Award Lecture

DESIGN RESEARCH

Both Theory and Strategy

The 1981 ASEE Chemical Engineering Division Lecturer is Arthur W. Westerberg of Carnegie-Mellon University. The 3M Company provides the financial support for this annual lecture award.

A native of Minnesota, Art received his B.Sc. from the University of Minnesota in 1960, his M.Sc. from Princeton in 1961 (both in chemical engineering), and his Ph.D. in 1964 from Imperial College, London.

Returning to Minnesota, he was president of a consulting company for nine months before joining Control Data Corporation as a senior analyst in their process control division. In 1967 an interest in teaching and research drew him to academia and he joined the chemical engineering department at the University of Florida.

In 1974-75, he spent a sabbatical at the Computer Aided Design Centre in Cambridge, England, at which time he coauthored Process Flowsheeting, *a unique book devoted to elucidating the underlying structures and their advantages for available and proposed flowsheeting programs.*

In 1976 Art joined Carnegie-Mellon University where he served as director of the Design Research Center until becoming head of the chemical engineering department in 1980.

In research, his publications emphasize optimization and synthesis in computer-aided design. Recent work includes developing a multileveled decomposition strategy to permit an optimization algorithm to be useful for engineering design calculations, the development of a new flowsheeting system, and a new approach for estimating minimum utility requirements.

He was on the CACHE Committee from its inception in 1970 until last year, and was program chairman for the ChE Division of ASEE Annual Conference in 1979. He gave the first invited "Tutorial Lecture" in 1978 at the Vancouver ASEE meeting and has authored several articles for CEE.

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THIS PRESENTATION is an opportunity to be philosophical about design, an opportunity not to be missed. The ideas to be given here are my version of ideas generated both in my own work and during several lively discussions with James Douglas (University of Massachusetts) and Bodo Linnhoff (Imperial Chemical Industries).

Design research is often narrowly viewed to be research to develop theory supporting computational methods useful for performing design calculations. The methods might be new convergence techniques, better stiff ODE integration methods, new optimization algorithms particularly well suited for systems of interconnected units, and so forth. Even the relatively new area of process synthesis is frequently viewed as solvable by using similar ideas, but perhaps using techniques which allow for a number of the variables to take on only discrete values.

The significant questions relating to synthesis were aptly stated by Simon (1969) and are further amplified in Motard and Westerberg (1978). They are 1) how does one represent the alterna-

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tive configurations permitted when developing a design, 2) how does one establish a value for each alternative so as to identify which are the better ones, and 3) how does one search among the enormous number of alternatives one is certain to create.

The guidelines we wish to state here speak principally to the third issue and partly to the second. We hope to show that powerful guidelines do exist which can be used to solve most open ended design problems directly or which can be used to design and evaluate aids and strategies which will be useful for solving such problems.

We conjecture that these guidelines can be taught; we (I. Grossmann and the author) attempt to do just that in our undergraduate and graduate design classes. We hope also to convince the reader that this aspect of design research is a valid contribution but one frequently avoided or understated when presenting new results.

THE GUIDELINES

WE OFFER THE FOLLOWING five guidelines to use when solving design problems.

1) **Evolve from simple to complex**
2) **Use a depth-first approach**
3) **Develop approximate criteria either as targets or heuristics for screening among alternatives**
4) **Use "top down" design techniques alternatively with "bottom up" ones.**
5) **All things being equal, make optimistic assumptions.**

We shall now explain each of these ideas in more detail and then, for the rest of the paper, examine their application to several examples. If the guidelines are true, then one should be able to use them to design a means to demonstrate their own validity; i.e., the ideas should be recursive.

Evolve from Simple to Complex

All earlier calculations for a design should be done using simple calculations even if one knows them to be quantitatively incorrect. The earlier calculations are for learning about the design qualitatively. Many of the major decisions can be made obvious by use of approximate calculations only. Hardly anyone experienced in design violates this guideline for long in practice, but when they do, failure to complete the needed calculations frequently results.

An obvious example is to prepare an outline to a research paper before writing it.

> **Douglas . . . conjectures that 99% of all initial design concepts will prove to be technologically or economically unsatisfactory . . . The correct mindset . . . is to try to prove concepts will** not **work.**

Use a Depth-First Approach

This guideline suggests one should go directly for a first feasible solution to the problem at hand, based on a sequence of best local decisions. One should *avoid the tendency to backtrack* at any point prior to finding an initial complete solution to the problem. (Outline the whole report.)

The reasoning is as follows. The initial design is an enormously effective learning device; it gives the designer his first glimpse as to the steps which are easy and to those which are the important difficulties to be encountered in the problem, with perhaps some difficulties being insurmountable. In this latter case, the design can be abandoned with minimal work expended.

"Depth first" is a term used to search a tree of decisions. It is a search strategy in opposition to "breadth first" searching. Breadth first allows backtracking prior to completing the first design if earlier decisions no longer appear to be likely winners.

To repeat this guideline—generally avoid backtracking. Go as quickly as possible to the first potential solution.

These first two guidelines permeate the recent publications by Douglas as well as the lecture notes for our own undergraduate design course.

Develop Approximate Criteria

One reason the design question is difficult to deal with is that design is caught in a dilemma. The final criteria used to assess the value of a design (if the criteria can be stated) cannot be evaluated without having in hand a completed design. Thus one must make initial decisions which one can only hope will result in solutions that are a good compromise with respect to the final criteria. To carry out the initial design, alternative approximate criteria must of necessity be used. Often these are in the form of heuristics. At other times they can be locally realizable targets.

A significant research contribution can be the discovery of effective approximate criteria, as we shall see has occurred in the synthesis of heat exchanger networks. The *targets themselves* may be considered the initial simple calculations needed for the earlier design stages. Linnhoff, in his research publications, is a vociferous advocate of target setting.

Use Top Down/Bottom Up Design Alternatively

Top down and bottom up design are forms used to describe how to design computer programs. The former, top down, refers to starting at the highest level with the overall goal of the design. This goal is then partitioned into subgoals, which, if solved, will accomplish the higher goal. These subgoals are then each treated as the top level goals to be further partitioned, etc., until lowest level subgoals are discovered which can be implemented without further partitioning.

Bottom up design is to design first the lowest level building blocks which one assumes will be necessary to accomplish the design. In computer programming, writing a linear equation solving subroutine first would be part of a bottom up strategy for designing a nonlinear equation solving package, where one assumes such a subroutine will be needed.

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What is being advocated here is to use the two strategies alternatively. The top down strategy should be used to scope out the alternatives in terms of high level tasks needed to solve the design. Once set, then bottom up design should be used to *locate bottom level subtasks which will preclude a solution.* Thus they will, for minimal effort, rule out an alternative suggested by top down design. To solve a bottom level subtask requires guessing the environment for the bottom level subtask.

Be Optimistic

Douglas (1979) conjectures that 99% of all initial design concepts will prove to be technologically or economically unsatisfactory—i.e., they will fail as concepts. The correct mindset, and one a designer usually fails to have, is to try to prove concepts will *not* work.

When attempting to use bottom up design to rule out design concepts, one should use optimistic guesses as to the environment for the bottom level task. If the task cannot succeed when being optimistic, then the failure to do the task can be used to rule out the top down concept requiring it. If one uses conservative guesses, and the bottom level task proves difficult, it may be because of the use of an overly conservative set of guesses as to the task environment, and thus one would be unable to use its behavior to rule out the concept.

A corollary to the above guidelines is that one should use the information learned from the original solution to move to subsequent improved solutions, using in one form or another a learning or evolutionary approach.

A second corollary to the above guidelines is that computer aided process design programs which do not cater to them will be significantly less useful than those which do.

The design problem is one of searching an enormous space of alternatives to select the correct building blocks and their interconnection, as well as also searching the space of continuous variables to establish the levels at which to operate any given structure. The guidelines are consistent with the following specific search strategy.

1) **Select a limited technology within which to solve the problem.**
2) **Using heuristics sketch a good initial solution from within the allowed technology.**
3) **Examine this solution and develop alternative solutions by revising within the allowed technology or within a modified allowed set of technology, where the initial solution suggests the allowed set modifications. Iterate from Step 2 until a "best" solution is found.**
4) **Repeat Steps 2 and 3 using more complete models.**

The guidelines also support the following specific strategy.

1) **Select a limited technology within which to solve the problem.**
2) **Within this technology set up a superstructure within which is embedded all the alternatives of interest. Use heuristics to eliminate obviously useless portions of the superstructure as it is being developed.**
3) **Use algorithmic methods to discover the best substructure from among the alternatives embedded in the superstructure.**
4) **Examine the solution and develop modifications to the allowed technology within which to search.**
5) **Return to Step 3 until no improvements are possible.**
6) **Iterate Steps 2 to 5 with more complete models.**

(Steps 3 and 4 can be very mathematical, giving rise to the development and use of sophisticated theorems, and thus perhaps satisfying many persons that quality abounds in the results.)

The advantage to this last approach is that parallel decisions are made in Step 3 so in a sense an optimal solution is found, but it is found by looking among a rather small set of alternatives. Fallible heuristics are used only to make the more riskfree problem reductions.

The sequential aspects to the approach are to learn which technological alternatives ought to be in the superstructure and to solve initially using simple models to get closer to the final solution before starting to do complex calculations.

EXAMPLES

WE SHALL NOW DESCRIBE four example "design" problems to illustrate the effectiveness of the guidelines.

An Entire Chemical Process

The first example is to scope out a process to hydrolyze ethylene (EL) to ethyl alcohol (EA) via the reaction at 560 k and 70 atm

$$CH_2 = CH_2 + H_2O \rightarrow CH_3CH_2OH$$

or

$$EL + W \rightarrow EA$$

The available ethylene feed contains one mole percent methane (M) and three mole percent propylene (PL). Propylene also hydrolyzes to isopropyl alcohol (IPA) but to a lesser extent at the given reactor conditions. Croton aldehyde (CA), a C_4 aldehyde, forms as a trace byproduct. Diethyl ether (DEE) forms in equilibrium with water and ethyl alcohol:

$$2CH_3CH_2OH \rightleftharpoons CH_3CH_2OCH_2CH_3 + H_2O$$

or

$$EA \rightleftharpoons DEE + W$$

Conversion of the ethylene is from 5 to 7%, with water in significant excess in the reactor feed.

Skipping lightly over many details, we start our design by scoping out the process using a top down view, getting at least the three structures illustrated in Fig. 1.

Remembering that the strategy being advocated suggests striking out for a completed design without backtracking, we must select one of these sketches (or a variant); we use a bottom up design technique to rule out alternatives. We look for reasons a concept will likely fail and do a quick bottom level calculation to validate our conjecture, guessing the most optimistic environment we can for that calculation.

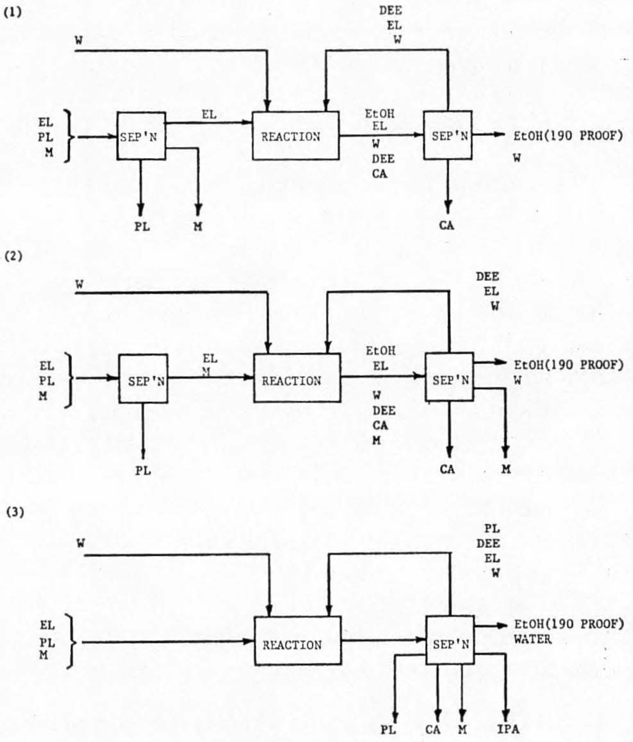

FIGURE 1. Top Down Sketches for Ethylene to Ethyl Alcohol Process.

The first two variants in Fig. 1 look as if they might fail because of the extremely low temperatures which may be required if we were to use distillation to effect the initial separation step. We need only a Mollier diagram for ethylene to see that at $P < P_c = 50.7$ atm, the highest temperature possible at the top of an ethylene/propylene column is 0°C. Refrigeration would be required, and, as an approximate criterion, we rule out using refrigeration if possible. The third option, if volatilities are examined, could be implemented to remove the methane and propylene by recycling them back with the ethylene to the reactor. Since methane is an inert here, it would build up and could be removed by bleeding it. The propylene will both convert to iso-propyl alcohol and be lost in part in the bleed. Finally comparing boiling points for water, iso-propyl alcohol, and the azeotope of water and ethyl alcohol suggests this separation is possible. All other separations look rather straightforward. We adopt option 3.

An automatic synthesis program for developing total flowsheets should be able to come quickly to this same result. If not, it must be working too hard. Remember this flowsheet is not purported to be the best one, only a good first one from which we intend to learn about the process so our second guess as to the solution is done with much improved insight.

Separation System Synthesis

The second process example we shall look at is separation system synthesis. We have an obvious candidate in our previous example, the separation of methane, propylene, ethylene, diethyl ether, ethyl alcohol, water, iso-propyl alcohol and croton aldehyde into the product ethyl alcohol, a recycle of ethylene, diethyl ether and water, and the by-products of methane, propylene, iso-propyl alcohol and croton aldehyde. The separation step of the third option in Figure 1 illustrates the problem. Note the feed to that step is vapor at high pressure and the recycle is also a vapor which needs to be returned at high pressure.

The strategy we now look at will be the first one stated earlier, one we claim is consistent with the guidelines given:

1) **Select a technology within which to solve the problem.**
2) **Using heuristics, sketch a good candidate solution. Evaluate it.**
3) **Examine the solution and develop alternate solutions by revising within the allowed technology or by adding new technology.**

If we were trying to develop our earlier flowsheet fully, we would likely skip Step 3 above because it represents backtracking. If, on the other hand, the separation problem is our entire design problem, Step 3 is a refinement step, one that follows our having a first complete solution.

Fig. 2 sketches a possible solution to the above separation problem using distillation technology.

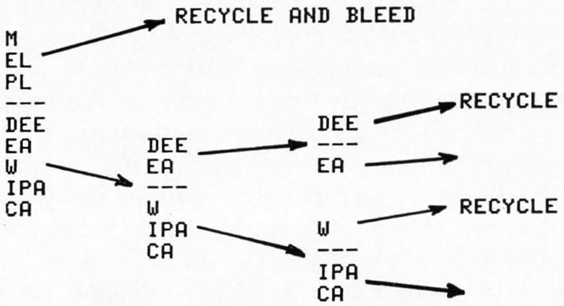

FIGURE 2. First Sketch for Separation System.

The heuristics used are ranked in order of importance and are a paraphrase and subset of those in Seader and Westerberg (1977). For the next separation

1) **do the easy split or**
2) **remove the most bountiful component or**
3) **remove the most volatile component.**

The split between diethyl ether and ethyl alcohol can be done easily; do it first. The recycle can tolerate methane and propylene so let them recycle, but then remove methane using a bleed stream. Go after the water which is plentiful next but, using heuristic 3 also, split above it to remove the ethyl alcohol. Finally split off the water from IPA and CA.

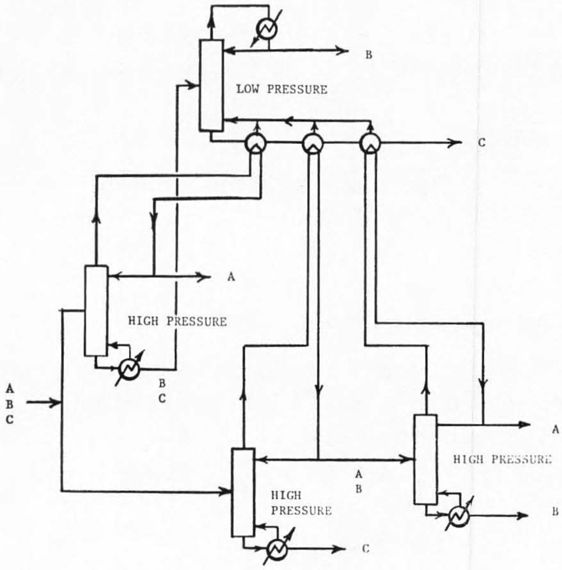

FIGURE 3. Highly Heat Integrated Distillation Scheme Using Multiple Effect Columns.

At this point let us consider the separation problem as the whole problem we are solving. For this problem Mark Andrecovich, a Ph.D. student of mine, is discovering that the second strategy stated earlier, where one creates a sequence of superstructures to be optimized, seems to be very effective. Figure 3 illustrates the solution found to a 3 component separation using this approach. It is 11% less expensive than all obvious competitors on an annualized cost basis which considers both investment and operating costs. Note the complexity of this structure. The research question is to establish a means to locate it quickly. □

EDITOR'S NOTE: The final two examples in this Award Lecture, and Professor Westerberg's concluding remarks will appear in the Spring '82 issue of Chemical Engineering Education.