A Research Program On

ARTIFICIAL INTELLIGENCE IN PROCESS ENGINEERING

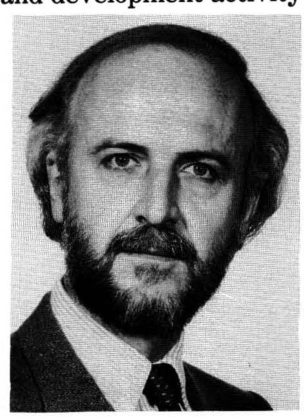
GEORGE STEPHANOPOULOS
Massachusetts Institute of Technology
Cambridge, MA 02139

THE REEMERGENCE of artificial intelligence as a viable and utilitarian discipline offers the potential of harvesting early promises on intelligent man-machine interaction. For process engineering, these promises have nurtured and disillusioned a generation of engineers. Presently, the mood is cautiously optimistic. The "novelty" of the technology has taken most by surprise and has found the large majority, even among the early devotees in artificial intelligence, unprepared for meaningful engineering applications. Nevertheless, idling skepticism has been replaced by a wide-spread activism, leading to a multitude of exploratory prototypes. But, what we observe as a feverish research and development activity in knowledge-based expert system is nothing else but a very serious effort in self-education. We will have to wait for the next phase of developments to see useful and practical products for process systems engineering purposes.

Existing prototypes of expert systems are interesting examples, and some of them have had significant economic impact in areas other than those related to chemical and biochemical engineering. They have provided certain paradigms which later efforts have tried to imitate. But, are these prototypes appropriate for process engineering?

- **Can they "model" the human activity during the conception of a chemical process, the design of a product, the development of a process flowsheet, or the synthesis of control configurations and operating procedures for complete processing plants?**
- **Can they support engineering activities, capitalizing on the innate "intelligence" of expert technologists and designers, as this intelligence is articulated within the context of the problem being solved?**
- **Do they provide high level, transparent communication between man and machine during the graphic generation of process flowsheets, or control configurations, or the analytic development of process models, the introduction of qualitative reasoning, or the formulation of design problems (assumptions, assertions, hypothesis testing, etc.)?**

It is our view that the existing paradigms cannot satisfy the above needs; after all, they were conceived to solve different problems. New prototypes are needed which should reflect the particularities of the process systems engineering problems.



George Stephanopoulos was an undergraduate at the National Technical University of Athens, Greece, received his ME at McMaster University, Canada, and did his doctoral studies in chemical engineering at the University of Florida. In 1974 he joined the faculty at the University of Minnesota, and from 1980 to 1983 he taught at the National Technical University of Athens. In 1984 he joined MIT, where he is presently the J.R. Mares professor of chemical engineering. He is the author of two books: *Chemical Process Control; An Introduction to Theory and Practice,* and *Synthesizing Networks of Heat Exchangers.* He has been a Dreyfus Scholar and he was awarded the Colburn Award (1982) of AIChE and the C. McGraw Research Award (1986) of ASEE. His research interests are in the area of process systems engineering, which he and his students have been recently interfacing with methodologies from artificial intelligence and technology from LISP computers.

THE M.I.T.-LISPE

The Laboratory for Intelligent Systems for Process Engineering (LISPE) at the Massachusetts Institute of Technology was recently established to advance the art of process engineering using current technological advances in the areas of artificial intelligence and LISP computers. It is the culmination of intensive preparatory work during the last 2 1/2 years, including extensive investment in education, hardware and software infrastructure, and communi-

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cation and collaboration with other research groups at MIT or industrial concerns, all of which have interests in artificial intelligence.

LISPE's present capabilities in research and education are at the forefront of the field, and encompass diversified expertise in various areas such as

- **Chemical or biochemical process development, design, control, or operations**
- **Methods of artificial intelligence**
- **Design and development of knowledge-based expert systems**
- **Structure and character of object-oriented programming**

In the remaining paragraphs of this section, we will discuss in more detail the present infrastructure of LISPE.

The MIT-LISPE is under the direction of Professor George Stephanopoulos and presently includes twelve graduate students working toward their PhD degree. It has also involved eight undergraduate research assistants through MIT's Undergraduate Research Opportunities Program (UROP).

The ability to amalgamate the most advanced knowledge and methods from many diverse areas important to process engineering depends upon close interaction with two important groups of people: 1) Other faculty members and investigators at MIT, and 2) Industrial practitioners from the chemical and biochemical industries as well as the computer industry (hardware and software).

Within MIT, the LISPE has established connections with groups such as the A.I. Laboratory, the Knowledge Systems Program of the Laboratory for Manufacturing and Productivity, the Intelligent Engineering Systems Laboratory in Civil Engineering, and various other independent researchers with interests in the fundamentals and applications of artificial intelligence.

Hardware Facilities. Present hardware facilities include

- **Two 3640 and two 3650 SYMBOLICS LISP computers, each equipped with 8 MB of memory and 280 or 360 Mb of disk capacity**
- **Two IBM PC AT (one with color and extended 2 Mb memory)**
- **Two printers (one laser, and one high quality dot matrix)**

Furthermore, we recently completed the networking of all machines as well as their connection to MIT's ATHENA system. Such networking capabilities allow us to expand the scope of the research projects by accessing a large multitude of databases, by communicating and reasoning with other intelligent systems, or by developing simulated environments of distributed, parallel intelligent systems.

Software Support. Current research developments in intelligent systems for process engineering are enjoying wide support from a multitude of generic and specific software facilities, such as

(a) The SYMBOLICS Zetalisp environment provides an extremely efficient medium for rapid prototyping of intelligent databases and interfaces with rudimentary natural language capabilities and extensive graphics, including active multiple windows, scrolling, menus, etc., and it allows an incremental mode of program development.

(b) An integrated software package, such as the Knowledge Engineering Environment (KEE), has been generously provided by IntelliCorp, and constitutes the integrated environment for the development of knowledge-based expert system support of our various research projects.

(c) The availability of LISP-based compilers for languages such as FORTRAN and PASCAL allows us to access, in a transparent way, a large number of software packages developed for various numerical process engineering needs such as: algorithms for the solution of equations, optimization algorithms, physical properties packages, simulators of process flowsheets, process design packages, packages for the design of control system, etc.

(d) The Lisp version of MACSYMA provides us with a powerful mathematical symbolic manipulator, which has found important applications on several projects.

(e) The GCLISP 286 Developer that we use in conjunction with the IBM PC AT computers provides an excellent environment for training in LISP. In addition, it provides an additional capability for the local development of small-scale, dedicated natural language interfaces, file editing in Common Lisp, and remote evaluation of Zetalisp functions.

THE PHILOSOPHY OF THE RESEARCH PROGRAM

The historical boundaries of process engineering activities are being pushed toward the "front-end" to include an important role in product design and development, as well as contributions in conceiving novel processing schemes and developing the appropriate technology, including the selection of mass separating agents, heat pump fluids, catalysts, etc. Within the scope of LISPE the following set comprises the process engineering activities of interest

New prototypes are needed which should reflect the particularities of the process systems engineering problems.

- **Design of molecules (products, or processing fluids) with desired physical or/and chemical properties**
- **Development of novel processing schemes**
- **Synthesis of process flowsheets for existing technologies**
- **Design of control systems for complete chemical plants**
- **Intelligent on-line controllers**
- **Planning and scheduling of operational procedures**
- **Development and design of biochemical processes**

All of the above problems are characterized by a series of common attributes which can be summarized as follows:

Each problem is multi-objective in nature. Thus, a new polymer should not only possess the desired thermal and mechanical properties, but it should also be easily processed while the production of the constituent monomers is chemically feasible and economic. The control structure of a complete chemical plant should not only provide good regulation, but it should also allow for easy plant-wide optimization and smooth start-up, change-over, or safe fall-back operations. The optimum trade-off of conflicting objectives has been the province of "experts," since a concrete formulation of such problems is very resistant to analytic treatment.

They use knowledge from different domains. This is a direct corollary of the multi-objective character of the problems and indicates the need for diversified expertise, which normally comes from different people. At the same time it is clear that we need to consult different data-bases with large amounts of diversified information. Coordinating the interaction of different "experts," and/or rationally using extensive data-bases with diverse scopes, is not a trivial problem. Current industrial practice is based on a rather inefficient segmentation of domain-responsibilities, where the control designer tries to make up for process design weaknesses, or the process developer attempts to conform the processing scheme to the chemist's dictation.

Required expertise is not easily articulated. The incisive knowledge that problems such as the above need for their solution cannot be easily articulated by the experts in the absence of a specific context. On the contrary, experience has demonstrated that "expertise" becomes active within the context of the particular problem they attempt to solve.

Imply a disciplined use of assumptions. For most of the above problems, the degree of success depends on the amount of available knowledge and the disciplined use of assumptions exercised by the "experts." Thus, the expert resorts to a series of assumptions, conjectures, hypotheses testing, reasoning by analogy to previous problems, assertion of intermediate goals, etc. The results of this procedure determine the next steps in the evolving design.

Employ models and quantitative information. In addition to expert qualitative knowledge, for the solution of the above problems designers often resort to quantitative information in the form of analytic (based on first principles) or short-cut models, correlations, tables of data from manuals or handbooks, etc. Accessing such information is normally slow and could be a serious inhibiting factor in their creative reasoning. Present day computing environments do not lend themselves easily to support such an activity. They require *ad hoc* programming by the experts, while the communication is mostly realized through cryptic text and command lines. Such an environment discourages the use of computers by the experts for the creative part of their work.

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The existing prototypes of expert systems acquire their knowledge by interviewing the experts, from manuals and from handbooks, etc. But the interview process reveals "bits" of knowledge, the so-called production rules. These rules reflect the expert's heuristic database, accumulated from past experience. Consequently, the extracted knowledge is limited to that which resides at the surface of the expert's cognitive abilities. Thus, rules stemming from repetitive tasks can be easily articulated. But, rules related to the synthesis of processing schemes, process flowsheets, control systems for complete plants, design of operating strategies, and other activities in process engineering, are highly "contextual" and thus very difficult to access and articulate.

Knowledge accumulated from interviews, handbooks, or manuals is very poor in terms of the reasoning strategy that an expert employs to solve various problems. Thus, the ill-defined formulations of the various process engineering problems imply unstructured reasoning methodologies, which normally are very inefficient and frustrating experiences. Within the scope of the available expert system prototypes it is extremely difficult to capture the reasoning procedures used by the experts, which are quite complex and highly contextual.

RESEARCH PROJECTS AND THE NEW PROTOTYPE OF AN INTELLIGENT SYSTEM

The two deficiencies discussed above are very restrictive and imply that one needs a different prototype in order to make artificial intelligence a viable technology in process engineering. The following are the principal characteristics of this prototype

- **Allows the designer to concentrate on the creative aspects of his/her work**
- **Facilitates the use of computers through rudimentary natural language interface, and intelligent databases and graphic interfaces**
- **Incorporates the features of standardized expert systems (heuristic knowledge extracted from interviews, handbooks, manuals, etc.)**
- **Contains facilities which permit the designer to articulate his/her knowledge within the context of the specific problem at hand, *e.g.* an on-line rule editor**
- **Allows the expert to formulate, on-line, during the solution of a particular problem, different reasoning strategies, activated by an *ad hoc* articulation of the designer's own "heuristics"**

Table 1 lists the research projects currently under way, all of which are implementing various forms of the prototype intelligent system under development. Unlike previous or parallel efforts in artificial intelligence, as Table 1 indicates, our research emphasis is on design-oriented intelligent systems. Let us now discuss in some more detail the main components for this new prototype:

Knowledge base: Knowledge is collected from three sources: (i) lists of experiential heuristics, (ii) quantitative models, and (iii) on-line heuristics activated and articulated by the designer within the context of the specific problem being solved. Facilities to capture the knowledge from the third source are absolutely necessary because such knowledge is very incisive and cannot be articulated out of context.

Reasoning strategies: The prototype intelligent system, under development, should have a rich repertory of reasoning strategies, which to a large extent are driven by the designer and are defined adaptively within the context of the problem being solved. Thus, the designer will be able, during the solution of a specific problem, to perform the following tasks automatically: test hypotheses; define conjectures; assert, online defined, intermediate goals; create alternatives; simultaneously carry several alternatives and evaluate them.

TABLE 1.
Current Research Projects at the MIT-LISPE

1. **"DESIGN-KIT": A System for Intelligent Engineering Interfaces and Databases**
2. **Process Development by Analogy**
3. **Synthesis of Process Flowsheets**
4. **Synthesis of Control Structures for Complete Chemical Plants**
5. **Planning and Scheduling Plant-Wide Process Control Operations**
6. **Intelligent Controllers**
7. **Operability Considerations in the Design and Control of Heat-Integrated Chemical Plants**
8. **Computer-Aided Modeling of Bacteria Cells for the Analysis and Development of Biochemical Processes.**
9. **Synthesis of Separation Systems for the Recovery and Purification of Proteins**
10. **Design of Molecules with Desired Properties**

Intelligent databases: The effective use of the proposed new prototype will be heavily dependent on the availability of an intelligent database which should allow: innate reasoning during the search of the database; conversational interaction with the designer through answering the designer's queries, or accepting new elements for the tables of data; easy expansion through permanent or temporary new entries, and identification of patterns among its elements. A rich repertory of alternative representations of knowledge and data is also indispenable.

Intelligent interfaces: The database system described above should be supported by a simple and transparent interface between the designer and the computer. Thus, the new prototype includes

- **Graphic interface with easy manipulation of graphic objects (*e.g.*, process flowsheets, control loop configurations, molecular structures, biochemical pathways, routes for operational procedures, etc.).**
- **Interaction with the graphic interface is supported by datamodels describing the available knowledge regarding the graphic objects. This is easily achievable through the frame description of all objects (graphic, models, etc.). Thus, the graphic objects are not empty of substance, but carry a rich content of inherited knowledge.**
- **The built-in "understanding" of the problem characteristics by the graphic objects, which allows the graphic interface to "draw" conclusions and to "provide" explanations, and allows the designer to concentrate on the creative aspects of his/her work.**

"Learning"—upgrade raw data: Process engineering problems are often characterized by the availability of large amounts of data accumulated from past experience, experiments, extensive numerical simulations, etc. The direct value of such information is normally very low because it is simple declarative

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information. Nevertheless, it can be upgraded and used within the context of specific problems. Thus

- **Accumulated data from past process designs (implemented in real life or not) can be upgraded to reveal the underlining patterns present in all similar flowsheets, as well as the sources of difference among different flowsheets.**
- **Analogous pattern recognition could reveal rules aiding the synthesis of control structures for complete plants.**
- **Extensive data on vapor-liquid, vapor-liquid-liquid equilibria (*e.g.*, DECHEMA series of experimental data) could be used to identify patterns between molecular structure and infinite dilution activity coefficients, etc.**

Therefore, the new prototype of an intelligent system should contain rudimentary capabilities of "learning" through a pattern recognition facility among large sets of accumulated data.

EPILOG

Artificial intelligence is expanding the scope of our problems and is enriching our capabilities to deliver viable solutions to otherwise hard and resistant problems. At the same time it is introducing new educational challenges that the research program at the MIT-LISPE is attempting to address and which are related to the computer-aided character of chemical process engineering, the rationalization of the man-machine interaction, and the role of fundamental science in engineering. Our research so far has produced more questions than it has answers, but the intellectual excitement and practical relevance have just started to permeate the programs of graduate research in chemical engineering.

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RESEARCH LANDMARKS

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to become more expert in surface physics, continuum mechanics, microbiology, biochemistry, large molecule chemistry, and other things I wish I could predict. We must change our educational perspective to include new things. For years, ever since I was a freshman in 1933, we have trained students as if they all were going to work for the DuPont Company. This was appropriate. The principles are no different for the future than they were for the past but we must find a new way to talk about chemical engineering if students are to be re-excited. We in chemical engineering have a marked advantage over all other engineers—we are the only ones who know anything about chemistry—an advantage we should work on diligently to parlay into future success.

When I was a young chap at Minnesota there were almost as large a number of students in the metallurgy department as there were undergraduates in chemical engineering. Not long after that, metallurgy disappeared as an undergraduate discipline and it took almost twenty-five years for materials science to emerge from the metallurgy grave. We must be sure that we do not allow a similar fate to befall chemical engineers.

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