ChE lecture

CHEMICAL PROCESS SYNTHESIS

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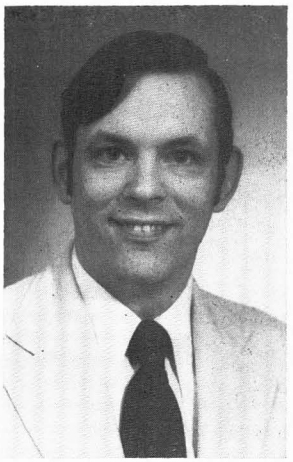

J. J. Siirola received his B.S. from the University of Utah and his Ph.D. from the University of Wisconsin-Madison in 1970 where he developed the AIDES process synthesis system and coauthored the introductory text, **Process Synthesis.** Besides a continuing involvement in synthesis technique development, implementation, and application, his research interests also include simulation and optimization aspects of computer-aided design, non-numeric programming, artificial intelligence, and technology assessment. He is currently a Research Associate in the Eastman Chemicals Division of Eastman Kodak Company.

STATE SPACE SEARCHING

Systematic generation approaches are variants of a problem-solving formalism known as the state space paradigm. Problems framed in this manner consist of an initial state (a set of streams at their initial temperatures or a multicomponent stream to be separated), a set of possible states (streams at intermediate temperatures or streams containing fewer components), a set of possible transformations (changing temperatures by heat transfer or separating multicomponent feeds into two streams of different compositions), descriptions of the states resulting from application of a transformation to a given state (design equations for determining exit temperatures from an exchanger or outlet compositions from a separator), and a final state (the set of streams at their desired temperatures or the set of separated streams). The number of possible states generally increases exponentially with problem size. A solution to the state space problem is any sequence of transformations that leads from the initial state to the final state subject to any constraints that may be applicable. Different paths through the state space may represent the same design. For the heat integration and separations sequencing synthesis problems considered here, the existence of a feasible path from the initial to the final state is usually not in question. Rather, what is sought are paths (designs) which arrive at the final state in some optimal manner.

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For sufficiently small problems, it may be possible to search exhaustively through the state space for solutions. Each feasible transformation may be applied to the initial state producing alternative intermediate states, followed by application of transformations to these states generating yet more states, and so on. A search strategy that considers states for transformation application in the same order in which they were generated is termed 'breadth first.' Alternatively, a search strategy can be implemented in which some transformation is applied to the initial state, followed immediately by another transformation applied to the resultant state, and so on. When the final state is reached, alternative transformations are applied to the penultimate state until

the final state is again reached. Only after all feasible transformations have been applied to a given state and followed through to the final state are alternative transformations applied to its predecessor, and so on, until all paths through the state space have been generated. This type of search is termed 'blind depth first.' However, if costs can be computed independently for each transformation, the smallest total cost for any complete path generated from initial to final states serves as an upper bound (if minimum cost is the design objective) for other desirable designs. Therefore, for the usual case where costs increase with each transformation, the search can be terminated without reaching the final state if the total cost of a partial path being developed exceeds the current bound.

Ideally, this 'branch-and-bound' technique is more efficient (avoiding a search through more of the feasible state space) if what proved to be the best path is generated early in the search. This might be accomplished by examining at each state all feasible transformations but choosing first the one with lowest cost. Searches which selectively apply state transformations are termed 'ordered depth first.' The technique may be refined by including in the transformation evaluation not only its cost but also an estimate of the costs of all remaining transformations to the final state resulting from its application. This 'predictor ordered search' generally examines the smallest subset of the state space in discovering optimum designs.

In situations where the application of at least some transformations are independent of each other, several different paths through the state space may result in the same design. As this is the case for sharp separations sequencing, it is sometimes more convenient to consider the dual of the usual state space representation in which the transformations become the nodes. This focuses attention on the alternative transformations to be performed rather than on the intermediate states. Each complete and consistent set of transformations joined by arcs of the dual graph represent a unique separations sequence.

Efficient use of state space search in systematic generation synthesis approaches requires at each state the identification of applicable transformations and an evaluation of the value (possibly considering effects on the remainder of the problem) of its application. In the previous examples, and in similar strategies applied to heat integration, as the objective function is taken simply as the sum of the transformation costs, the search is guaranteed to find the optimal design for the classes of transformations available. Searches in this situation have been termed 'algorithmic.'

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However, in many cases involving for example subjective multivariable design criteria, extremely complex transformation evaluations, or very large state spaces, it may not be desirable or even possible to search analytically. The selection or evaluation of transformations can then be made on an empirical basis by using previous experience embodied in design rule-of-thumb. These rules, or 'heuristics,' reflect generally successful strategies, although they carry no guarantees of optimality. Their value is that they often limit the growth of the state space to only a polynomial function of problem size. Heuristic searches are among the oldest systematic process synthesis techniques, having been applied very early to separations selection and sequencing. For this problem, at least 14 such rules are now in common use, including 'remove the most volatile species next', 'remove the species in highest concentration next', 'perform the separation which results in an approximately equimolal split', 'perform separations with high recover fractions last', and 'perform the cheapest separation next.' Similar design heuristics have been proposed for other synthesis subproblems including complex refrigeration cycles and heat integration.

Since the design that results from a heuristic search often becomes the initial point in an evolutionary structural improvement procedure, it is important that the heuristically developed design be as near to optimal as possible. Unfortunately, the advice offered at each state by alternative heuristics is sometimes contradictory. Adaptive heuristic selection procedures can be modified on the basis of the success of repeated heuristic ordered depth first searches. However, for large problems such iteration may not be practical. As an alternative, situation dependent preference ordering of the selection rules has been proposed

for once-through heuristic search procedures which terminate when the final state is reached and for guidance in altering the ordering during any subsequent evolutionary modification.

Much synthesis research continues into the search for more powerful design heuristics and more precise definitions of conditions which delimit their applicability. For example, heuristics have been developed which, given only a description of the initial state (and assumed for the final state), completely specify the optimal path without examining the intermediate states for three-component separations that involve simple ordinary and thermally coupled distillation. In heat integration, utility and capital economic factors have led to the realization that better (from a cost criterion) designs generally result from efforts to maximize heat transfer among process streams, while simultaneously minimizing the number of exchangers employed to accomplish it. That maximum integration is consistent with the thermodynamic desirability to minimize network irreversibilities led to a minimum temperature driving force match heuristic. Methods to minimize the number of exchangers have also been investigated. The most significant recent result in heat integration is the fact that maximum integration (and hence minimum utility requirement) and the likely minimum number of exchangers can both be calculated for a given problem before the generation of any networks. This analysis provides additional bounds and targets which can be used to limit the size of the search space, estimate the potential for evolutionary improvement of a candidate design, or estimate the cost of accomplishing heat transfer tasks for a process without actually synthesizing any networks. Similar performance targets, often the result of simplified thermodynamic analysis, are being developed for other synthesis subproblems.

Another critical factor in the application of state space problem-solving approaches in process synthesis is the choice of representation for describing the states and the transformations among them. It is desirable from search efficiency considerations to develop representations which do not include states that cannot possibly be part of the optimal path. On the other hand, care must be exercised so that the experience, prejudice, heuristics, or assumptions embedded into a representation for efficiency do not inadvertently constrain or otherwise exclude truly novel 'creative' optimal solutions from consideration.

COMPLEX SYNTHESIS

Although the previous discussion has drawn examples only from heat integration and separations sequencing, state space systematic generation approaches have also been applied to other synthesis subproblems including reaction paths, control systems, and safety systems. Each of these subproblems is fairly well defined and each has a sizable state space. However, these synthesis subproblems are not necessarily independent. For example, if thermal energy is employed to effect a multicomponent separation as in distillation, the separations sequencing and heat integration subproblems interact closely. The optimal design and operation of a column (operating pressure, degree of feed vaporization, number of stages, reflux ratio, etc.) depend on energy costs and, hence, on heat integration. Heat integration opportunities, however, depend upon column temperatures and heat loads, which are functions of operating pressure and reflux ratio which is, in turn, influenced by pressure effects on the exploited property difference, relative volatility. Further, the identity of the streams available for integration is not known until the complete separation sequence has been generated.

Early procedures for solving this combined problem required excessive effort, largely because of the incompatibility of the dynamic programming approach used for column sequencing with the interactions resulting from heat integration and the large state space of even the restricted integration problem. Later developments in heuristic search improved both the capacity and speed of heat integration syntheses. These improvements allowed all sources and sinks including sensible streams to be considered by an integration procedure fast enough to be included within a design variable optimization of each synthesized separation sequence subject to the same simplifying assumptions. Evaluations of many case studies verified that, although the resultant objective surfaces are very irregular, significant improvements are achieved when designs for these two subproblems are synthesized simultaneously in comparison with independent sequential synthesis. Current efforts, based on the development of improved bounding strategies, seek to generate optimal designs for this combined problem without necessarily generating all paths through the separations sequencing state space.

The design of complete flowsheets is another complex synthesis problem that perhaps embodies all the other synthesis subproblems discussed. Ideally, based on experience with the combined problems of separations sequencing and heat integration, it may be desirable to solve all the subproblems simultaneously. Development of such a formulation is a formidable task and may never be accomplished. Several simplified approaches, however, have been suggested.

One scheme, like other systematic generation approaches, decomposes the problem in such a way that at least one task is immediately recognizable as achievable with available technology such as a reactor, distillation column, or heat exchanger. Given descriptions of the desired product, potential raw materials, pertinent chemistry, and available technology, the binary resolution procedure of predicate calculus was adapted to prove constructively the existence of a path through the state space. Since for most real design problems the existence of a solution is not in question, resolution was replaced with a goal-directed depth first search (proceeding backwards from the desired products) followed by evolutionary improvements involving recycles and energy recovery to generate efficient overall designs.

Alternatively, a decomposition scheme is possible that does not result in the immediate recognition of available technology but rather a multilevel series of subproblems similar to the synthesis subproblems identified previously. The innermost level subproblem involves the selection of chemical transformations by which available raw materials are to be converted into the desired product. Once approximate conversions and yields of the chosen reactions are determined, a rough material balance can be calculated. In the next subproblem, the fate of each chemical species in every raw material and reactor effluent is assigned. Decisions to recycle unconverted reactants, remove contaminants before or after reaction, allow them in the product, send them to waste treatment, or process them into byproducts, etc. are made. The implementation of this species allocation is addressed in the next subproblem by using means-ends analysis to detect required temperature-changing, pressure-changing, stream-splitting, species-separating and or other physical transformation tasks. The outermost level subproblem specifies processing equipment and control strategies to effect the required tasks, integrating as appropriate consecutive or complementary tasks for capital and operating cost efficiencies. Each of these subproblems interact. Correct reaction choices depend upon how the reaction path will be implemented. Optimal species allocation to support the reaction path depends in part upon the separation problems which arise as a result of the allocation. The selection of physical transformation tasks and their operating conditions may depend upon the degree of task integration, etc. At each level, choices are made as a result of an analysis of the bounds defined by actions taken in previous levels and by heuristic estimates of the probable effects of the choice selected on subsequent levels.

STATE OF THE ART

The level of sophistication exhibited by the systematic chemical process synthesis techniques so far developed ranges from primitive to moderate. From an industrial point of view, heat integration synthesis is the most mature, although no single technique is universally superior in all applications. The prediction of utility bounds, minimum number of exchangers, and identification of evolutionary structural improvements are significant design tools. Some computer programs are commercially available. Heat-integrated separations sequencing also has industrial applicability, although at present is somewhat limited by simplifying assumptions. The total flowsheet synthesis computer programs are strictly experimental. It is, of course, not necessary that successful process synthesis techniques be computerized, although in research the development of computer implementations sometimes forces more careful attention to logic detail.

Industrial interest in continued progress in process synthesis techniques is strong. Well-attended symposia sponsored by AIChE and others throughout the world are becoming more frequent and serve as a forum for discussion of latest results. Current research needs include relaxing the restrictive assumptions particularly related to type and component distribution in separations sequencing techniques and developing improved representations to account for phase equlibria and possibly reactions occurring within separations equipment. Additional work is needed in the development of complex synthesis strategies and of heuristic transformation selection and evaluation functions for efficient state space searches which avoid unnecessary prejudice or constraints. Improved performance targets and

bounding properties will be required for search space reduction and dual-level design optimizations. Also work needs to continue on combined synthesis problems such as control strategies and heat integration.

As more difficult synthesis problems are examined, more problem-solving techniques may be required for their solution. Although the goal of chemical process synthesis research is definitely not the computerization of the design invention activity, some powerful paradigms have been developed within the computer science discipline of artificial intelligence. For example, pattern recognition and semantic information processing were once considered as a means for coding and retrieving the historical experience of the profession for application to new problems, but were abandoned because of the feeling that novel, creative solutions were unlikely. Likewise, theorem proving was the foundation of resolution based flowsheet synthesis but was ultimately rejected when structural optimization rather than proof of feasible design existence was sought. Learning techniques were incorporated into heuristic transformation selection functions and goal-directed state space search techniques. It is expected that these and other artificial intelligence strategies such as planning, reasoning, and game playing may be an important part of the solution procedure for more difficult synthesis problems.

Finally, synthesis is a fundamental part of the synthesis-analysis-evaluation-optimization process design activity. Although once the exclusive domain of the experienced practitioner, the results of the research reviewed here indicate that at least some concepts such as decomposition and state space search can be formalized. And as such, it seems definitely desirable to incorporate these as well as some of the specific procedures for selected subproblems such as heat integration, separations selection and sequencing, or control systems along with discussions of concept discovery aids and descriptive chemical engineering into traditional design courses. In less detailed form, basic synthesis concepts would seem to be an excellent introduction to the nature of chemical engineering, providing an overview and foundation for the rest of the curriculum.

CONCLUSIONS

Chemical process synthesis is an activity concerned with the invention of structurally and operationally superior design alternatives. This activity has generally been performed by experienced, creative engineers assisted by several design aids based primarily on analogy.

Several approaches not necessarily patterned after existing concept discovery practice have been proposed for systematic process synthesis. Optimization approaches attempt to apply traditional mathematical methods for operations optimization to structural optimization. Evolutionary approaches identify features for possible modification or rearrangement. These approaches require some preinvented design. This invention can be accomplished with decomposition or systematic generation approaches. Perhaps a truly competent process synthesizer should contain elements of all three approaches.

Systematic generation involves decomposition and a subsequent search through very large state spaces. For some synthesis subproblems, these searches have become tractable through the development of efficient state representations, search heuristics, and bounds on the state space containing optimal designs.

Industrially significant results have been obtained in the area of heat integration. Other useful techniques have been demonstrated in reaction path selection, separations sequencing (particularly combined with heat integration), control systems, and complete flowsheets. Traditional concept discovery aids and newer systematic synthesis approaches should be included in process design instruction.

Significant research opportunities remain, particularly in the area of combined synthesis subproblems. Solution techniques for more difficult problems may require greater application of artificial intelligence techniques. Tradeoffs between level of detail and search efficiency will be difficult and representation and heuristic search developments must be made carefully to avoid unnecessary or unintentional constraints. □

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