THE STATE OF THE S AMERICAN INSTITUTE OF CHEMICAL ENGINEERS 1989 SPRING NATIONAL MEETING **AND** GEORGE R. BROWN CONVENTION CENTER HOUSTON, TX **APRIL 2-6, 1989** 

W. J. Parkinson, G. F. Luger, and R. E. Bretz, "Using PC-Based Shells to Write an Expert Assistant for Use with the ASPEN Computer Code," Paper presented at the AIChE Annual Meeting, Session on Applications of Artificial Intelligence in Chemical Engineering (April 2-6, 1989, Houston, Texas).

# USING PC-BASED SHELLS TO WRITE AN EXPERT ASSISTANT FOR USE WITH THE ASPEN COMPUTER CODE

by

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#### ABSTRACT

Many engineers argue against using expert systems to solve problems because of the relatively high cost of specialized LISP machines and the large expert system shells written for them. This paper demonstrates how small, but useful, expert systems can be written with inexpensive shells and run on inexpensive personal computers (PCs). Two such shells are CLIPS and EXSHELL. CLIPS, developed by NASA, is a forward-chaining, rule-based system. It is written in the C language, but the rules are entered in a LISP-like format. EXSHELL, developed by the Computer Science Department at the University of New Mexico, is a backwardchaining, rule-based system written in PROLOG. Each of these shells was used to write an expert assistant to aid the design engineer in using the ASPEN (Advanced System for Process ENgineering) computer code. ASPEN is a large computer code used to design chemical plants and refineries. Among other things, ASPEN computes mass and energy balances for the plant design.

Unfortunately, an expert, or several experts, are required to use ASPEN to its full potential. For example, choosing the proper thermodynamic package to represent a given process is important in developing the correct mass and energy balances. An ASPEN user may be an expert in plant design, yet may not be expert enough at thermodynamics to pick the proper package from the many offered by ASPEN. CLIPS and EXSHELL were used to develop a useful expert assistant to help process plant designers pick the proper thermodynamic package to be used with particular operating conditions at various points in the ASPEN plant simulation. This paper also demonstrates the utility and ease of use of these inexpensive shells and compares the approach used by each.

#### INTRODUCTION

Our goal for this project was to develop a small computer-based expert assistant to help engineers in choosing the proper thermodynamic model to be used with a large flowsheet simulator. Such simulators are often used in chemical plant and refinery design and often provide the user with several thermodynamic model options. Design engineers frequently use the ideal gas and ideal liquid options because they do not have the knowledge and experience to determine the necessary criterion for making another choice. This is unfortunate because other more appropriate options are available that will yield better solutions.

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, in this

late 1980s time frame, any usable expert system should be executable with an inexpensive shell and an easily available computer. At the time we began this project, KEE was not portable to a PC, and it is not inexpensive. 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 system we envisioned. We were pleasantly surprised when we found two shells that could handle the task at an affordable price.

# TWO PC-BASED EXPERT SYSTEM SHELLS

After an extensive search for an appropriate PC-based shell, we made two observations. The first was that powerful expert system shells are expensive, and when written for use on a PC, they often include special purpose computer chips that add special features to the PC. The costs of these shells varied from just under \$1000 to several thousands of dollars. The second observation was that PC-based shells that cost around \$100 were not adequate for our job. Nevertheless, we were fortunate to find two shells, CLIPS<sup>1</sup> and EXSHELL,<sup>2</sup> that met our low cost criteria and were adequate for our problems. Both shells were supplied to us essentially without cost, and both have performed well. Neither has shown any sign of degradation or reduced performance with our applications (about 200 rules).

CLIPS was developed by NASA. It is a forward chaining, rule-based shell written in the C programming language that emulates the LISP programming language. To use the CLIPS shell, it is helpful, though not essential, to know both the C and LISP programming languages.

EXSHELL was developed by the University of New Mexico
Computer Science Department. It is a backward chaining, rulebased shell written in the PROLOG programming language. One
must know some PROLOG to use EXSHELL.

Both of these shells are valuable tools, even though they have different features. One significant result of our shell comparisons is that the comparisons may be useful to other investigators in the future. For this reason, examples and comparisons are included in the Appendix and in the section on Shell Comparisons.

Our 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<sup>3</sup> (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

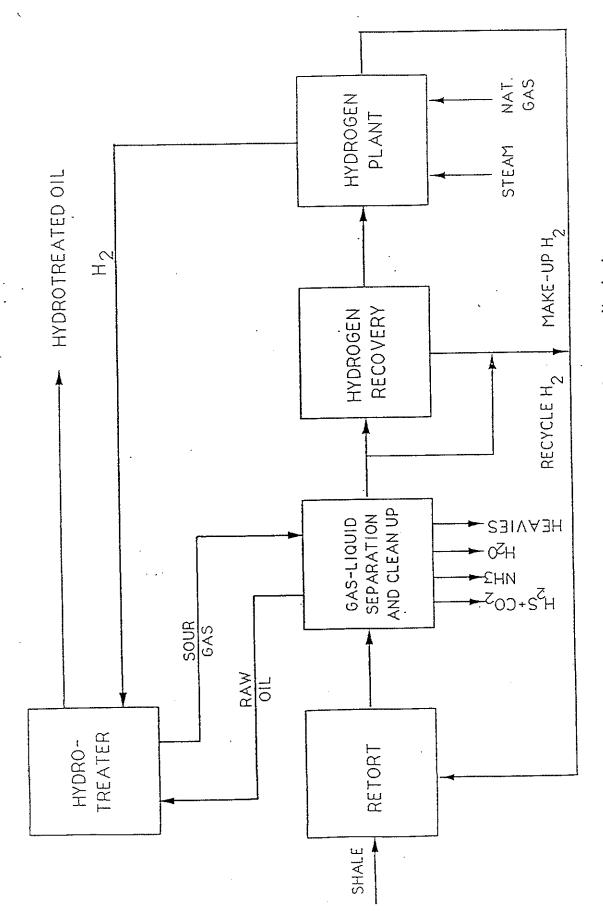
suitable for the design of coal and oil shale processing units. Thus, ASPEN was the product of choice for use in LANL's recent coal and shale oil projects.

To demonstrate why an expert system is useful and how such an expert system is used, 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,

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

conditions and rates of raw materials, and operating conditions, and identify the modules 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 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

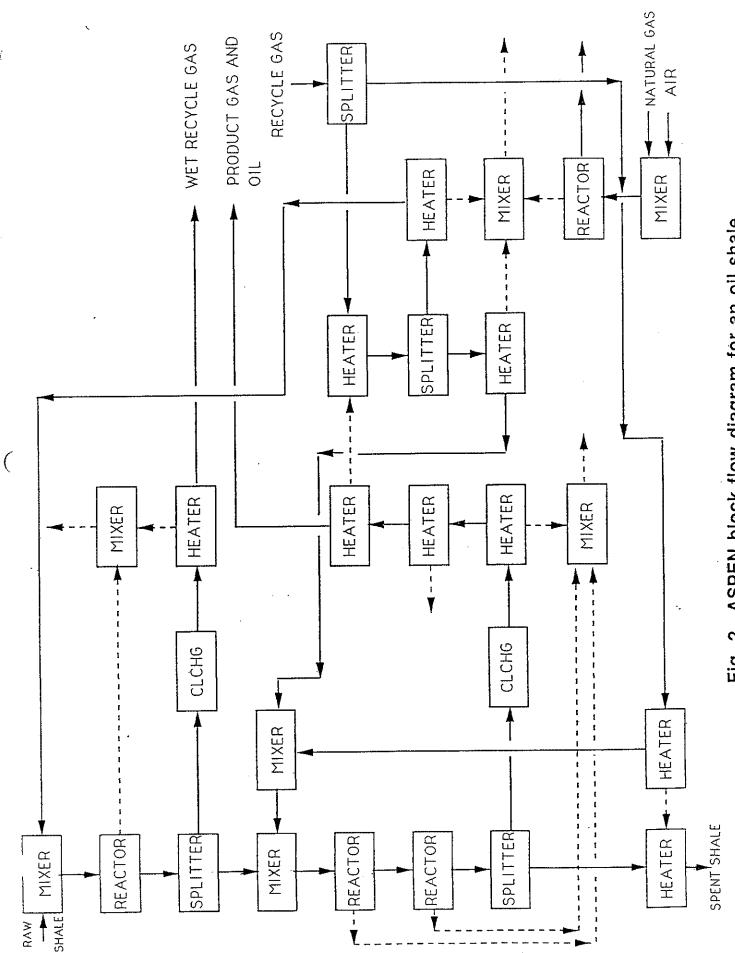


Fig. 2. ASPEN block flow diagram for an oil shale retort.

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, 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 gasliquid 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 processes 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 differ 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

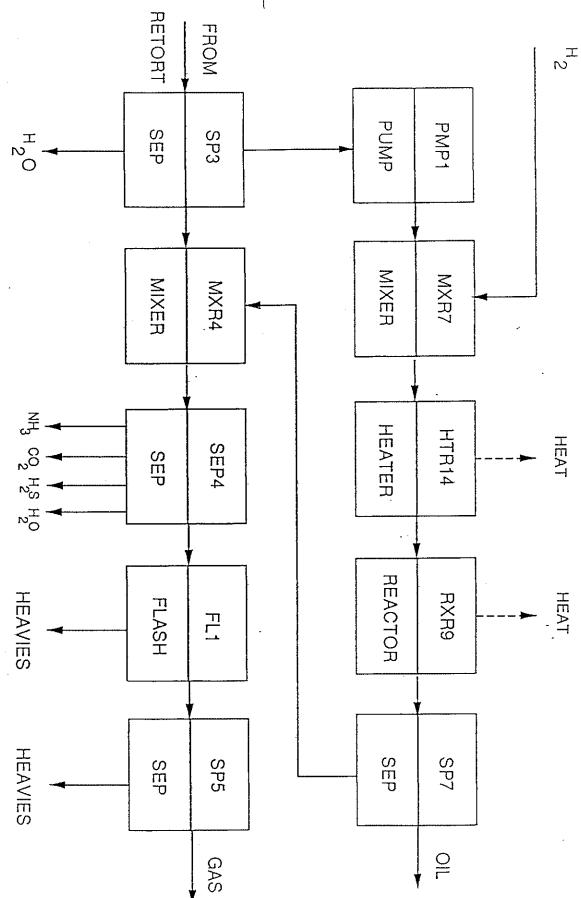


Fig. 3. ASPEN block flow diagram of a gas-liquid separation and clean-up unit.

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 Kvalues, that is,

$$K_i = y_i/x_i = \emptyset_i^{L}/\emptyset_i^{V} , \qquad (1)$$

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,

 $\phi_i^L$  = the fugacity coefficient of component i in the liquid phase, and

 $\emptyset_i^V$  = 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 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 equation,<sup>4</sup>

$$K_{i} = v_{i}^{o} \gamma_{i} / \emptyset_{i}^{V} , \qquad (2)$$

where  $v_i^0$  = the liquid fugacity coefficient of the pure component (this coefficient is different from  $\emptyset_i^L$ , which is the liquid fugacity coefficient of component i in the liquid mixture), and

 $\gamma_i$  = the liquid phase activity coefficient.

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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

$$-\Delta G_i = RTlnK_i$$
, (3)

where  $\Delta G_i$  = 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

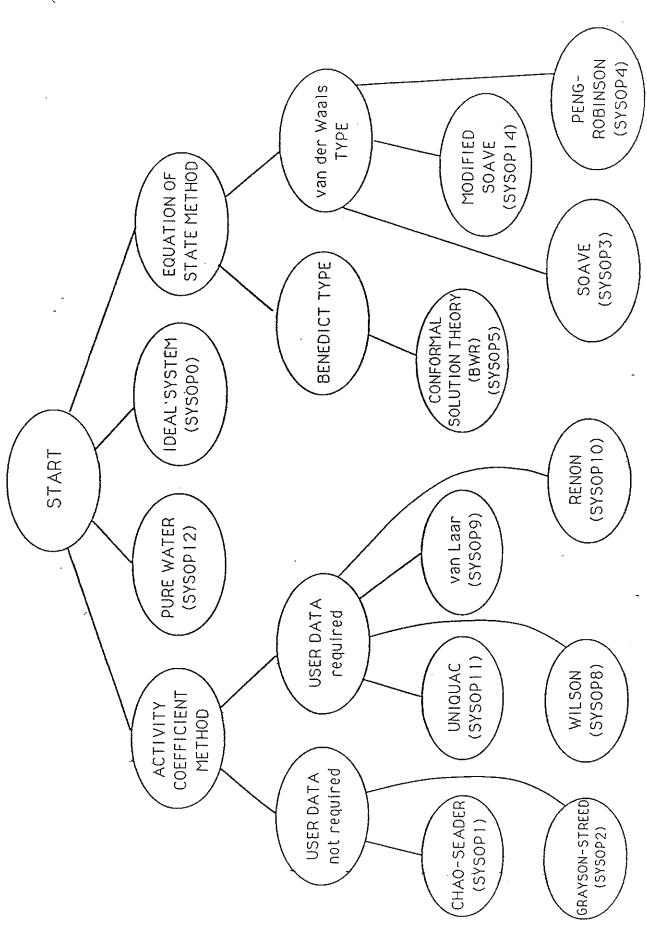
$$\Delta H_i = \Delta G_i + T \Delta S_i , \qquad (4)$$

where  $\Delta H_i$  = the enthalpy of component i relative to a reference state,

 $\Delta S_i$  = 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 (SYSOP0), ASPEN contains two additional major model types: EOS and activity coefficient models. These major model types



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

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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<sup>5-11</sup> and personal experience. References 5 and 6 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 I are the model numbers, which are related to SYSOP numbers.

TABLE I
ASPEN FUGACITY COEFFICIENT MODELS

Model <u>Number</u>	<u>Name</u>
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 lists the possible substitutions for which we have compiled rules.

POSSIBLE FUGACITY COEFFICIENT SUBSTITUTIONS
FOR THE PROJECT TWO EXPERT SYSTEM

SYSOP Number	SYSOP Name	Vapor Fugacity Coefficient Model Number	Liquid Fugacity Coefficient Model Number
0	Ideal solutions		26
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 <sup>a</sup> ,7 <sup>a</sup>	6 <sup>a</sup> ,7 <sup>a</sup>
4	Peng-Robinson	2,6a,7a	6a,7a
5	BWR	2,6 <sup>a</sup> ,7 <sup>a</sup>	6a,7a
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	2,6a,7a	6a,7a

<sup>&</sup>lt;sup>a</sup>If models 6 or 7 are used for the vapor phase, the same model must be used for the liquid phase and vice-versa.

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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.

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

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SYSOP Number	SYSOP Name	Vapor Fugacity Coefficient Model Number	Liquid Fugacity Coefficient Model Number
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8 9 10 11 12 14	Wilson van Laar Renon (NRTL) UNIQUAC Water Modified Soave	2,3,4,5,6,7,14 2,3,4,5,6,7,14 2,3,4,5,6,7,14 2,3,4,5,6,7,14 2,6a,7a	22,26 23,24,26 26 25,26 26 6a,7a

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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.

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 THE SHELLS WORK

We have picked a simple example to demonstrate how CLIPS and EXSHELL work 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 the features of both shells. 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). The entire dialogue with both CLIPS and EXSHELL is presented in the Appendix for the interested reader. A portion of the search space used by the EXSHELL expert assistant that contains this example is shown in Fig. 6. A portion of the search-space used by the CLIPS expert assistant that contains the same example is shown in Fig. 7. The solution to the example problem is shown on both figures in bold face. Figure 6 is an "and/or" graph. (It is called an and/or graph because the branches connected by an arc are "and" branches, that is, all

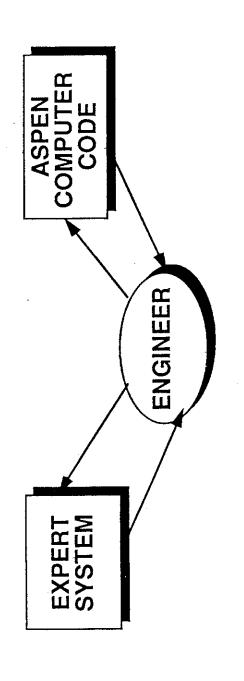
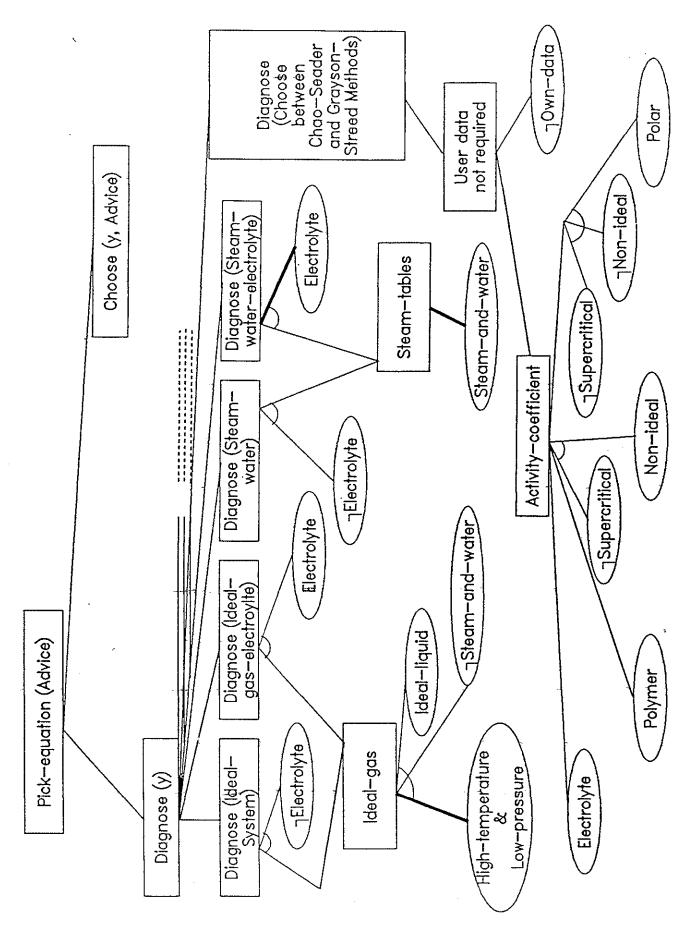


Fig. 5. The engineers use of the expert assistant with the ASPEN computer code.



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Fig. 6. And/or graph for a portion of the search space for the EXSHELL version of the plant design expert assistant.

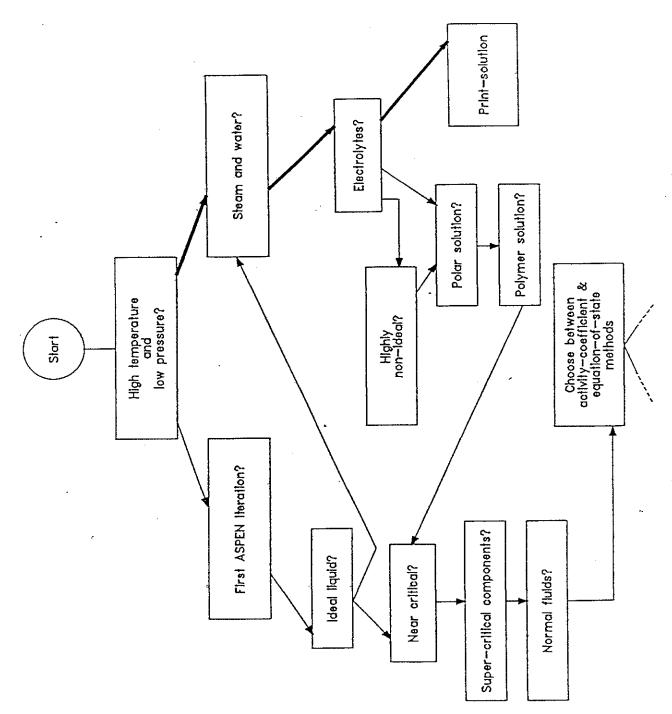


Fig. 7. A portion of the search space of the plant design expert assistant using CLIPS.

leaves must be true before the branch is resolved. The unarced branches are "or" branches. They require a single truth for resolution.) The problem solution can be traced using the backchaining technique found in EXSHELL. Figure 7 demonstrates the forward-chaining technique found in CLIPS.

The important observations that should be made from the sample sessions in the Appendix are as follows. The EXSHELL version has an explanation facility. The user may ask why to any query. EXSHELL will present the rule it is trying to resolve with that particular query. The user may also ask how when he wants to know how EXSHELL obtained a particular fact. EXSHELL will present the branch of the search tree (the list of rules) that led to that fact. When the solution is found, EXSHELL will ask the user if he wants a trace. EXSHELL can give the entire logic set that led to the solution.

The CLIPS version of the expert system presents more verbose queries to the user. These queries are easier to understand than the relatively cryptic queries presented by EXSHELL.

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Although it is not apparent from the simple example shown in the Appendix, careful examination of Figs. 6 and 7 shows that in more complicated examples, CLIPS asks more questions than EXSHELL does before making a decision. The EXSHELL version tries to quickly eliminate all possibilities except the "correct" answer. The CLIPS version attempts to obtain enough information to give a

score to the top candidates and present the user with an ordered list of possible solutions.

#### SHELL COMPARISON AND SUMMARY

Both CLIPS and EXSHELL were adequate for our programming needs, but each has its strengths and weaknesses. With CLIPS, it is easier to exert program control. Thus, it is easy, for example, to allow the CLIPS expert system to help the user choose whether to use his own data or to accept the built-in activity coefficient methods. Control can either be a curse or a blessing. It is nice to be able to easily force the program to follow any desired path, but when you add new rules to an over-controlled system, you will have to do a lot more programming than with a program that requires less control. We took advantage of the additional control in CLIPS, but it was much more difficult to medify the CLIPS program than the EXSHELL program. It is easier to program the user interface with CLIPS. The questions to the user are more verbose and more explanatory.

With EXSHELL, the explanation facility comes free. We have not programmed an explanation facility into the CLIPS version because to do so would require considerably more work. It is easier to handle probabilities or confidence factors with EXSHELL than with CLIPS; therefore, we constructed a scoring system with the CLIPS version. Actually, the scoring system (with rated lists of possible

models) is a good method for some applications. But the scoring system would be harder to implement with EXSHELL. Finally, EXSHELL is easier to program than CLIPS. Figure 8 is a rule programmed in CLIPS and Fig. 9 is a similar rule programmed in EXSHELL. The EXSHELL rule is much shorter.

An expert system is a good approach to the ASPEN assistant. As new methods and new rules are introduced, they can be added to an expert system shell without changing the entire program. This is important in our application because even though we had experience in two areas, chemical plant design and oil field operations, and conducted a literature search, our expert system is still strong in some areas and weak in others. We will need to update it often in the future. An expert system with an explanation facility can help relatively inexperienced people learn and use complicated numerical programs with minimal assistance from human experts.

# APPENDIX-SAMPLE SESSION WITH THE EXPERT SYSTEM SHELLS

In Fig. 10, the user initiates the session with go(X)! EXSHELL responds with a question high temperature and low pressure? The user types No. This satisfies EXSHELL that an ideal system method should not be used (see Fig. 6). Now EXSHELL tries to decide if a steam table correlation method should be used, so it asks the question steam and water? The user responds Yes. This establishes that a

```
then (bind ?equation-of-state (+ ?equation-of-state 1.0))
(assert (operating-conditions supercritical-components))
(if (eq ?supercritical-components no)
then (bind ?equation-of-state (- ?equation-of-state 1.0))
(fprintout t "Equation of state,= "?equation-of-state crlf)
                                              ?s-c <-(supercritical-components ?equation-of-state)
                                                                                                                             (fprintout t "Are supercritical components present?
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    assert (normal-fluids ?equation-of-state)
(defrule supercritical-components) "Rule 3"
                                                                                                                                                                        (yes/no/\"don't, know"\" crlf)
bind ?supercritical-components (read))
                                                                                                                                                                                                                                                                   (if (eq ?supercritical-components yes)
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          retract ?s-c))
```

Fig. 8. A rule from the CLIPS expert assistant.

Fig. 9. A rule from the EXSHELL expert assistant.

steam table correlation will be used for at least the gas phase. EXSHELL then tries to establish whether electrolytes are present (this is the only option that we have allowed for the steam table correlation), so it asks the question electrolyte? To demonstrate the explanation facility, the user types Why. (Why are you asking this question?) Remember, that the user will not normally have a copy of the search space, as shown in Fig. 6. To a why query, EXSHELL responds by presenting the if...then rule it is trying to satisfy together with the facts that are known and the certainty with which they are known. The rule that EXSHELL is trying to satisfy in this example is shown in both Figs. 6 and 10. The rule is "if the major-type is steamtables and electrolyte, then diagnose steam-water-electrolyte." The fact "major-type (steam-tables)" is known with 100% certainty. EXSHELL has satisfied the why query, so it again asks the question electrolyte? The user wants to know more, so he asks how (majortype (steam-tables)), or how do you know that it is major-type (steamtables)? To respond to a how query, EXSHELL lists and explains the if...then rules that form the branch of the and/or graph that led to the fact in question. In this case, EXSHELL points out that the fact major-type (steam-tables) was established with the if...then rule "if steam-and-water then major-type (steam-tables)." The fact "steamand-water" was given by the user. In this simple example, only one rule is presented by the how query. In a real problem, the user should be prepared to see many rules when asking how. When the

```
go (X)!
high temperature_and_low_pressure? > mo.
steam_ and _ water? > yes.
electrolyte? > why.
                               ***Known, Certainty = 100
IF major_type(steam_tables)
 AND electrolyte
THEN diagnose(steam_water_electrolyte)
\mathbf{CF}
    100
electrolyte? > how(major_type(steam_tables)).
major_type(steam_tables) CF = 100
was proved using the rule
                               ***Known, Certainty = 100
IF steam and water
THEN major_type(steam_tables)
\mathbf{CF}
     100
steam_and_water was given. CF = 100
electrolyte? > yes.
Solved pick_equation('Use Steam Tables (SYSOP12) with
electrolyte correction
(liquid-fugacity model 26)') With Certainty = 100
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Fig. 10. Dialogue with EXSHELL.

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how query is satisfied, EXSHELL again asks the question, electrolyte? This time the user answers Yes. EXSHELL now has enough information to solve this simple example, and gives the solution "Use Steam Tables (SYSOP12) with electrolyte correction (liquid-fugacity model 26)." This solution is given with a 100% certainty factor because the given combination is the only model that will handle this particular problem.

The example was set up to be as simple as possible and still convey the necessary information. In Fig. 11, EXSHELL asks the question, Trace of reasoning to goal? In this case, the user entered yes for demonstration purposes. This is part of the EXSHELL explanation facility. It traces the rules of the search space graph from the beginning to the solution. The dialogue is shown in Fig. 11. In this case, the rules and facts and the way in which the facts were ascertained are the same as the combination of the how and why queries shown earlier. This would probably not be the case for more difficult problems.

Figure 12 shows the dialogue between a user and CLIPS. The reader can follow in Fig. 7, which is a portion of the search space used by the expert system shell CLIPS, that contains the answer to the same problem. Even though the problem is the same, the approach is different because CLIPS uses forward rather than backward chaining. One difference that is not apparent from the dialogue in this simple problem can be seen by comparing Figs. 6 and 7.

\*

Trace of reasoning to goal? > yes.

pick\_equation('Use Steam Tables (SYSOP12) with electrolyte correction (liquid-fugacity model 26)') CF = 100 was proved using the rule

IF diagnose(steam\_water\_electrolyte) \*\*\*Known, Certainty = 100

AND choose(steam\_water\_electrolyte, "Use Steam Tables (SYSOP12) with electrolyte correction (liquid-fugacity model 26)') \*\*\* Known, Certainty = 100

THEN pick\_equation('Use Steam Tables (SYSOP12) with electrolyte correction (liquid-fugacity model 26)')

CF 100

diagnose(steam\_water\_electrolyte) CF = 100 was proved using the rule

IF major\_type(steam\_tables) \*\*\*Known, Certainty = 100
AND electrolyte \*\*\*Known, Certainty = 100
THEN diagnose(steam\_water\_electrolyte)
CF 100
major\_type(steam\_tables) CF = 100
was proved using the rule

IF steam\_and\_water \*\*\*Known, Certainty = 100
THEN major\_type(steam\_tables)
CF 100

steam\_and\_water was given. CF = 100 electrolyte was given. CF = 100 choose(steam\_water\_electrolyte, "Use Steam Tables (SYSOP12) with electrolyte correction (liquid-fugacity model 26)') is a fact, CF = 100

Fig. 11. Dialogue with EXSHELL (continued).

CLIPS > (reset)
CLIPS > (run)
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

5 rules fired

Fig. 12. Dialogue with CLIPS.

With CLIPS, more questions are asked up front. Because of the forward-chaining technique, we use a different approach with CLIPS. With this system, instead of picking the best solution, we use a scoring technique and supply the user with a list of rated solutions. To do this, we ask more question in the beginning and give each choice a score based on the answer to the question. In this example, however, the questions are the same as in the EXSHELL example. Another difference is that the questions asked by CLIPS are more verbose and descriptive than those asked by EXSHELL.

The dialogue with CLIPS begins with the user typing (reset) and (run). CLIPS then asks 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 in the same way as before: "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 and is related to the EXSHELL confidence factor of 100. This is in this example, we really do not have much 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.

# REFERENCES

- J. C. Giarratano, <u>Clips User's Guide</u>, Version 4.1 of CLIPS, Artificial Intelligence Section (Lyndon B. Johnson Space Center, October 13, 1987).
- G. F. Luger and W. A. Stubblefield, <u>Artificial Intelligence and</u> the Design of Expert System (The Benjamin/Cummings Publishing Company, Inc., Redwood City, CA, 1989).
- 3. \_\_\_\_\_\_, <u>ASPEN User Manual</u>, Department of
  Chemical Engineering, Massachusetts Institute of
  Technology, Cambridge, Massachusetts, December 1981
  (ASPEN Project for the USDOE, Contract Numbers E(49-18)2295, Task No. 9, and DE-AC21-81MC16481).
- 4. K. C. Chao and J. D. Seader, "A General Correlation of Vapor-Liquid Equilibria in Hydrocarbon Mixtures," AIChE Journal, Vol. 7, No. 4, (December 1961) pp. 598-605.
- R. Banares-Alcantara, "Development of a Consultant for Physical Property Predictions, "Master's Thesis, Department of Chemical Engineering, Carnegie Mellon University (1982).

- R. Banares-Alcantara, A. W. Westerberg, and M. D.
   Rychener, "Development of an Expert System for Physical Property Predictions," Computers and Chemical Engineering, Vol. 9, No.2 (1985) pp. 127-142.
- R. F. Wilcox and S. L. White, "Selecting the Proper Model to Simulate Vapor-Liquid Equilibrium," Chemical Engineering (October 27, 1986) pp. 141-144.
- 8. J. M. Prausnitz, <u>Molecular Thermodynamics of Fluid-Phase</u>

  <u>Equilibria</u>, (Prentice-Hall Inc., Englewood Cliffs, New Jersey, 1969).
- R. C. Reid, J. M. Prausnitz, and B. E. Poling, <u>The Properties of Gases and Liquids</u>, 4th Ed. (McGraw-Hill Book Company, New York, 1987).
- D. R. Hart, "Liquid Activity Coefficients," Chemical Engineering (November 23, 1987) pp. 131-138.

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11. H. G. Grayson and C. W. Streed, "Vapor-Liquid Equilibria for High Temperature, High Pressure Hydrogen-Hydrocarbon Systems," paper presented at the Sixth World Petroleum Conference, Frankfurt, West Germany (June 19-26, 1963).