Award Lecture

DESIGN RESEARCH

Both Theory and Strategy

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EDITOR'S NOTEs This is the second and concluding installment of Professor Westerberg's 1981 ASEE Award Lecture. The first installment appeared in the Winter 1982 issue of Chemical Engineering Education *(Vol. 16, No. 1, page 12).*

Arthur W. Westerberg received his degrees in chemical engineering at Minnesota, Princeton, and Imperial College, London. He then joined Control Data Corporation in their process control division for two years. In 1967 he joined the University of Florida where he remained for nine years. In 1976 he joined the faculty at Carnegie-Mellon University. He was Director of the Design Research Center from 1978 to 1980 and just became Head of Chemical Engineering this January.

ASCEND-II: An Analysis Aid for Arbitrarily Configured Processes

We shall move off on an entirely new tack at this point and describe briefly the ASCEND-II flowsheeting system (Locke, et al (1980)) that we are developing in my research group at Carnegie-Mellon University. The persons involved are Michael Locke (Locke (1981)), Selahattin Kuru (Kuru (1981)), Peter Clark (Clark (1980)), Dean Benjamin and Andrew Hrymak. The messages to be conveyed by this example are two: the breadth of research activities which support this project and a description of the use of this system to develop a working analysis model for a process in a manner which is consistent with the design strategy that has been the main theme of this paper.

To examine ASCEND-II we need first to establish what we mean by analysis. We include the following types of analysis for a given but arbitrarily configured process flowsheet.

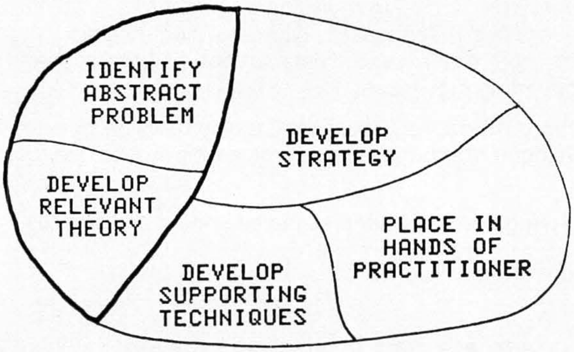

FIGURE 4. Aspects of Design Research.

1) **Simulation. The inputs to the process, the temperature and pressure levels at which to operate and the equipment sizes are fixed. The calculation is to discover how the equipment performs, a rating calculation.**
2) **Design. Some outputs from the process and some intermediate stream variable values may be specified in exchange for calculating an equal number of the inputs, levels of operation and/or equipment sizes.**
3) **Dynamics. The dynamic behavior of a process may be required.**
4) **Optimization. We may wish to optimize the process over the set of continuous variables that describe equipment sizes and process operating levels.**

Fig. 4 illustrates the breadth of questions which one can address in the area of design research. Many persons identify design research

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with only the two aspects highlighted with a dark line: 1) Identify Abstract Problem and 2) Develop Relevant Mathematical Theory. We have been arguing all along about the importance of developing a correct design strategy. Support techniques are often shrugged off as not fundamental enough, but, if not done correctly, the implementation of the theory will likely prove too complex to be practical. Finally one should not overlook the problem of placing sophisticated tools into the hands of unsophisticated users. There is research lurking there too.

The abstract problem for developing ASCEND-II is how to solve large sets of simultaneous nonlinear, sparse algebraic, ordinary and partial differential equations, perhaps subject to inequality constraints and perhaps containing discrete variables. There is certainly enough of a problem here to require considerable effort.

Relevant theory includes convergence proofs, analysis techniques to take advantage of structure and Lagrange theory. We have already discussed strategy ideas at length. The supporting techniques include consideration of data structures, problem decompositions (see Westerberg and Berna (1978), Berna, et al (1980), Clark (1980)), data bases and use of network computing. Finally the ideas involved in placing the tools into the hands of the practitioner include language design, level of interaction, online documentation system design and use of graphics. We are making considerable progress at dealing with the above ideas and others in the development of ASCEND-II.

Fig. 5 illustrates the underlying evolutionary aspect of ASCEND-II.

ASCEND-II is intended to help a process engineer "design" a computer model for his process, using the available building blocks provided within the program. "Design" here refers to finding and solving a model of the needed complexity to answer the questions being asked of the process, where the engineer is learning both about the questions he should ask and about the model as he proceeds. We could broaden the meaning of design to that of designing the process for which the model is being developed, a task for which ASCEND-II is also well suited, but we want to limit ourselves here to the narrower model design problem.

The axes in Fig. 5 are axes along which the model design can evolve. Model complexity can evolve from simple to complex, where simple models consist of only a few units and the use of the simplest of physical property models; e.g., a flash unit using constant relative volatilities.

With each model a range of analysis types can be performed, starting with simulation, moving to design and finally (when ASCEND-II is further developed) to optimization. Simulation is intuitively the easiest mode to use for the engineer. In that mode he can usually establish a set of specifications which will lead to a solution for the remaining variables. For example, one has some confidence that, if he fixes the feed stream to a flash unit, fixes the fraction of the feed which will vaporize and the flash pressure, then the flash unit will have to operate and so will the corresponding calculation. Why not allow the user to start then with this "comfortable" calculation? Once he can simulate the flash unit ASCEND-II allows him to alter the set of variables to be specified. For example, he could require that the recovery fraction of one of the components be specified and that the pressure be calculated. If the trade is illegal, he will be warned immediately.

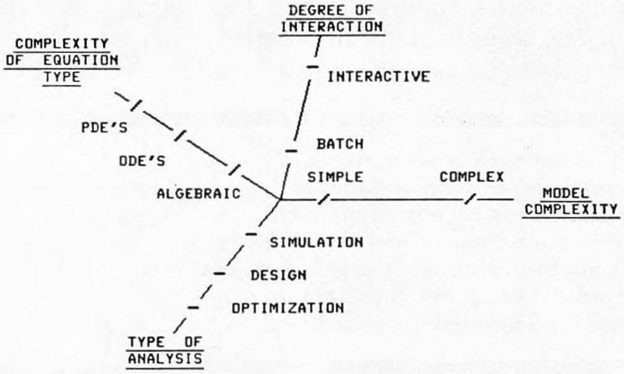

FIGURE 5. The ASCEND-II Flowsheeting System.

Running through a few design calculations will acquaint him with the shape of the solution space and when he gets near to a good solution, he can switch into doing an optimization calculation.

Once this sequence is solved using simple algebraic models, he can selectively add more complexity to the model by adding more units and/or more sophisticated physical property calculations and continue.

A type of complexity which can be added is to broaden the type of equations which are used to model portions or all of the process, i.e., by allowing models involving ODE's (Kuru (1981)) and PDE's to be introduced. With ODE's and PDE's one can consider doing dynamic studies.

The last axis is that reflecting the degree of interaction ASCEND-II will have with the user. In ASCEND-II a standard command file can be created which will attempt to solve any model once it is set up. Invoking this "standard" file is like running the problem in batch mode on a computer. At the other extreme, the commands can be executed interactively one at a time in fairly arbitrary order. (The computer is a DEC-20 which provides a very friendly interactive environment.)

Examples of the types of commands available are 1) to input some more structure to the flowsheet, 2) to delete some of the existing structure, 3) to save and retrieve variable values, 4) to initialize variable values (selectively), 5) to change the set of variables whose values are to remain fixed, 6) to cause variables and equations to be rescaled to reflect current variable values, 7) to do one or more Newton-Raphson iterations, 8) to determine the constrained derivative of one variable with respect to another, 9) to display variables selectively, and 10) to display equation errors selectively.

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With this structure for ASCEND-II, the user can "drive" his computation around computational obstacles much as he drives a car and can become very effective at getting solutions quickly, even for stubborn problems.

We have set the stage now to argue that ASCEND-II allows the model for a given process to be designed using our earlier guidelines. Clearly the first guideline is dealt with: evolving from simple to complex. The depth first strategy can be followed by developing first a simple model for the entire process.

Unlike conventional flowsheeting systems, each unit within a flowsheet can be tested by itself in ASCEND-II, permitting a bottom up solving of the units at any time. In this mode and using the simple model as the base case design, much testing can be done to see where to add complexity, and where perhaps to remove complexity. Answers can be obtained to a simpler version of the problem to use as a starting solution point for the more complex versions, a strategy often needed when solving highly nonlinear equations. The notion of developing and using approximate criteria is also possible. One usually gets a solution to the equations, perhaps far from the desired solution point. This solution may be from doing a simulation rather than the desired design calculation. Not unlike the idea behind a continuation method, the calculation can be converted to the desired design calculation in terms of which variables are specified. Then one can move to the solution point desired through a series of small steps, converging to the solution at each step.

While it is obvious that much of the power of a program like ASCEND-II comes from its being interactive, it is equally as obvious when using it that the ability to find a base case solution and then to move from that solution in almost any manner desired (top down/bottom up, simulation/design, etc.) is the heart of the rest of its power. It is the learning that can occur which helps to decide the nature of the next calculation, to see its impact and to alter one's path as a consequence, that makes ASCEND-II so useful. Traditional flowsheeting systems (and for that matter, traditional equation solving packages) do not offer the flexibility provided by ASCEND-II for this approach.

ASCEND-II has been designed under the assumption that calculations will often fail until one learns about the problem. Diagnostic tools are thus provided to allow the user a chance to detect where the failures are occurring. As mentioned only briefly before, these include interactive access at any time to *every* variable in the problem by a convenient name and similarly to every *equation error*. This latter access allows one to note, for example, that the phase equilibrium equations on stage 3 of the diethyl ether column are not converging. The variables around that stage can

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then be examined to see if one is perhaps too large or worse yet, negative. Having located the problem, the user can then start to work on correcting it.

Interestingly, the current version of this system is a third generation version. We designed ASCEND-II following our guidelines by prototyping it twice, at each step improving the design based on the previous version. This was and remains a deliberate policy for creating ASCEND-II.

Heat and Power Integration of a Process

THE LAST PROCESS PROBLEM to be considered is to integrate the heat and power requirements for a process for which one has just set temperature and pressure levels for each of the units and has solved the process heat and material balances (using ASCEND-II for example). Great progress has been made for solving this problem. The heat integration portion is usually called a heat exchange network synthesis problem. See Nishida et al (1981) for an extensive review of the heat exchanger network synthesis problem.

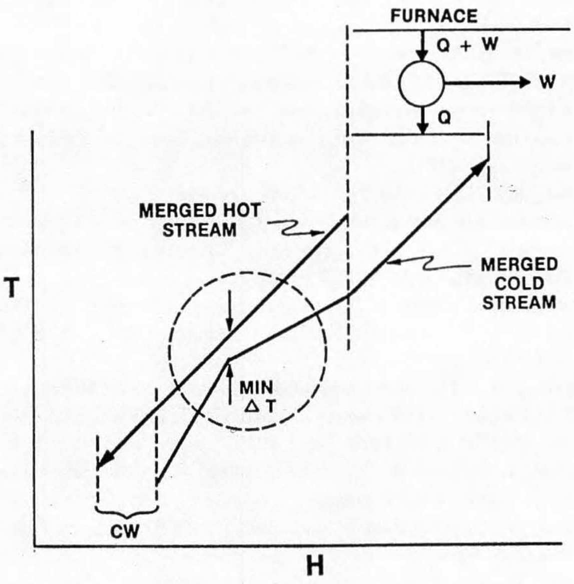

FIGURE 6. Minimum Utility Calculation. Upper right illustrates how to extract "work" efficiently from process.

The heat exchanger network synthesis problem epitomizes the effective use of approximate criteria to locate excellent final network designs. Using thermodynamic arguments, one can predict a priori the least amount and kind of utilities needed to solve this problem. Also using graph theoretic ideas one can guess the fewest number of heat exchanger units likely to be needed. Experience has shown that the better designs meet these goals, or come very close to meeting them. Finally, effective design techniques exist to aid one to find such designs.

In preanalyzing the heat integration problem, one discovers for most problems a bottleneck will occur to further heat integration in the form of a temperature pinch. Fig. 6 illustrates the way Hohmann (1971) located this pinch. He merged all hot streams into a single "super" hot stream and all cold into a single "super" cold stream. Placing them as illustrated on a temperature versus total enthalpy diagram reflects the opposing hot and cold stream temperature profiles one would see if these super streams met in a single counter current heat exchanger. The pinch is the point which precludes further integration. Cerda (1980) from our group and, in parallel, Mason and Linnhoff at ICI recently developed an approach which generalizes this minimum utility calculation.

Umeda et al (1979) have exploited the pinch to aid in locating where in a process the reestablishing of temperature and pressure levels will permit more heat integration. Very recently Linnhoff and coworkers (Townsend and Linnhoff (1981), Dunford and Linnhoff (1981)) have shown how to exploit large temperature differences between these super streams which occur either entirely above or entirely below the pinch. They show how to convert heat entirely to mechanical work or obtain some "free" separation work within a process. For example, the upper right part of Figure 6 shows how one can place a turbine to get 100% of the thermal energy which must be added into the process converted to the desired mechanical work. The cost is the degrading of the thermal energy which enters and is later rejected by the turbine. If that energy can be degraded and still be rejected at a temperature where it is useful as heat input to the process *and* if that heat can be extracted and rejected entirely above or entirely below the pinch, then 100% of the extra energy added to drive the turbine is converted to work.

The design strategy is to establish first a process design not yet heat integrated. Then by examining the process, one finds the pinch temperature and predicts the minimum utility costs associated with the process. Next one can modify the process near the pinch if further heat integration is desired. Finally one can place some turbines if possible so they degrade thermal energy either entirely above or below the pinch. The design can then be reassessed and improved from this thermally integrated base case.

PROVING THE STRATEGY ITSELF

How would one "prove" that the design guidelines are basically sound? That problem is itself a design problem and should be (if we are correct) solved using a strategy consistent with the guidelines themselves. The concept should be recursive. In our case it is leading to the design and testing of the ASCEND-II system. We are only at present proving we are right by demonstrating how rapidly one can put together a working computer model for a process using this system. In one example a model was constructed using a conventional flowsheeting system and the exercise took two full time days. Using ASCEND-II, it took two hours.

Since teaching these guidelines to our students in the undergraduate design course, we see a noticeable reduction in the time needed to get realistic designs.

IN CONCLUSION

The guidelines suggested to aid one to do design more efficiently have been illustrated on several diverse problem types. Only qualitative "proof" exists as to their correctness. If correct a principal use can be to examine a proposed or existing design tool (or design effort) to see if it abides by them. Where it fails should suggest modifications to the tool which could significantly change its effectiveness. Designers have to make a conscious effort to stick to the guidelines as they do not always coincide with the most natural approach. They can be taught; we try to do so in the undergraduate design class. □

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