

MARIANA — A SIMPLE CHEMICAL EQUILIBRIUM MODULE

VERSION 1.0

Prepared for

**Nuclear Regulatory Commission
Contract NRC-02-88-005**

Prepared by

**Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas**

August 1992

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1 INTRODUCTION

In accordance with the provisions of the Nuclear Waste Policy Act (NWPA), as amended, the Nuclear Regulatory Commission (NRC) has the responsibility of granting a license for the first (and subsequent, if any) geologic repository for high-level nuclear waste (HLW). The Center for Nuclear Waste Regulatory Analyses (CNWRA) at Southwest Research Institute (SwRI) is a Federally Funded Research and Development Center (FFRDC) created to support the NRC in its mission of licensing the repository. To meet its licensing function, the NRC will review the application submitted by the Department of Energy (DOE). One of the critical sections of the license application will deal with the assessment of the future performance of the repository system which has to meet the system requirements in 10 CFR 60.112 and the subsystem Particular Barriers requirements in 10 CFR 60.113.

In order to develop capabilities to review the performance assessment in DOE's license application, the staffs of the NRC and the CNWRA are engaged in developing and applying performance assessment methods and models to existing data. Later, at the time of license application review, these methods may be used to conduct an independent performance assessment, if the NRC elects to do so.

This work addresses the subsystem performance requirements of 10 CFR 60.113 for containment and gradual release of radionuclides from the engineered barriers subsystem. To support the evaluation of these requirements, software development activities are under way at the CNWRA. The detailed mechanistic modeling in support of the containment and gradual release performance assessment is the aim of the EBSPAC analysis program. Together with the system source term code, *SOTEC*, and the EBSPAC development, comprehensive and integrated system/subsystem performance assessments can be conducted. *Mariana* represents work developed under the EBSPAC program.

Calculations related to engineered barriers behavior must often consider chemical equilibrium in conjunction with other simultaneous processes such as mass transport of radionuclides, corrosion, colloid generation, and waste form alteration. In recognition of the requirement for equilibrium and other calculations in a variety of engineered barriers performance and research models, the CNWRA is developing a set of modules that can be easily incorporated into multiple codes. *Mariana* is intended as a simple equilibrium solver that can be called as a subroutine from other codes. The equilibrium solver is designed to react the input solution to equilibrium including all homogeneous and heterogeneous reactions specified in the stoichiometric matrix.

Chemical equilibrium problems have been solved by a number of analysts (Smith, 1982), and many stand alone codes for aqueous equilibria are available (e.g., EQ 3/6, PHREEQE). While existing codes such as EQ3/6 (Wolery, 1983, Wolery *et al.*, 1990) or PHREEQE (Parkhurst, Thorstenson and Plummer, 1987) are appropriate for detailed analysis of closed systems, codes of this size and complexity are not easily coupled with other processes. Small, compact, and simpler codes are more appropriate for solving the coupled problem. A small and compact code requires significantly smaller computer resources and is easier to customize for specific problems.

Mariana solves the chemical equilibrium problem through stoichiometric Gibbs free energy minimization. The solution is written in terms of the reaction progress variables for the reactions under consideration. All reactions considered are solved to equilibrium. In order to keep the code compact and general, *Mariana* has no built-in database of thermodynamic data or reactions. Instead, the main calling

program passes the required thermodynamic data and stoichiometric matrix for the problem to be solved to *Mariana* in a common block.

The specification of the stoichiometric matrix of reactions in the calling program adds flexibility to the solver. For example, individual redox reactions may be either included or omitted from the stoichiometric matrix depending upon whether the compounds are electroactive in the system under consideration. In other situations, some reactions will be considered on a rate basis in the calling program with *Mariana* applied only to a subset of fast reactions (e.g., hydrolysis). Activity coefficients can be calculated by the B-dot equation, the Davies equation, or assumed to be equal to one (ideal solution).

2 THEORY

Mariana solves the chemical reaction equations by stoichiometric Gibbs free energy minimization (Smith, 1982). The Gibbs free energy of formation of a system is given by

$$G = \sum_i n_i \mu_i = \sum_i n_i (\mu_i^o + RT \ln \{a_i\}) \quad (2-1)$$

where:

G	=	Gibbs free energy (J/mole)
n_i	=	moles of i in 1 kg of water (mole/kg)
μ_i	=	chemical potential of i (J/mole)
μ_i^o	=	standard state chemical potential of i (J/mole)
R	=	gas law constant (J/mole/°K)
T	=	absolute temperature (°K)
a_i	=	activity of species i .

Simply put, the free energy of the system is equal to the sum of the chemical potentials contributed by each species in the solution. This equation arises from the definition of the chemical potential of a species:

$$\mu_i = \left(\frac{\partial G}{\partial n_i} \right)_{T,P} \quad (2-2)$$

The chemical potential is defined to be that portion of the Gibbs free energy contributed by a particular species. The moles of a particular species i in the system can be related to the reaction progress variable:

$$n_i = n_i^o + \sum_r \nu_{i,r} \xi_r \quad (2-3)$$

where:

n_i^o	=	moles of i in 1 kg of water at initial time (mole/kg)
$\nu_{i,r}$	=	stoichiometric coefficient of species i in reaction r
ξ_r	=	reaction progress variable for reaction r (moles).

This states that the number of moles of species i present is equal to the number of moles originally present plus the number of moles produced or lost through multiple chemical reactions. The reaction progress variable for any reaction is unconstrained and can be either positive or negative.

The activity, a_i , of an aqueous species, or its effective concentration, is equal to the product of its molal concentration and its activity coefficient:

$$a_i = \gamma_i n_i \quad (2-4)$$

The activity of solids is assumed to be unity in the current version of *Mariana*. Consideration of solid solutions may be added in future updates.

Minimization of Gibbs free energy is accomplished by taking the derivative of G with respect to each reaction progress variable and setting the result equal to zero:

$$\frac{\partial G}{\partial \xi_r} = \sum_i \left(\frac{\partial G}{\partial n_i} \right)_{T,P} \cdot \frac{\partial n_i}{\partial \xi_r} = \sum_i \mu_i \cdot v_{i,r} = \sum_i v_{i,r} (\mu_i^o + RT \ln a_i) = 0 \quad (2-5)$$

One equation is written for each chemical reaction considered. Simultaneously solving the resulting set of equations for the reaction progress variables yields the extent of each reaction, which in turn yields the equilibrium concentration of each species.

For aqueous species, by combining Eqs. (2-3), (2-4), and (2-5), the term inside the summation becomes:

$$v_{i,r} \left(\mu_i^o + RT \ln \left[\gamma_i \left(n_i^o + \sum_{\hat{r}} v_{i,\hat{r}} \xi_{\hat{r}} \right) \right] \right) \quad (2-6)$$

For pure solids, the activity is defined to be 1, so the summation term reduces to:

$$\mu_i^o v_{i,r} \quad (2-7)$$

Thus, Eq. (2-5) becomes:

$$\sum_i^{aqueous} v_{i,r} \left(\mu_i^o + RT \ln \left[\gamma_i \left(n_i^o + \sum_{\hat{r}} v_{i,\hat{r}} \xi_{\hat{r}} \right) \right] \right) + \sum_j^{solid} \mu_j^o v_{j,r} = 0 \quad (2-8)$$

Several subscripts are used for the summations in Eqs. (2-8) and (2-9); i is the summation variable for all aqueous species, j is used for solids, r and k refer to chemical reactions the particular equation applies to, and \hat{r} refers to summation over all chemical reactions.

Mariana solves this set of nonlinear algebraic equations using the Newton-Raphson method, which requires calculation of the Jacobian matrix. The derivatives for the Jacobian are obtained by taking a second derivative of G with respect to the various reaction progress variables:

$$\frac{\partial}{\partial \xi_k} \left(\frac{\partial G}{\partial \xi_r} \right) = \sum_i^{aqueous} v_{i,r} \frac{RT \cdot \gamma_i \cdot v_{i,k}}{\left[\gamma_i \left(n_i^o + \sum_{\hat{r}} v_{i,\hat{r}} \xi_{\hat{r}} \right) \right]} + 0$$

(2-9)

$$= \sum_i^{aqueous} v_{i,r} v_{i,k} \frac{RT}{\left(n_i^o + \sum_{\hat{r}} v_{i,\hat{r}} \xi_{\hat{r}} \right)}$$

3 CALCULATION OF ACTIVITY COEFFICIENTS

Mariana currently has three options for determining activity coefficients: (i) assume ideal solution ($\gamma_i = 1$), (ii) calculate using B-dot equation, and (iii) calculate using Davies equation. The Davies equation is (Stumm and Morgan, 1981)

$$\log (\gamma_i) = -Az_i^2 \left(\frac{\sqrt{I}}{1 + \sqrt{I}} - 0.3I \right) \quad (3-1)$$

$$I = \frac{1}{2} \sum_i C_i z_i^2 \quad (3-2)$$

The B-dot equation is given by (Helgeson, 1969):

$$\log (\gamma_i) = -Az_i^2 \frac{\sqrt{I}}{1 + a_i^o B \sqrt{I}} + \dot{B}I \quad (3-3)$$

where

- A = Debye-Huckel parameter
- I = ionic strength
- C_i = concentration of aqueous species i (moles/kg)
- B = Debye-Huckel parameter
- a_i^o = ion size parameter for species i
- \dot{B} = B-dot parameter
- z_i = charge of species i

The Debye-Huckel and B-dot parameters are calculated as a function of temperature in *Mariana* based upon data in the EQ3/6 database version: (data0.com.R12) (Wolery, 1983; Wolery et al., 1990). The correlations are valid over the range 0 to 250 °C. Uncharged species, water, and solids are currently assumed to have activity coefficients of 1.

Figure 1 demonstrates how the activity coefficient of calcium chloride varies with concentration at 25 °C. The vertical axis denotes the base-10 logarithm of the activity coefficient and the horizontal axis denotes the molal concentration of calcium chloride. The dotted line represents experimental data collected by Staples and Nuttal (1977). The dashed line represents the Davies equation; the solid line is the B-dot equation.

Figure 2 is a close-up of Figure 1 at low molal concentrations. The B-dot equation accurately predicts the activity coefficient out to a concentration of almost 0.3 molal, while the Davies equation is only accurate for concentrations of 0.1 molal or below. Interestingly, the B-dot equation remains qualitatively correct at high ionic strengths, exhibiting slow divergence from the experimental data as ionic strength increases. Calculation of the Davies equation is quicker, and the values of a_i^o are not required. The range of accuracy of the Davies equation can be expanded somewhat by adjusting the coefficient in the second term. Figure 3 illustrates the results when 0.2 is substituted for this value. The results follow the

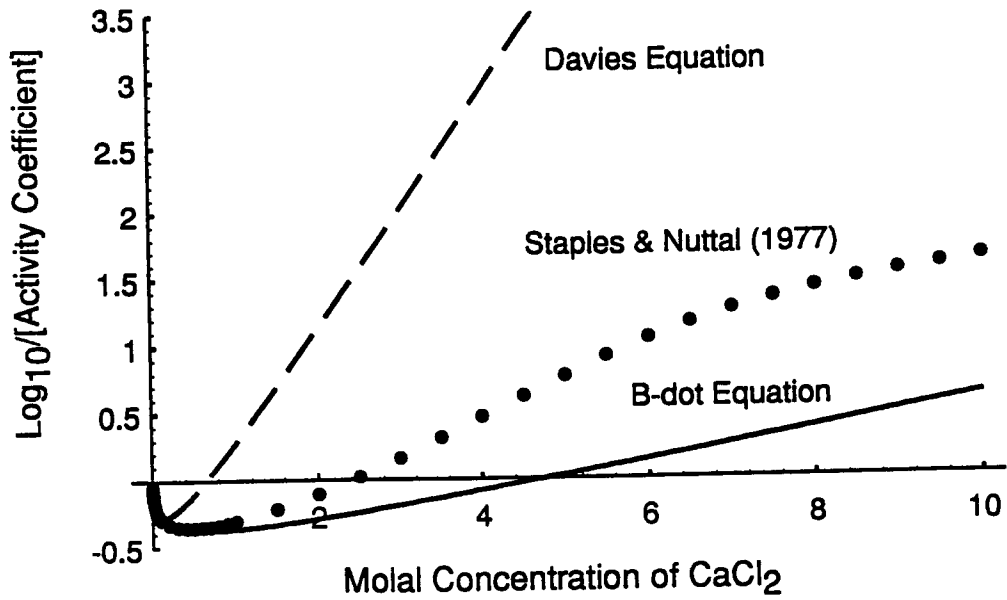


Figure 1. Comparison of calculated activity coefficients for calcium chloride with experimental data at 25 °C

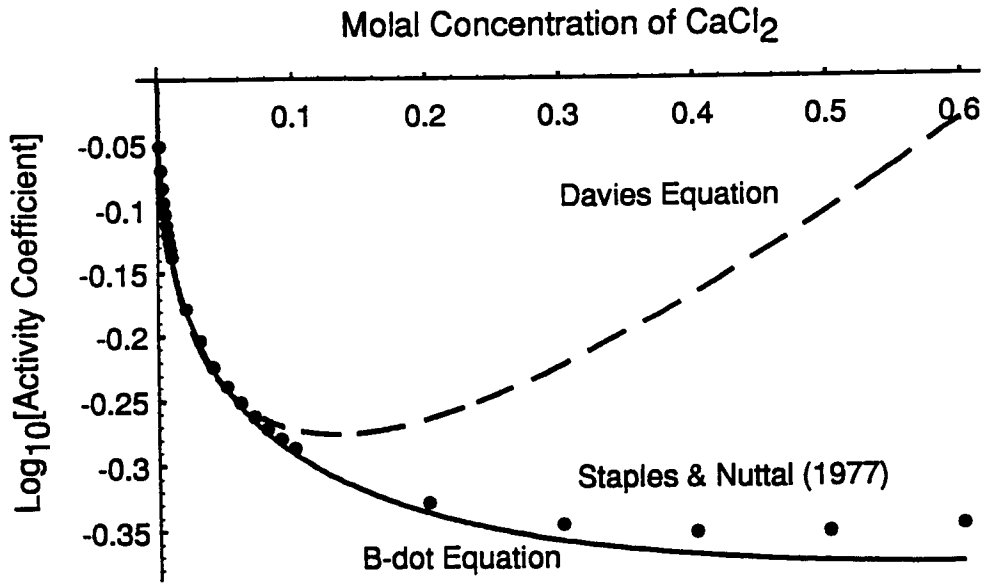


Figure 2. Comparison of calculated activity coefficients for calcium chloride with experimental data at low molal concentrations

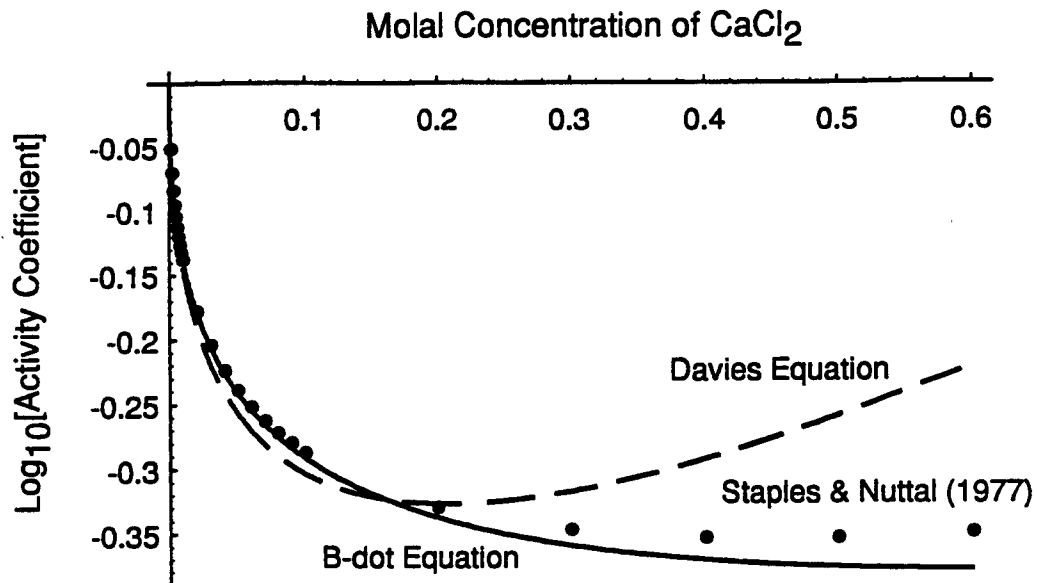


Figure 3. Comparison of calculated activity coefficients for calcium chloride with experimental results using modified Davies equation.

experimental data out to a concentration of 0.2 molal before diverging, but the accuracy at lower concentrations has suffered somewhat.

The Davies equation may be used if the user does not know the values of a_i° . The ideal case (activity coefficients equal to 1.0) requires no calculation or parameters. The B-dot equation should be used otherwise. The user may strike a balance between calculation time and reasonable accuracy over a larger range by changing the 0.3 parameter in the Davies equation to 0.2.

The method of estimating activity coefficients appropriate for each simulation cannot be established *a priori*. The amount of error in the estimate that is acceptable depends upon many factors such as the specific type of application and other inherent uncertainties in the problem. Assumptions considered completely inadequate for analysis of carefully controlled laboratory experiments may be acceptable in simulation of a complex field situation where many key parameters are estimated. At high ionic strengths, the question will often not be: Is the B-dot equation accurate in this range? (it is not), but whether the B-dot equation provides a better approximation than no activity coefficients at all.

4 IMPLEMENTATION OF THEORY

Mariana is written in standard FORTRAN 77 with real*8 variables. The code assumes that a maximum of one solid species is present in any reaction. The only other limitation is that the reactions must consist of a linearly independent set of complete chemical reactions. Half reactions are not allowed. Only reactions specifically entered in the stoichiometric matrix will be considered. This includes simple reactions such as the dissociation of water. Generally, water will be entered as a species just like any other. The amount of water present is not important as long as it is present in excess. Solids may be input in zero, limited, or excess amounts. The code will precipitate or dissolve solids as required to reach equilibrium. Currently the code assumes that water is present at unit activity and the concentration of everything else is per 1,000 gm of water.

All parameters except the reaction progress variables are passed to and from *Mariana* in the common block "eq.f", which is dimensioned by another common block, "param.f". The reaction progress variables, "xi()", are passed in the calling sequence "call *Mariana*(xi,iwork)". *Mariana* will iterate around a solution until either convergence is achieved or the maximum number of iterations is exceeded. Absence of convergence is indicated in the "iwork" variable. The variable returns a 1 upon successful completion. Failure to converge can result from either a pathological condition or lack of required precision. Pathological conditions can occur, for example, when the stoichiometric matrix contains errors such as incomplete reactions or equations that are not linearly independent. The solver requires that the reaction progress variable, ξ , be specified with sufficient precision to cover the changes in concentration of each species in moving from the initial solution composition to the equilibrium state. If a particular species changes by many orders of magnitude during the iterations (e.g., an insoluble species with a high starting concentration), the proper solution may not be obtained. This infrequent problem can be addressed by resetting the solution composition to the partially converged solution and the reaction progress variables to zero. A second call to *Mariana* should lead to convergence. In reactive transport codes, the solution composition should not change dramatically during an individual time step; thus, the starting composition should be a good guess for the equilibrium composition and numerical precision of the reaction progress variables should not be a significant problem.

The most difficult situation is when the code attempts to give a negative concentration for a single species phase (i.e., a mineral). The chemical potential of an aqueous species tends to go through a natural minimum according to the calculation of $G-n_i \ln(n_i)$. Unfortunately, the equation for solids is $G-n_i$, which does not pass through a minimum prior to zero leading to negative concentrations. To eliminate the problem of negative concentrations, two simple modifications were made to the solver. If an aqueous species is predicted to go negative in an iteration, the step size for all reactions calculated with the Newton-Raphson equations is reduced until the negative condition is eliminated. For solid species, negative concentrations are avoided by setting the iteration step size to a value where the problem solid has a mass of zero. This can be attained by inversion of Eq. (2-3). The Jacobian matrix and first derivative for zero amount solids are modified to reflect the direction of reaction suggested by the first derivative. Simply put, if the solid is not present and wants to precipitate, it is included in the calculations. If the solid is not present and wants to dissolve, the terms for the solid are removed from the matrix.

The governing equations in the code are electrically balanced because iteration is on the reaction progress variable and all reactions are electroneutral (i.e., half reactions are not allowed); as such, they are designed to conserve the electrical state of the system. If the solution is electroneutral going into the

calculations, it will be electroneutral (within roundoff errors) coming out of *Mariana*. Any initial deviations from electroneutrality are also preserved. Since the *Mariana* governing equations will not change the electrical state of the system, the task of dealing with any deviations from electroneutrality are left to the calling program.

The iterative solution process followed by *Mariana* is summarized as follows and as illustrated in Figure 4:

- Calculate the current activity of each species
- Determine the value of the second derivative
- Perform a Newton-Raphson iteration
- Check for negative concentrations and make appropriate adjustments
- Update the species concentrations according to the stoichiometric matrix and reaction progress variables
- Repeat all of above until convergence is reached or maximum number of iterations exceeded

The *DoReact* subroutine is responsible for this last step. The Newton-Raphson iterations are performed by the *LUDCMP* and *LUBKSB* subroutines from Press *et al.*, (1980), and the value of the first and second derivatives are determined by the *ddfunc* and *dfunc* subroutines. The *Activity* subroutine calculates the activity of each species by multiplying concentration by activity coefficient. Activity coefficients are calculated in the *Gamma* subroutine.

The following list summarizes the subroutine hierarchy of each *Mariana* iteration:

- I. *Mariana*
 - A. *Activity*
 1. *Gamma*
 - B. *ddfunc*
 1. *dfunc*
 - C. *LUDCMP*
 - D. *LUBKSB*
 - E. *DoReact*

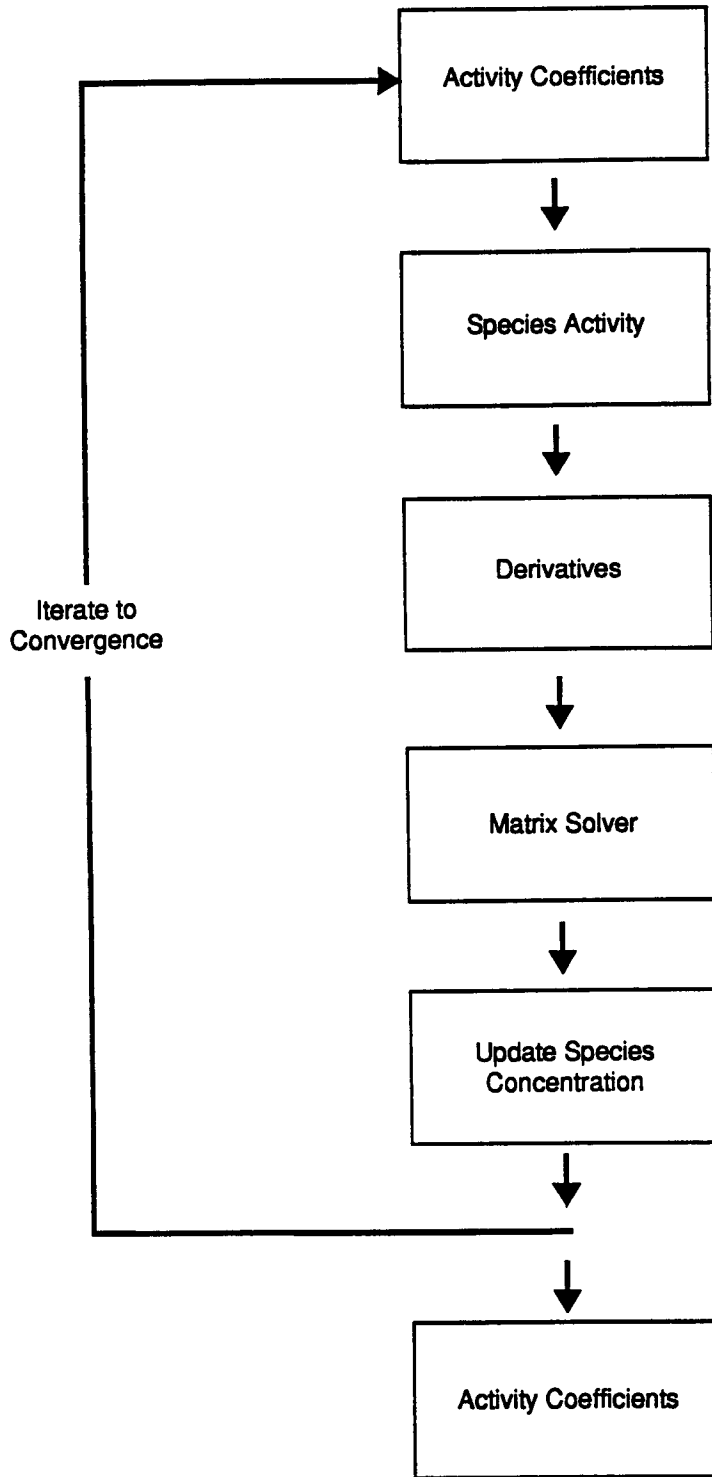


Figure 4. Flowchart

5 INTERFACING WITH *MARIANA*

As stated before, all parameters except the reaction progress variables are passed to and from *Mariana* in the common block "eq.f", which is dimensioned by another common block, "param.f". The reaction progress variables "xi()" are passed in the calling sequence "call *Mariana*(xi)". Normally, the subroutine is invoked with the line "call *Mariana* (xi)", where all the elements of the array "xi" have been set to zero. Routines or programs which call *Mariana* must also contain the common blocks, 'param.f'" and "include 'eq.f'" in order to pass variables to *Mariana*.

The text below is a copy of the file "param.f":

```
c
c param.f contains all the parameter statements to dimension the
c problem.
c 4/13/92/ John Walton
c
c   parameter(maxX = 100, maxR = 25, maxS = 30)
c
c Definitions:
c   maxX = maximum number of nodes
c   maxR = maximum number of chemical reactions
c   maxS = maximum number of species
c
```

These values are used by the compiler in dimensioning the variable arrays. If these values are changed, the program must be recompiled before the changes take effect. *Mariana* currently does not use the maxX parameter included in the example above.

The following text is a copy of the file "eq.f". The comment statements identify the variables and indicate whether they are inputs or outputs. Variables labeled as flags are given a value of "1" for true and "0" for false unless otherwise specified. Variables with "maxS" in parentheses are given values for each species present while variables dimensioned with "maxR" are given values for each reaction considered. If the system under consideration is partitioned into nodes, *Mariana* must be called separately for each node, with the parameters passed to it specific to each node as well. Input and output parameters are clearly identified in the code listing.

```
c
c   common /react/ u0(maxS), smass(maxS), sact(maxS), scalc(maxS),
c   & dgdxi(maxR), iphase(maxS), sto(maxS,maxR), nspec, nreact,
c   & ineg(maxR), isolid(maxR), isolsp(maxR), rgas, temp, farad,
c   & u(maxS), a0(maxS), sgamma(maxS), igamma
c
c Definitions:
c   u0 = Gibbs Free Energy of Formation (standard state chemical
c   potential) (input)
c   smass = moles of species i in one Kg of water (input)
```

c sact = species activity (output)
 c scalc = estimated new moles of species i in one Kg of water (output)
 c dgdxi = partial G with respect to reaction progress variable (output)
 c iphase = phase of species (1=aqueous, 2= solid, 3=gas, 4= water)
 c (input)
 c sto = stoichiometric matrix: sto(species, reaction) (input)
 c nspec = number of species (input)
 c nreact = number of reactions (input)
 c ineg = flag for reactions with negative species mass (output)
 c isolid = flag for reactions with solids (output)
 c isolsp = species in reaction isolid that is the solid (note: only
 c one solid is allowed per equation) (output)
 c rgas = gas law constant (units consistent with u0) (input)
 c temp = absolute temperature (input)
 c farad = Faraday constant (input)
 c u = chemical potential (output)
 c a0 = "effective diameter" correction factor for Debye-Huckel (input)
 c sgamma = species activity coefficient (output)
 c igamma = activity calculation flag (0=ideal, 1=Bdot, 2= Davies)
 c (input)
 c

Care should be taken to insure that the units of "u0", "smass", "rgas", "temp" and "farad" are consistent. The units of "sact", "scalc", and "u" will be consistent with the values provided.

6 CONCLUSION

A simple chemical equilibrium module has been developed. The module will be incorporated as a subroutine in several Engineered Barriers codes. The initial version of the module has undergone limited testing. The testing verifies that the code conserves mass and sets all reactions to equilibrium; however, only a few sets of reactions have been checked. In particular, much care must be taken with heterogeneous reactions. Although the code has been able to successfully sort out the appropriate solid assemblage in limited tests, it is *not* guaranteed to work in every situation. The design goal for the solver was to work rapidly to calculate equilibrium for simple systems. The implicit assumption is made that more sophisticated equilibrium solvers (e.g., EQ/6) have been used prior to *Mariana*. The more sophisticated solver should be used to sort out the most important reactions for the system. The simplified set of equations can then be solved with *Mariana* in a coupled fashion with other processes. Additional testing of the code including benchmarking against EQ3/6 is anticipated in the future.

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8 NOMENCLATURE

G	=	Gibbs free energy (J/mole)
n_i	=	moles of i in 1 kg of water (mole/kg)
μ_i	=	chemical potential of i (J/mole)
μ_i^b	=	standard state chemical potential of i (J/mole)
R	=	gas law constant (J/mole/°K)
T	=	absolute temperature (°K)
a_i	=	activity of species i
$\nu_{i,r}$	=	stoichiometric coefficient of species i in reaction r
ξ_r	=	reaction progress variable for reaction (moles) r
A	=	Debye-Huckel parameter
I	=	ionic strength
C_i	=	concentration of aqueous species i (moles/hg)
B	=	Debye-Huckel parameter
a_i^o	=	ion size parameter for species i
\dot{B}	=	B-dot parameter
z_i	=	charge of species i