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PREFACE

The Proceedings of COPE-91 (Computer-Oriented Process Engineering) represent the continuing effort of both the scientific and industrial community to make known what is new in research and development in the increasingly important interdisciplinary field of computers in Chemical Engineering. Thus it follows the tradition of the Symposium series initiated by the Working Party on the Use of Computers in Chemical Engineering of which the most recent ones were CHEMDATA'88 in Goteborg, Sweden, CACHI'89 in Erlangen, Germany, and ComChem'90 in The Hague, The Netherlands. COPE-91 is the 22nd event of the Working Party and the 449th of the European Federation of Chemical Engineering. A Call for Papers has already been issued for the next symposium of the Working Party, ESCAPE-1, in Elsinore, Denmark, May 25-28, 1992.

In essence, the scope of COPE-91 focused on the following topics:

- Artificial Intelligence in Chemical Engineering
- Computer Integrated Process Engineering
- Reliability and Risk Assessment
- Process Design under Uncertainty
- Education and Training in Computer Applications

Keynote lectures were presented by prominent invited speakers to introduce each selected topic. A total of 61 papers representing 21 countries (Argentina, Austria, Belgium, Bulgaria, China, Czechoslovakia, Denmark, Finland, France, Germany, Hungary, Italy, Japan, The Netherlands, Norway, Poland, Spain, Switzerland, United Kingdom, United States of America and Yugoslavia) were chosen by the COPE-91 Scientific Committee from the 118 submitted. The criteria for choice being originality, scientific contribution, long-term significance and the quality of presentation. All the selected papers and the keynotes are included in this volume grouped by topic and type of contribution. An effort was made to have the most deserving papers accessible to all congress participants in plenary sessions (10), while the others were presented and discussed in parallel (30) and poster (21) sessions. In this way maximum interaction between all participants was realised. This Symposium tried to create a forum for debate on the new developments in chemical engineering, rather than attempting to forecast the future. We want to thank all of the authors for their valuable contributions to this Symposium.

On behalf of the international community, we wish to thank the Spanish Society of Industrial Chemistry (SEQUI), the Catalonian Institution of Industrial Engineers, the Department of Chemical Engineering of the Universitat Politècnica de Catalunya and, of course, to all members of the Organizing and Scientific Committees.

With respect to the financial aspects of this Symposium, we would like to express our gratitude towards those contributing to make this Symposium a reality: Hoechst Ibérica, Dow Chemical Ibérica, Solvay and IBM SAE

The theoretical and practical aspects of the use of computers in Chemical Engineering covered in this book should find wide use in libraries and research facilities, and a direct impact in the chemical industry, particularly in production automation, utility networks and computer integrated process engineering.

L. Puigjaner
A. Espuña

COPE-91

EUROPEAN SYMPOSIUM ON COMPUTER APPLICATIONS IN CHEMICAL ENGINEERING

Barcelona, Spain, October 14-16, 1991

Organised by:
The Spanish Society of Industrial Chemistry (SEQUI)
The Catalonian Institution of Industrial Engineers
The Department of Chemical Engineering of the Universitat Politècnica de Catalunya (UPC)

in collaboration with The Working Party on the Use of Computers in Chemical Engineering (22nd Event) of the European Federation of Chemical Engineering (449th Event)

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Session 1

ARTIFICIAL INTELLIGENCE IN CHEMICAL ENGINEERING

Computer-Oriented Process Engineering, edited by L. Puigjaner and A. Espuña
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Artificial Intelligence in Process Engineering, 1969 to 1991 and the future: some Pertinent Questions.

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Abstract

The first appearance of 'intelligence' in process engineering software was in the field of heat exchanger network synthesis in 1969. With the subsequent expansion of AI as a discipline a plethora of techniques became available for application to process design, operation and analysis. After more than twenty years of research it seems appropriate to ask some critical questions. What can we now do better as a result of AI technology? Can we expect future quantum improvements in our ability to design and operate chemical plants through the use of AI techniques? What should be the relationship between process engineers and the mainstream of AI workers? Are there requirements which we should be urging the AI community to address to achieve the major breakthrough which still appears to be needed?

1 Introduction

In 1969 Masso and Rudd [1] described computer software to synthesise heat recovery networks. This used what has subsequently become known as an 'expert system'. It had a series of rules for generating alternative networks, and it 'learned' by changing weights which directed the choice of rule, these being changed to favour successful strategies.

The method did not produce very good networks, and although many subsequent workers used this 'rule based' approach to process synthesis it was never entirely successful.

In the early 1980's the expansion of the field of Artificial Intelligence caused a number of chemical engineers to re-examine the rule based approach. While Masso and Rudd had written their programs, with great ingenuity and probably pain, in Fortran, later workers had available a range of new languages [1] and techniques from the AI community. However, the same rules rewritten using more sophisticated tools appeared, unsuprisingly, to work no better than before.

The point I wish to make here is that to date AI has supplied us mainly with *tools*. However, as chemical engineers we are concerned ultimately with *principles* and *understanding of phenomena*. The application of new tools, however sophisticated cannot advance engineering practice, unless it leads to, or is combined with, improved understanding.

2 The Techniques and Achievements of AI

I will discuss some of the techniques which the chemical engineering community have so far taken from AI and use this as a framework to address my first two questions:

- What can we now do better as a result of AI techniques, and
- What significant improvements might we expect in future?

2.1 Rule Based Systems

The AI technique which most clearly caught the popular imagination in the early 1980s was the so called 'expert system'. At one time practically every meeting I attended seemed to include the discussion of some highly intractable and little understood problem. This discussion would be terminated by the remark 'What we need is an Expert System'. This was in fact the very last thing that was needed in most cases; the real

[1] Well, newish; LISP appeared about 1960. Given that is has probably evolved less since then than has FORTRAN it might be regarded as the oldest programming language still in use!

requirement was a proper understanding of the problem. The rule based or 'expert' system is a technique for avoiding the need for understanding by programming a large set of empirical rules. Such an approach does not require any deep systematic knowledge, and indeed the most effective applications have been in areas dominated by experience and 'rules of thumb' such as materials selection. An 'expert' in this context is someone who succeeds without actually knowing why.

The importance of the rule based system to process engineers was not its ability to be an automated rule book for plant design or operation, although this has been a useful and practical facility, particularly in the operations area.

I believe we learned two lessons from the efforts which were expended on these systems.

Firstly, we confirmed the overwhelming importance of knowledge as opposed to technique, i.e. the rules themselves and not the method of programming them. This has already been mentioned in the content of heat exchanger network synthesis. It is useful to complete this discussion.

Following the work of Masso and Rudd and others, we produced in 1972 [11] a rule based system with only *one* rule, the 'hottest-highest' heuristic. This worked at least as well as any other technique available at that date, clearly illustrating the importance of getting the rules correct! However the method was still unsatisfactory, and the deficiencies of the approach were not fully exposed until the work of Flower and Linnhoff [3] led to a more thorough understanding of the nature of the problem.

Thus experimentation with rule based systems did promote efforts to understand both phenomena and methods. An example of the latter is seen in the work of Douglas [4] in the development of hierarchical rules for process design. I believe that the systematisation which Douglas has brought to the area of conceptual process design will in future be extended to other complex design tasks, such as control systems [12] and the immensely timeconsuming area of hazard and operability studies.

The second lesson from attempts to apply rule based techniques to the phenomena of process engineering is that rules alone were shown to be inadequate to represent the complexity of the subject. We thus learned that we require means of representing the knowledge of the process engineer, especially in process design, in a systematic manner, and that this task is neither simple nor straightforward. Different workers have drawn different conclusion as to the best approach to the problem of knowledge representation. Some have concentrated on techniques, e.g, the use of object oriented programming, discussed below. However, I believe a more fundamental conclusion was drawn by a minority of workers.

This important conclusion is that the appropriate representation for most engineering knowledge is a *model.* I believe that most engineers think in terms of models. The idea of design as modelling was proposed by Westerberg [2]. It is notable that attempts to use rules to handle fault diagnosis [16], [17] and 'hazop' analysis [10] in fact constructed models, in some cases out of rules. The method of constructing the model is of secondary importance, the key concept is that of the model itself.

2.2 Object Oriented Programming

The examples quoted above [17], [10] were less than entirely successful because of the limitation of models built only from if ... then rules. The deficiency of the rule based approach was recognised by Stephanopoulos and his co-workers when they developed DESIGN KIT [5]. One of the most important developments in this work was the use of object oriented programming. In a sense all programming languages are object oriented, only in most cases the type and complexity of the objects available is highly restricted, e.g. to numbers. Object orientation can be regarded as the ultimate conclusion of user defined types and general structures which have been available, in restricted form, in languages such as PL/1 and Pascal. There are also many similarities between hierarchical objects and databases. However, the idea is greatly extended by allowing objects to be active agents as well as just data items; they can be computer code which does does things. Thus object orientated programming provides an ideal vehicle for modelling. However, it is only a means to an end. The model itself, the knowledge which underlies it, and how it is used is still remains the crucial factor.

2.3 Blackboard Systems

Another technique which emerged from the AI community was the blackboard system, embodying the idea of cooperating agents each contributing its own particular expertise to the solution of a common problem. This approach may be used successfully in areas where many diverse and apparently unrelated factors need to be considered, as for example in the design of catalysts [8].

This is also a good model of how a design team or large design project works, and one could regard an

environment for co-operative design as a blackboard system on a large scale [2].
While undoubtedly true, the concept that complex problems require co-operative solution is not a fundamental insight. The difficulty remains of ensuring consistency between the various contributors. Here, I believe, the use of a model to provide a global representation of the problem can provide the way forward.

2.4 Planning

Are most AI planning methods merely inferior ways of solving LP problems? The relationship between some AI and optimisation techniques is probably closer than the very different terminology might suggest. An early comparison by Johns [13] showed that efficiency was comparable, and more recently Grossman [15] has shown a more formal relationship.
I have only seen one major scheduling problem which has been successfully solved using AI planning and which was genuinely too large for realistic solution by classical methods, [14]. Thus developments in this area seem to lead to improvements which are marginal at best. However, I think that there should be useful synergy between the two approaches; one profitable development would seem to be in the superstructure approach to MINLP, where AI techniques can be used to construct the superstructure.

2.5 Achievements

What can be now do better? Not a lot I fear. Some useful, practical 'automated manuals' have been provided, but these have not really addressed problems that were either of large scale or real complexity.
One large scale problem, a whole plant diagnostic system, was tackled in the Falcon project [17], a joint industry/university exercise which cost a very large amount of money and seems, despite initial optimism, to have yielded only modest returns. Although the project was large in scope, its detailed implementation seems to have been rather simplistic, and none of the participants has gone on to further similar projects.
We have seen some demonstration design systems on a rather larger scale, like DESIGN KIT [5] and the distillation design system of Myers etal [6], but significant practical complex systems have not yet resulted from these efforts.
However, we have learned things about the nature of process engineering knowledge, particularly in the domain of design, and this may help us to the missing quantum leap in the future. To summarise, we now know that:

- process engineering knowledge is diverse and complex.
- it must be structured hierarchically
- problems must be solved cooperatively
- heuristic and mathematical techniques must be combined

And what will we be able to do better in future? If we extrapolate from present state of the art, then our expectations will have to be modest. More selection systems, showing only the 'intelligence' of a low to medium grade technician or plant operator, or perhaps at best a horrendously expensive large scale system applicable only in the particular domain for which it was constructed, and effectively impossible to modify or extend.

3 Future Developments and Possibilities

The Reader may by now have gained the impression that I am somewhat disappointed by the outcome of AI work in process engineering. I do indeed believe that there have been no major innovative achievments and that the effort and ingenuity invested so far has not yielded a commensurate return.
What did I expect? I should have hoped for something on a much broader scale. I would be hard pressed to define *intelligence*, but whatever it is, I do not see it in rule based systems which can handle only restricted or intellectually trivial problems of a 'rule book' nature. Nor do any larger systems so far produced appear to have the ability to handle a real problem in depth.
Why have rule based systems not been developed to handle larger problems, such the integration of various activities in process design? One important reason for this has already been noted, namely that rules are inadequate to represent all but a rather restricted type of knowledge. However, more sophisticated techniques, such as frames, also have severe deficiencies, which suggest that there is at present no adequate methodology to represent the kind of knowledge with which we are concerned [18]. However, one direction in which we might go to find a solution has already been suggested, namely by the use of models.
The other major problem is that of sheer scale and complexity. It is not possible to contemplate the creation of a rule base for a really large system for the same reason that it is not possible to sit down and write a ten thousand line program without subroutines. The answer to this might appear to be the

same as to the programming problem, namely structure [23], through the decomposition of tasks and the use of a blackboard system. However this gives rise to another problem, that of consistency. Concepts such as 'pressure', will be used by different modules in their own context. The interpretation of 'pressure' in, say, a flash calculation, will almost certainly differ from the use of the concept in the design of a pressure vessel. It will however be the same concept, and may even be the same value. We became aware of this difficulty in the course of an attempt to construct blackboard system for integrated process design [7] when it became clear that it was necessary to define such fundamental concepts in a consistent manner for all modules. Although this is a more structured task than the construction of a monolithic rule base, to define all necessary concepts will be a task at least as daunting.

The problems identified here, namely the use of models for knowledge representation and the resolution of conflicts without overwhelming complexity are intractable and have not been addressed by process engineers working with AI. Nor have they been much examined by what most process engineers would regard as 'mainstream' workers in AI, with the exception of Brachman and his coworkers [18]. However, these are problems which humans deal with regularly, and I believe it is to the areas of cognitive science, psychology and linguistics that we must turn for their solution.

To answer my last two questions I shall discuss the above problems in the light of work from these disciplines. I must emphasise that the ideas I am going to report are almost entirely due to the insight of Struthers [7], who appears to have been the only process engineer to approach the problem of knowledge based process systems from this point of view.

3.1 Models

Most process engineers can accept readily that models of all sorts play an important part in our understanding of complex phenomena. What is not necessarily so obvious is that models are a rich means of knowledge representation which can be used for reasoning. The ability of models to form the basis of knowledge representation and reasoning was identified some time ago in a more general context by Johnson-Laird [20], who developed the idea of 'mental models' from an even earlier suggestion by Craik [21].

Briefly, the idea is that we reason using 'working models' of the world. Like engineering models, these are neither complete nor exact. The key feature is that in order to work the models do not have to be exact. It appears that we can make correct deductions using models which are not quite correct, and even, with their aid, make logical deductions without the use of formal syllogisms. We also use our model in different contexts and are able to switch contexts without confusion.

Although this work has had little influence on engineering applications of AI, it has been applied effectively elsewhere, for example in the domain of computer aided language translation. Rather than pursuing the ever moving goal of semantic analysis, one can seek to construct a model of the sense of a text, interacting with the speaker if necessary by asking questions to resolve ambiguity [22].

The need for something of this sort became apparent to us while trying to construct our large scale design system. The conventional rule based system with a general purpose 'dumb' rule interpreter seemed to be too inflexible and restrictive. Instead, we moved towards a system of specialised interpreters and a guiding model. Such techniques might be used to construct the knowledge base both of a process design and of the design method itself. [2] An important feature of any useful knowledge representation will be its ability to change with time, i.e. it must be dynamic and not static. Our models must be able to extend and refine themselves as we add to our knowledge of the current problem and refine our objectives.

3.2 Categorisation

As mentioned above, we discovered that the provision of consistent global definitions of fundamental concepts for a large scale blackboard system was an apparently overwhelming task. This appears to be inherent and not related to the technique used to implement the system. We might still have to accept that this must be done anyway; large scale systems may just require very large scale and complex knowledge bases, but before wading in with a sledgehammer it is worth looking for alternative solutions. There is good reason to suppose that there must be a better way. Studies of human cognition suggest that it operates by more effective mechanisms.

The difficulty with creating global definitions is that to cover all possible eventualities they need to be pro-

[2] It should be apparent that we are concerned with two rather different, but related types of knowledge in most engineering situations, namely knowledge about our process, its chemistry and physics etc., and knowledge about calculation and design methods. We thus need two kinds of model, a model of the process itself, and also knowledge about design procedures and the design process [9].

hibitively extensive and complex. Even then, it is not practical to ensure that every contingency has been covered. At a later date we are bound to have to add to our knowledge base. The problem of adding to, say, the rule base of a conventional 'expert system' is that of ensuring consistency of the new rules with the old, and is impractical on combinatorial grounds. In whatever form we choose to represent our knowledge we will have this same problem.

These difficulties apply not only to abstract concepts. Consider what we must do if in a process design system we wish to represent the concept 'heat exchanger'. We must include all types of heat exchanger: shell and tube, plate etc., and all their properties: geometry, material of construction and so on. In reasoning about heat exchangers in different contexts we will use different aspects of these properties depending on whether we are interested in, say, the process flowsheet structure, equipment costs or plant layout. All heat exchangers will share some properties, but not others; they will still be 'heat exchangers' even if lacking certain properties. We may find that we have forgotten to allow for a particular type of heat exchanger, e.g. graphite block, and wish to add it at a later date. We face substantial problems if in designing our original knowledge base we assumed implicitly that all heat exchangers were to be made of metal. There are so many facets of 'heat exchangers' or 'pressure' that we cannot realistically expect to construct a representation which deals with them all consistently. Indeed, we are likely to find inconsistencies in the way in which we need to handle these concepts, for example in circumstances when we can, or must, assume pressure to be a function of other variables. Humans are able to handle inconsistencies and incompleteness of this sort readily; can we make use of the experience of cognitive psychologists?

As long ago as 1956, J S Bruner and his coworkers [19] proposed their theory of *conceptual categorisation*. According to this theory, *concepts* may be categorised in terms of their *attributes*, these attributes being of various types having a different role and importance in the assignment of a concept to a category. The theory was constructed in an effort to explain how we are able, for example, to recognise a person from a series of photographs taken in different lighting conditions, wearing different clothes or even taken several years apart. We identify all these as falling into the category of that person because they have some essential attribute of 'person-ness'.

Although this may sound esoteric, I believe that the approach offers useful guidelines to the construction of knowledge based systems for process engineering. For example, following the ideas of different types of category, of *equivalence categories* of things that are the same in particular circumstances, and especially of *functional equivalence*, of things, like heat exchangers, which are equivalent, at the flowsheet level at least, because they perform the same function, viz to transfer heat. Similarly there are different types of attribute which heat exchangers possess, some of which, *criterial attributes*, enable us to assign an entity to the class of 'heat exchanger' or 'constant pressure process' even in the presence of other conflicting information. The ideas also suggest the definition of *typical* and *generic* instances; these are used extensively by engineers in design. An 'ideal gas' is a *generic* gas. On the other hand nitrogen is a *typical* gas.

A knowledge based system making use of these ideas could overcome many of the problems of complexity since categories might be manipulated as entities. The ability to allow certain inconsistencies reduces the problem of adding new information. The idea of categorising has obvious implications in learning, when an entity is recognised as belonging to an existing category then we have 'learned' how to deal with this new entity.

4 Conclusions

The problem of constructing a 'real' knowledge based system remains a significant one, and I hope I have not given the impression that I know how to do it! However, I believe there are fundamental insights to be obtained, especially from the field of cognitive science, which will do more to bring about such an achievement than a concentration on the use of tools and techniques.

I am thus able to propose answers to my last two questions.

- What should be the relationship between process engineers and the AI community ? We should be talking to theoreticians and cognitive scientists as well as those whose 'practical' work might appear to be of more direct relevance to our immediate needs.

- Are there requirements we should be urging on the AI community to address? Yes. We need practical tools to implement the esoteric ideas of cognitive science, and AI workers are best placed to develop them. These tools will be useful to us and also in nonengineering applications; translating from a design concept to a design is a task comparable to translation from English into Spanish and at least as intellectually challenging!

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