ChE curriculum

DESIGN EDUCATION IN CHEMICAL ENGINEERING

PART 1: Deriving Conceptual Design Tools

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MOST OF THE CHEMICAL engineering curriculum is focused on the analysis of either engineering science problems or single unit operations. That is, very well-defined physical systems that normally involve chemical (or biological) reactions and/or separations, are investigated in considerable detail. Students usually do not encounter any synthesis problems until their senior year design course, where one of the goals is to integrate the complete curriculum by demonstrating how the individual process units fit togther into a large system, *i.e.*, a chemical process. However, because of time constraints, usually only a narrow range of design problems is considered.

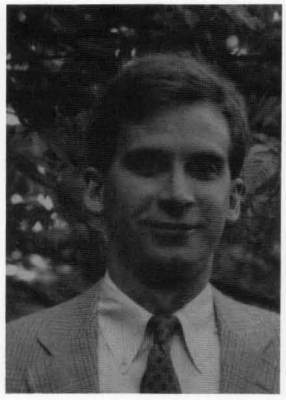
The purpose of this paper is to describe the spectrum of process design problems and to suggest a methodology for teaching the important concepts used in design. The topics that will be considered are: the types of processes considered and their designs, some new tools that are useful in conceptual design, and a strategy for developing conceptual designs.

CLASSIFICATION OF PROCESSES

We can classify processes in a variety of ways, including the type of operation, what they produce, and the types of products they make. There are two main types of operations: continuous and batch. Continuous processes are designed to operate twenty-four hours a day, seven days a week, for 300 to 350 days a year, and hopefully, nothing changes with time. In contrast, batch plants contain units that are deliberately started and stopped according to some schedule. They may operate twenty-four hours a day, or they might be designed to operate for only a single shift. Batch plants are more flexible, but they are usually less efficient than continuous processes. In general, continuous processes are associated with large production capacities, whereas batch plants are associated with specialty chemicals.

Another way of classifying processes depends on the number of products they produce. Some plants produce only a single product stream, whereas others might produce several products simultaneously. Still others might produce different products in the same equipment, but at different times of the year.

We can further define a process based on the characteristics of the product. Sometimes we may wish to produce pure chemical compounds (petrochemical processes), while at other times the final product is a mixture (there are hundreds of com-



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Experience indicates that less than 1% of the ideas for new designs ever becomes commercialized. In order to avoid expensive failures, it is common practice for process engineers to develop a heirarchy of designs where the accuracy of the design calculations and the amount of detail considered increases as the next level in the heirarchy is considered.

pounds in gasoline or furnace oil streams). In still other instances we produce materials that are described by distribution functions (solid products are usually characterized by a particle size distribution, and polymer products are normally characterized as a function of their molecular weight distribution.

Since such a wide variety of processes exists, it is not surprising that different design techniques and criteria are applicable. Moreover, it should be apparent that there is not enough time in an undergraduate's program to discuss all of these types of problems. Thus, it has been common practice to have undergraduates consider the design of only one type process (usually a petrochemical process that produces a single, pure product) in the design course.

A GENERAL STRATEGY FOR APPROACHING DESIGN PROBLEMS

Experience indicates that less than 1% of the ideas for new designs ever becomes commercialized. In order to avoid expensive failures, it is common practice for process engineers to develop a hierarchy of designs where the accuracy of the design calculations and the amount of detail considered increases as the next level in the hierarchy is considered (see Table 1, from [2]). The design course in chemical engineering looks at Level 2 for a single process. That is, the students are given a flowsheet, *i.e.*, a description of the process units and the interconnections between these units. They calculate the process material and energy balances, the required equipment sizes, the utility flows, the capital and operating costs, and the process profitability. The design calculation routines used are fairly rigorous so that obtaining a solution normally requires extensive iteration, which often becomes quite tedious.

Most design research has focused on Levels 2 and 3 in the hierarchy. The emphasis has been on the development of improved algorithms for the rigorous design of a variety of types of equipment or complete flowsheets. Similarly, improved optimization procedures for various types of problems have received considerable attention.

Level 1 in the hierarchy of Table 1, also known as the conceptual design phase, is usually undertaken by experienced engineers. They use numerous heuristics and back-of-the-envelope calculations to develop the first design, *i.e.*, the base-case design, and then to screen the process alternatives. In some companies an engineer is sent to a chemist's laboratory as soon as the chemist has discovered a new reaction or a new catalyst, and the engineer is expected to complete a base-case design within a period of two days to one week. The results of this design study are then used to help guide the development of the project.

TABLE 1
Types of Designs

1. Order of magnitude estimate *(Error about 40%)*
2. Factored estimate *(Error about 25%)*
3. Budget authorization estimate *(Error about 12%)*
4. Project control estimate *(Error about 6%)*
5. Contractor's estimate *(Error about 3%)*

TEACHING CONCEPTUAL DESIGN

Conceptual design is a creative activity where the goal is to find the best flowsheet from a large number of process alternatives. If one were to blindly consider all of the possible alternatives, it would be necessary to consider something like 10^4 to 10^9 flowsheets. According to Westerberg [4], each flowsheet is described by about 10,000 to 20,000 equations, and there are usually ten to twenty optimization variables associated with each alternative. It is necessary to compare these alternatives at close to the optimum design conditions in order to determine the best flowsheet. Typical of design problems in other disciplines, chemical process design problems are characterized by the combinatorially explosive nature of the possible solutions.

The question then arises as to whether it is possible to teach undergraduates how to complete a first design in a two-day to one-week period, and how to determine the best flowsheet in another two-day to one-week time frame. This requirement implies that it will be necessary to teach them how to derive back-of-the-envelope calculation procedures and how to derive heuristics, since these are the tools used by experienced engineers. It will also be necessary to teach the undergraduates a systems approach to synthesis which emphasizes the interactions that may occur when we put a complete process together. A discussion of some new tools of this type follows.

DERIVING BACK-OF-THE-ENVELOPE DESIGN MODELS

Chemical engineers are used to having a hierarchy of models, with increasing orders of complexity and accuracy, available for solving various problems. For example, the Navier-Stokes equations used in fluid mechanics are sufficiently complex that it is necessary to use order-of-magnitude (or scaling) arguments to simplify them in order to obtain an answer. It is surprising that no one seems to have attempted to use this same approach to simplify models in other problem areas, such as equipment or process design.

One could use order-of-magnitude arguments to derive a back-of-the-envelope model for an isothermal, plate-type gas absorber used to recover solutes from a dilute feed stream. For this special class of absorber problems there is an analytical solution, called the Kremser equation [1], which most undergraduates have studied.

$$N + 1 = \frac{\ln\left\{\left[\frac{L}{mG} - 1\right]\left[\frac{Y_{in} - mX_{in}}{Y_{out} - mX_{in}}\right] + 1\right\}}{\ln\left[\frac{L}{mG}\right]} \qquad (1)$$

We would like to develop a short-form of this equation to further simplify our analysis. Since we do not need great accuracy for conceptual design (see Level 1 in Table 1) our criterion will be to drop any term that does not affect the answer by more than 10%.

We first note that most gas absorbers encountered in practice contain 10 to 20 trays, and therefore we are interested in obtaining accurate solutions when N is of the order of 10 to 20. When we examine Eq. (1) we see that order-of-magnitude arguments yield

$$N + 1 = N \qquad (2)$$

For gas absorbers with pure solvent streams, $X_{in} = 0$. From other arguments it can be shown that $L/mG = 1.4$, approximately, and that $Y_{in}/Y_{out} = 100$, or so. When we compare the orders-of-magnitude of the terms in the numerator on the right-hand-side of Eq. (1), we see that

$$\ln\left\{\left[\frac{L}{mG} - 1\right]\left[\frac{Y_{in}}{Y_{out}}\right] + 1\right\} = \ln\left[\frac{L}{mG} - 1\right]\left[\frac{Y_{in}}{Y_{out}}\right] \qquad (3)$$

Since $L/mG = 1.4$, we could replace the denominator in Eq. (1) by its Taylor series expansion and write, approximately

$$\ln\left[\frac{L}{mG}\right] = \left[\frac{L}{mG} - 1\right] = 0.4 \qquad (4)$$

Our result becomes, after replacing $\ln$ by $\log$

$$N = \frac{2.3 \log\left[\frac{L}{mG} - 1\right]\left[\frac{Y_{in}}{Y_{out}}\right]}{0.4} \qquad (5)$$

If we are willing to sacrifice accuracy for simplicity, the final form is

$$N + 2 = 6 \log \frac{Y_{in}}{Y_{out}} \qquad (6)$$

and we have achieved our goal of developing a back-of-the-envelope model.

Of course, it is essential to check our simple model against the more rigorous expression. For the case of 99% recoveries, where $Y_{in}/Y_{out} = 100$, Eq. (6) predicts 10 trays versus the rigorous value of 10.1, and for 99.9% recoveries where $Y_{in}/Y_{out} = 1000$, Eq. (6) gives $N = 16$ versus the correct value of 16.6. We have used this same procedure to develop short-cut models for process material and energy balances, a variety of equipment design procedures, cost expressions, *etc.*

DERIVING ERROR BOUNDS FOR DESIGN MODELS

The simple models used to describe process units or other physical relationships normally have specific limitations (*i.e.*, the Kremser equation is valid for isothermal, dilute systems and the ideal gas law is valid only for low molecular weight, non-polar materials at low pressure). Of course, students need to know when they can use these simplified models and it is easy to quantify when these approximations are valid simply by applying Taylor series expansions. For example, in order to assess the validity of the assumption of dilute, isothermal operation in a plate-type gas absorber, we can use Taylor series expansions around the condition of infinite dilution, along with some back-of-the-envelope approximations (*i.e.*, that high recoveries are equivalent to complete recovery) to show that the value of the distribution coefficient will change by less than 10% if

$$Y_{in}\left(1 + \left\{2\left(A_{21} - 2A_{12}\right) + \frac{\Delta H_v^2}{RC_p T_L^2}\right\}\right) < 0.1 \qquad (7)$$

Thus, the dilute, isothermal assumption depends on the heat of vaporization of the solvent, as well as the inlet solute composition. We can develop a similar expression for how this assumption affects the number of plates required in the absorber by considering how

changes in m affect N in Eq. (1). This approach is simple to teach, and it provides a way of making decisions that can be used instead of experience.

DERIVING DESIGN HEURISTICS

Design heuristics were originally proposed by experienced engineers who solved similar problems many times, and then noticed common features of the solution. At the present time, however, they are being developed by graduate students who solve hundreds of case studies on a computer and then attempt to generalize the results (see Tedder and Rudd [3]). The fact that heuristics exist implies that their solutions must be insensitive to almost all of the design and cost parameters. Therefore, by eliminating these insensitive terms using order-of-magnitude arguments, it should be possible to derive heuristics.

As an example of a derivation of a heuristic, we again look at the design of the simple gas absorber problem that we considered above. The number of trays selected for the gas absorber depends on an economic trade-off, *i.e.*, as we increase the number of trays we increase the cost of the absorber, but we decrease the amount (and therefore the value) of the material that is not recovered. If we express the capital cost of the absorber on an annualized basis and assume that the total cost depends only on the number of trays and the annual value of the lost solute, we obtain

$$TAC = (C_s)(G)(Y_{in})\left(\frac{Y_{out}}{Y_{in}}\right)(8150\ hr/yr) + (C_N)(N) \quad (8)$$

Now if we substitute Eq. (6) for N and find the optimum value of Y_{out}/Y_{in}, we obtain

$$\frac{Y_{out}}{Y_{in}} = \frac{(6)(C_N)}{(C_s)(G)(Y_{in})(8150\ hr/yr)} \quad (9)$$

and by substituting some reasonable values for the parameters, we find

$$\frac{Y_{out}}{Y_{in}} = \frac{(6)(850)}{(15.4)(10)(8150)} = 0.004 \quad (10)$$

The important feature of this result is not the expression for the optimum, but the insensitivity of the solution. We note that if we make a 100% change in any of the values in either the numerator or denominator, the answer changes only from 0.002 to 0.008, which corresponds to fractional recoveries in the range from 99.2% to 99.8%. This is the basis for the well known heuristic:

It is desirable to recover more than 99% of all valuable materials.

With this simple procedure we have been able to derive most of the current heuristics used in process design, and have also been able to discover new heuristics for other design problems. Again, since we derive our heuristics, the assumptions made in the derivations will help to indicate the limitations of their applicability.

CONCLUSIONS

With the new techniques described above, the engineer now has the tools available to quickly evaluate flowsheet alternatives. In Part II of this article [which will be published in the next issue of *CEE*] we will describe how these tools, along with a hierarchical decomposition procedure to generate flowsheet alternatives, are used in a systems approach to conceptual design.

NOMENCLATURE

A_{ij} = Margules constants of the solute and solvent at infinite dilution
C_N = annualized absorber cost per plate, \$/plate
C_p = heat capacity, Btu/mol-F
C_s = value of solute, \$/mol
G = carrier gas flowrate, mol/hr
ΔH_v = heat of vaporization of solute, Btu/mol
L = solvent flowrate, mol/hr
m = slope of equilibrium line
N = number of theoretical plates
R = ideal gas constant, Btu/mol-F
TAC = total annualized cost, \$/yr
T_L = solvent temperature, deg. F.
X = mole fraction of solute in liquid
Y = mole fraction of solute in gas

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