

## A GEOCHEMICAL EXPERT SYSTEM PROTOTYPE USING OBJECT-ORIENTED KNOWLEDGE REPRESENTATION AND A PRODUCTION RULE SYSTEM

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**Abstract**—This paper presents the design and development of a Geochemical Expert System prototype (GES) for analyzing solution–mineral interactions in nature. The emphasis is placed on expert system design and knowledge representation. One of the most challenging and research-intensive steps was the identification of the key geochemical characteristics that would enable the expert system to identify salient features of any user-defined geochemical composition. Moreover, developing a system to create geochemical interpretations similar to those written by expert geochemists proved to be difficult. Important geochemical characteristics and their interrelationships which were “discovered” during knowledge acquisition and conceptualization are presented. These characteristics have been organized and documented within the expert system to emulate the skills of an expert geochemist. Examples of expert system-generated analyses are presented.

**Key Words:** Artificial Intelligence (AI), Expert systems, Geochemistry, Geochemical modeling, MINEQL, Geochemical Expert System (GES).

### INTRODUCTION

Computer-based models are used by chemists, geochemists, hydrologists, environmental engineers, and waste-management professionals to determine chemical and hydrological conditions in nature. These models are important for assessing the chemical reactivity and transport potential of contaminants in soil and groundwater. Accurate construction and use of these models (i.e. problem formulation, preparation of correct input data, and model execution) requires not only that the user fully understands the model, but also that he/she has a wide range of knowledge including statistics, numerical methods, and computational techniques, in addition to the knowledge of his/her own discipline. This knowledge is even more critical when the individual attempts to interpret the results of a model and to make decisions based upon those interpretations. At the same time, the increasing demand for waste management professionals, financial constraints, and the large number of contaminated sites have made affording expert advice at all times impractical. In response to these problems, Oak Ridge National Laboratory developed the Geochemical Expert System (GES). This prototype interacts with geochemical models, makes expert interpretation of model results, and provides decision support to persons responsible for waste management and environmental restoration.

### BACKGROUND

#### *Geochemical modeling*

Geochemical models are used to assess the rate and extent of geochemical interactions (Stumm and Morgan, 1981). Because of the limited amount of information available about the rates at which chemical reactions occur (kinetics) in nature, geochemical models usually employ the equilibrium thermodynamics approach. Equilibrium models—including MINEQL (Westall, Zachary, and Morel, 1976), PHREEQE (Parkhurst, 1983), EQ3/6 (Wolery, 1984), and MINTEQ (Felmy, Girvin, and Jenne, 1984)—are imperfect because of an incomplete understanding of important chemical processes and inadequate thermochemical data for quantification of known processes. However, they are used widely and offer the best available tools for quantitative assessment of geochemical processes at this time. GES uses a modified version of MINEQL as the geochemical model; however, other geochemical models could be incorporated easily into the expert system without compromising the integrity of the knowledge base and rule base.

#### *Development strategies*

Unlike expert systems which are based on qualitative classification and diagnosis, GES calculates as much information as possible to account for all

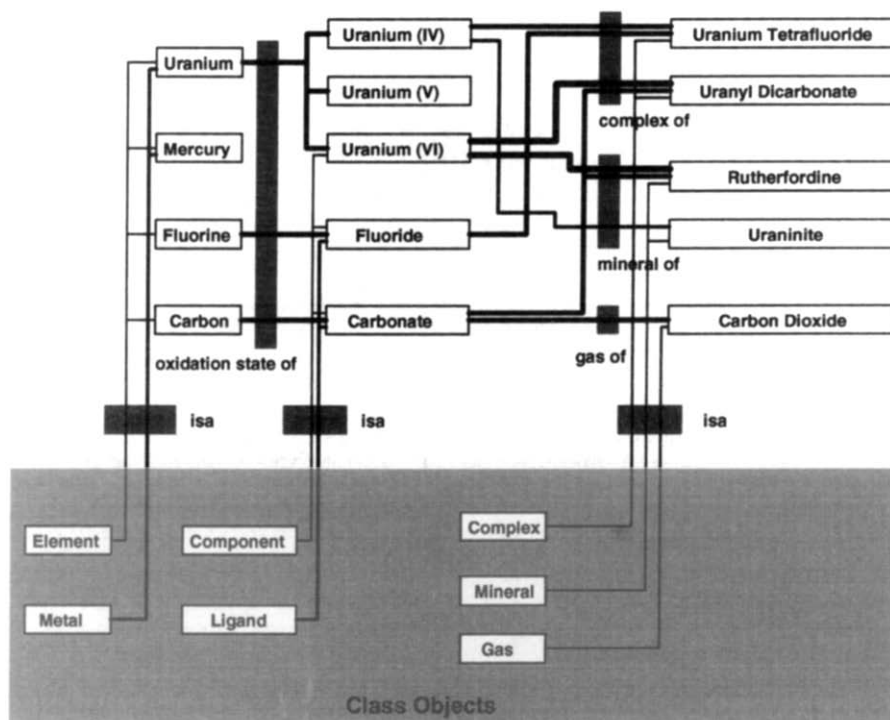


Figure 1. Subset of "first-principles" chemistry objects and their relationships as represented in GES knowledge base. Note that relations in figure read from right to left (i.e. Uranium isa Element).

possible reactions. When processes or characteristics cannot be calculated, heuristics and qualitative classifications in the form of rules are used for analysis. This strategy has provided GES with both quantitative and qualitative methods of mimicking the thoughts, analytical skills, and interpretations of expert geochemists.

#### Tool selection

Laser\* was selected as the expert system development shell to meet the following criteria: (1) availability on a wide range of computer hardware, (2) modularity so that knowledge of different disciplines (chemistry, geochemistry, and hydrology) can be kept separately and so that modules can be developed independently, (3) provision of facilities for calling other programs and communicating over networks, (4) sophisticated forward-chaining production (rule) system, and (5) ability to perform complex mathematical operations within rules.

Laser (Reddy and others, 1986) is available on a wide range of computers including microcomputers, minicomputers, workstations, and mainframes. Laser employs both semantic network and frame-based knowledge representation schemes in its Knowledge Representation (KR) module. The Rule Production System (RPS) of Laser (Raman, 1985) provides a forward-chaining inference engine which uses special classes of objects represented in the KR module.

\*Laser is a registered trademark of Bell Atlantic Knowledge Systems, Inc.

These rule objects can be related into groups to provide better modularity and to increase speed during the evaluation cycle of the inference engine. Laser is written in C and can be called from or make calls to user-written programs; therefore, the expert system can communicate over a network and can be linked and used in conjunction with other software tools. RPS interprets its rules right out of the objects which allows the expert system to alter its own rule base. This feature is not available in most expert system shells. Although extensive use of this feature is not made in the current prototype, it has implications for learning systems which may be developed in future prototypes.

### EXPERT SYSTEM DESCRIPTION

#### Knowledge representation

To build the GES knowledge base, each chemical element of interest is represented as an individual object. Because some elements can occur in different oxidation (valence) states in nature, each valence state was added as an individual object and related to its parent element as child objects. Next, complexes, minerals, and gases which are required by the model when solving for equilibrium were created and added to the knowledge base. These objects were related to all of their parent components as child objects.

A small subset of the objects represented in the knowledge base is shown, with hierarchical relationships, in Figure 1. The uranium, mercury, fluorine,

and carbon objects are related to the element object through an isa relationship because they are all examples of elements. Additionally, uranium and mercury also are descendants of the metal object because they are examples of metals. Objects such as element and metal are termed *class objects* because they classify groups of other objects. The elements then have child objects which represent their oxidation states. These oxidation states in-turn have child objects which are the complexes, minerals, and gases formed from combinations of oxidation states. Class objects are used to group components and ligands on the oxidation state level and to group complexes, minerals, and gases on the final level. This *object-oriented* approach carries much chemical information because each object also contains characteristic properties of the element, oxidation state, complex, mineral, or gas. These properties include (1) atomic weights, (2) stoichiometries, (3) charges, (4) scientific names and symbols, and (5) formation (free energy) constants.

In order to provide additional structure to the many objects in the GES knowledge base, sample compositions of rivers, groundwaters, soils, and other natural and man-made environments were created in the knowledge base. The two additional class objects are the basis (or components) groups and the natural systems.

Basis groups contain lists of similar chemical components or components which occur together in nature or in man-made chemical systems. These objects not only contain typical components, but also specify typical concentrations of these components. The radionuclides object is an example of a component group. This object contains a list of typical radionuclides: uranium (VI), neptunium (V), plutonium (V), thorium (IV), and strontium (II). It also contains their typical concentrations in areas near waste-storage sites. In future versions, the user will have the ability to customize these objects to reflect local conditions or inventories of chemicals.

Natural geochemical systems, such as component groups, specify typical components and concentrations in natural environments; however, they also provide typical pH and pE values and have a hierarchy which is useful for creating submenus in the GES when the user specifies a composition. Groundwater is a natural system, but was given a wide range of pH and pE values for groundwater environments. In order to restrict these ranges, compositional sub-categories of groundwater were created as child objects of the primary groundwater object. The oxidizing groundwater has higher pE values; the acidic groundwater has lower pH values; and the oxidizing acidic groundwater has both higher pE and lower pH values. Because these child objects inherit the component list and concentrations from the groundwater object, only the changed or restricted values need to be included in the child objects.

#### *Expert system output*

It was initially thought that, in order to have the expert system communicate results in logical, grammatical, and useful English, a rule for every possible outcome would be needed. Because almost 34,000 possible combinations exist for the small subset of interpretations in the preliminary GES prototype this was not feasible. Alternately, a rule was created for every classification of a geochemical property, and English phrases concerned only with that classification were stored in that rule. During execution, if an output is expected (i.e. the model run suggests chemical behavior that is verified by derived characteristics) a phrase describing the outcome is stored in a list of expected phrases. If the model has calculated an unexpected outcome (i.e. the model run calculates an outcome that the heuristic rules do not verify), GES generates a phrase which describes that outcome and stores it in a list of unexpected phrases. For example, a given species may be classified as strong, but, because of competition from other species, it may turn out to be insignificant. Phrases from other classifications which were neither expected nor unexpected are added to the list of neutral phrases. Neutral phrases provide additional information about speciation which may be of interest to the user. Finally, these collected phrases are combined into sentences which fully describe the modeled outcome.

#### *Expert system analysis*

The three major areas of analysis performed by GES are oxidation (reduction), complexation, and precipitation (dissolution). Derived properties, which were "discovered" during knowledge acquisition sessions, are described for each of these areas of analysis. Sample explanations, taken directly from GES output, are included here after the discussion of the derived properties. For a more detailed explanation of the geochemical concepts, see Tripathi and Hoffman (1990).

*Oxidation analysis.* The first area of analysis provided by GES is that for chemical oxidation. If an element has only one oxidation state, its total concentration is described; however, if more than one oxidation state exists, the abundance of all oxidation states is described and explained. Because the equilibrium model has completed the computations, its answers are explained in view of the chemical composition of the system and the thermodynamic properties of relevant complexes and minerals. The methods by which the explanation is performed are described next.

The oxidation states are sorted in order of their free concentrations. A table then is generated containing the oxidation states, the free concentrations, the dissolved concentrations, the precipitated concentrations, and the total concentrations.

Each oxidation state is interpreted individually. First, the total concentration of an oxidation state is

compared to the concentration of the total element. The oxidation state then will be described as significant (with a percent of total element given), negligible, or its percent of total element concentration will be printed. Second, any extrema associated with the oxidation state—minimum or maximum free, dissolved, precipitated, and total concentrations—will be described. Finally, the oxidation state is described in terms of the next oxidation state of the element and its ranking is explained based on the composition's pE and pH.

Using the stored stoichiometry information, the expert system can describe any oxidation state as a function of any other oxidation state plus electrons and possibly hydronium (protons). The oxidation analysis rule base takes advantage of this capability to determine threshold pE's and pH's that would lead to the calculated distribution of oxidation states. The expert system first will attempt to explain the results based solely on pE; however, if the system pE is such that another result should have occurred, the expert system will use the pH to explain the model results.

Finally, if the dissolved concentration of the second oxidation state is greater than that of the first oxidation state, the expert system will infer that the complexation potential of the second oxidation state is higher than the complexation potential of the first oxidation state.

The following paragraph shows the expert system describing the oxidation of uranium using threshold pH's and pE's.

for the basis chemicals involved in the complexation with a component. Although the complexes are not described individually, the basis chemicals involved in solution with the component are interpreted. The derived properties of complexation are attributed to the basis chemical for the sake of analysis. In this way, limits are placed on the strengths and the complexation potentials of basis chemicals. These properties and their derivations are described next.

The strength of a complex is calculated as:

$$\text{strength} = \frac{\log \beta}{\text{number of constituent ions} - 1} \quad (1)$$

Classifications of strength are made as follows:

Strength	Classification
$\geq 10$	Very strong
$< 10$ and $\geq 7$	Strong
$< 7$ and $\geq 4$	Moderately strong
$< 4$ and $\geq 2$	Weak
$< 2$ and $\geq 0$	Very weak
$< 0$	Extremely weak

The strength of a basis chemical's complexation with the component under consideration is that of the strongest complex involving both the basis chemical and the component.

During analysis, the strengths associated with each basis chemical are compared. While describing the

Uranium				
Concentrations				
Oxidation states	Free	Dissolved	Precipitated	Total
Uranium (V)	$1.18 \times 10^{-12}$	$1.18 \times 10^{-12}$	0.00	$1.18 \times 10^{-12}$
Uranium (VI)	$1.93 \times 10^{-18}$	$1.98 \times 10^{-15}$	$2.50 \times 10^{-03}$	$2.50 \times 10^{-03}$
Uranium (IV)	$2.02 \times 10^{-28}$	$4.50 \times 10^{-10}$	$7.50 \times 10^{-03}$	$7.50 \times 10^{-03}$
Total uranium	$1.18 \times 10^{-12}$	$4.52 \times 10^{-10}$	$1.00 \times 10^{-02}$	$1.00 \times 10^{-02}$

Uranium (V) constitutes a negligible fraction of total uranium. Of the uranium valences, uranium (V) has the largest free concentration despite this fact. The pE is reducing enough (below 2.79) to allow free uranium (V) to dominate free uranium (VI).

Uranium (VI) constitutes only 25.0% of total uranium. Of the uranium valences, uranium (VI) has the smallest dissolved concentration. Although the pE is not oxidizing enough (above 4.61) to make free uranium (VI) greater than free uranium (IV), the pH is high enough (above 3.80) to cause this to occur. The complexation potential of uranium (IV) is greater than the complexation potential of uranium (VI); therefore, dissolved uranium (IV) is greater than dissolved uranium (VI).

Uranium (IV) is significant and constitutes 75.0% of total uranium. Of the uranium valences, uranium (IV) has the largest dissolved concentration and has the largest solid concentration, but it has the smallest free concentration.

**Complexation analysis.** For the second area of analysis, the complexation of each oxidation state is described. In the following discussion, the term "component" will be used to indicate the oxidation state being analyzed and the term "basis chemicals" will be used to indicate all of the oxidation states which form complexes with the oxidation state being analyzed. The complex concentrations are added up

strongest and weakest basis chemicals, the expert system notes that the basis chemical is the strongest or the weakest of all basis chemicals which form complexes with the component being analyzed. The strength used for comparison, the same one used for the strength classification as described, is that of the strongest complex involving both the basis chemical and the component.

The complexation potential of a complex is a measure of the extent to which the complex is likely to form. It is a derived quantity which was "discovered" during knowledge acquisition and it reflects the thermodynamic strength of the complex and the composition of the system. The complex with the greatest complexation potential is the most significant complex for a component. The calculation of the complexation potential for triuranyl tetrahydroxide  $(\text{UO}_2)_3\text{OH}_3^+$  is:

$$\text{complexation potential} = \frac{\beta \times [\text{UO}_2]^3 \times [\text{OH}]^5 \times 3}{[\text{UO}_2]} \quad (2)$$

where  $\beta$  is the formation (free energy) constant and the quantities in brackets are the free concentrations of the components within the brackets. The complexation potential of a basis chemical with the component under consideration is that of the largest complexation potential involving both the basis chemical and the component.

If the complexation potential is the largest or the smallest for the basis chemical being interpreted, its fraction of the maximum complexation potential is calculated and described. This quantity is especially useful for conveying the effectiveness with which a basis chemical competes in complexation for the component being interpreted.

The pH of hydrolysis of a metal is calculated as:

$$\text{pH of hydrolysis} = -\log \beta \text{ of (1,1) hydroxo species} + 13.99 \quad (3)$$

where  $\beta$  is the formation (free energy) constant as in Equation (3). The pH of protonation of a ligand is the  $\log \beta$  of HL, the (1,1) protonated ligand species. GES uses the pH of hydrolysis when interpreting complexes involving hydroxide and the pH of protonation when interpreting complexes involving hydronium (protons).

The relative concentrations of aqueous basis chemicals and aqueous components are used to explain model results. If there is little complexation with a basis chemical and the component concentration is significantly higher than the basis chemical concentration, then this result is supported. Likewise, if there is significant complexation of a component with a basis chemical and the basis chemical concentration is significantly higher than the component concentration, then this result is supported.

The free concentrations of all basis chemicals involved in complexation with the component under consideration are compared. The system points out which basis chemicals have the largest and which have the smallest free concentrations.

Each basis chemical is described as constituting some percentage of the total dissolved concentration of the component under consideration. If this number is small, the system will merely say that the basis chemical constitutes a negligible fraction of the dissolved component. If this number is  $> 85\%$ , the

system will state that the basis chemical dominates the complexation of the dissolved component. Actual percentages are printed for the other classifications. Classifications of significance are made as follows:

Percent of dissolved component	Classification
$\leq 0.1\%$	Negligible
$< 15\%$ and $> 0.1\%$	Not important
$< 85\%$ and $\geq 15\%$	Important
$\geq 85\%$	Dominant

The next paragraph shows the expert system explanation using strength, relative complexation potential, relative aqueous concentration, and basis amount of component (i.e. dominant or  $> 85\%$ ).

Under these conditions, the  $\text{CO}_3^{2-}$  complexes of  $\text{UO}_2^{2+}$  in this system are strong and the  $\text{CO}_3^{2-}$  complexation potential is the highest for  $\text{UO}_2^{2+}$  and the total aqueous  $\text{CO}_3^{2-}$  concentration is over 1000 times the total aqueous  $\text{UO}_2^{2+}$  concentration; therefore, complexes with carbonate dominate the complexation of uranium (VI).

The following paragraph shows the expert system output using relative aqueous concentration, strength, pH of hydrolysis, complexation potential fraction of maximum, and basis amount of component.

Although the total aqueous  $\text{OH}^-$  concentration is over 1000 times the total aqueous  $\text{UO}_2^{2+}$  concentration and the  $\text{OH}^-$  complexes of  $\text{UO}_2^{2+}$  in this system are strong and the pH is favorable for significant hydrolysis of  $\text{UO}_2^{2+}$ , the  $\text{OH}^-$  complexation potential is 1/68 of the highest complexation potential for  $\text{UO}_2^{2+}$ ; therefore, complexes with hydroxide are not important and constitute only 1.0% of total aqueous uranium (VI).

The next paragraph shows the expert system explanation using relative aqueous concentration, relative free basis chemical concentration, strength, relative strength, relative complexation potential, and basis amount of component (i.e. negligible).

Although the total aqueous  $\text{Cl}^-$  concentration is over 1000 times the total aqueous  $\text{UO}_2^{2+}$  concentration and the free  $\text{Cl}^-$  concentration is greater than that of other components which form complexes with  $\text{UO}_2^{2+}$ , the  $\text{Cl}^-$  complexes of  $\text{UO}_2^{2+}$  in this system are very weak and the  $\text{Cl}^-$  complexes are the weakest complexes of  $\text{UO}_2^{2+}$  in this system and the  $\text{Cl}^-$  complexation potential is the lowest for  $\text{UO}_2^{2+}$ ; therefore, complexes with chloride are not important and constitute a negligible fraction of total aqueous uranium (VI).

*Precipitation analysis.* The third area of analysis is precipitation. When analyzing precipitation, the expert system will perform additional model runs in order to determine the correct equilibrium composition. Because of phase rule violation problems which may occur when the model considers all minerals for precipitation, an initial run is made with all minerals ignored (except those that are specified to be available in an unlimited supply). The model computes saturation indices for all possible minerals. Next, another model run is made with supersaturated minerals (saturation index  $> 1$ ) considered for

precipitation. This process continues until all the ignored minerals are undersaturated (saturation index < 1).

Minerals, unlike complexes, are interpreted on an individual basis. Each mineral is interpreted according to its properties. These properties are strength, relative strength, saturation index, relative saturation index, and percentage of component.

Mineral strengths, like complex strengths, are calculated using Equation (1). Mineral strength classifications are made as follows:

Strength	Classification
$\geq 12$	Very strong
$< 12$ and $\geq 9$	Strong
$< 9$ and $\geq 6$	Moderately strong
$< 6$ and $\geq 4$	Weak
$< 4$ and $\geq 2$	Very weak
$< 2$	Extremely weak

In addition to describing the strength of a mineral, the expert system notes if the mineral is the strongest or the weakest of all minerals which form with the component being analyzed.

The saturation index of a mineral, which is computed by the geochemical model, is:

$$\text{Saturation index} = \frac{\text{ion activity product (IAP)}}{\text{solubility product (KSP)}} \quad (4)$$

Every mineral is classified into a category according to the  $\log_{10}$  of its saturation index. The following table lists the classifications:

$\log_{10}$ of saturation index	Classification
$\geq 10$	Extremely supersaturated
$< 10$ and $\geq 4.0$	Very supersaturated
$< 4.0$ and $\geq 1.0$	Moderately supersaturated
$< 1.0$ and $\geq 0.5$	Slightly supersaturated
$< 0.5$ and $> -0.5$	Near equilibrium
$\leq -0.5$ and $> -1.0$	Slightly undersaturated
$\leq -1.0$ and $> -4.0$	Moderately undersaturated
$\leq -4.0$ and $> -10.0$	Very undersaturated
$\leq -10.0$	Extremely undersaturated

Minerals whose saturation index is  $> 1$  form at equilibrium (are supersaturated), whereas minerals whose saturation index is  $< 1$  do not form (are undersaturated). If a mineral has the largest or smallest saturation index of all the minerals of the component considered, the expert system indicates the condition while interpreting the mineral. Finally, statistical information is provided. Each mineral which is supersaturated is described as constituting some percentage of the total component based on concentrations. Undersaturated minerals do not constitute any amount of the total element because they do not form at equilibrium.

For example,  $U_4O_9$  is described using strength, saturation, relative saturation index, and mineral percentage of component as follows:

$U_4O_9$  ( $U_4O_9$ ) is very strong and is extremely supersaturated when no other minerals are allowed to precipitate and has the largest saturation index of all the uranium (VI)

minerals considered for precipitation when no other minerals are allowed to precipitate; as a result, it constitutes 100.0% of total uranium (VI).

The next paragraph illustrates the expert system explanation using strength and saturation index to describe pitchblende.

While pitchblende ( $\alpha U_3O_8$ ) is strong and is very supersaturated when no other minerals are allowed to precipitate; it is extremely undersaturated when other minerals are allowed to precipitate.

The paragraph below shows the expert system discussion using strength and saturation index to describe uranophane.

While uranophane ( $Ca(UO_2)_2H_2SiO_4$ ) is strong; it is extremely undersaturated when no other minerals are allowed to precipitate and the saturation remains unchanged when other minerals are allowed to precipitate.

## INTEGRATED SOFTWARE

The chemical equilibrium model currently used by the expert system, MINEQL, is written in FORTRAN but has been combined with code written in C which allows the expert system and the model, which run as separate processes (client/server scenario), to communicate. Using Berkeley sockets across a TCP/IP network, the C-portion of the model waits to receive input from the expert system. Upon receiving the input, the C-portion loads up the arrays necessary for the model and calls MINEQL. After MINEQL solves the equilibrium problem, control returns to the C-portion of code which passes the output data back across the network to the waiting expert system. This design is extremely flexible because the model can be running on a massively parallel machine or on a supercomputer for fast floating-point computations while the expert system runs on a workstation or departmental computer with a high integer performance.

The user interface of the expert system consists of dynamic menus written in the X Window environment (Scheifler and Gettys, 1986; Scheifler, Gettys, and Newman, 1988). The X Window system, developed and made available by the Massachusetts Institute of Technology, was selected because it can be used on networks between computers and organizations and because it is written in C, can be compiled with and called from the expert system. The network capabilities are especially important because a GES user may use a local workstation to display the user interface in one part of the country or in the field while GES is running on a high-speed computer in another part of the country or at the primary research facility. The menu screen (see Fig. 2) is constructed from the knowledge base so that the state of the knowledge base determines how the user interface behaves and what it displays. Unlike traditional user interfaces which require all menu items to be specified before development, this interface builds its menus from the data passed from the expert system. This

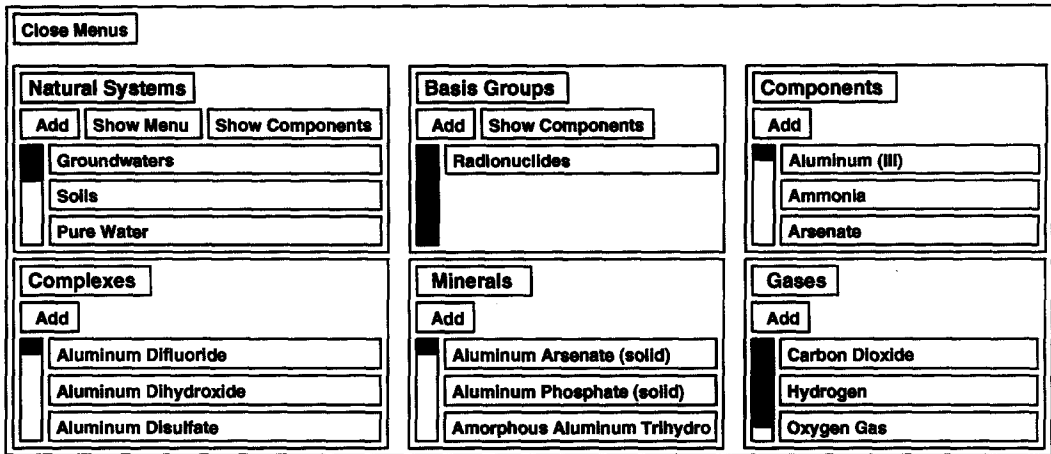


Figure 2. GES menu screen.

*dynamic user interface* is extremely flexible and requires almost no maintenance because, as more capabilities are added to the expert system, a simple change in the knowledge base results in an updated user interface. The status screen (see Fig. 3), which also is dynamic, shows the chemical composition, including all components, species, elements, the pH, and the pE, that the user has selected for analysis.

runs, kinetics computations, and uncertainty analysis—will be added before it becomes a field prototype, at which time field testing on real problems will occur. In addition, modules for presenting results graphically and for performing hydrological computations will be added in later prototypes. As models for reaction and transport of organic compounds improve, expert system modules for handling such processes will be developed.

**FUTURE DEVELOPMENTS**

GES is currently a research prototype. It has over 600 rules and generates reasonable, but not perfect, answers to the problems presented to it. Additional features—such as merging the results of many model

**SUMMARY**

The research and development efforts to date have shown that, by employing currently available expert system development technologies, it is possible to

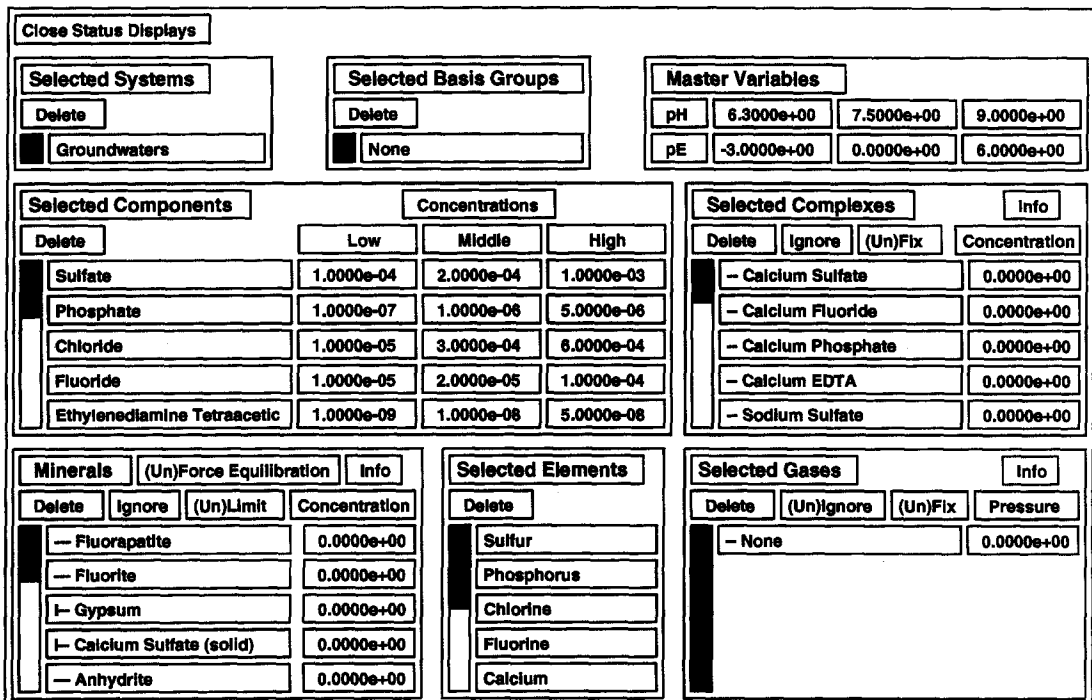


Figure 3. GES status display.

perform a comprehensive analysis of geochemical behavior of interest to contaminant transport, waste management, and related areas. Numerous problems involved in the direct use of geochemical models have been totally eliminated. Unlike traditional expert systems, GES uses dynamic information (model results) and provides explanations and justifications in terms of thermodynamic properties, the chemical composition, and the equilibrium state of the chemical system. The work has provided a solid foundation for continued development aimed at solving and analyzing, in more detail, more significant problems about chemical behavior and interactions. Additionally, the same techniques can be applied to other problems including hydrological, and kinetic modeling.

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