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THREE CLIPS-BASED EXPERT SYSTEMS FOR SOLVING ENGINEERING PROBLEMS

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ABSTRACT

We have written three expert systems, using the CLIPS PC-based expert system shell. These three expert systems are rule based and are relatively small, with the largest containing slightly less than 200 rules. The first expert system is an expert assistant that was written to help users of the ASPEN computer code choose the proper thermodynamic package to use with their particular vapor-liquid equilibrium problem.

The second expert system was designed to help petroleum engineers choose the proper enhanced oil recovery method to be used with a given reservoir. The effectiveness of each technique is highly dependent upon the reservoir conditions.

The third expert system is a combination consultant and control system. This system was designed specifically for silicon carbide whisker growth. Silicon carbide whiskers are an extremely strong product used to make ceramic and metal composites. The manufacture of whiskers is a very complicated process, which to date, has defied a good mathematical model. The process was run by experts who had gained their expertise by trial and error. A system of rules was devised by these experts both for procedure setup and for the process control. In this paper we discuss the three problem areas of the design, development, and evaluation of the CLIPS-based programs.

INTRODUCTION

Our goal for these projects was to develop small computer-based expert assistants to help some of the less-experienced engineers at Los Alamos National Laboratory make expert decisions about particular tasks for which they may not otherwise have the expertise.

Although we had available a LISP machine and the sophisticated hybrid expert system shell, KEE, we felt that the "frame" or "object-based" simulation expert system designs were unnecessary and overly complex for our application. We further felt that any usable expert system should be executable with an inexpensive shell and an easily available computer. We therefore focused our search on rule-based shells for the PC family of computers. But we were not sure that the PC-based shells available to us would be adequate for the expert systems that we envisioned. We were pleasantly surprised when we found that CLIPS[1] could handle our tasks.

We have written three expert systems using the CLIPS expert system shell. These three expert systems are rule-based and relatively small. The largest is slightly less than 200 rules. Their size, however, does not preclude them from being useful. The first expert system is an expert assistant that was written to help users of the ASPEN computer code pick the proper thermodynamic package to be used with their particular vapor-liquid equilibrium problem. ASPEN is a large computer code used to design chemical plants and refineries. Vapor-liquid equilibrium and associated energy balance problems are an important part of chemical plant and refinery design. There are 144 possible correlations for vapor-liquid equilibrium calculations that can be obtained using combinations of the built-in ASPEN options. Picking the proper combination requires some expertise in thermodynamics, which may not be a strong area for the plant designer. If the designer uses the wrong correlation, the plant design will be wrong.

The second expert system was designed to help petroleum engineers pick the proper enhanced oil recovery method to be used with a given reservoir. There are several different techniques used for enhanced oil recovery. The effectiveness of each one is highly dependent upon the reservoir conditions. Ultimately, the choice of an enhanced oil recovery technique will be based upon economics. However, there are many techniques and many variations of conditions within each technique. It is therefore impractical to do an economic analysis of each case. This expert system helps the user screen the methods and reduce the required number of economic calculations to just a few.

The third expert system is a combination consultant and control system. This system was designed specifically for the silicon carbide whisker growth. Silicon carbide whiskers are an extremely strong product that are used to make ceramic and metal composites. The manufacture of the whiskers is a very complicated process, which to date has defied a good mathematical model. The process was run by experts who had gained their expertise by trial and error. A system of rules was devised by these experts both for procedure set up and for process control. These rules make up the expert system used for this process. This expert system is especially useful because the silicon carbide whisker process is a candidate for technology transfer. With the expert system, we can transfer complicated technology that is not well enough understood to model mathematically without transferring the experts as well.

THE ASPEN COMPUTER CODE

One goal was to develop an expert system to help engineers design refinery and chemical processes. The modern design of refinery or chemical plant operations requires a chemical process simulation computer code. The simulation

code used by Los Alamos is ASPEN[2] (Advanced System for Process ENgineering). It was developed for the United States Department of Energy at the Massachusetts Institute of Technology. Similar software products are available in the commercial marketplace, but because of ASPEN's solids handling capability and its wide choice of built-in thermodynamic packages, it was considered to be the only product suitable for the design of coal and oil shale processing units. Thus, ASPEN was the product of choice for use in LANL's recent coal and shale oil projects.

To demonstrate why an expert system is useful, it is first necessary to give a brief description of how ASPEN works. Then the descriptions of thermodynamic packages and of our expert system for determining the proper thermodynamic package for use with ASPEN will demonstrate why and how this program is useful.

With ASPEN, a chemical plant is represented by modules that are tied together by material flow streams. The modules may, in turn, be represented by building blocks that are unit operations common to many different types of processing modules. The ASPEN package also includes a large thermodynamic database and a code that allows mass and energy balances to be performed to aid the designer in sizing, specifying, and selecting equipment and/or determining optimum processing conditions.

For example, Fig. 1 is a block flow diagram of an oil shale processing plant. Each block represents a major plant module, including modules for a retort, a gas-liquid separation and cleanup unit, a hydrogen recovery unit, a hydrogen plant, and a hydrotreater unit. The solid lines represent material flow streams in the plant. In developing a block flow diagram like that in Fig. 1, the designer supplies instructions to ASPEN that specify the compositions, conditions and rates of raw materials, and operating conditions, and identify the module and the flow streams between modules. Output from ASPEN contains information on the rates, temperatures, pressures, and compositions of the flow streams between and from the modules.

Figure 2 is the building block, or unit operation, flow diagram for the retort module of Fig. 1. In Fig. 2, the unit operation blocks, pumps, mixers, heaters, reactors, etc., are displayed in a logical design sequence. The solid lines represent mass flow, and the dotted lines represent energy flow. When the flow stream information and conditions are specified and calculated for the block diagram of Fig. 1 and additional instructions are supplied for each building block, calculations can be performed in ASPEN to yield rate, temperature, pressure, composition, and energy requirements for each building block and for the flow streams between the building blocks. This output is used by the designer to make economic calculations, to specify equipment, or to set the optimum operating parameters for the unit.

In the retort module, the oil shale unit undergoes processes of heating, thermal decomposition, combustion, and vaporization to name a few. Calculations involving these processes require information on enthalpy, heat capacities, heats of reaction, and vaporization for materials that contain so many components that the compositions must often be expressed in terms of fractions containing components with nearly like-properties. Measured thermodynamic data are often sparse over the range of compositions and conditions encountered, and even if available, would be clumsy or time consuming for use with computer codes. Thus,

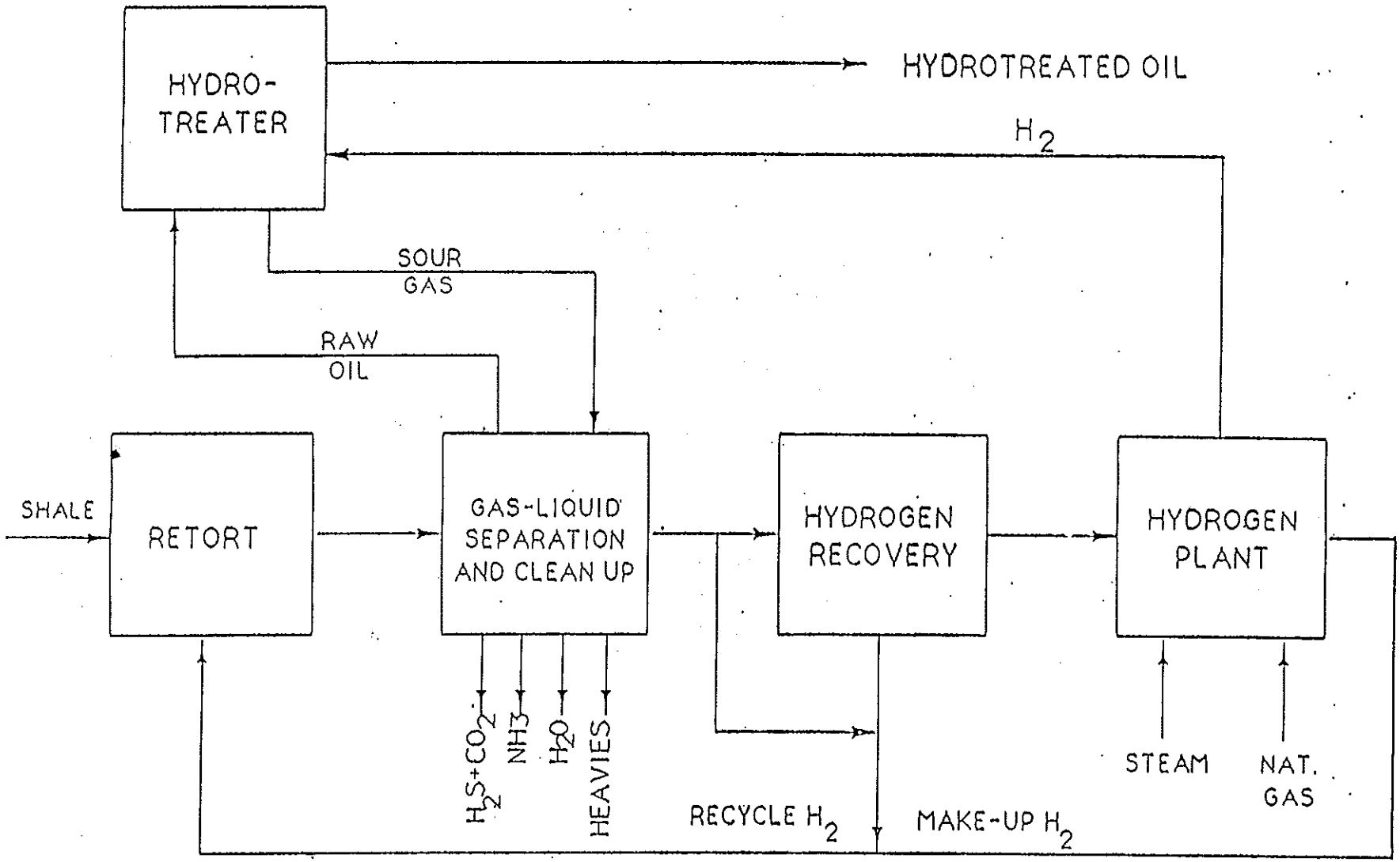

Fig. 1. ASPEN block flow diagram for an oil shale plant.

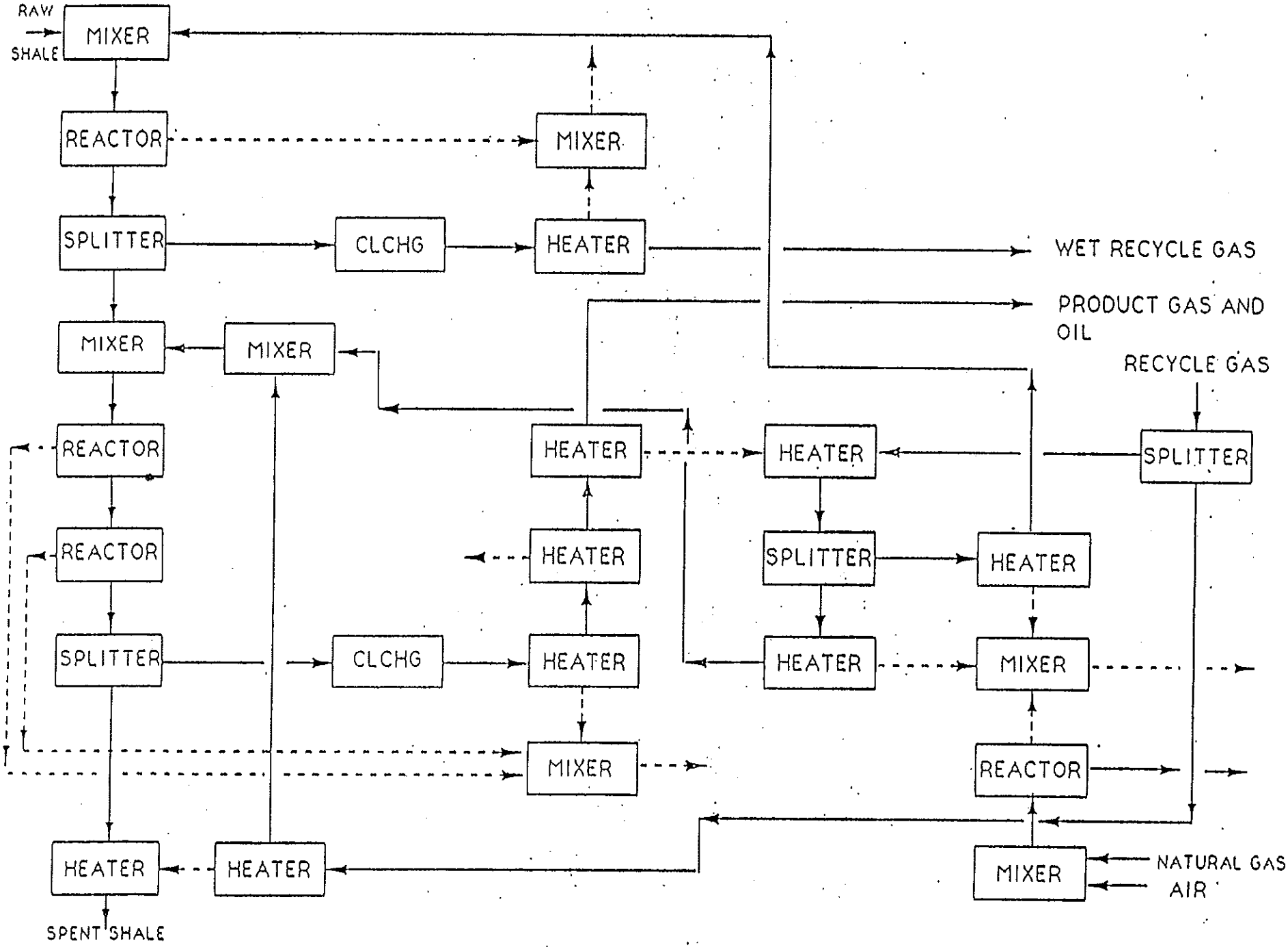

Fig. 2. ASPEN block flow diagram for an oil shale retort.

the ASPEN code provides the designer with several thermodynamic models, or packages, that provide data for the calculations described above.

Figure 3 is the ASPEN building block diagram for the gas-liquid separation and cleanup module. The diagram requires less equipment than the retort, but, more importantly, it differs from the diagram for retort (Fig. 2) in the type of process being carried out. As shown in Fig. 3, like the retort module there are heating, pumping, and mixing blocks, but in addition, here there are water separation, hydrocarbon phase separations, and impurity removal processes. Although these separations also require thermodynamic data for modeling, the nature of these processes differs significantly from those in the retort module.

Not surprisingly, the thermodynamic package that is appropriate for use with calculations in the retort module is likely very different from the appropriate package for use with the gas-liquid and cleanup module. Even within the gas-liquid separation and cleanup module, the best thermodynamic package for use in performing calculations on the different unit operations may differ. For instance, the best package to use in separating impurities, which may be highly polar compounds, might be different from that used with the flash unit in which the liquid-vapor phase behavior of relatively nonpolar compounds is described.

Also not surprisingly, many designers, when first assigned the task of using ASPEN, do not have the necessary experience and training to know the strengths and weaknesses of the different thermodynamic packages available to them. Those neophytes often must rely on the advice of more experienced designers until they gain their own knowledge and experience.

As an example of the computations involved, ASPEN contains two basic thermodynamic model types for predicting equilibrium K-values, that is,

$$K_i = y_i/x_i = \phi_i^L/\phi_i^V \quad , \qquad (1)$$

where y_i = the mole fraction of component i in the vapor phase,
x_i = the mole fraction of component i in the liquid phase,
ϕ_i^L = the fugacity coefficient of component i in the liquid phase, and
ϕ_i^V = the fugacity coefficient of component i in the vapor phase.

In K-value calculations, the vapor phase fugacity coefficients are always calculated using an equation of state (EOS) thermodynamic model. For liquids that are ideal mixtures or nearly ideal mixtures, such as mixtures of hydrocarbons, EOS are also used to predict liquid fugacities. When both the liquid and vapor phase fugacities are predicted using an EOS, the model is called an EOS model. Several such EOS models are available with ASPEN. Many EOS are based, at least in part, on fundamental concepts of the physical properties of matter, while others may be purely empirical. And each different EOS offers an advantage over

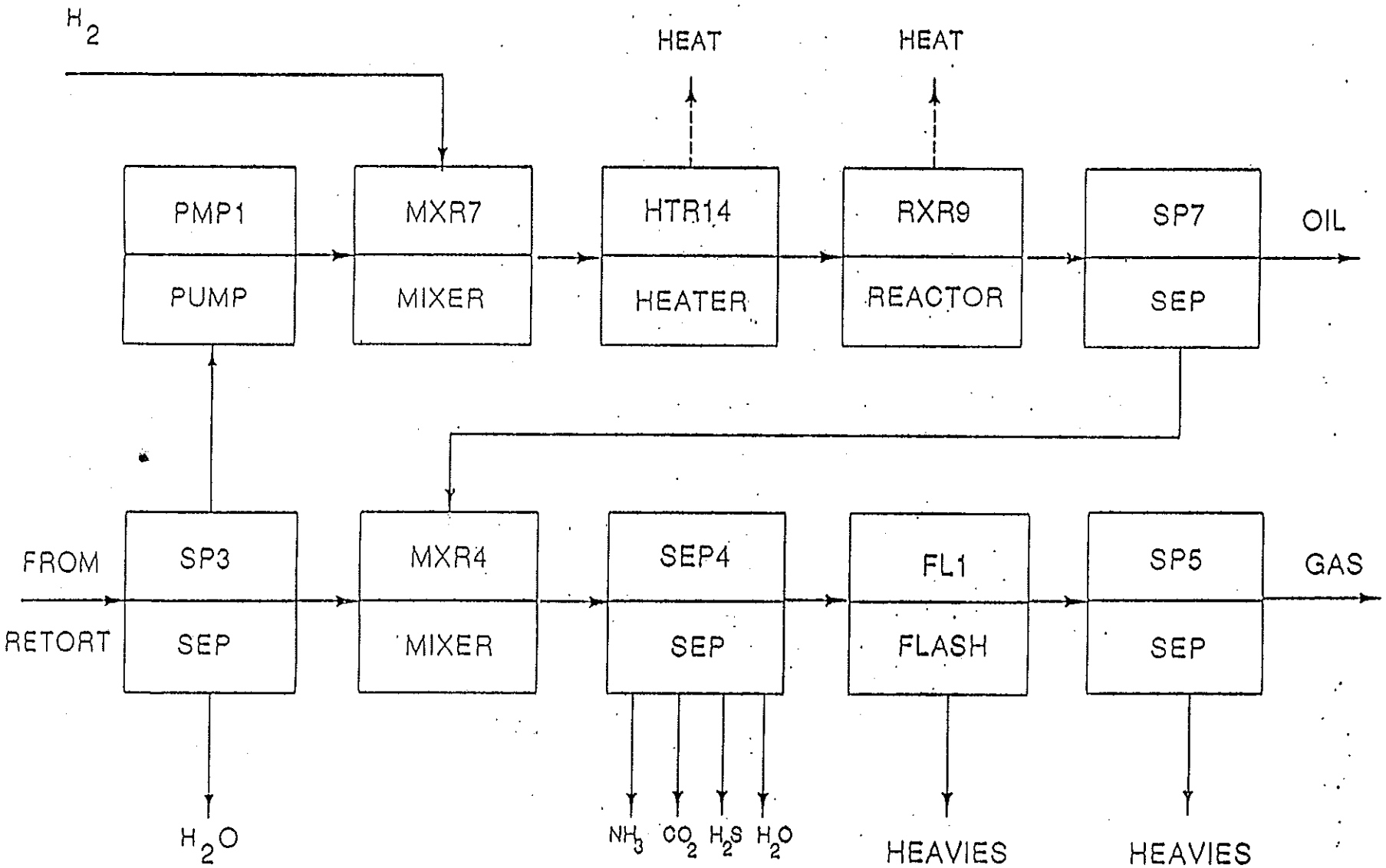

Fig. 3. ASPEN block flow diagram of a gas-liquid separation and clean-up unit.

the other EOS for one (or more) type of prediction. But no EOS has been demonstrated to be superior to all other EOS for every design situation.

For nonideal liquid mixtures, such as aqueous electrolyte solutions, a type of thermodynamic model called an activity coefficient model is often used to predict liquid phase fugacity coefficients. An example of this type of model is Eq. (2), the famous Chao-Seader Eq. (3),

$$K_i = \nu_i^o \gamma_i / \phi_i^V \quad , \tag{2}$$

where ν_i^o = the liquid fugacity coefficient of the pure component (this coefficient is different from ϕ_i^L, which is the liquid fugacity coefficient of component i in the liquid mixture), and

γ_i = the liquid phase activity coefficient.

Typically, with an EOS model, both the liquid- and vapor-phase fugacity coefficients are calculated using the same EOS. With the activity coefficient model, the pure component liquid fugacity coefficient model is usually matched with a particular activity coefficient model. In this model, however, one may choose the calculation for the vapor-phase fugacity coefficient from many EOS, independently from the activity coefficient calculation. Thus, many models and many combinations of models are available from which to choose, and in a given situation, one choice is often better than any other.

In addition to the equilibrium K-values, other important thermodynamic functions are also used in ASPEN. For example, the Gibbs free-energy function is related to the equilibrium K-value by Eq. (3), as

$$-\Delta G_i = RT \ln K_i \quad , \tag{3}$$

where ΔG_i = the Gibbs free energy of component i at a given state relative to the reference state,
R = the gas law constant, and
T = the absolute temperature.

The enthalpy is related to the entropy and the Gibbs free energy by Eq. (4), as

$$\Delta H_i = \Delta G_i + T\Delta S_i \quad , \tag{4}$$

where ΔH_i = the enthalpy of component i relative to a reference state,
ΔS_i = the entropy of component i relative to a reference state, and where enthalpy, entropy, and Gibbs free energy are all defined for a given state relative to a reference state.

Correct enthalpy values are necessary for proper energy balances. Therefore, it is important to pick the correct K-value model and to pick thermodynamic models that are consistent with the K-value model. This is necessary for the proper use of ASPEN because the major tasks performed by ASPEN are to obtain energy balances and mass balances (phase compositions) at all points in a chemical plant or refinery. The expert assistant helps the ASPEN user to pick the correct K-value and thermodynamic models.

Figure 4 shows the search tree for the expert assistant. The leaves on the tree are the ASPEN system options, or SYSOPs, which are the models that can be used for predicting K-values. In addition to the steam tables for pure water (SYSOP12) and the ideal gas and liquid model (SYSOPO), ASPEN contains two additional major model types: EOS and activity coefficient models. These major model types are further subdivided. The EOS models vary from the empirical Benedict-type equations to the more theoretical-type van der Waals equations. The activity coefficient models are divided into two groups: the models for which the ASPEN user is not required to supply his own system data and the models for which the user is required to supply the system data. The expert assistant asks the user questions about the situation in question. On the basis of the answers given, the assistant recommends the most appropriate model for that situation. The rules for determining the correct model were obtained from the literature[4-10] and and personal experience. References 4 and 5 are exceptionally good.

Each ASPEN SYSOP has provisions for calculating the following thermodynamic properties for the solid, liquid, and vapor phases in a thermodynamically consistent manner.

Fugacity coefficient
Enthalpy
Gibbs Free Energy
Entropy
Volume (density)
Viscosity (no solid correlation)
Thermal conductivity
Diffusivity (no solid correlation)
Surface tension (liquid correlation only)

Within each SYSOP, the code allows changing of thermodynamic models used to calculate the individual phase properties. We have compiled rules in our expert assistant that will allow the user to choose changes to the vapor and liquid fugacity coefficients. This is the most important correlation because it leads directly to the plant mass balance. In a later paper, it would be worthwhile to explore different correlations for all of the other properties. The ASPEN-supplied alternate thermodynamic models for calculating liquid and vapor fugacity coefficients that may be substituted into the system options are listed in Table I. Also listed in Table are the model numbers, which are related to SYSOP numbers.

Table II lists the possible substitutions for which we have compiled rules.

There are 144 possible combinations of models in Table II that may be suggested by using our compiled rules. Each model will be better than any other in a given situation.

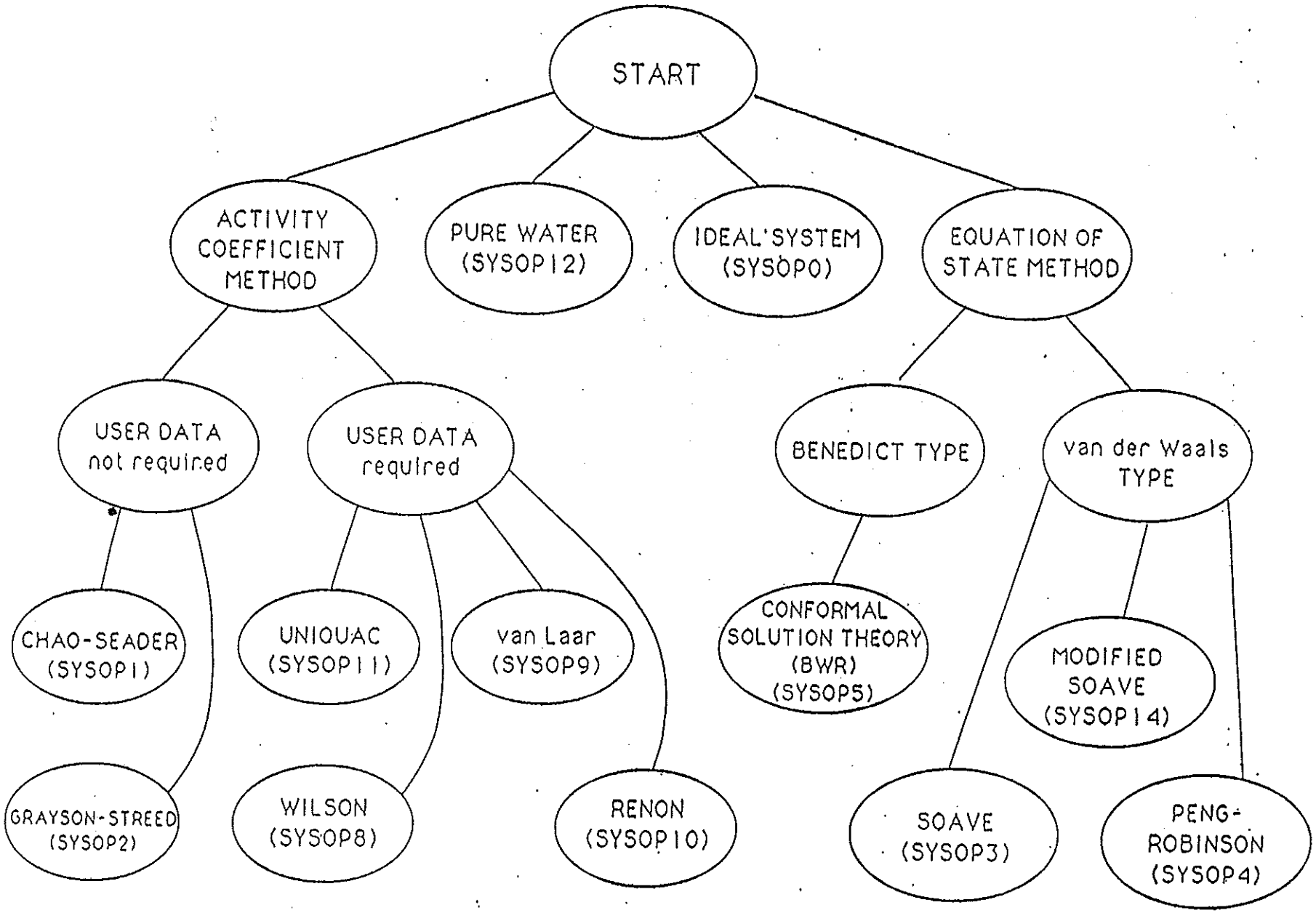

Fig. 4. Search tree for the plant design expert assistant.

TABLE I

ASPEN FUGACITY COEFFICIENT MODELS

Model Number	Name
2	Hayden-O'Connell
3	Redlich-Kwong-Soave
4	Peng-Robinson
5	Conformal Solution Theory (BWR)
6	Perturbed Hard Chain (nonpolar)
7	Perturbed Hard Chain
14	Modified Redlich-Kwong-Soave
21	Scatchard-Hildebrand (temperature dependent)
22	Wilson (temperature dependent)
23	van Laar (temperature dependent)
24	Renon (temperature dependent)
25	UNIQUAC (temperature dependent)
26	Electrolytes

TABLE II

POSSIBLE FUGACITY COEFFICIENT SUBSTITUTIONS FOR THE PROJECT TWO EXPERT SYSTEM

SYSOP Number	SYSOP Name	Vapor Fugacity Coefficient Model Number	Liquid Fugacity Coefficient Model Number
	Ideal solutions		26
0			
1	Chao-Seader	2,3,4,5,6,7,14	21
2	Grayson-Streed	2,3,4,5,6,7,14	21
3	Soave	2,6[a],7[a]	6[a],7[a]
4	Peng-Robinson	2,6[a],7[a]	6[a],7[a]
5	BWR	2,6[a],7[a]	6[a],7[a]
8	Wilson	2,3,4,5,6,7,14	22,26
9	van Laar	2,3,4,5,6,7,14	23,24,26
10	Renon (NRTL)	2,3,4,5,6,7,14	26
11	UNIQUAC	2,3,4,5,6,7,14	25,26
12	Water		26
14	Modified Soave	2,6[a],7[a]	6[a],7[a]

[a] If models 6 or 7 are used for the vapor phase, the same model must be used for the liquid phase and vice-versa.

After the ASPEN user has chosen the best thermodynamic models for each situation in the plant, he can run the code. Unfortunately, since the temperature, pressures, and compositions of many of the internal flow streams were initially only estimates, the ASPEN computation will change these values. These changes may be great enough to require model changes for subsequent ASPEN iterations. Typically, several ASPEN runs are required to obtain the desired product. Figure 5 characterizes how a design engineer can interactively use an expert system with the ASPEN computer code.

EXAMPLE--HOW CLIPS WORKS

We have picked a simple example to demonstrate how CLIPS works with this expert system. In the example, the ASPEN user wants to know which model to use for a desalination plant. Although this is a trivial problem for the expert system it demonstrates well how CLIPS solves a problem. With the answers to only three questions, the expert system picks the steam tables (SYSOP12) and suggests using the electrolyte model for the liquid phase fugacity coefficient (model 26 in Table I). A portion of the search space used by the CLIPS expert assistant that contains this example is shown in Fig. 6. The solution to the example problem is shown on the figure in bold face.

Figure 7 shows the dialogue between a user and CLIPS. The reader can follow in Fig. 6, which is a portion of the search space used by CLIPS.

With this system, instead of just picking the best solution for the more complicated problems, we use a scoring technique and supply the user with a list of rated solutions. To do this, simply score the answer to each question asked by CLIPS.

The dialogue with CLIPS begins with the following questions: *"Are the system conditions low pressure and high temperature?" "Is your system almost all steam and water?"* and *"Are electrolytes present in the mixture?"* The user responds with *No, Yes, Yes.* In this case, this is enough information to allow CLIPS to make a final decision: *"Use SYSOP12 for steam, the score is 5.0. Use liquid phase fugacity coefficient option number 26 for electrolytes."* The score of 5.0 is high. In this example, we really have little choice. With most problems, at this point CLIPS would give a list of possible choices with their relative scores. These scores will be more meaningful as one uses the system more often.

EXPERT ASSISTANT FOR ENHANCED OIL RECOVERY

Some of the reasons to study enhanced oil recovery (EOR) are listed in a 1986 paper by Stosur (11). At the time of the printing of his paper only 27% of the oil ever discovered in the United States had been produced. About 6% more will be produced using existing technology; under current economic conditions. This leaves the remaining 67% as a target for EOR. Currently, only about 6 % of our daily oil production comes from EOR. These figures indicate, even in these times of reduced awareness of an impending energy crisis, that the study of EOR can be rewarding because of the high potential pay-off.

EOR is expensive. It is necessary for engineers to pick the best EOR recovery method for the reservoir in question in order to optimize or even make

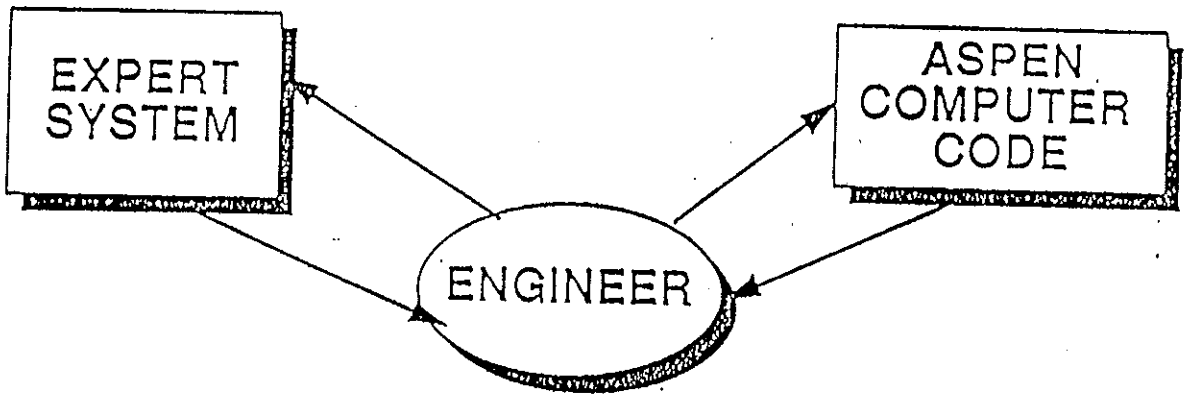

Fig. 5. The engineers use of the expert assistant with the ASPEN computer code.

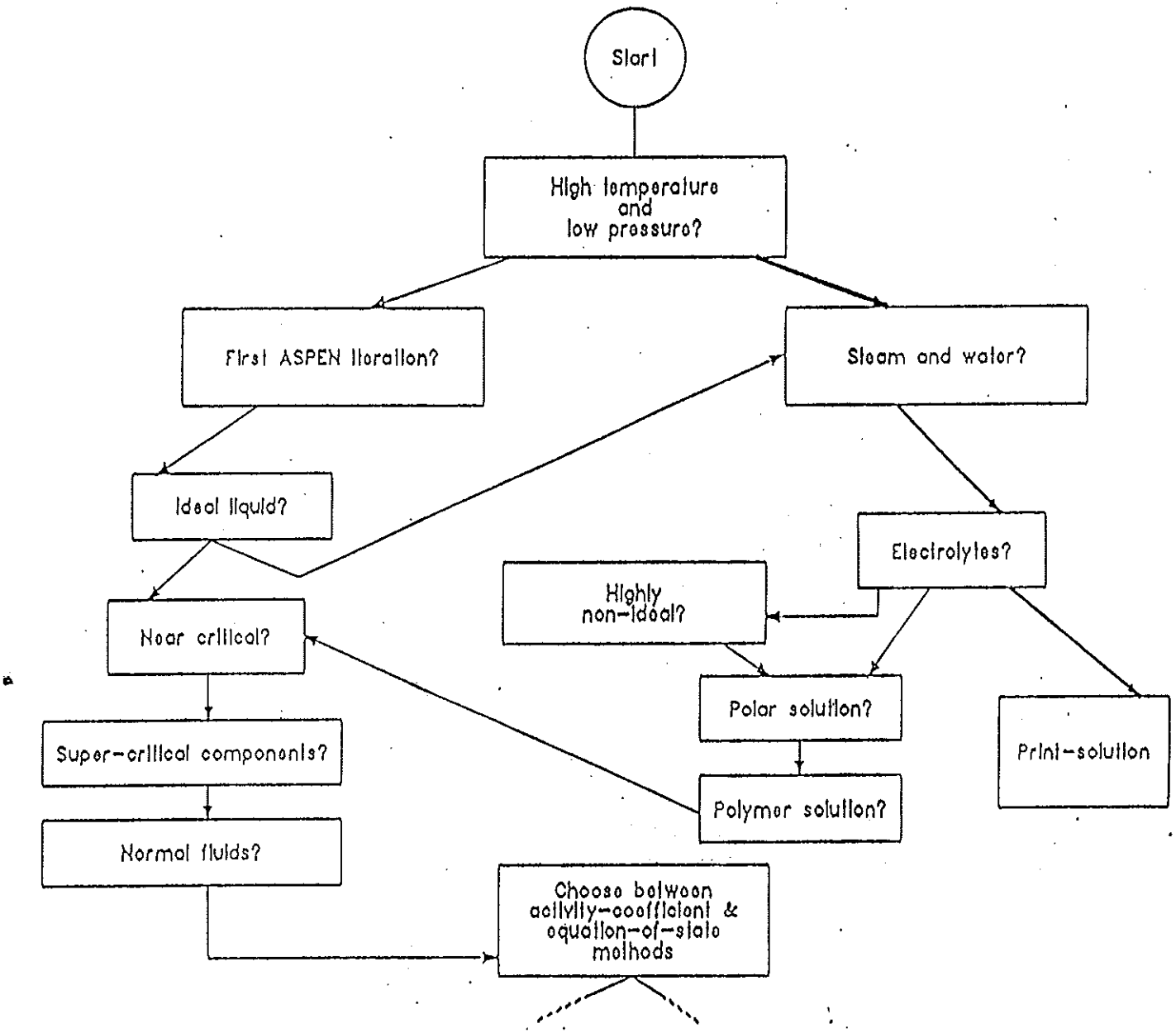

Fig. 6. A portion of the search space of the plant design expert assistant using CLIPS.

Are the system conditions, low pressure and high temperature?

(yes/no/"don't know")

no

Is your system almost all steam and water ? (yes/no)

yes

Are electrolytes present in the mixture?

(yes/no/"don't know")

yes

Use SYSOP12 for steam, the score is 5.0

Use liquid-phase fugacity coefficient option number 26 for electrolytes

Fig. 7. Dialogue with CLIPS.

profits. The entire screening method itself is expensive. It typically involves many steps. The first step is to consult a technical screening guide. Screening guides consist of a table or several charts that list rules of thumb for picking the proper EOR technique as a function of reservoir and crude oil properties. The candidate techniques are often subjected to laboratory flow studies. Data from these studies are then often used in computer simulations of the reservoir. Finally, a pilot project may be used to demonstrate the viability of the selected technique. Economic evaluations are usually carried out throughout the screening process.

Our expert assistant was developed to replace the table and the graphs used in the technical screening guides or to replace step one in the screening process. It provides essentially the same information as the old table and graph method, but it is more comprehensive than graphs and easier to use than the tables. It provides the user with a weighted list of potential techniques at the end of the run, which is quite hard to do with the tables. The expert assistant is user friendly in that it asks all the questions and leads the user through the first stage of the screening process. It is understood that the final choice of a technique will be based upon economics, but it is obvious that the first screening step is quite important because of the high cost of the entire screening process and the absolute necessity of choosing the most economically optimum EOR technique.

For this study we define EOR as any technique that goes beyond water flooding or gas recycling to increase oil well production. This includes only the injection of material not usually found in the reservoir. The program we have developed relies mainly on the work of Taber and Martin (12) and Goodlet et al. (13) for its rules.

EOR techniques can be divided into four general categories: thermal, gas injection, chemical flooding, and microbial. Thermal techniques usually require reservoirs with fairly high permeability. Steam flooding is a thermal technique that has traditionally been the most used EOR method. In the past it has been applied only for relatively shallow reservoirs containing viscous oils. This is one area where screening criteria are changing because improved injection methods now allow us to go deeper, and because new studies have pointed out that steam temperatures affect other reservoir and oil properties, than just viscosity. The expert system format is a good one to use here because we can easily change the program as the technology changes. On the other hand, gas injection techniques are the opposite extreme of steam flooding. Gas injection techniques tend to work best in deep reservoirs containing light oils. Chemical flooding is usually used with low- to medium-viscosity oils, and reservoir depth is usually not a problem. Microbial techniques are new and primarily experimental at this time, and little is known about them. Chemical flooding is divided into polymer, surfactant-polymer, and alkaline recovery techniques. Gas injection is divided into hydrocarbon, nitrogen and flue gas, and carbon dioxide. Thermal flooding is further subdivided into *in situ* combustion and steam flooding techniques. The microbial category is not subdivided. Figure 8 shows the search tree for the expert system.

Expert system users, are quizzed by the system about their particular problems. Typical questions are about the rock formation type, well depth, reservoir temperature and pressure, reservoir thickness, reservoir permeability, oil saturation, oil gravity, viscosity, and composition. Based on the answers to these questions, the system presents users with an ordered list of preferred techniques for their particular wells.

The solid lines in Fig. 8 represent the most common calculated paths to the solution method. The dotted lines show other possible paths to the same solution method. In other words, with this particular expert system a final solution can be found before the system has zeroed in on the correct EOR category. Our search tree is really a directed graph. The reason for this is probably that this system should really be goal driven or use a backward chaining search instead of the normal forward chaining approach used in CLIPS. Although the CLIPS User's Guide (1) shows how to force CLIPS to do backward chaining we did not use this approach. Instead, we forced it into the forward chaining mode by using a scoring system and following a data-driven approach. It would be an interesting exercise to try a goal-driven approach and see if it is easier to program.

Figure 9 is a portion of the search space used by this expert system. Figure 10 shows a portion of the dialog with CLIPS that is used in solving a simple problem.

CLIPS asks the user the following questions:

What is the well depth?

The user answers, *2000 feet*, this is a relatively shallow well.

CLIPS asks *what is the formation type?*

The user answers *Sandstone.*

CLIPS asks questions about payzone thickness, reservoir temperature, permeability, porosity, and oil saturation. The well is at a low temperature corresponding to the relatively shallow depth and has a high permeability. The last two questions shown in Fig. 10 have to do with oil gravity and viscosity. In this case the oil is heavy and quite viscous. The shallow well, high permeability, and heavy high-viscosity oil lead to the conclusion that thermal techniques will work well with this reservoir. The printed list shows the two thermal techniques, steam flooding and *in situ* combustion rate very high on the list to be considered for further study, with scores of 17 and 15, respectively. Two other possibilities are Alkaline flood and microbial drive, with scores of 9 and 7 respectively. To make this expert system work in the forward chaining mode, we decided to ask a lot of questions up front, score the answer to each question, and make decisions based on these scores. The scoring system is empirical and works like this. If the answer to a question presents a condition for which it is impossible for a given method to work, that method will receive a score of -100. If it is very difficult for that method to work at those conditions, a score of -5 is assigned to that method for that question. Other levels of difficulty are assigned -3 and -1 for difficult and just slightly difficult. The method gets a 0 if the answer to the question is not important for that particular method. Scores of 1, 3, and 5 are given for fair,

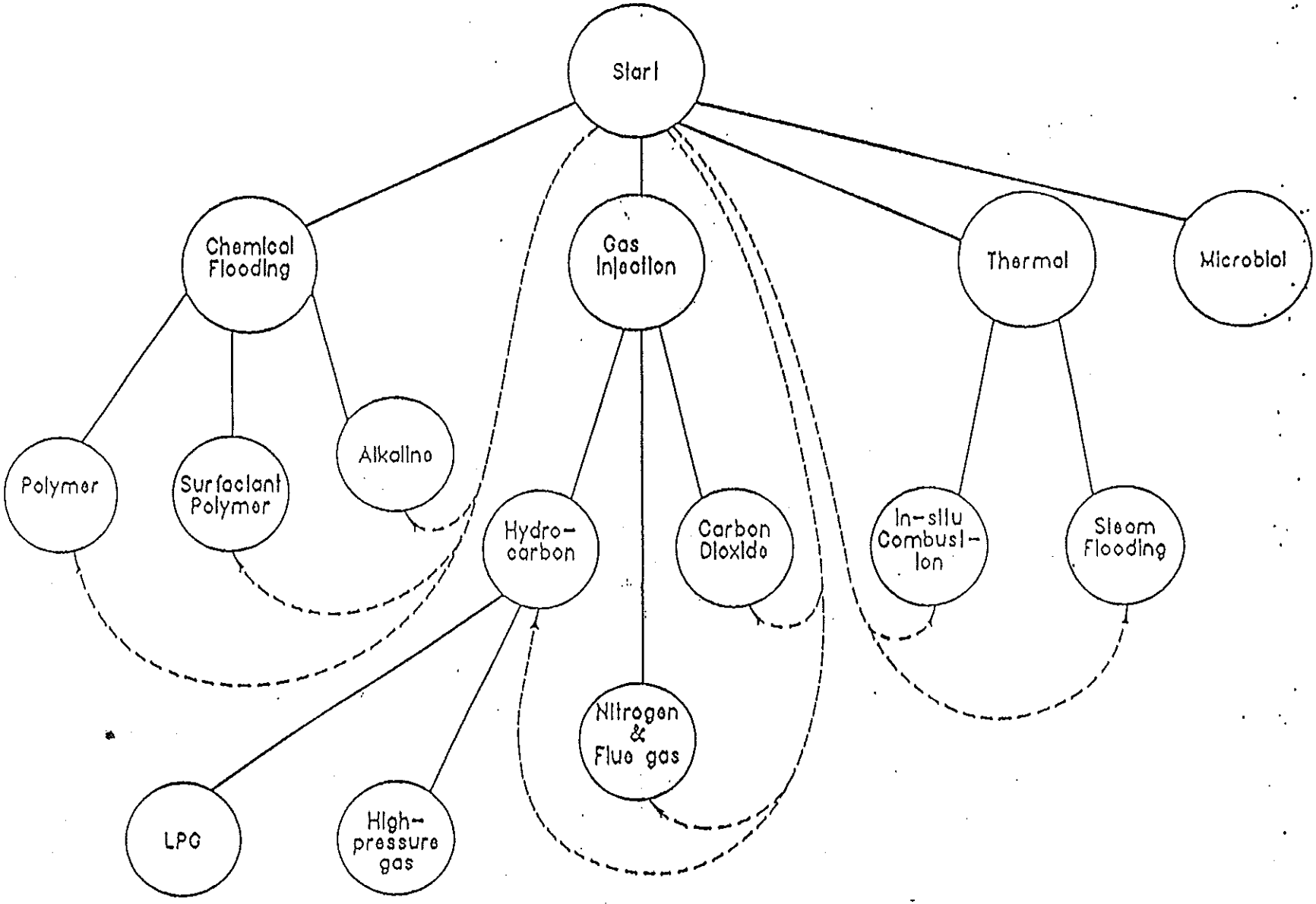

Fig. 8. Search tree for EOR expert assistant.

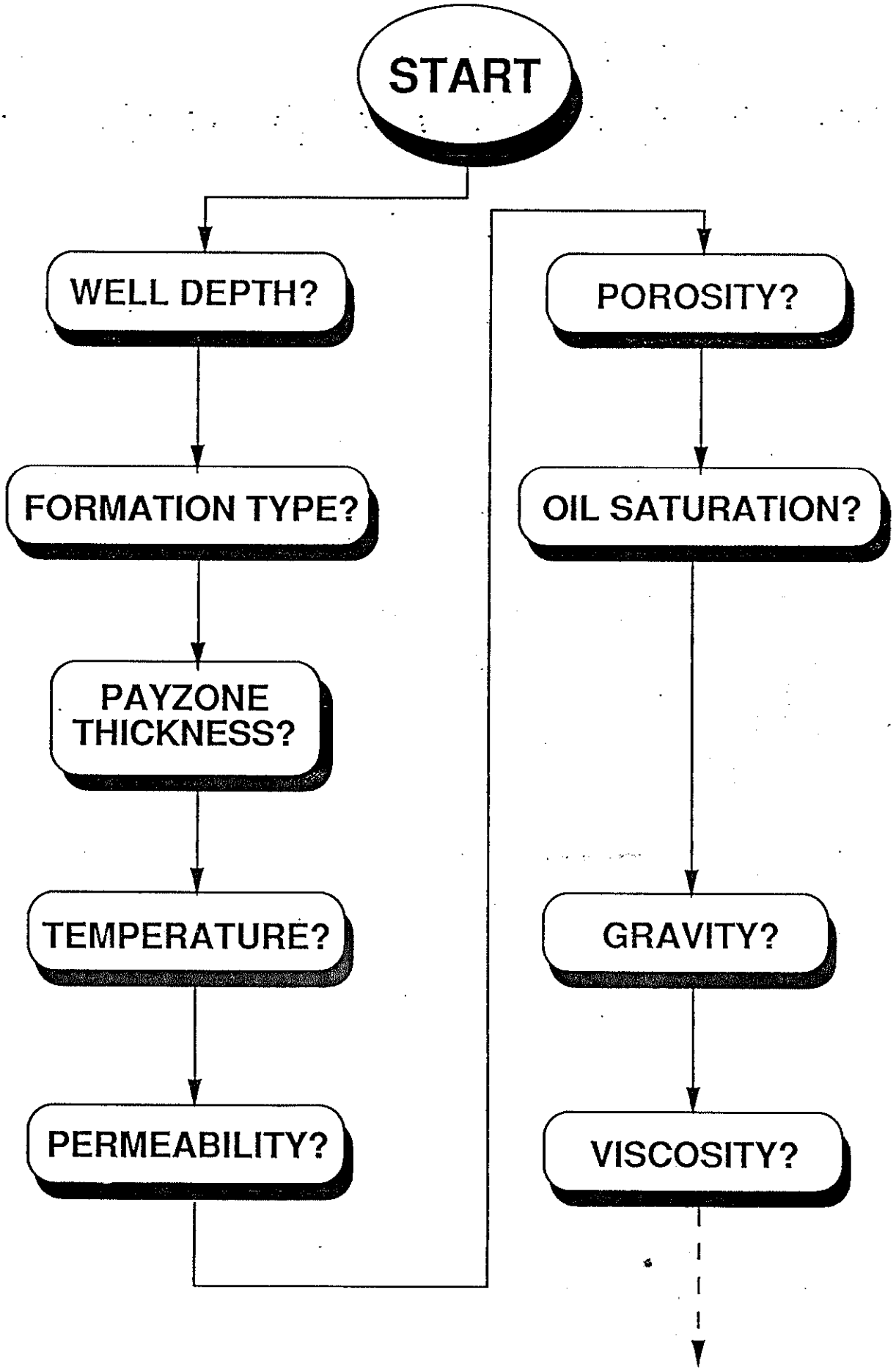

Fig. 9. A portion of the search space for the EOR expert system.

What is the well depth ? (feet)

2000

What is the formation type ?
(Sandstone, Carbonate, or Unconsolidated-sand)

Sandstone

What is the payzone thickness ? (feet)

30

What is the reservoir temperature ? (F)

110

What is the reservoir permeability ? (md)

1000

What is the reservoir porosity ? (%)

28

What is the reservoir oil saturation ? (%)

50

What is the oil gravity at 60 F ? (degrees API)

18

What is the oil viscosity at reservoir temperature ? (cp)

500

.
.
.

The following list contains the candidate EOR methods and their relative scores

Steam flood score = 17
In-situ combustion score = 15
Alkaline flood score = 9
Microbial drive score = 7

Fig. 10. A portion of the dialogue with the EOR expert system.

good, and optimal operating conditions for a given method. As an example, the hydrocarbon gas injection technique and the surfactant-polymer chemical flood technique cannot be used with as high a viscosity as 400 centipoise, so they both score -100 for this question. On the other hand, this is an optimal condition for the thermal techniques steam flooding and *in situ* combustion, both of which score 5's. Microbial drive scores a 1 on this question, and all other methods score a -5.

At the end of the session, the scores are tallied. Any method with a score greater than 5 makes the list of candidates for further consideration. So far, this approach has given realistic results.

Some of the other questions that are asked that are not shown in Figs. 9 and 10 have to do with reservoir pressure, oil composition, salinity, rock wetability, etc.

In this system, because different operating conditions are required as different methods are used, one question can lead to as many as eight rules. The entire expert system currently has about 50 rules.

EXPERT CONSULTANT AND CONTROL SYSTEM FOR THE SILICON CARBIDE WHISKER GROWTH PROCESS

Silicon carbide whiskers are a very strong material that resemble cat's whiskers. They are produced primarily as a reinforcing material for strengthening ceramic or metallic composite materials. Whiskers can be used as randomly oriented chopped fibers or they can be grown in long lengths, which can be made into yarns and woven. When woven, these fibers create an even more effective directional reinforcement. Although the primary purpose of the whiskers is for the compositing of materials for strength, other uses are also being considered.

Whisker-production is a semi-batch process that is extremely difficult to model mathematically. We are using rules accumulated from many years of trial and error experience to successfully set up and run the process. Two catalyst types, two reactor configurations, and several sets of process conditions are available. When the proper combination of these variables is chosen, the desired result can be attained.

In the past, as long as one person would set up and operate the whisker production runs each time, it was considered adequate for that person to keep the rules in his or her head. But because the whiskers process is now a candidate for technology transfer, we are faced with the problem of how to transfer the expertise to industry without transferring the expert. We therefore designed an expert system to organize and assist in the solution process.

The first phase of the expert system design was to build an expert consultant to provide the user with enough information to correctly set up the run and produce the desired results. The setup information was then incorporated into the rule base to make up the second phase, the control system. The control system corrects perturbations in the process conditions to ensure that the proper corrections can be made and to ensure that the desired product will be obtained at the end of the run.

The SiO (the ingredient used to make silicon carbide) production rate is proportional to the concentration of SiO_2 and CO in the brick, and those concentrations are diminishing with time. This is the transient batch portion of the process. As shown in Fig. 11, a mixture of gases containing methane, the carbon source for the silicon carbide production, is forced through the reactor. For many situations, the composition and flow rate of this gas mixture does not vary throughout the length of a production run. This is the steady-state portion of the process. The silicon carbide is formed by Eq. (2).

$$SIO + CH_4 \text{ ----------> } SIC + H_2O + H_2 \qquad (2)$$

An idealized growth sequence for a silicon carbide whisker is shown in Fig. 12.

The SIO formed by Reaction 1 must mix with CH_4 in the process gas stream. These gases must find their way to a whisker growth surface, as shown in Fig. 11. Flow-visualization studies (14) have shown that this path is tortuous, involving several different modes of mass transfer. Figure 13 shows the modes of mass transport from the SiO generator to the whisker growth surface. Figure 14 shows the steps involved in the overall kinetic process for growth the whiskers.

We have learned a great deal about the silicon carbide whisker growth process and we can now grow them quite well. The foregoing discussion indicates how hard this process is to model with normal mathematical-algorithmic techniques. In fact, we first tried the mathematical modeling approach and found that our models would not adequately predict whisker yield and type from a particular experimental setup. Furthermore, they were inadequate for process control. We had to ask the question "*How can we grow whiskers as well as we do, when we do not understand the physics and chemistry of the process any better than we do?*"

The answer to this question is that our expert operators have learned excellent rules of thumb, through years of trial-and-error experiences, for setting up and running whisker growth experiments. Our next question was "*How do we capture this expertise so that the process can be set up and run by people who are not experienced experts?*" This question is especially important since the technology of the whiskers process has been earmarked for transfer to industry. We would like to be able to transfer the technology without transferring our experts as well. So the answer to this question was to write an expert system or systems to capture this expertise.

THE EXPERT SYSTEMS

Our goal for this stage of the project was to develop a small PC-based expert system in two phases, as shown in Fig. 15. In Phase I, we developed a whisker growth consultant to help the operator set up a whisker run for the desired whisker type and quantity. The knowledge developed during this phase was entered into a knowledge base that could be used with the expert control system. The expert consultant developed in this phase can be used with the expert control system developed in Phase II, or it can stand alone. The expert control system developed in Phase II uses rules to control our laboratory-scale silicon carbide whisker growth process. The expert control system uses rules and facts

Because our system is a "laboratory-scale" project, we have not added elaborate sensory devices to test for perturbations or upsets. Instead, we use a human sensor: the operator. After observing the controlled variable readings, the operator asks the expert system whether the process is behaving correctly. The expert system responds and suggests which, if any, corrections should be made. The operator then makes the corrections. This system is designed so that automatic controls and sensors can easily be added at a later date or for a larger operation.

The expert system is rule-based, and it is designed to run on a PC. For easy access by the operator, the PC is kept in the laboratory associated with the whisker process equipment.

THE SILICON CARBIDE WHISKER GROWTH PROCESS

On the laboratory scale, the silicon carbide whisker process is a semi-batch process. That is, part of the process is run in the transient batch mode and part of the process is run in the steady-state continuous flow mode. Figure 11 is a diagram of the silicon carbide whisker reactor. Silicon dioxide bricks impregnated with graphite are placed inside the reactor. After they are heated, these bricks produce silicon monoxide by reaction (1).

$$SiO_2 + C \text{ ----------> } SiO + CO \qquad (1)$$

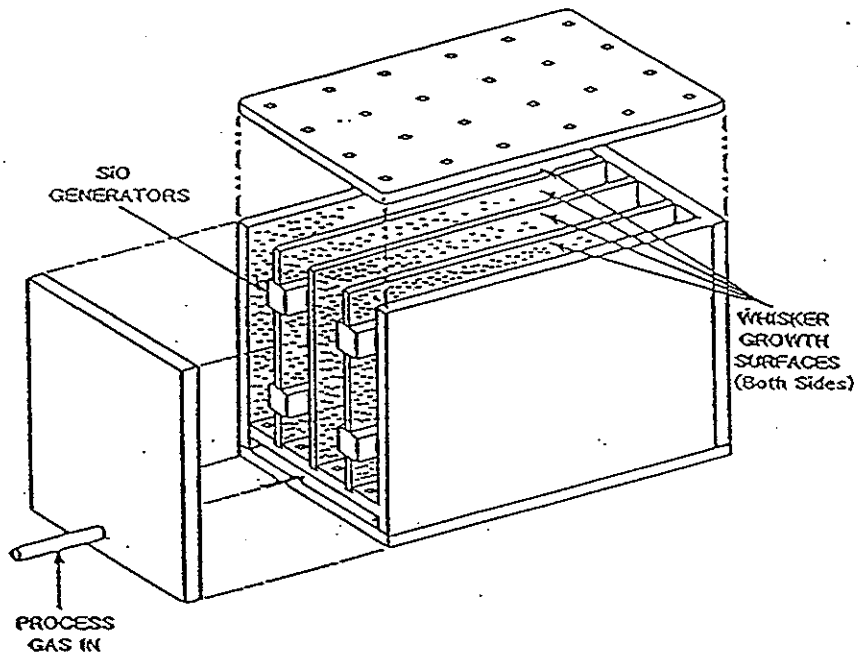

Fig. 11. The Los Alamos silicon carbide whisker production reactor.

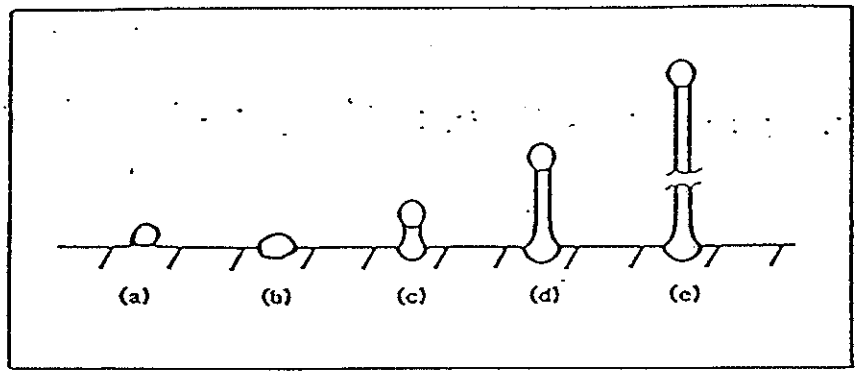

Fig. 12. Idealized growth sequence for the Los Alamos silicon carbide whisker production: (a) metallic catalyst is melted on a substrate, (b) catalyst forms a crater in the substrate, (c) silicon carbide whisker is nucleated, and (d,e) whisker grows away from the substrate with liquid catalyst ball at the tip.

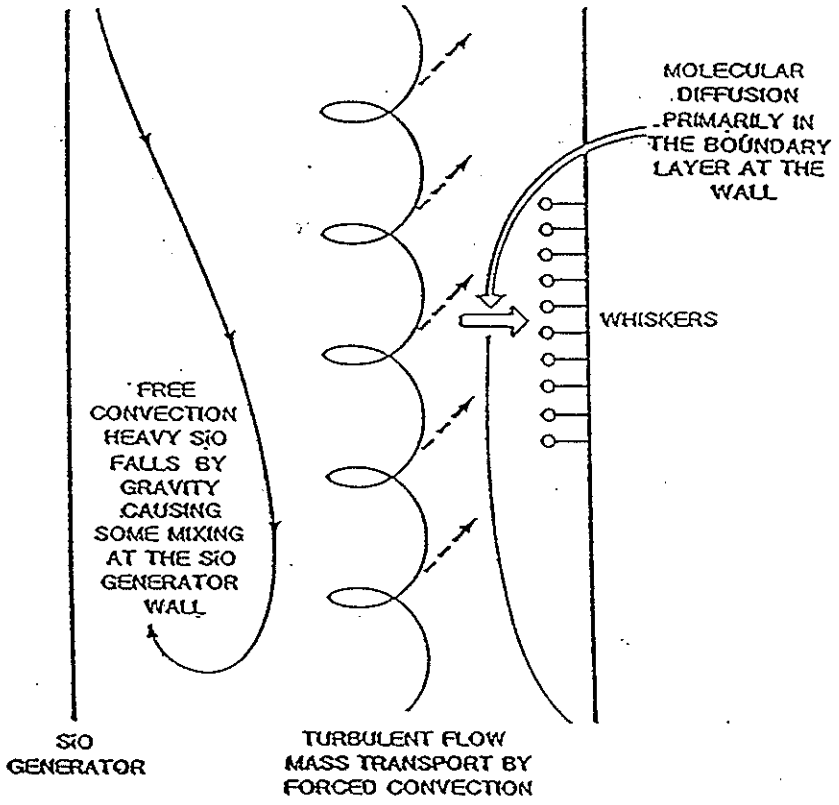

Fig. 13. Gas-phase mass transport modes.

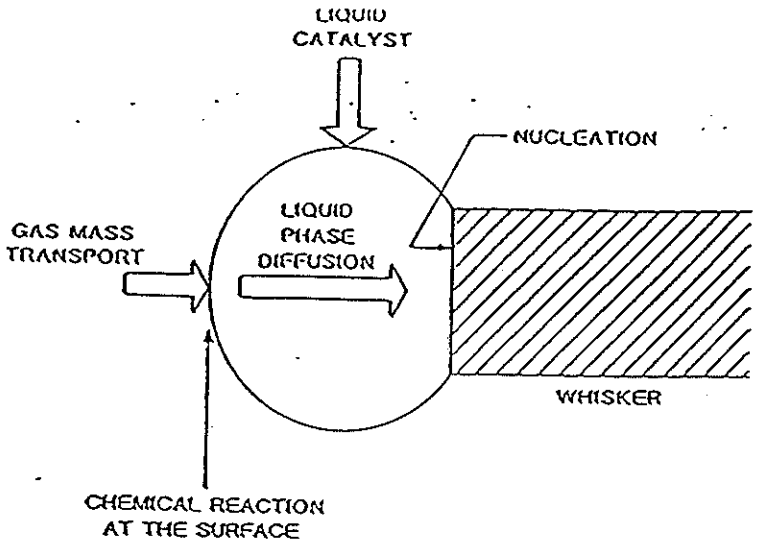

Fig. 14. Steps in the overall kinetic process for growing silicon carbide whiskers.

from the knowledge base shown in Fig. 15. Because our process is "laboratory-scale," our controls are manually operated and our sensor output is manually observed. This means that our control system is somewhat limited because it cannot work without an operator interface. This scenario is depicted in Fig. 16. Although this system is adequate for our current process, it would fall short for a full-scale whisker production plant. The full-scale plant scenario is depicted in Fig. 17. This type of of control system is the ultimate goal of future work.

Figure 18, taken from Ref. (15) shows an empirical phase diagram for the growth, and the types of whiskers that can be produced as a function of gas composition. The abscissa represents a change from silicon-rich to carbon-rich gas mixtures. The ordinate represents the silicon monoxide concentration in the gas phase. The properties for the whiskers from categories one through seven, shown at the top of the chart, depend primarily on the whisker diameter. To date, there is some commercial interest in all sections of the chart except areas E and F. These are the combined species and the large bent needles.

For this study we have lumped the whisker types into slightly different groups, based on lengths and diameters. The whisker lengths vary from about 1/8 in. to about 3-1/2 in., which we have divided into three categories: short, medium length, and very long. The whisker diameters vary from 0.1 to 15 in. We have divided them into three groups: small, medium, and large. With short whiskers we are interested only in small diameters. With long and medium length whiskers, we are interested only in those with medium and large diameters.

In addition to developing rules to produce a particular whisker type, we have developed some rules to help maximize the production of those whiskers under various operating constraints. These rules can be divided into three categories: (1) how to obtain the maximum yield with new growth plates, (2) how to obtain the maximum yield with used growth plates, and (3) how to obtain a

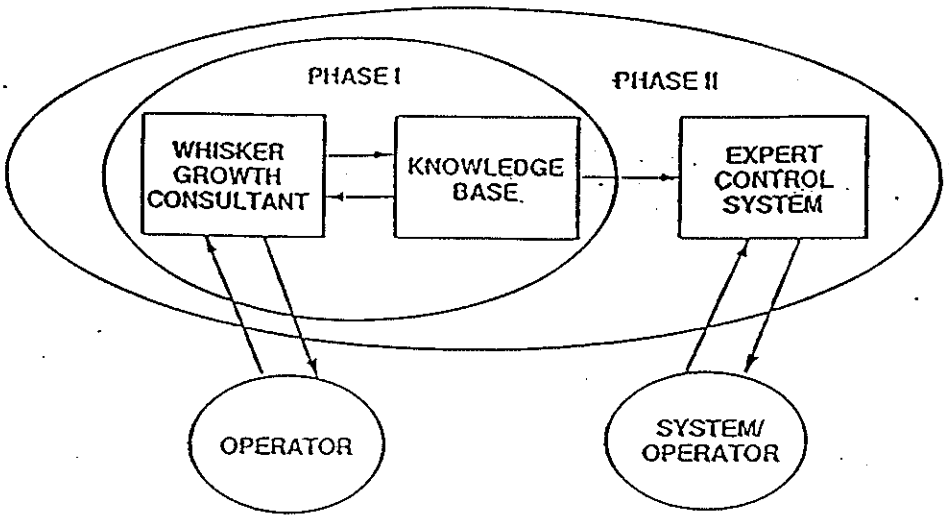

Fig. 15. The two phases of the expert system design.

Fig. 16. Demonstration of the operator interface between the current expert system and the process.

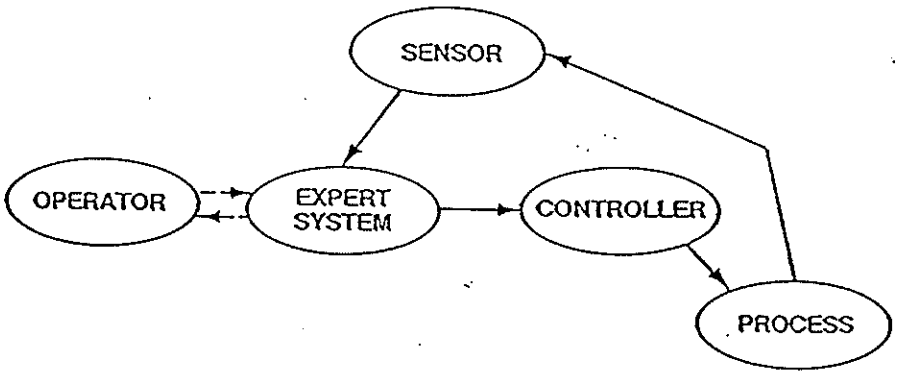

Fig. 17. Desired expert system/process interface for full-scale plants.

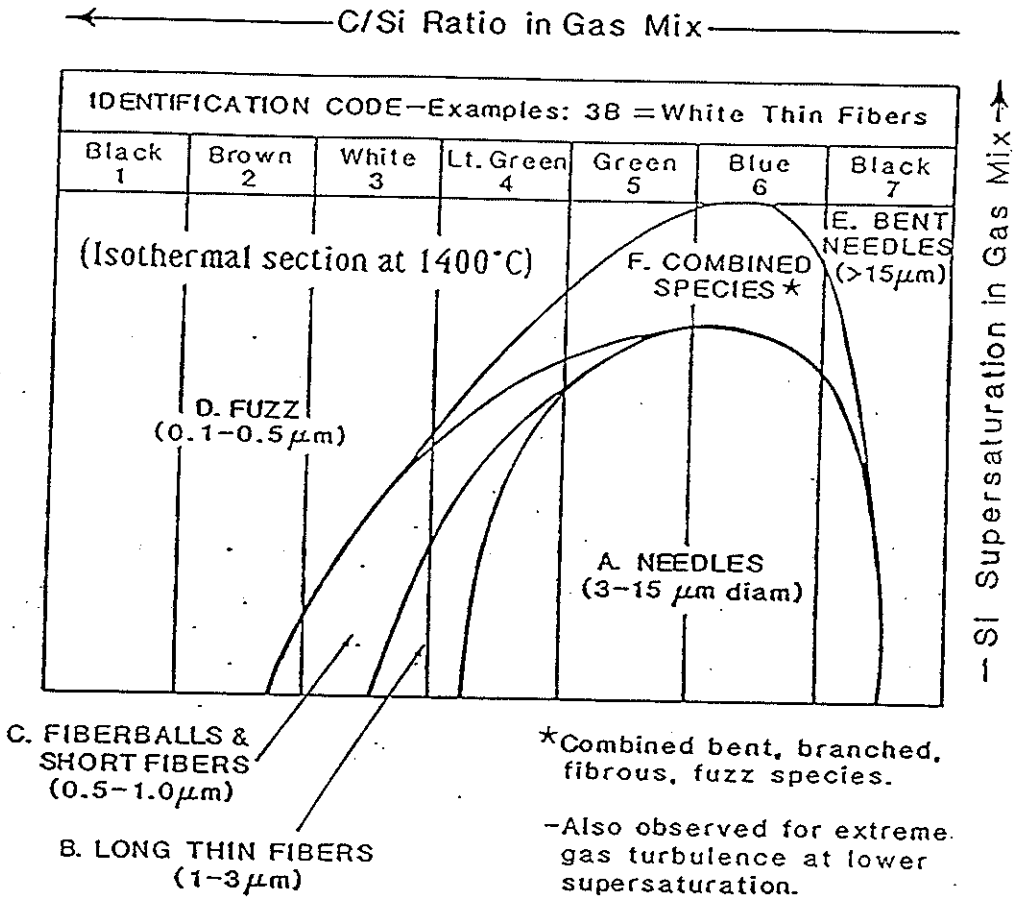

Fig. 18. Empirical phase diagram for the growth of silicon carbide whiskers.

maximum yield in a limited run time. We can also have combinations of these three categories. These rules depend upon the type of whisker that we are trying to produce and are included in our whisker growth consultant expert system.

For our laboratory scale operation, we have been primarily concerned with Categories (1) and (2). New growth plates require different gas compositions than used growth plates to produce the same quantity of whiskers. After one run, the new growth plates are coated with silicon carbide, and from then on the silicon carbide participates in the process chemistry. After about four runs the whisker production degrades to the degree that we must replace the plates. We have developed some cost analyses of our process and find it to be labor and material intensive. Replacing growth plates after every run is too expensive, even for a "laboratory-scale" process. Figure 19 shows the general shape of the time-versus-whisker yield curve. Because we are a laboratory operation, our approach is to run the reactor as long as possible to produce the maximum yield.

Figure 19 suggests that a point of diminishing returns is reached before the reactor is shut down. Because this process is a candidate for technology transfer to industry, we have developed some production rules for maximizing yields with shorter run times based on the curve shown in Fig. 19. We assume that an industrial process, even if a batch process similar to ours, would be optimized in a different manner. For example, if several batches were run in one day to the point of diminishing returns, more whiskers would be produced than in our previous maximum production run, yet in the same amount of time.

Figure 20 is a simplified search tree for our whisker growth consultant. The leaves of the tree represent operating conditions that will produce the type of whiskers we want to make. We can change the production from medium length to long whiskers by changing the reactor and catalyst type. To produce short whiskers, we must change the gas composition. Whisker diameter depends primarily on catalyst choice and particle size. At first glance picking the proper production rules for a given run seems straight forward. However, rules obtained from our database have shown that this procedure is more complicated to set up and run optimally than it appears at first observation. For example, gas compositions and temperatures should be different, depending upon the catalyst and the particle size used. The rules for maximizing the whisker yield in a shorter period of time depend upon the intended whisker diameter and length. Long whiskers are not normally produced in shorter run times, and so on.

The expert control system requires the information given to the knowledge base by the operator and the expert consultant. Because, in our system, sensors do not communicate directly with the expert control system, the operator must observe the sensor output, communicate with the control program, and then, if necessary, adjust the system controls manually. The current system has only eleven sensed variables and eight possible control adjustment actions. Three of the sensed variables are temperature, pressure, and total inlet flow. The other eight variables are the inlet and outlet compositions of the four process gases, hydrogen, carbon monoxide, nitrogen, and methane. The eight control adjustment actions are shutdown; adjust temperature; adjust total inlet flow; adjust the flow of the four individual inlet gases (hydrogen, carbon monoxide, nitrogen, and methane); or take no action. The amount of adjustment is highly

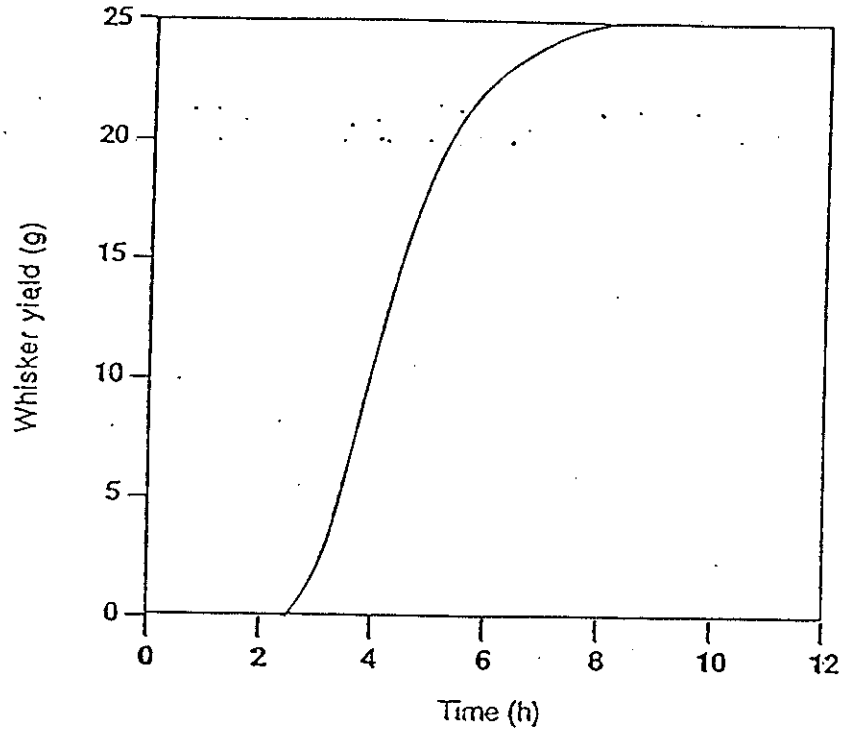

Fig. 19. A time-vs-yield curve for the silicon carbide whisker growth process.

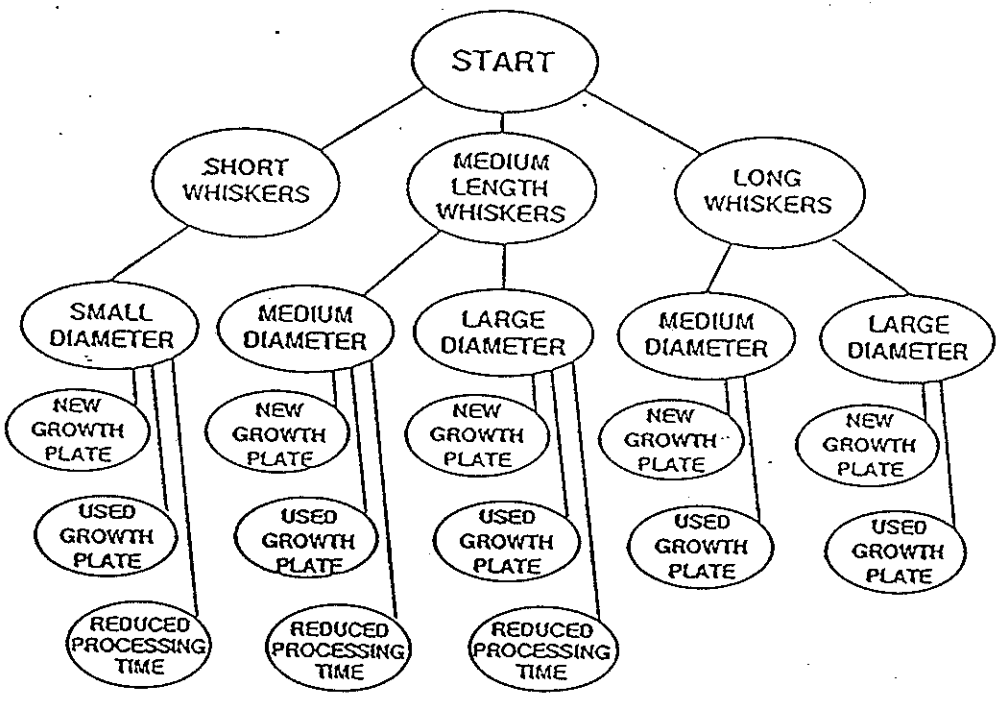

Fig. 20. A search tree for the whisker growth consultant.

dependent upon the current reading and the run setup conditions supplied by the expert whisker growth consultant. Figure 21 shows part of the search tree for the expert control system.

Figure 22 is a simplified search space diagram for our expert consultant. The rectangular blocks represent the major decision points in the program. Figure 23 shows the CLIPS dialogue with the whisker growth consultant. It follows the search space shown in Fig. 22. Some of the values given in Fig. 23 are fictitious, because the whisker process falls under the purview of United States Export Control Laws and some information is subject to limited access. The questions in Fig. 23 are questions asked by the expert system with user supplied answers. Note that, at each decision point, the user is given the opportunity to use values other than those recommended. The system was set up this way because, at the end of the consulting session, the correct values must be available for use by the control system.

Figure 24 is a search space diagram for the expert control system. Figure 25 shows the CLIPS dialogue with the expert control system. Note that the control system makes many of its decisions based on parameter values given during the session with the expert consultant.

It should be pointed out that our laboratory scale process is relatively simple. Our operation is not subject to some of the problems of a full-scale plant, such as real-time time-constraint problems caused by the need to search through thousands of rules before an urgent decision can be made. Our expert system works fast enough for the whisker process at this scale. Evidence for this is given in the last line of Fig. 25, "*Reduce the inlet composition... and check with me again in forty minutes.*" In the laboratory environment, gas-stream compositions are only monitored every 40 minutes. This is adequate.

CONCLUSIONS

The expert systems discussed here have been useful. In each case, we intend to expaned the systems to be even more useful. In the case of the expert assistant used with the ASPEN code, we intend to upgrade the expert system to add more capability. With the expert control system, we plan to fully automate the system and take the operator out of the loop, as shown in Fig. 17. The EOR expert screening assistant requires updates to the methodology as the technology improves. An example of this, as pointed out in the paper, is how the use of steam flooding as an EOR technique is expanding.

The expert system shell is a very good vehicle for this kind of programming, that is, for writing programs that have to be changed and updated regularly; because it is easy to just add rules to the existing code. To date CLIPS has worked very well on these problems, and the PC has been an adequate, if not preferred, platform for the work. We intend to expand our work and explore other approaches to these problems, as discussed in Ref. 16. For example the goal-driven or backward-chaining approach may work better on some of these problems than the data-driven or forward-chaining approach used in CLIPS. As the problem space becomes larger, there may be significant performance differences between these paradigms. CLIPS can be programmed in this mode, but it may be easier to go to other shells if this is the case.

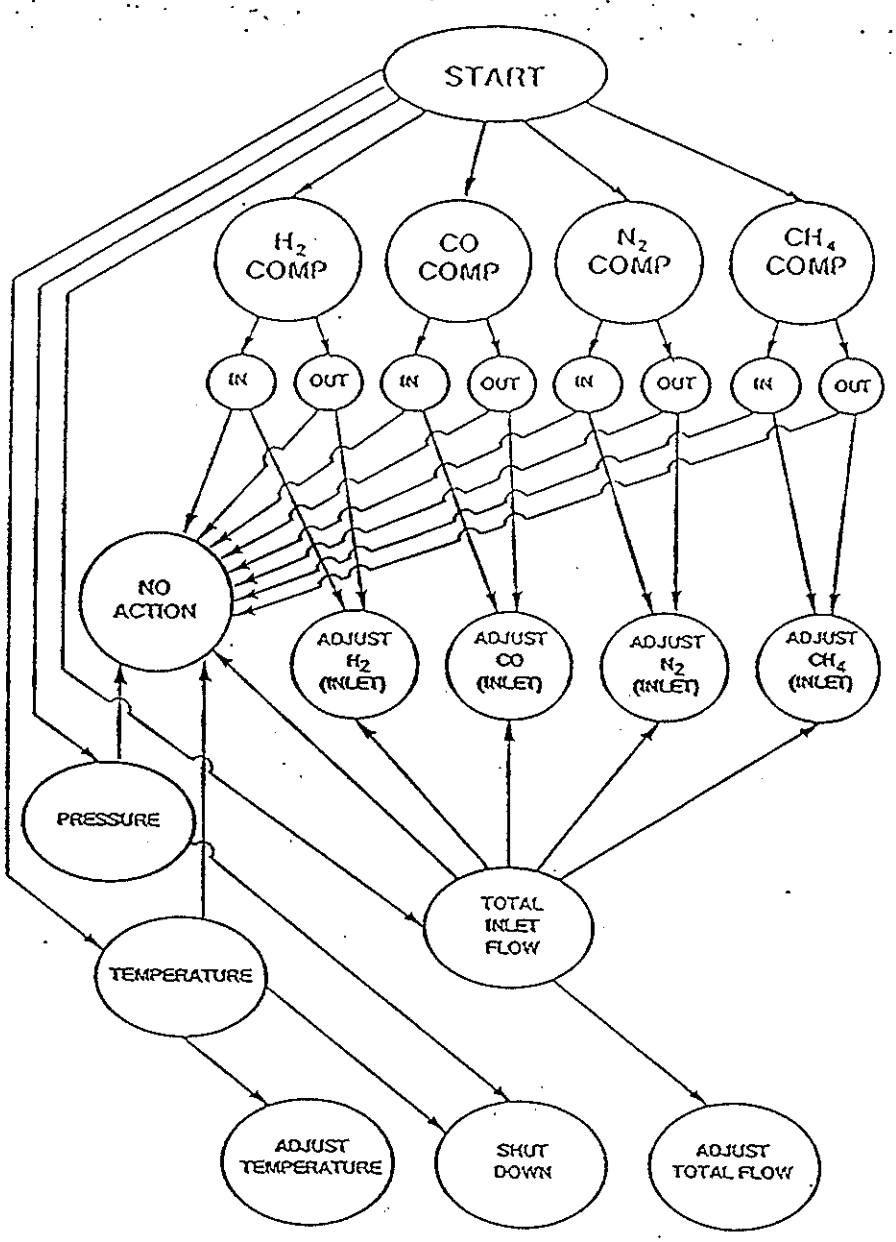

Fig. 21. A search tree for the expert control system.

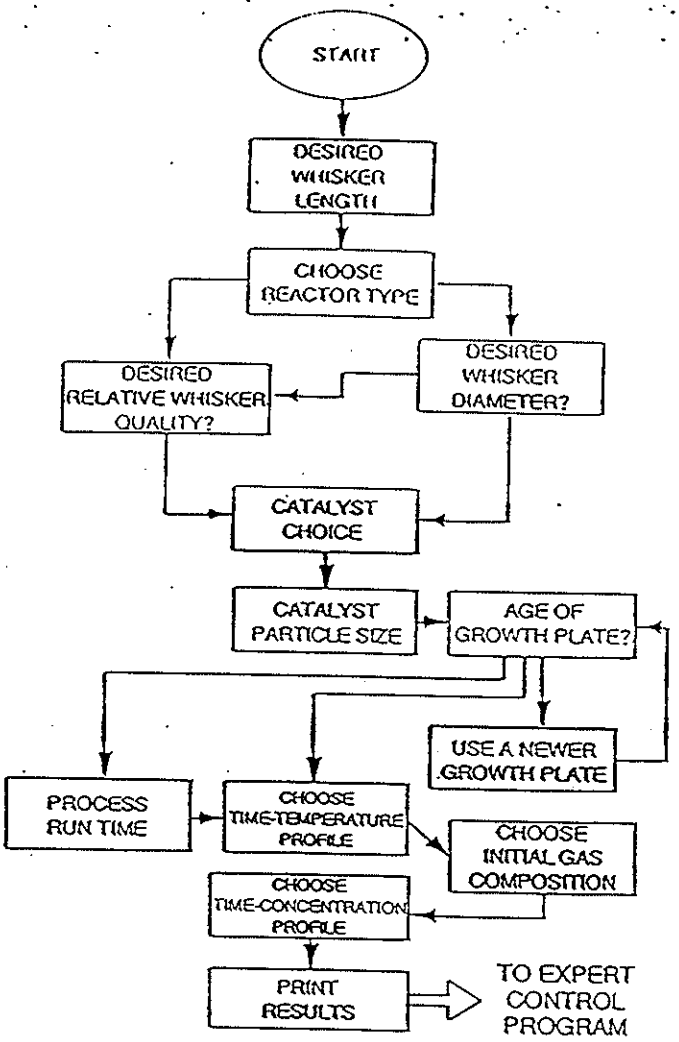

Fig. 22. The search space diagram for the expert consultant.

```
What is the desired average whisker length ?
(in inches 0. to 3.5)

3.0

We recommend reactor type B, which will you use ?
(A or B)

B

What is the desired average whisker diameter ?
(in microns, 0 to 12)

10

We recommend the manganese based catalyst, which
one will you choose ? (manganese or iron)

manganese

We recommend sieve size 20-25, what will you use ?
(25-32, 20-25, or 15-20)

20-25

How many times have you used the reactor growth plate ?
(0 or greater)

0

We recommend time-temperature profile A, which will you use ?
(A, B, C, or D)

A

We recommend that you use the following initial gas composition:
H2 = 80.0 %
CO = 5.5 %
N2 = 14 %
CH4 = 0.5 %

Will you use this ? (yes or no)

yes

We recommend that you vary the CO concentration according to
time-concentration profile A. What profile will you use ?

(A, B, C, or D)

A
```

Fig. 23. Dialogue with the expert consultant.

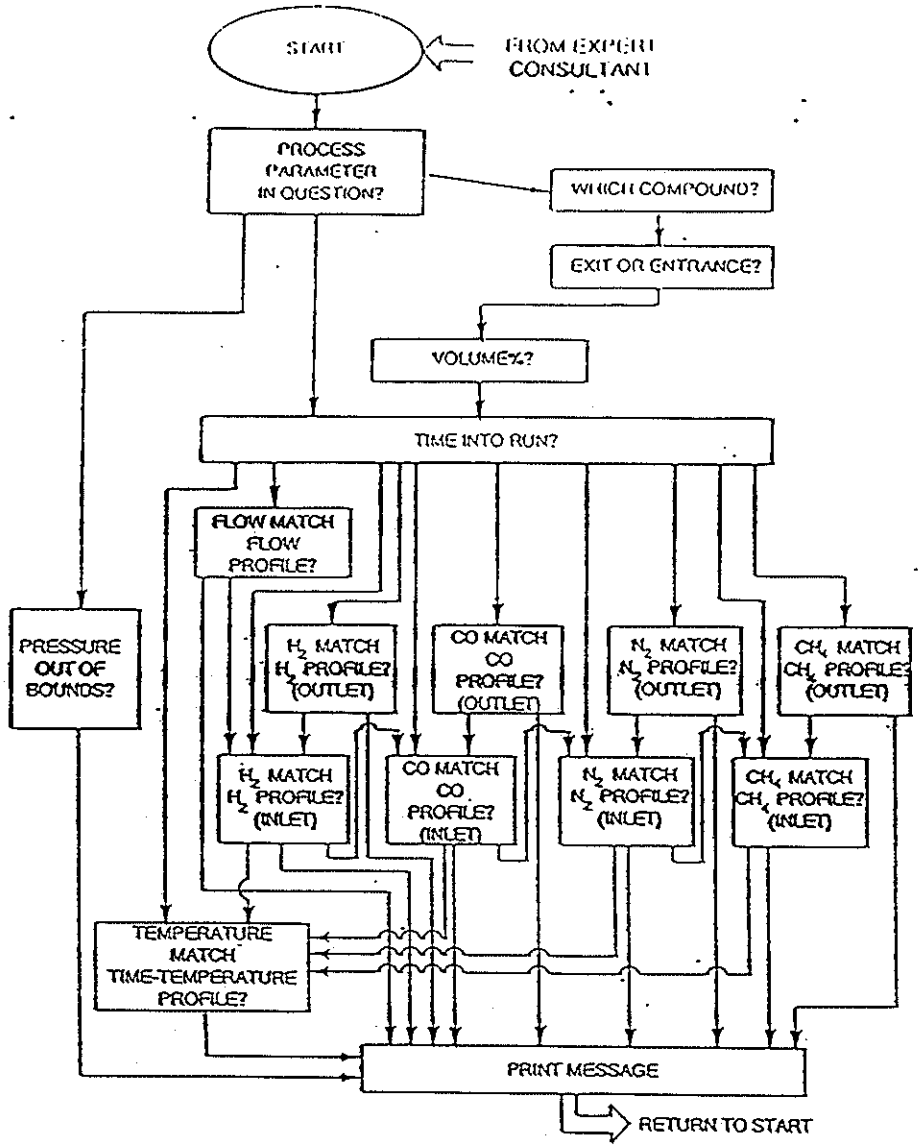

Fig. 24. The search space diagram for the expert control system.

What process parameter do you wish to question ?
(Temperature/ Pressure/ Total-Flow/ Gas-Composition)

Gas-Composition

Which component ? (H2/ CO/ N2/ CH4)

CO

Exit or Entrance Composition ? (Exit/ Entrance)

Exit

What is the volume percent ?

5

How many minutes since the run began ?

420

The volume percent is too high.

What is the inlet CO volume percent ?

4.6

What is the reactor temperature in degrees centigrade ?

1400

The temperature is OK.

Reduce the inlet composition to 2.9 volume percent and check with me again in forty minutes.

Fig. 25. Dialogue with the expert control system.

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