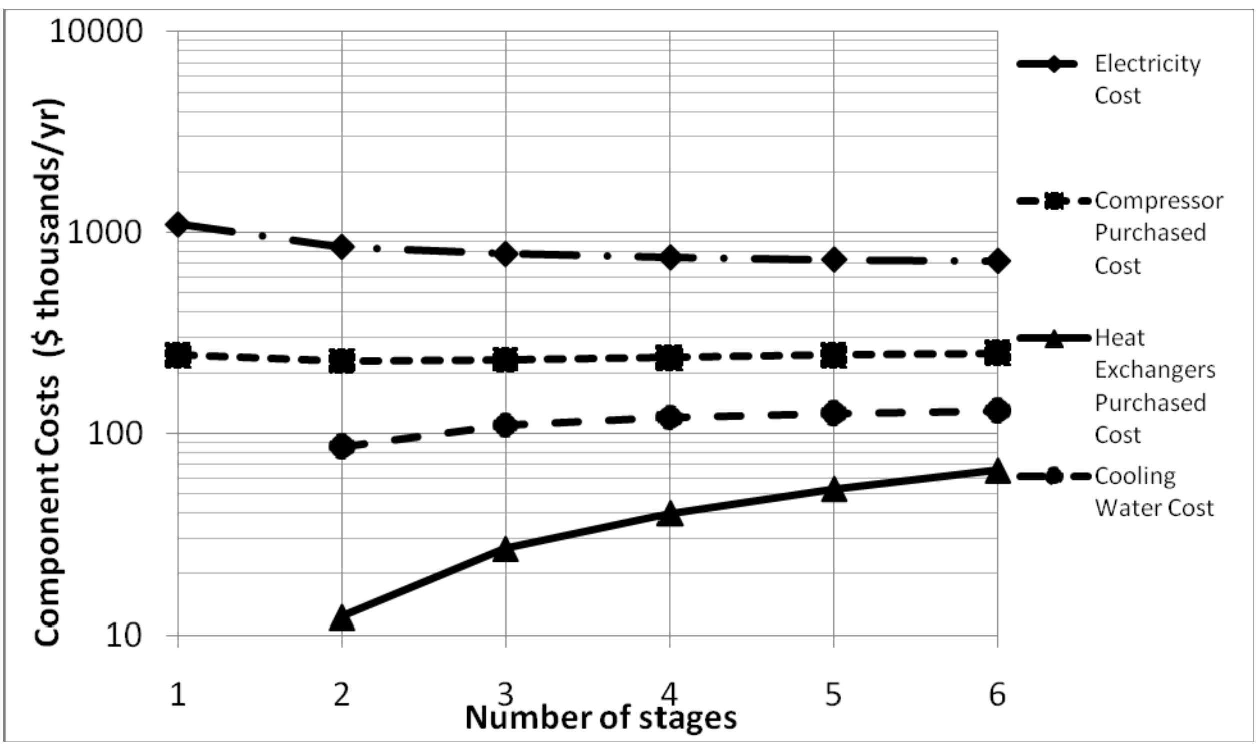

Figure 2: Annual Cost of Components of EAOC for Multi-stage Compression

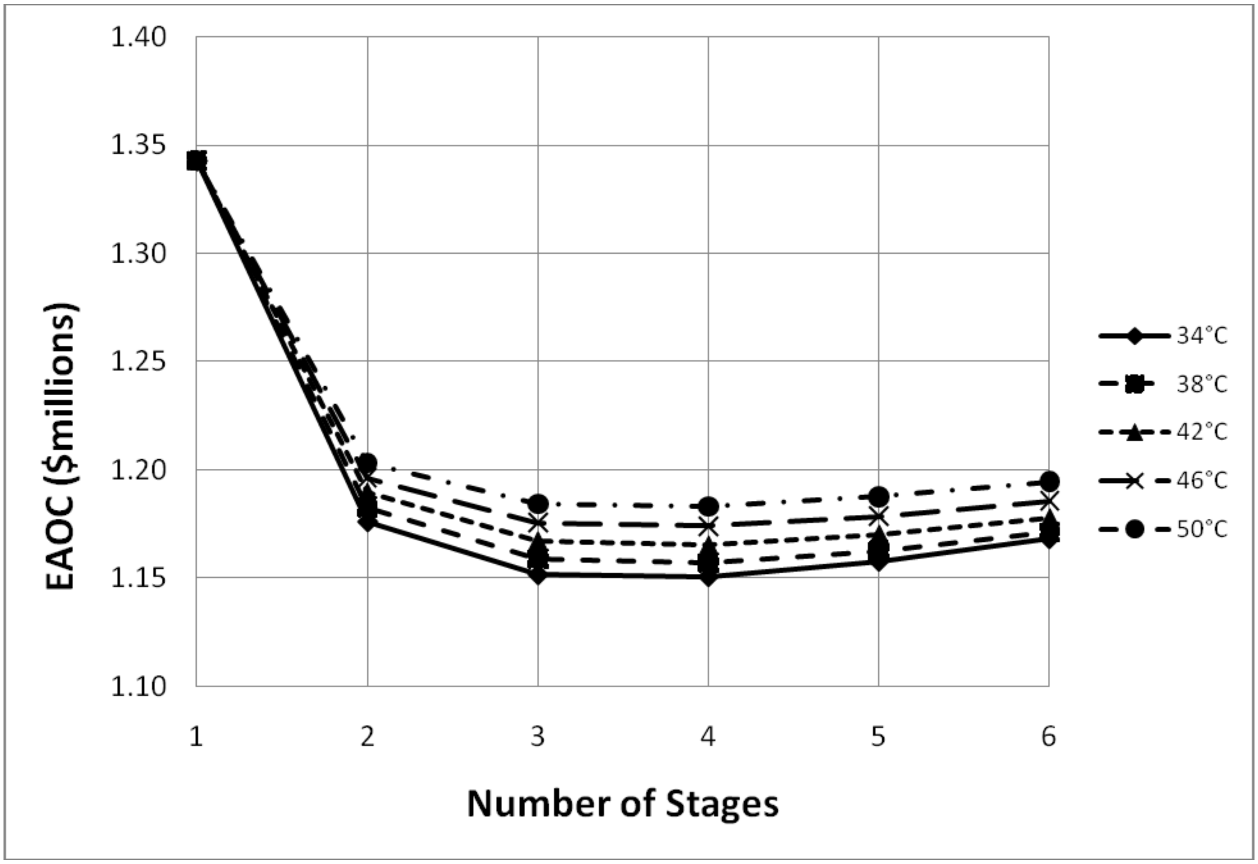

Figure 3: Bivariate Optimization Plot for Compressor Optimization

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Problem 2: Chemical Process

Problem Statement

Introduction

All chemical and biochemical processes have a similar structure. The goal is to create a more-valuable product from a less-valuable raw material while maximizing the profit. The generic process structure involves five steps: 1. reactor feed preparation, 2. reaction, 3. separator feed preparation, 4. separation, and 5. recycle. In this project, you will analyze a generic process to determine the optimum process parameters.

Background

The generic process flow diagram is shown in Figure 4. The raw material is A, but the feed stream contains 20 mole% inerts, I (non-reactive impurities), at a total flowrate of 100 kmol/h and 50°C. The feed stream is mixed with recycled, unreacted A and then preheated to at least

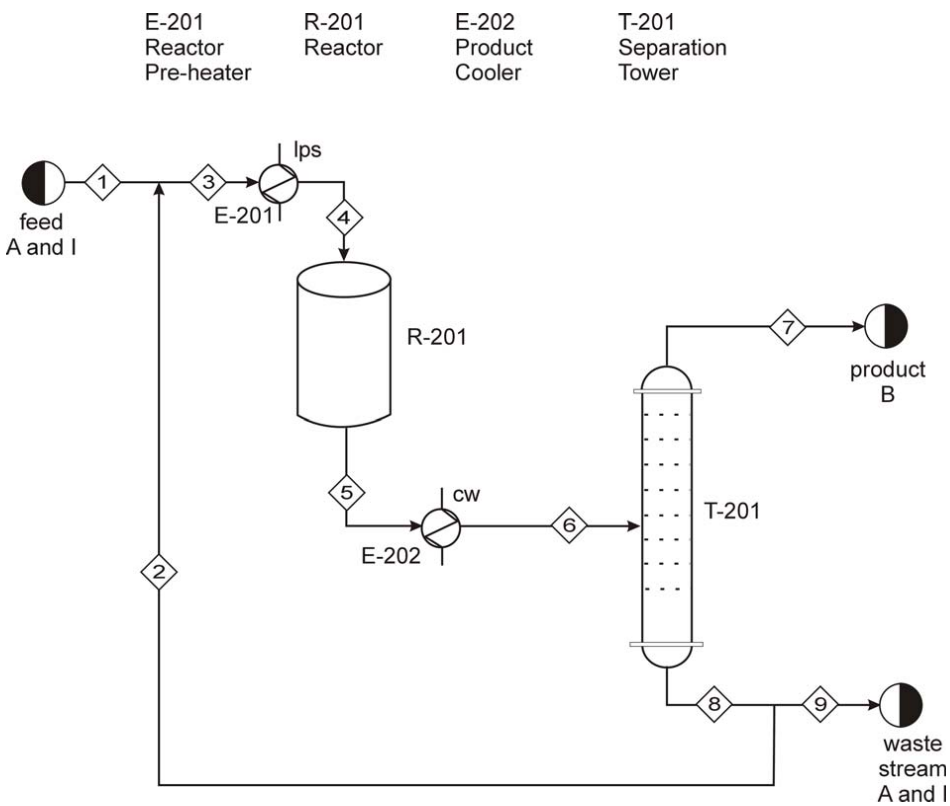

Figure 4: Generic Process Flow Diagram for Unit 200

75°C but no more than 155°C before entering the reactor. The heat source is low-pressure steam at 160°C that condenses at constant temperature. In the reactor, the reaction that occurs is A→B, with a maximum possible conversion of 95%. The reactor is adiabatic (meaning that no heat is added or removed), and it may be assumed that the temperature rise within the reactor is 50°C. The reactor effluent must be cooled to 50°C, in E-202, using cooling water (C_p = 4.184 kJ/kg°C) entering at 30°C and exiting at 40°C. The separator is assumed to be ideal (There is no such thing in reality!), and pure product B leaves in Stream 7, while all A and I go to Stream 8. Since not all of the valuable reactant, A, is reacted, it can be recycled rather than discarded (Stream 2). However, since there is some inert, *i.e.*, a component that does not react, there must be a purge stream (Stream 9) to avoid an uncontrolled increase of I in the system. It may be assumed that all process streams have the same properties: ρ = 900 kg/m^3 and C_p = 2.1 kJ/kg°C. The molecular weights of A and B are 100 kg/kmol and the molecular weight of I is 50 kg/kmol. The heat of vaporization of condensing steam is 2100 kJ/kg.

An Excel file has been provided that does the material balance calculations for this process. As you change the fractional conversion in the reactor and/or the fraction of Stream 8 that is recycled to Stream 2, the molar flowrates of each stream are updated. You should use this spreadsheet as your starting point and add the additional calculations necessary to optimize the process.

Economic Data

As in previous projects, the objective function for your optimizations is the equivalent annual operating cost (EAOC) of purchasing and installing the equipment and operating the process.

$$EAOC[\$/\text{y}] = \sum PC_i[\$](A/P,i,n)[1/y] + \sum OC_i[\$/y] \tag{10}$$

where PC_i is the cost of each piece of equipment, and OC_i is each operating "cost," which includes the revenue from selling B (a negative cost), the cost of purchasing A, the cost of steam, and the cost of cooling water.

You should assume that the project lifetime is 12 years at an interest rate of 11%. A year is assumed to be 8000 hours

Capital Investment Costs and Method for Calculation

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

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

where

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

and T is the average temperature in the reactor. The design equation for the reactor is given by:

$$V = \frac{v_o X_A}{k(1 - X_A)} \tag{13}$$

where V is the reactor volume (m^3), v_o is the volumetric flowrate of fluid into the reactor (m^3/s), and X_A is the fractional conversion. The design equation for the heat exchangers is given by

$$Q[\mathrm{W}] = \dot{m}_i[\mathrm{kg/s}]C_{p,i}[\mathrm{J/kg\ K}]\left(\left|T_{out} - T_{in}\right|\right) = U[\mathrm{W/m^2K}]A[\mathrm{m}^2]F\Delta T_{lm} \tag{14}$$

for streams undergoing a temperature change, or for streams undergoing a phase change (either evaporating or condensing)

$$Q[\mathrm{W}] = \dot{m}_i[\mathrm{kg/s}]\left|\Delta H_{vap}\right|[\mathrm{kJ/kg}] = U[\mathrm{W/m^2K}]A[\mathrm{m}^2]\Delta T_{lm} \tag{15}$$

where

$$\Delta T_{lm} = \frac{\left(T_{h,in} - T_{c,out}\right) - \left(T_{h,out} - T_{c,in}\right)}{\ln\left[\frac{T_{h,in} - T_{c,out}}{T_{h,out} - T_{c,in}}\right]} \tag{16}$$

and

F = 1.0 for E-201, F = 0.8 for E-202
U = overall heat transfer coefficient = 1000 W/m^{2}K
c, h = cold and hot stream, respectively

The cost of a heat exchanger is based on its area, which can be calculated by solving for A in either Equation 14 or 15. The cost equation is

$$PC_{hx}[\$] = \$12{,}000\left(A[\mathrm{m}^2]\right)^{0.57} \tag{17}$$

The cost of the reactor may be estimated by

$$PC_{reactor}[\$] = \$20{,}000\left(V[\mathrm{m}^3]\right)^{0.85} \tag{18}$$

The cost of the separator may be estimated by

$$PC_{tower}[\$] = 2{,}000\left(\dot{m}[\mathrm{kg/h}]\right)^{0.65} \tag{19}$$

Operating Costs

The cost of cooling water is

$$UC_{cw}[\$/\mathrm{kg}] = 1.48 \times 10^{-5} \tag{20}$$

and the cost of steam is

$$UC_{stm}[\$/\text{GJ}] = \$13.00 \tag{21}$$

The raw material A (containing I) is valued at \$0.50/kg (total stream flowrate), and the product B is valued at \$0.70/kg (revenue, hence a negative cost).

Stream 9 is a waste stream, and its fate must be considered. At this time, we are unsure of how this stream will be handled. If it can be burned for fuel, the fuel value is

$$UC_{burn}[\$/\text{kg of A}] = \$0.6 \tag{22}$$

based on the amount of A in the stream, since the inert will not burn. This is a revenue (a negative cost). If it has to be treated, the cost is

$$UC_{treat}[\$/\text{kg}] = \$0.036 \tag{23}$$

You should feel free to suggest additional process improvements that would enhance profitability.

Discussion of Problem 2

In this problem, there are three decision variables, the single-pass conversion, the recycle/purge split, and the reactor inlet temperature. Therefore, it is difficult to illustrate the solution on a single plot. Figure 5 is a plot of the effect of reactor inlet temperature on the EAOC for different recycle fractions (fraction of Stream 8 recycled). The fractional, single-pass conversion is at a constant value of 0.93, which further investigation would demonstrate is the optimum. Illustration of this three-variable optimum would require either multiple plots or a three-dimensional plot. Figure 5 is illustrative, because the optimum is not an absolute maximum or minimum with temperature. In this problem, since low-pressure steam at 160°C is the heating utility, 155°C was set as the maximum allowable reactor inlet temperature. Of course, the problem could be changed to allow different steam levels.

The trade offs are as follows. The highest reactor temperature is best because the reactor cost is large and the highest allowable temperature minimizes the reactor cost. If the single-pass conversion is too low at a fixed recycle/purge split, more reactant is needed to produce a fixed amount of product, or less product is produced for a fixed feed. As the recycle/purge split increases, the load on the reactor preheater increases as does the reactor volume, due to the larger amount of material within the recycle loop. As the recycle split decreases, more reactant is lost, so the cost increases.

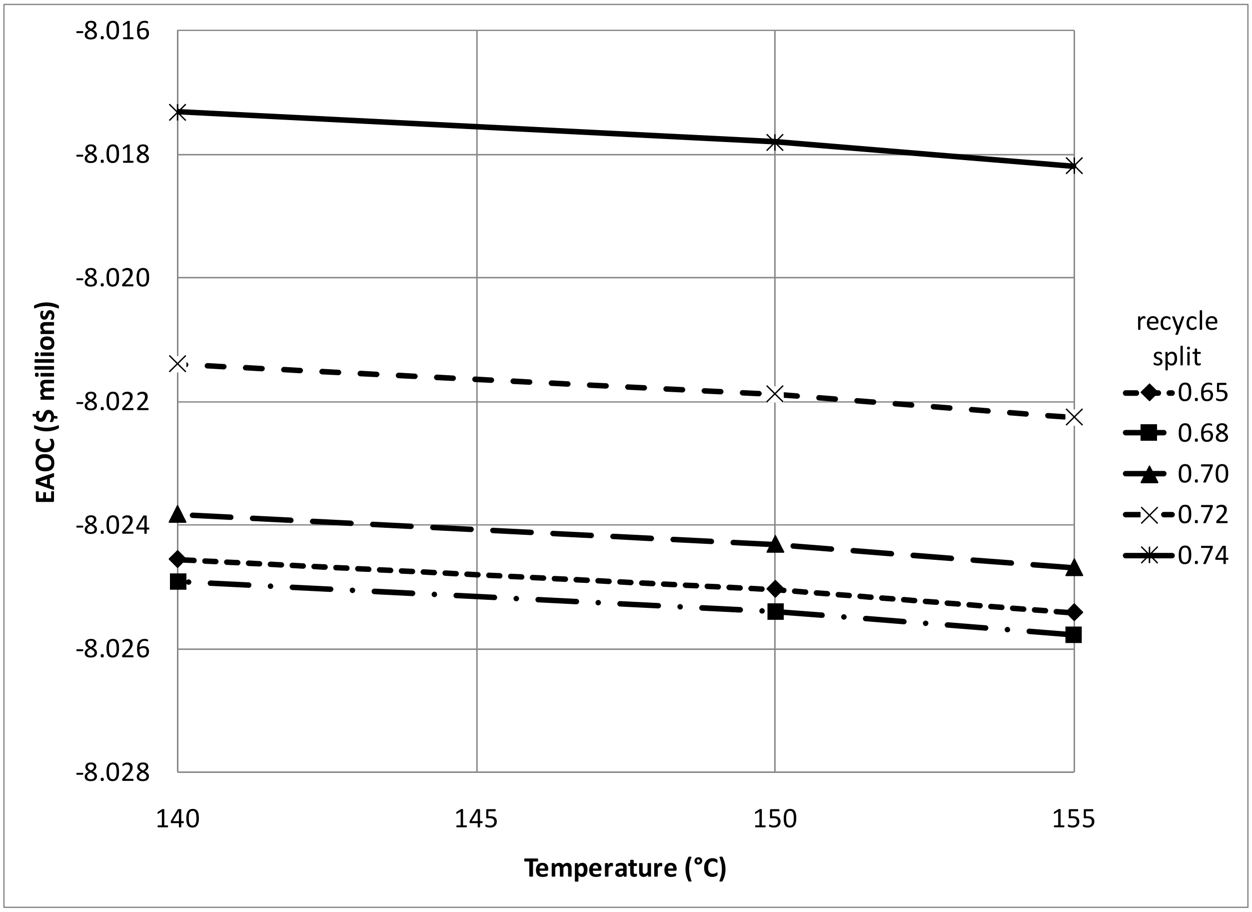

Figure 5: Parametric Optimization of Reactor Inlet Temperature and Recycle Fraction

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General Discussion

The problems discussed here are among the more complex of the optimization problems available. Univariate optimization problems like reflux ratio optimization and pipe diameter optimization are available on the web site,[2] and a univariate optimization problem is discussed in more detail elsewhere.[1] In these simpler problems, it is expected that students would be able to explain the trade off between number of stages and reflux ratio, or the trade-off between pump cost plus pumping utility cost and pipe cost.

It is also observed that these problems have been simplified somewhat, since they are used mostly in a freshman class. It would not be difficult to add complexity to these problems in higher level classes. For example, the compressor problem could be made more complex by allowing refrigerated water as an option, and the chemical process problem could be made more complex by allowing different types of steam. Our seniors are expected to be able to analyze an entire chemical process, taking results from a process simulator and performing a comprehensive economic analysis to that in Problem 2. Problems like those illustrated here provide training so that students can perform the more advanced process economic analysis.

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, the Excel solver can be used to obtain a more exact value of the optimum.

Assessment

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. Since these problems have been used successfully in a freshman class for several years, we believe they can be used anywhere in the curriculum. Some of these problems also appear as end-of-chapter problems in our design textbook.[9]

The successful use of these problems in the freshman class, where successful is defined as the students being able to obtain a valid solution, is the only assessment currently available. When a "simple" optimization problem (usually single variable, perhaps some two-variable problems for students in our Honors College) is assigned, students are coached until they obtain a valid solution. The level of coaching required differs, depending on the individual's computing background and ability. When a more complex, multivariate problem is subsequently assigned, there is less coaching needed on the optimization portion, but more coaching needed on the technical aspects of the problem, since the students are only freshmen. Feedback suggests that the freshmen appreciate the chemical engineering applications compared to their peers in the programming class. Design problems involving optimization are assigned throughout our curriculum.[10] Optimization is taught again in a sophomore numerical methods class, and we believe that optimization is a skill that all of our graduates possess. Since all students in chemical engineering do not take the freshman class in which these problems are assigned, and since the topic is taught again, assessment of the long-term impact of including these problems in the freshman class is difficult.

Conclusion

An array of optimization problems that are believed to be suitable for all levels of chemical engineering students are available. 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 component capital and operating cost terms. An important part of the pedagogy of these problems is an understanding 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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