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WIPP PA

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User's Manual

for

NONLIN, Version 2.0

Document Version 1.0

WPO #30740

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Table of Contents

1.0 INTRODUCTION
1.1 SOFTWARE IDENTIFIER
1.2 POINTS OF CONTACT
1.2.1 Code Sponsor
1.2.2 Code Consultants
1.2.3 Code Author
2.0 FUNCTIONAL REQUIREMENTS
3.0 REQUIRED USER TRAINING AND/OR BACKGROUND
4.0 DESCRIPTION OF THE MODELS AND METHODS
4.1 GMIN CHEMICAL EQUILIBRIUM MODEL
4.1.1 Thermodynamic Model
4.1.2 The Pitzer Activity Coefficient Formalism
4.1.3 Free-Energy Minimization Approach
4.2 NONLIN PARAMETER CALCULATION
5.0 CAPABILITIES AND LIMITATIONS OF THE SOFTWARE
6.0 USER INTERACTIONS WITH THE SOFTWARE
6.1 OVERVIEW
6.2 USER-SUPPLIED INPUT FILES
6.3 EXECUTING NONLIN
6.3.1 DEC Environment
6.3.2 Macintosh Environment
6.4 SETTING UP AND RUNNING SOLUBILITY PROBLEM
6.5 SETTING UP AND RUNNING APPARENT STABILITY CONSTANT PROBLEM
6.6 SETTING UP AND KUNNING EXTRACTION PROBLEM
7.0 DESCRIPTION OF INPUT FILES
7.1 GMIN
7.2 INPUT
7.3 COMP DATA BASE FILE
7.4 BINARYP DATA BASE FILE
7.5 TERNARYP DATA BASE FILE
7.6 LAMBDA DATA BASE FILE
8.0 ERROR MESSAGES
9.0 DESCRIPTION OF OUTPUT FILE
10.0 REFERENCES
11.0 APPENDICES
APPENDIX A - EXAMPLE FOR CALCULATING THERMODYNAMIC PARAMETERS FROM APPARENT STABILITY CONSTANTS
APPENDIX B - SAMPLE INPUT FILE: EXTR_00.GMIN
APPENDIX C - SAMPLE INPUT FILE: EXTR_07_EXACT.IN
APPENDIX D - SAMPLE INPUT FILE: SOLUB_00 GMIN
APPENDIX E - SAMPLE INPUT FILE: SOLUB_01.IN
APPENDIX F - LISTING OF COMP.DAT
APPENDIX G - LISTING OF BINARYP.DAT

APPENDIX H - LISTING OF TERNARYP.DAT	. 65
APPENDIX I - LISTING OF LAMBDA.DAT	. 66
APPENDIX J - SAMPLE OUTPUT FILE: EXTR_07_EXACT.OUT	. 67
APPENDIX K - SAMPLE OUTPUT FILE: SOLUB_01.OUT	. 72
APPENDIX L - REVIEW FORMS	. 75

κ.



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List of Figures

FIGURE 6-1. INPUT AND OUTPUT FILES FOR NONLIN	14
FIGURE 6-2. SUGGESTED DATA BASE FOLDER ORGANIZATION FOR MACINTOSH ENVIRONMENT	17
FIGURE 6-3. SUGGESTED PROBLEM FOLDER ORGANIZATION FOR MACINTOSH ENVIRONMENT	17
FIGURE 7-1. FORMAT FOR SIX-DIGIT SPECIES ID NUMBER	19
FIGURE 7-2. SECTIONS OF THE INPUT FILE.	21
FIGURE A-1. SAMPLE INPUT FILE: AM_ACET.GMIN	45
FIGURE A-2. SAMPLE INPUT FILE: AM_ACET.IN	45
FIGURE A-3. LISTING OF AM_ACET_COMP.DAT	46
FIGURE A-4. SAMPLE LISTING OF AM_ACET_BINARYP.DAT.	47
FIGURE A-5. SAMPLE OUTPUT FILE: AM_ACET.OUT (1 OF 3)	48
FIGURE A-6. SAMPLE INPUT FILE: AM_ACET_POST_ABN.GMIN	51
FIGURE A-7. SAMPLE INPUT FILE: AM_ACET_POST.IN	51
FIGURE A-8. SAMPLE INPUT FILE: AM_ACET_COMP_POST_ABN.DAT	52
FIGURE A-9. SAMPLE OUTPUT FILE: AM_ACET_POST_ABN.OUT (1 OF 2)	53
FIGURE A-10. APPARENT STABILITY CONSTANT FOR AMAC IN NACL MEDIA: COMPARISON OF THE	
MODEL WITH DATA	55
FIGURE A-11. SAMPLE INPUT FILE: AM_ACET_POST_NORM.GMIN.	56
FIGURE A-12. SAMPLE INPUT FILE: AM_ACET_COMP_POST_NORM.DAT	57
FIGURE A-13. SAMPLE OUTPUT FILE: AM_ACET_POST_NORM.OUT (1 OF 3)	58

List of Tables

TABLE 7-1.	GMIN FILE PARAMETERS (LINE NUMBERS CORRESPOND TO SAMPLE LISTING IN APPENDIX	
	B)	20
TABLE 7-2.	PARAMETER KEY INDEX TABLE	22
TABLE 7-3.	INPUT FILE PARAMETERS (LINE NUMBERS CORRESPOND TO SAMPLE LISTING IN APPENDIX	
	C)	24
TABLE 7-4.	COMP FILE PARAMETERS (LINE NUMBERS CORRESPOND TO SAMPLE LISING IN APPENDIX	
	F)	26
TABLE 7-5.	BINARYP FILE PARAMETERS (LINE NUMBERS CORRESPOND TO SAMPLE LISTING IN	
	APPENDIX G)	27
TABLE 7-6.	TERNARYP FILE PARAMETERS (LINE NUMBERS CORRESPOND TO SAMPLE LISTING IN	
	APPENDIX H)	28
TABLE 7-7.	LAMBDA FILE PARAMETERS (LINE NUMBERS CORRESPOND TO SAMPLE LISTING IN	
	APPENDIX I)	29
TABLE 9-1.	OUTPUT FILE DESCRIPTION (LINE NUMBERS CORRESPOND TO SAMPLE LISTING IN	
	APPENDIX J)	31



1.0 INTRODUCTION

The program NONLIN fits parameters for a designated aqueous electrolyte model to experimental data on osmotic coefficients, mineral solubility, emf, or solvent extraction. Although NONLIN has two aqueous electrolyte models for excess free energy available, the Davies equations (Davies, 1962) and Pitzer's aqueous electrolyte model (Pitzer [1973] and coworkers), this document will discuss only the Pitzer model, which is used to support the 1996 WIPP Performance Assessment (PA) calculations.

For the 1996 WIPP PA calculation, NONLIN is used to calculate Pitzer parameters and standard chemical potentials of actinide chemical species. The calculated values will be added to the CHEMDAT data base used by a program called FMT. CHEMDAT contains the Harvie-Møller-Weare (HMW) database (Harvie et al., 1984; Felmy and Weare, 1986) for nonradioactive electrolyte systems and the actinide series of radioactive elements, such as americium(III) and neptunium(V). FMT is a chemical equilibrium modeling code, also used to support the 1996 WIPP PA calculations. The FMT User's Manual, WPO 28119, documents both the CHEMDAT data base and the FMT code.

1.1 Software Identifier

Code Name: NONLIN WIPP Prefix: NL_ Version Number: 2.0 08/23/96 Platforms: FORTRAN 77 for Open VMS AXP, version 6.1, on DEC Alpha machines and Power Macintosh 7100

1.2 Points of Contact

1.2.1 Code Sponsor

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2.0 FUNCTIONAL REQUIREMENTS

- **R.1** NONLIN fits parameters for Pitzer's aqueous electrolyte model to experimental data on mineral solubility.
- **R.2** NONLIN fits parameters for Pitzer's aqueous electrolyte model to experimental data on solvent extraction.
- **R.3** NONLIN fits parameters for Pitzer's aqueous electrolyte model to experimental data for apparent stability.

3.0 REQUIRED USER TRAINING AND/OR BACKGROUND

In order to run the NONLIN code successfully, the user will need a basic knowledge of one of the following platforms:

- Open VMS and Digital Equipment Co.'s (DEC's) Digital Command Language (DCL), if running the code on the DEC platform
- Power Macintosh 7100 operation, if running the code on a Macintosh platform.

To interpret the results of NONLIN, a chemistry background is required. A user should have a:

- BS in Chemistry, or the equivalent
- familiarity with the Pitzer model for activity coefficient of electrolytes
- sound understanding of chemical reaction equilibrium analysis.

To understand how the NONLIN code works and the theory and algorithms upon which NONLIN is based, the user should also have a basic understanding of:

- equilibrium thermodynamics and solution chemistry
- linear algebra (through senior undergraduate level)
- numerical methods (graduate or senior level undergraduate level).

4.0 DESCRIPTION OF THE MODELS AND METHODS

NONLIN solves chemical equilibrium problems, as defined by the linear material balance equations and the nonlinear reaction equilibrium equations as given in standard chemical thermodynamics texts such as Denbigh (1981) and Smith and Van Ness (1975).

More specifically, NONLIN couples the GMIN free-energy chemical equilibrium program with the MINPACK least squares minimization routines. NONLIN can be used to interpret (i.e., fit) experimental concentration data such as

• solubility (i.e., the total dissolved concentration of element X in aqueous electrolyte of composition Y)

- electromotive force (emf)
- isopiestic data
- solvent extraction data (i.e., the distribution of element X between an aqueous and an organic phase)
- ion exchange data
- apparent stability constant data (i.e., the molal ion quotients for intra-aqueous reactions).

4.1 GMIN Chemical Equilibrium Model

The GMIN chemical equilibrium program is explained in detail by Felmy (1990) and Felmy (1995). Sections 4.1.1 and 4.1.3 of the following discussion are largely excerpted from that source. Section 4.1.2, which explains the Pitzer activity coefficient formalism, is excerpted from Felmy and Weare (1986).

4.1.1 Thermodynamic Model

The mathematical basis of GMIN is based on the development of an algorithm for solving the chemical equilibrium problem that is based on a constrained minimization of the Gibbs free energy.

NONLIN, as used in support of the 1996 WIPP PA calculation, makes use of the following general equations that GMIN can solve:

• chemical potential for water solvent in aqueous phase:

$$\frac{\mu_{\rm H_2O}}{RT} = \frac{\mu_{\rm H_2O}^0}{RT} - \frac{W}{1000} \left(\sum_{i=1}^{\rm ns} m_i\right) \phi$$
(4-1)

• chemical potential for solute species in aqueous phase:

$$\frac{\mu_i}{RT} = \frac{\mu_i^0}{RT} + \ln m_i + \ln \gamma_i$$
(4-2)

where

- μ_i = chemical potential of species *i*
- μ_i^0 = standard chemical potential of species *i*
- R = the gas constant
- T = absolute temperature

W = molecular weight of wa

- ns = the total number of chemical species
- m_i = molality of species *i*
- ϕ = osmotic coefficient

 γ_i = activity coefficient of species *i*.

While GMIN contains two formulations for activity coefficients for aqueous species, only one formulation is used in support of the WIPP PA calculation. This model is based on the work by Pitzer (1979) and coworkers. In this model, the activity coefficients are expressed in a virial-type expansion.

4.1.2 The Pitzer Activity Coefficient Formalism

The Pitzer activity coefficient formalism is a set of mathematical equations for calculating activity coefficients for aqueous species, and is valid from dilute systems through the concentrated brine concentrations observed at the WIPP Site. The theoretical and historical development of this formalism can be traced though Pitzer (1991), particularly Chapter 3, and references therein.

The implementation of the Pitzer activity coefficient formalism within NONLIN is based on the forms of the equations as presented in Harvie and Weare (1980), Harvie et al. (1984), and Felmy and Weare (1986). Because there is no difference in the mathematical formulation provided by these references, only the equations in Felmy and Weare (1986) are presented below. The interested reader will find a comprehensive presentation of these equations in the three cited publications.

The activities of the species a_i can be defined by the following equation:

$$\left(\frac{\partial G}{\partial n_i}\right)_{T,P,n} = \mu_i = \mu_i^0 + RT \ln a_i.$$
(4-3)

where G = Gibbs free-energy function, P = pressure, $n_i = number of moles of species i, and activity is defined for each solute species i by$

$$a_i = \gamma_i \mathbf{m}_i \tag{4-4}$$

and, for the solvent, by

$$\ln a_{\rm H_2O} = \frac{-W}{1000} \left(\sum_i m_i \right) \phi, \qquad (4-5)$$

where

 m_i = the molality of the solute species,

W = the molecular weight of water,

 $\sum m_i$ = the sum over all solutes (cations (c), anions (a), and neutrals(n)), and

 ϕ = the osmotic coefficient.

While the chemical potentials for pure phases (e.g., minerals) are constant at fixed temperature and pressure, the fugacity of gas-phase species, f_i , is defined as follows:

$$\frac{\mu_i}{RT} = \frac{\mu_i^0}{RT} + \ln(f_i). \tag{4-6}$$

n a

The remaining variables that lack explicit definition are the excess functions γ_i and $(\phi-1)$. These functions, rewritten below, are modeled using the semiempirical equations of Pitzer (1973) and co-workers. (Note that, in the Pitzer equations presented below, I = ionic strength, and that subscripts M, X, and N refer to cations, anions, and neutrals, respectively. The remaining terms are explained following the presentation of the Pitzer equations.)

$$(\phi-1) = \frac{2}{\left(\sum_{i} m_{i}\right)} \left\{ -\frac{A^{\phi}I^{3/2}}{1+bI^{1/2}} + \sum_{c} \sum_{a} m_{c}m_{a}\left(B^{\phi}_{ca} + ZC_{ca}\right) + \sum_{c} \sum_{c'} m_{c}m_{c'}\left(\Phi^{\phi}_{cc'} + \sum_{a} m_{a}\psi_{cc'a}\right) \right\}$$

$$+ \sum_{a} \sum_{a'} m_{a}m_{a'}\left(\Phi^{\phi}_{aa'} + \sum_{c} m_{c}\psi_{aa'c}\right) + \sum_{n} \sum_{c} m_{n}m_{c}\lambda_{nc} \qquad (4-7)$$

$$+ \sum_{n} \sum_{a} m_{n}m_{a}\lambda_{na} + \sum_{n} \sum_{c} \sum_{a} m_{n}m_{c}m_{a}\zeta_{nca} \right\}$$

$$\ln\gamma_{M} = z_{M}^{2}F + \sum_{a} m_{a}\left(2B_{Ma} + ZC_{Ma}\right) + \sum_{c} m_{c}\left(2\Phi_{Mc} + \sum_{a} m_{a}\psi_{Mca}\right)$$

$$+ \sum_{a} \sum_{c} m_{a}m_{a'}\psi_{aa'M} + |z_{M}|\sum_{c} \sum_{a} m_{c}m_{a}C_{ca} + \sum_{n} m_{n}(2\lambda_{nM}) + \sum_{n} \sum_{a} m_{n}m_{a}\zeta_{naM} \qquad (4-8)$$

n

$$\ln\gamma_{X} = z_{M}^{2}F + \sum_{c} m_{c} \left(2B_{Xc} + ZC_{Xc}\right) + \sum_{a} m_{a} \left(2\Phi_{Xa} + \sum_{c} m_{c}\psi_{Xca}\right)$$

$$+ \sum_{c} \sum_{c'} m_{c} m_{c'}\psi_{cc'X} + \left|z_{X}\right| \sum_{c} \sum_{a} m_{c} m_{a}C_{ca} + \sum_{n} m_{n}(2\lambda_{nX}) + \sum_{n} \sum_{c} m_{n}m_{c}\zeta_{ncX}$$

$$(4-9)$$

$$\ln \gamma_N = \sum_c m_c (2\lambda_{Nc}) + \sum_a m_a (2\lambda_{Na}) + \sum_c \sum_a m_c m_a \zeta_{Nca}$$
(4-10)

$$F = -A^{\phi} \left(\frac{I^{1/2}}{1+bI^{1/2}} + \frac{2}{b} \ln(1+bI^{1/2}) \right) + \sum_{c} \sum_{a} m_{c} m_{a} B'_{ca} + \sum_{c} \sum_{c'} m_{c} m_{c'} \Phi'_{cc'} + \sum_{a} \sum_{a'} m_{a} m_{a'} \Phi'_{aa'}$$
(4-11)

where b = 1.2 for all electrolyes.

$$C_{MX} = \frac{C_{MX}^{\phi}}{2|Z_M Z_X|^{1/2}}$$
(4-12)
$$Z = \sum_i |z_i| m_i$$
(4-13)

 A^{ϕ} is one third of the Debye-Hückel limiting slope (A in the following empirical equation):

$$\ln \gamma_i^{\rm DH} = -\frac{A\sqrt{I}}{1 + Ba_i\sqrt{I}} + \dot{B}_i I, \qquad (4-14)$$

as presented on page 981 of Harvie and Weare [1980].) Here A^{ϕ} is a function of temperature and equals 0.39 at 25°C. The second virial coefficients, *B*, are empirical expansions and are given the following ionic strength dependence:

$$B_{MX}^{\phi} = \beta_{MX}^{(0)} + \beta_{MX}^{(1)} e^{-\alpha_1 \sqrt{1}} + \beta_{MX}^{(2)} e^{-\alpha_2 \sqrt{1}}$$
(4-15)

$$B_{MX} = \beta_{MX}^{(0)} + \beta_{MX}^{(1)} g(\alpha_1 \sqrt{I}) + \beta_{MX}^{(2)} g(\alpha_2 \sqrt{I})$$
(4-16)

$$B'_{MX} = \beta_{MX}^{(1)} \frac{g'(\alpha_1 \sqrt{I})}{I} + \beta_{MX}^{(2)} \frac{g'(\alpha_2 \sqrt{I})}{I}$$
(4-17)

The functions g and g' are defined by

$$g(x) = 2\frac{\left(1 - (1 + x)e^{-x}\right)}{x^2} \tag{4-18}$$

$$g'(x) = -2 \frac{\left(1 - \left(1 + x + \frac{x^2}{2}\right)e^{-x}\right)}{x^2}$$
(4-19)

with $x = \alpha_1 \sqrt{I}$ or $= \alpha_2 \sqrt{I}$. When either cation *M* or anion *X* is univalent, $\alpha_1 = 2.0$ and $\alpha_2 = 12$. For 2 - 2 pairs, $\alpha_1 = 1.4$ and $\alpha_2 = 12$. For 2 - 3 and higher pairs, $\alpha_1 = 1.4$ and $\alpha_2 = 50$. The dimensions of α_1 and α_2 are kg^{1/2}mole^{-1/2}. The virial coefficients, Φ , which depend upon ionic strength, are given the following form:

$$\Phi_{ij}^{\phi} = \theta_{ij} + E \theta_{ij}(\mathbf{I}) + \mathbf{I}^{E} \theta_{ij}'(\mathbf{I})$$
(4-20)



The functions, ${}^{E}\theta_{ii}(I)$ and ${}^{E}\theta'_{ii}(I)$, are functions only of ionic strength and the electrolyte pair type.

The activity coefficient parameters, λ_{ni} and ζ_{nij} , represent the interactions between ions and neutral species. The third virial coefficients, C_{MX}^{ϕ} and ψ_{ijk} , are also assumed to be independent of ionic strength.

The following is the complete set of parameters that define the model for nonideal behavior of electrolyte solutions:

- $\beta_{MX}^{(0)}$, $\beta_{MX}^{(1)}$, $\beta_{MX}^{(2)}$, and C_{MX}^{ϕ} for each cation-anion pair
- θ_{ii} for each cation-cation and anion-anion pair
- Ψ_{iik} for each cation-cation-anion and anion-anion-cation triplet
- λ_{ni} and ζ_{nii} for ion-neutral and ion-ion-neutral interactions.

NONLIN minimizes the sum of the errors squared for the standard chemical potential of userspecified species by adjusting the values of the thermodynamic parameters specified by the user.

These are the Pitzer parameters NONLIN solves for using thermodynamic data.

4.1.3 Free-Energy Minimization Approach

The free-energy minimization problem in GMIN is formulated as

minimize
$$G = \sum_{j=1}^{n_s} \mu_j n_j$$
 (4-23)

subject to the following mass-balance constraint

$$\sum_{j=1}^{n_s} a_{ji} n_j = b_i, \qquad i = 1, \dots, m_c$$
(4-24)

and the following charge-balance constraint

$$\sum_{j=1}^{nas} z_j n_j = 0 \tag{4-25}$$

and

$$n_j \ge 0$$
 for all species j (4-26)

where

ns	=	the total number of chemical species	And the second s
n_j	=	mole number of species j	
a _{ji}	=	number of moles of component i in species j	

b _i	=	total number of moles of element i
m _c	=	number of linearly independent mass-balance constraints
nas	=	total number of aqueous species j
z _j	=	charge on species j

The free-energy minimization approach is fully documented in Harvie, Greenberg, and Weare (1987).

4.2 NONLIN Parameter Calculation

NONLIN calculates the Pitzer ion interaction parameters by using a non-linear least squares fitting algorithm. The code calculates values for user-specified aqueous solution and solid thermodynamic parameters, including the standard chemical potentials for ion pairs. NONLIN calculates the function to be minimized; i.e., the difference between solid and solution chemical potentials, and the Jacobian (the derivative of the chemical potential difference with respect to the adjustable parameters). The adjustable parameters, discussed in detail in Section 7.1, are the Pitzer parameters and the standard chemical potential of the chemical species to be fitted. Andrew R. Felmy is the code author of both NONLIN and GMIN, a chemical equilibrium code called by NONLIN. Pacific Northwest Laboratory maintains MINPACK, a set of matrix routines called by GMIN.

5.0 CAPABILITIES AND LIMITATIONS OF THE SOFTWARE

The chemical data base files and the problem definition files must be compatible; i.e., the species must be characterized in the data base before it is referenced in the problem. NONLIN capabilities are discussed at the beginning of Section 1.

6.0 USER INTERACTIONS WITH THE SOFTWARE

6.1 Overview

NONLIN requires six input data files— GMIN, INPUT, COMP, BINARYP, TERNARYP, and LAMBDA. The problem is defined by the GMIN and INPUT files. The GMIN file defines the chemical species to be considered. The INPUT file contains the experimental data and initial estimates for the Pitzer parameters or standard chemical potentials to be fitted. The last four files COMP, BINARYP, TERNARYP, and LAMBDA are the chemical data base files. These files contain species names and unique ID numbers, chemical characteristics, and Pitzer parameters. All the input files are discussed in detail in Section 7.0.

NONLIN generates one file OUTPUT. This file lists the problem definition as read from the GMIN and INPUT files, chemical species considered, and the best fit to the experimental data set(s).

Figure 6-1 illustrates all the input and output files used by NONLIN.





Figure 6-1. Input and Output Files for NONLIN.

6.2 User-Supplied Input Files

Using a convenient editor, the user creates the GMIN file and the INPUT file for a problem. The user should check the COMP, BINARYP, TERNARYP, and LAMBDA files to be sure that the required species and Pitzer parameters are included there.

6.3 Executing NONLIN

6.3.1 DEC Environment

The user can access the command file NL_NONLINC.COM to run NONLIN on the Sandia NWER network, using Digital's Alpha machine BEATLE. This file is located in the NL library. All files in the library are under control of Digital's Configuration Management System (CMS). This library contains NONLIN data base files, source code, and command files. The user can retrieve the command file NL_NONLINC.COM from the NL library using the CMS "fetch" command. For ease in executing NONLIN, the command file should be in the same directory where the input files reside.



 ^{1}X

6.3.1.1 Fetching the Command File NL_NONLINC.COM from CMS

To retrieve the command file NL_NONLINC.COM, the user logs into BEATLE and types the symbol "nonpa_cms_syms" to define other CMS symbols, followed by the command "libnl" to specify the NL library. Then the user locates the directory/subdirectory where his/her input files reside by typing in a "set default (sd)" command. The command "cfe nl_nonlinc.com" copies the command file into the user's current directory. The lines are:

\$nonpa_cms_syms
\$libnl
\$sd [username.user_inputfile_directory]
\$cfe nl nonlinc.com

The command file can be copied from directory to directory. The user does not need to fetch the file each time. NL_NONLINC.COM also issues the lines "nonpa_cms_syms" and "libnl" automatically, making typing them unnecessary.

6.3.1.2 Running NL_NONLINC.COM

To execute "@NL_NONLINC" the user must always be logged into BEATLE. The user should be in the directory that contains the .IN and .GMIN files before starting NL_NONLINC. To execute the command, the user types:

\$@ NL_NONLINC

The user will be prompted to supply a **substring** for the COMP, BINARYP, TERNARYP, and LAMBDA files and the GMIN and INPUT file names. To retrieve a list of all data base files, the user can simply type in ".DAT" since all of the NONLIN data base files have the string ".DAT" as the extension. Or, the user can type in any substring of the data base file name (e.g., COMP_960130). The GMIN and INPUT filestem names can be independent (e.g., SOLUB_01.IN and SOLUB_00.GMIN) or the same (e.g., AM_ACET.IN and AM_ACET.GMIN).

After listing the data base files that match the substring specified, the user is prompted to select each data base file. The user may select a file by copying and pasting the file name to the waiting request, by double clicking on one of the file names listed, or by typing the entire name.

WARNING: The NL_NONLINC command deletes all data base files with the "NL_" prefix and ".DAT" extension from the user's current directory before fetching any of the four data base files.

6.3.2 Macintosh Environment

The Macintosh executable icon for NONLIN is called PMacNonlin. To start the code, the user double clicks, either with a mouse or track ball, on the PMacNonlin icon. The chemical data base files must be located in the same folder that contains the executable icon. After starting the icon, the program will use the files explicitly labeled BINARYP, COMP, TERNARYP, and LAMBDA in the icon's folder.

A suggested method for organizing folders or directories while running NONLIN on the Macintosh is shown in Figure 6-2 and Figure 6-3. Using this approach, files are grouped as follows:

- all chemical data base files (BINARYP, COMP, TERNARYP and LAMBDA) and the PMacNonlin icon in one folder labeled "HMW_ACTINIDE_DB," as shown in Figure 6-2. New species can be added to these existing chemical database files without affecting the results of calculations performed using previous versions of these database files, as long as a consistent ID numbering scheme is maintained (Sections 7.3 through 7.6).
- the GMIN and INPUT files in another folder. Beneath a major folder labeled "TEST CASES," Figure 6-3 shows two problem-labeled folders, "Am_Acet" and "SOLUB," each containing the GMIN and INPUT files for the solvent extraction and mineral solubility problems, respectively. By default, the OUTPUT file will be placed in the same folder that contains the GMIN and INPUT files.

A screen titled "Output from PMacNonlin" displays the file prompts and writes the file names on the screen after the user has responded to all prompts. The user makes a selection through a window display by navigating the folders or directory tree and double clicking on a file name.

The user can set a folder or directory before selecting or naming any file. The prompts direct the user to:

- 1. Select INPUT File
- 2. Select GMIN File
- 3. Enter OUTPUT File Name

6.4 Setting up and Running Solubility Problem

The user supplies the GMIN and INPUT files. The HMW_ACTINIDE_DB chemical data base files are defined in COMP, BINARYP, TERNARYP, and LAMBDA. The INPUT file has a variable named "ndtyp," which defines the type of experimental data. Solubility data is denoted by setting the "ndtyp" variable to -1.

6.5 Setting up and Running Apparent Stability Constant Problem

NONLIN may be used to fit apparent stability constant data by setting up the problem as a solubility calculation. A detailed discussion and an example problem are provided in Appendix A.

6.6 Setting up and Running Extraction Problem

For a solvent extraction problem, the input files are the same as those for an solubility problem (as listed in Section 6.4). Solvent extraction data is denoted by setting the "ndtyp" variable to -4 in the INPUT file.



Figure 6-2. Suggested data base folder organization for Macintosh environment.



Figure 6-3. Suggested problem folder organization for Macintosh environment.

7.0 DESCRIPTION OF INPUT FILES

Of the six input files for NONLIN (see Figure 6-1), the user sets up the problem in the two files GMIN and INPUT. The other four files COMP, BINARYP, TERNARYP, and LAMBDA are the input chemical data base files. All files are text-based files and can be edited by the user using a convenient text editor.

Although NONLIN reads the INPUT file with both fixed-field and free field-formats¹, it reads all other data files using fixed-field formats only. There are two distinct independent numbers - the parameter key number and the species ID number. Although both numbers have six digits, they are not related in any way. The parameter key number is used only in the INPUT file while the species ID number is used in the other five files. To allow a species to be added or deleted easily, files are terminated by either a zero or a minus one in the ID number field. Blank lines and comments can be inserted with caution. Comments may be placed at the bottom of the file, or, in some cases, at the end of a line where NONLIN does not read them. Comments are used throughout the chemical data base files and the sample files to help the human reader identify the species on a line and document the source of the data or the fields in the file.

A description of all six input files follows.

7.1 GMIN

The GMIN file species are the chemical species to be considered in a particular computer run. The species ID numbers used in GMIN must correspond to species definitions in the COMP file. In addition, aqueous species may have ion interaction parameters specified in BINARYP, TERNARYP, or LAMBDA, but these are not required.

The six-digit ID number is assigned by the user. The first digit is the phase indicator, and can be 0, 1, 2, 3, or 4 for aqueous, solid, solid solution, and two types of adsorbed species, respectively. Only aqueous and solid species are relevant to WIPP use of this code, so only phase types 0 and 1 will be considered henceforth.

The assignment of the remaining five digits is arbitrary, with the only constraint being that each six-digit combination must be unique. The following conventions are suggested to help provide a method to assign ID numbers. Let the second and third digits correspond to the atomic number of the metallic portion of the species (if any) and the fourth and fifth digits correspond to the nonmetallic portion (if any). Use the final digit is used to break redundancies. These scheme is illustrated in Figure 7-1.

For example, the species IDs could be 012000 for aqueous Mg $^{++}$, 000170 for aqueous Cl $^{-}$, and 012170 for the MgCl $^{+}$ pair.

¹ "Fixed-field format" means that input data is read precisely in the columns specified by the code; "free-field format" means that the input numbers are independent of column formatting (i.e., the numbers in the input file are simply separated by spaces, tabs, or carriage returns). For example, in the sample INPUT file provided in Appendix C, lines 1 through 3, only the first 16 columns are read using a fixed-field format; lines 6 - 37 are read using the free-field format. However, the sample GMIN file provided in Appendix B must be read in its entirety using a fixed-field format input specification.

The order of the species in the file is important. The first species must be water, followed by cations, and neutral species. The solid species are listed last.

The mole numbers for the species are read from the INPUT file. The mole numbers in GMIN file should be set to zero for aqueous species, and nonzero for solid species.

Table 7-1 lists the GMIN file parameters. The "LINE" column refers to the line numbers listed in the EXTR_00.GMIN file. The "Variable Name" column corresponds to the NONLIN program variables. "Permissible Value" column is the only set of values permitted for use with this program. Any other values have unknown consequences.

The EXTR_07.GMIN listing shows a "-1" on line 11 denoting the end of all species. NONLIN will ignore any lines that follow line 11. On lines 3-8 and line 10, NONLIN ignores the comment at the end of the lines following the species ID and mole number.

In Appendix D the sample input file SOLUB_00.GMIN lists six aqueous species and one solid species. NONLIN ignores any lines after line 11.



Figure 7-1. Format for six-digit species ID number.

Table 7-1. GMIN File Parameters (Line Numbers Correspond to Sample Listing in Appendix B)

Line	Frmt	Col	Variable Name	Регтіssible Value	Description	
1	1x,15	1-6	idebg1	0 or	normal mode or	
				1	debug mode, prints intermediate calculations while iterating	
	15	7-11	isopt	0	flag setting the Pitzer ion interaction model	
	15	12-16	idopt	0	flag setting the non-ideal free energy model	
	15	17-21	iphopt	0 or	flag for printing species concentrations at end of iterative cycle	
,				1	print after each iteration	
2	13	1-3	iads	0	no adsorption option	
3	16	1-6	id(1)	001080	species ID number for water (water must be listed first)	
	F15.3	7-21	x(1)	0.0	unused mole number (read from INPUT file)	
4-8	I 6	1-6	id(i)		list of aqueous species	
	F15.3	7-21	x(i)	0.0	unused mole number (read from INPUT file)	
9	I6	1-6	id(i)	000000	end of aqueous species	
10	16	1-6	id(i)	200000- 299999	list of solid species	
	F15.3	7-21	x(i)	0.0	unused mole number (read from INPUT file)	
11	16	1-6	id(i)	-1	end of all species	
12	+				comment line	
	I	1	L	,		

7.2 INPUT

The INPUT file is used to specify the experimental data and the thermodynamic parameter(s) to be fitted to the data. The first section lists the parameters to be fitted. In the first two columns, a "-1" is used to signal the end of the parameter list. The next section contains one or two data sets that are used to fit the parameters. Figure 7-2 illustrates the sectioning of an INPUT file using the lines in EXTR_07_EXACT.IN, Appendix C as an example. If there were another experimental data set, it would start on line 22.

In the first section the parameter key is a six-digit number whose structure is divided into three fields where

first and second digits	=	type of parameter
third and fourth digits	=	first ion number
fifth and sixth digits	=	second ion number

The parameter key index table relevant to WIPP use of NONLIN is shown in Table 7-2.





Figure 7-2. Sections of the INPUT file.

Table 7-2. Parameter Key Index Table



Adjustable parameter	Туре	First Ion	Second Ion	
µ°/RT (standard chemical potential)	00	00	species position number	
$\beta^{(0)}$ (cation-anion pair)	01	cation number	anion number	
$\beta^{(1)}$ (cation-anion pair)	02	cation number	anion number	
$\beta^{(2)}$ (cation-anion pair)	03	cation number	anion number	
C _{MX} (cation-anion pair)*	04	cation number	anion number	
θ_{ij} (cation-cation pair)	05	00	cation-cation number	
θ_{ij} (anion-anion pair)	06	00	anion-anion number	
Ψ_{ijk} (cation-cation-anion triplet)	07	cation-cation number	anion number	
Ψ_{ijk} (anion-anion-cation triplet)	08	anion-anion number	cation number	
λ (cation-neutral)	09	neutral number	cation number	
λ (anion-neutral)	10	neutral number	anion number	
λ (neutral-neutral)	11	neutral number	neutral number	
ζ_{ijk} (ion-ion-neutral)	12	neutral-cation number	anion number	
C [] _{MX} may be computed from (C _{MX} by usin	g equation 12 (Section 4.1	.2).	· · ·

To illustrate, consider the species list in Appendix C, i.e.,

	** .7.8 * 2 M/P				
	Cation Number	Anion Number	Species Position Number		
H ₂ 0			01		
Na ⁺	01		02		
Th++++	02		03		
H ⁺	03		04		
OH		01	05		
ClO ₄		02	06		

Na⁺, Th⁺⁺⁺⁺, and H⁺ have cation numbers 01, 02, and 03, respectively; OH⁻ and ClO₄⁻ have anion numbers 01 and 02, respectively. (The number must be 2 digits.) Neutral species follow the same pattern.

Cation-cation, anion-anion, and neutral-cation numbers are more complicated to specify. These are assigned as follows, illustrated for the cations above. The first cation (Na+) is taken pairwise with the other cations (Th++++, H+) in the order in the list; i.e., Na+ - Th++++ is pairwise interaction 01, Na+ - H+ is pairwise interaction 02. With these, all Na+- cation interactions are specified. The next cation (Th++++) is then taken pairwise with the remaining cations, which in this case is only H+; i.e., Th++++ - H+ is pairwise interaction 03. (Th++++ - Na+ is the same as Na+ - Th++++). Anion-anion and neutral-cation numbers are handled similarly. If the above illustration contained a neutral aqueous species, here called NeuSpec#1, the numbering would be as given in the table below:

	Cation-Cation Number	Anion-Anion Number	Neutral-Cation Number
Na ⁺ - Th ⁺⁺⁺⁺	01		
$Na^+ - H^+$	02		
Th++++ - H+	03		
$OH^{-} - ClO_{4}^{-}$		01	
NeuSpec#1 - Na ⁺			01
NeuSpec#1 - Th ⁺⁺⁺⁺			02
NeuSpec#1 - H ⁺			03

Therefore, for this illustration, $\theta_{Na^+-Th^{++++}}$ is represented by 050001, and $\psi_{H^+-Th^{++++}-Clo_4^-}$ is represented by 070302.

The OUTPUT file in the section titled "ADJUSTED PARAMETERS" echo prints the parameters that are being fitted by listing the parameters and the species names. This section should be examined to verify that the parameter numbers were selected correctly. This section is listed in Appendix J, lines 102-105; Appendix K, lines 94-95; and Figure A-5, lines 99-103.

When a species parameter is to be fitted, NONLIN ignores the value assigned to that species in the appropriate data base file(s).

The second section of the INPUT file lists an experimental data set, the number of data points, and the data type on one line followed by the data points. A "-1", "0", or a blank line may be used to signal the end of all experimental data sets. A line-by-line description of the INPUT file is provided below in Table 7-3, using the sample listing of EXTR_07_EXACT.IN in Appendix C.

Table 7-3 lists the INPUT file parameters. The "LINE" column refers to the line numbers listed in the EXTR_07_EXACT.IN file. The "Variable Name" column corresponds to the NONLIN program variables. The "Permissible Value" column is the only set of values permitted for use with this program. Any other values have unknown consequences.

Table 7-3. INPUT File Parameters (Line Numbers Correspond to Sample Listing in Appendix C)

Line	Frmt	Col	Variable Name	Permissible Value	Description
1-3	312	1-6	ipar1(i), ipar2(i), ipar3(i)	000000- 9999999	ID of the i th parameter to adjust
	F10.4	7-16	parv(i)	real number	estimate of the i th parameter value (best guess)
4	12	1-2	ipar1(i)	-1	end of parameters to fit
5	в	1-5	ndata(k)	1-99999	number of data points in the k th data set
	Ľ	6-10	ndtyp(k)	1,0,-1,-2,-3, or -4	type of experimental data (1=emf data, 0=osmotic data, -1=solubility data or solid solution data, -2=solid solution data in stoichiometric saturation, -3=adsorption data, -4=solvent extraction data)
6-21	free field		y(i)	positive real number	molar concentration in organic phase for extraction data otherwise set to 0.0 for all other data types
	free field		pph(i)	positive real number	target ph value if a fixed ph value is desired otherwise set to 0.0
	free field		mole(i, j), j=2,naș	positive real number>0	mole numbers for all species except water where water as $mole(i,1)$ is set to 55.508373 within the code
22	15	1-5	ndata(k)	0 or -1	end of all data sets
23					comment line (not read by NONLIN)

The next data set, if any, would begin on line 22 and would include the number of data points, the type of data, and all of its data points, following the format provided in lines 5 through 21. However, the EXTR_07_EXACT.IN listing shows a "-1" on line 22, which denotes the end of all data sets. NONLIN will ignore any lines that follow line 22. On lines 1-3 NONLIN also ignores the comment following each estimate. The EXTR_07_EXACT.IN shows that the user has

specified three parameters to be fitted (the standard chemical potential μ°/RT , $\beta^{(0)}$, and C_{MX}) with an experimental extraction data set of 16 points.

Line 25 in the IN file of Appendix C, included only for the benefit of the user, shows the value type in each column for data specification. The first column, for extraction problems, is the concentration of the extracted species in the organic phase, here represented by mORG. The second column represents the pH (= $-\log_{10} a_{H^*}$) in all problem types, but is used only when the pH is to remain fixed, which is not the case in either Appendix C or E. The remaining columns give initial estimate molalities for all the aqueous species (except H₂O) from the GMIN file, and in the same order. (By definition, water is always 55.5 moles H₂O/kg H₂O.) These initial estimates should be charge balanced to best represent the chemical system.

In Appendix E the sample input file SOLUB_01.IN shows one parameter, μ°/RT , to be fitted with an experimental solubility data set of 7 data points. On line 3 the data type is set to "-1" for solubility data. NONLIN ignores lines 12-15.

The file SOLUB_01.IN in Appendix E is similar to EXTR_07_EXACT.IN in Appendix C. The first two entries on line 1 indicate that the standard chemical potential of species number 6 (199001 in the GMIN file, corresponding to $H_2Ox \cdot 2 H_2O(s)$) is to be fitted. The -1 (line 2) terminates the list of parameters to be fitted. Line 3 indicates that there are seven data points of type -1 (solubility data). Lines 4 - 10 provide the following data:

- The first column is zero by definition in solubility problems.
- The second column is pH, which is only used when pH is fixed (not in this run).
- The remaining columns correspont to (charge-balanced) species molalities.

These are illustrated in comment line 15 in Appendix E.

The apparent constant stability sample input file AM_ACET.IN in Appendix A, Figure A-2 shows four parameters to be fitted (μ°/RT , $\beta^{(0)}$, $\beta^{(1)}$ and C_{MX}) using the solubility data set of 6 data points. On line 6 the data type is set to "-1" for solubility data.

7.3 COMP Data Base File

Table 7-4 lists the COMP file parameters. The COMP file contains a list of chemical species, the species stoichiometry and charge, and the dimensionless standard chemical potential. The temperature of the thermodynamic data is specified at 25 °C. The COMP file contains all the species that could be considered by NONLIN in its calculations. The species list must begin with water, followed by other aqueous species, and then the solid species. The list of all chemical species must end with a "-1".

NOTE

The COMP file listed in Appendix F is not necessarily the file that will be used to support the WIPP 1996 PA calculations. Additional species and elements may be added to the file that will be used to support the 1996 WIPP PA calculations.

 Table 7-4. COMP File Parameters (Line Numbers Correspond to Sample Lising in Appendix

 F)

Line	Frmt	Col	Variable Name	Permissible Value	Description
1-40	I6	1-6	idtmp	000000- 999999	six digit species ID number where H ₂ O must always be the first species declared
	A12	7-16	intmp		name of species
	1x	18			
	12	19-20	iztmp		charge of species
	F15.3	21-35	uOtmp		standard chemical potential of the species (μ_i°/RT)
	1x	36			
	10(12, F4.1)	37-96	nt(j),v(j), j=1,10	0-99, 0.0-9999.	atomic number and stoichiometric coefficients for elements comprising the species (i.e. $H = 1$, $O = 8$, $Np = 93$, etc.)
41	I6	1-6	idtmp	000000	blank line (species $ID = 0$)
42	I6	1-6	idtmp	-1	denotes the end of species list

A blank line may be inserted anywhere in the COMP file and the species ID will be assigned the value 0. In this file, the blank line can be used to separate groups of species to improve file readability, e.g., lines 6, 11, and 13. A "-1" on line 42 denotes the end of all species. NONLIN will ignore any comments that follow after the end of species list.

7.4 BINARYP Data Base File

The BINARYP file contains the species ID number in each binary interaction considered (e.g., Na⁺-Cl⁻, K⁺-Cl⁻) and the Pitzer ion-interaction parameters ($\beta^{(0)}$, $\beta^{(1)}$, $\beta^{(2)}$, and C_{MX}) for binary systems. The binary interaction list must end with a "000000". A cation anion pair and their Pitzer parameters may be inserted anywhere in this file. Blank lines are not allowed in this file until the end of the list.

In Table 7-5, which describes the input parameters for BINARYP, the "Variable Name" column lists the NONLIN program variables.



NOTE

The BINARYP file listed in Appendix G is not necessarily the file that will be used to support the WIPP 1996 PA calculations. Additional species and elements may be added to the file that will be used to support the 1996 WIPP PA calculations.

Table 7-5.	BINARYP File Parameters (Line Numbers	Correspond to Sample Listing in
	Appendix G)	

Line	Frmt	Col	Variable Name	Permissible Value	Description
1-20	I6	1-6	id1	000000- 9999999	ID of the cation species
	1x	7			
	16	8-13	id2	000000- 999999	ID of the anion species
	F7.3	14-20	tb0		$\beta^{(0)}$ parameter for the cation-anion interaction
	F7.3	21-27	tb1		$\beta^{(1)}$ parameter for the cation-anion interaction
	F7.3	28-34	tb2		$\beta^{(2)}$ parameter for the cation-anion interaction
	F7.3	35-41	tcmx		C _{MX} parameter
21	16	1-6	idl	000000	end of binary interactions
22-23					comments

NONLIN will ignore any lines following a blank line or a species ID number of "000000".

7.5 TERNARYP Data Base File

The TERNARYP file contains Pitzer ion-interaction parameters θ_{ij} for anion-anion and cationcation systems and ψ_{ijk} for anion-anion-cation and cation-cation-anion systems. Species can be inserted in any order. For the file listed in Appendix I, the same species ID numbers in the first column were grouped together. Blank lines are not allowed in this file until the end of the list.

In Table 7-6, which describes the parameters in the TERNARYP file, the "Variable Name" column lists the NONLIN program variables.

NONLIN will ignore any comments that follow after species ID number 000000, the end of all ternary species parameters.

NOTE

The TERNARYP file listed in Appendix H is not necessarily the file that will be used to support the WIPP 1996 PA calculations. Additional species and elements may be added to the file that will be used to support the 1996 WIPP PA calculations.

Table 7-6.	TERNARYP File Parameters (Line Numbers Correspond to Sample Listing in
	Appendix H)

Line	Frmt	Col	Variable Name	Permissible Value	Description
1-5, 10-11	16	1-6	id1	000000- 999999	ID of cation species
	1x	7			
	16	8-13	id2	000000- 999999	ID of cation species
	F7.3	14-20	ttc		θ_{ij} for cation-cation species
	1x	21			
	20(I6,1x,F7.3,1x)	22-320	id3(j1), tpsic(j1), j1=1,20		ID of anion species and Ψ_{ijk} for cation- cation-anion species
6-9	16	1-6	id1	00000- 999999	ID of anion species
	1x	7			
	16	8-13	id2	000000- 999999	ID of anion species
	F7.3	14-20	ttc		θ_{ij} for anion-anion species
	lx	21			
	20(I6,1x,F7.3,1x)	22-320	id3(j1), tpsic(j1), j1=1,20		ID of cation species and Ψ_{ijk} for anion- anion-cation species
12	16	1-6		000000	end of all neutral parameters



7.6 LAMBDA Data Base File

The LAMBDA file (described in Table 7-7) contains Pitzer ion-interaction lambda parameters for neutral species. The species interactions include: neutral-cation, neutral-cation-anion, neutral-anion, and neutral-neutral.

NOTE

The LAMBDA file listed in Appendix I is not necessarily the file that will be used to support the WIPP 1996 PA calculations. Additional species and elements may be added to the file that will be used to support the 1996 WIPP PA calculations.

Table 7-7.	LAMBDA	File Parameters	(Line Numbers	Correspond to	Sample	Listing in
		Ap	pendix I)	-	-	-

Line	Frmt	Col	Variable Name	Permis- sible Value	Description
1-2	I6	1-6	idl	00000- 999999	ID of the neutral species
	1x	7			······································
	16	8-13	id2	000000- 9999999	ID of cation species
	F7.3	14-20	tlambda		λ parameter for neutral-cation species
	lx	21			
	20(I6,1x,F7.3,1x)	22-27	id3(j1), thol(j1), j1=1,20		for neutral-cation species, ID of anion species and λ parameter for neutral-cation- anion species; a neutral-cation pair may have from zero to twenty anion species and lambda values
None ²	16	1-6	id1	00000- 999999	ID of the neutral species
	1x,I6	7-13	id2	000000- 999999	ID of anion species
	F7.3	14-20	tlambda		λ parameter for neutral-anion species
None ³	16	1-6	id1	000000- 999999	ID of the neutral species
	1x, I 6	7-13	id2	000000- 9999999	ID of neutral species
	F7.3	14-20	tlambda		λ parameter for neutral-neutral pair
3	16	1-6	1	000000	end of neutral species list

² No corresponding line numbers in Appendix I since there are no neutral-anion species in the file.

³ No corresponding line numbers in Appendix I since there are no neutral-neutral species in the file.

In Table 7-7, the "Variable Name" column lists the NONLIN program variables. The neutral species can be inserted in any order. A value for a neutral-cation pair, even if it is zero, must be assigned in order to specify a triplet neutral-cation-anion interaction. For the file in Appendix H, the same neutral species were grouped together with the cations first, and then the anions. There are no neutral-neutral parameters considered in NONLIN. Blank lines are not allowed in this file until the end of the list.

NONLIN will ignore any lines that follow after species ID number 000000, the end of all lambda parameters.

8.0 ERROR MESSAGES

NONLIN is not a particularly user-friendly code. NONLIN will detect errors in species ID numbers and in counting the total number of allowed species. The code will not automatically detect all errors in preparing the GMIN or INPUT files, or the interaction of these input files with the chemical model data files. Therefore, care should be taken to avoid errors. It is important that output from NONLIN be examined to see if it makes sense.

At the end of the OUTPUT file, a successful NONLIN run will display a set of lines with the header "FINAL APPROXIMATE SOLUTION" and the species ID with the converged parameter value. However, the presence of these lines may not necessarily indicate a set of valid values. There may still be errors in any of the files and the entire OUTPUT listing should be scanned carefully.

Error messages are usually listed at the end of the OUTPUT file before NONLIN terminates. A pair of single quotes within a message enclosing a phrase starting with 'value of ...' indicates that the run time value in NONLIN will be listed. A listing of the error messages follows.

• The following messages are printed when the nonlinear routine does not converge:

********** ITERATION DID NOT CONVERGE ****** **** MATRIX WITH ZERO ROW IN DECOMP NO CONVERGENCE IN IMPROV MATRIX NEARLY SINGULAR **** SINGULAR MATRIX IN DECOMP, ZERO DIVIDE IN SOLVE ********** ITERATION DID NOT CONVERGE ******

If any of the above messages are displayed, the user should start with another set of initial estimates in the INPUT file. If the second message "MATRIX WITH ZERO ROW IN DECOMP" is displayed, the charge balance may be incorrect.

• The following messages are printed when there are more than two solid solution data sets in the INPUT file:

** MORE THAN TWO SOLID SOLUTION DATA SETS *** ***** ONLY TWO DATA SETS WITH EQUAL POINTS ALLOWED **

If any of the above messages are displayed, the user should limit the number of solubility data sets to two in the INPUT file. In addition, for a data type of -2, the number of data points must be the same in both sets. However, this mode of running NONLIN is not used for the WIPP.

• The following message is printed when a species is listed in the GMIN file and is not in the chemical model data files:

SPECIES 'value for ID' NOT FOUND IN DATA FILE

If the above message is displayed, the user may have an incorrect species ID in the GMIN file or may need to add the species and its Pitzer parameters to the chemical model data files, i.e., the COMP, BINARYP, LAMBDA, and TERNARYP files.

• The following message is printed when the species listed in the GMIN file exceeds 16:

TOO MANY AQUEOUS AND ADSORBED SPECIES

If the above message is displayed in the GMIN file, the user should verify that the "000000" species or a blank line separates the aqueous from the solid species or the user should reduce the number of aqueous and adsorbed species.

9.0 DESCRIPTION OF OUTPUT FILE

NONLIN generates an OUTPUT (.OUT) file. The OUTPUT file lists the problem identity, echo prints the input data, computes the goodness of fit using the initial estimates (before any adjustments are made to the key parameters), continues to iterate until the absolute value of the error tolerance test converges to a value $\leq 10^{-5}$, and then prints the final solution.

Table 9-1 explains the OUTPUT (.OUT) file generated from the problem called EXTR_07_EXACT. The "Line" column refers to the line numbers listed in EXTR_07_EXACT.OUT. "Variable Name" column shows applicable NONLIN program variables and some formulas.

Table 9-1.	OUTPUT	'File Descr	iption (Line	Numbers	Correspond to	Sample]	Listing in
			- Appendix	к J)	-	-	-

Line	Variable	Name	Description
1	versn		notation; program name 'NONLIN' and version number
3			notation; code author
5-7	infnm, oufnm	gmfnm,	user-supplied input file name, GMIN file name and output file name
9-21			table of aqueous and solid species and characteristics
	id(i), a(i,j), j=1,	name(i), ncomp	species from GMIN, name from COMP, mole number from GMIN, charge and standard chemical potential from COMP
23			title for table of constraint equations
I	L		

24	ncol(j), j=1,ncomp	column labels where 0 is charge and all others are elemental atomic numbers
25-31	name(i), a(i,j) j=1,ncomp	for each speciesname, charge, and number of atoms in one molecule or ion
33		notation; closed two files
35-38	cofnm, bifnm, tefnm, lafnm	chemical data base file names
40		notation; Pitzer activity coefficient model used
42-48	name(jpc(i)), name(jpa(j)), b0(i,j), b1(i,j), b2(i,j),cmx(i,j)	table of single electrolyte parameters; listing cation-anion binary interactions, $\beta^{(0)}$, $\beta^{(1)}$, $\beta^{(2)}$, and C_{MX} parameters for i th cation, j th anion interactions
50-58		table of ternary electrolyte parameters; listing cation-cation-anion, if any; anion- anion-cation, if any
52	name(jpa(k)), k=1,na	column labels of anion species
53-55	name(jpc(i), name(jpc(j), tc(nt), (psic(nt,k), k=1,na)	cation-cation ternary interaction parameter, θ_{ij} and any cation-cation-anion ternary interaction parameters, Ψ_{ijk}
57	name(jpc(k)), k=1,nc	column labels of cation species
58	name(jpa(i), name(jpa(j), ta(nt), (psia(nt,k), k=1,nc)	anion-anion ternary interaction parameters, θ_{ij} and any anion-anion-cation ternary interaction parameters, Ψ_{ijk}
None ⁴		table of neutral ion parameters, if any
	name(jpn(k), k=1,nn	column labels of neutral species
	name(jpc(i)), (clamb(j,i), j=1,nn)	neutral-cation species and binary interaction values, λ_{ij}
	name(jpa(i)), (alamb(j,i), j=1,nn)	neutral-anion species and binary interaction values, λ_{ij}
	۱	

 $^{^4}$ No corresponding line numbers in Appendix J since there are no neutral ion parameters in the file.

	name(jpn(i)), (nlamb(j,i), j=1,nn)	neutral-neutral species and binary interaction values, λ_{ij}
None ⁵		table of higher order lambdas, if any
	name(jpa(k)), k=1,na	column labels of anion species
	name(jpn(i), name(jpc(j), (holamb(nt,k), k=1,na)	neutral-cation-anion species and ternary interaction values, ζ_{ijk}
50-62	ns, ncomp, irank	count of species, components and independent constraints
64	ndtyp(k)	type of experimental data for data set #1
56-85		table listing the experimental data points
59	name(i),i=2,nas	column labels of species
70-85	mole(i,j),j=2,nas	input molality of each species
		type of experimental data for data set $\#k$ with table $\#k$, where $k=2n$ dataset
37-99	parv(j),j=1,npar, fnorm	solution vector and norm from evaluating function at the initial estimates and each subsequent adjustment to the estimates
02- 106	ipar1(i), name1, name2, name3, parv(i)	table of adjusted parameters: the parameter, species either (name1) or (name1 and name2) or (name1, name2 and name3) of first and second ions, and final fit value
07- 25	y(m),sigma	calculated difference for data set #1, using the initial estimates
27- 29	adev,sdev	$adev = \sum abs(sigma)/ndatat; sdev = (\sum(sigma*sigma)/ndatat)^{0.5}$
		calculated difference for data set #k, where k=2ndataset; adev,sdev
31- 49	<u> </u>	table of final molalities
33	names(i),i=2,nas	column labels of species names

⁵ No corresponding line numbers in Appendix J since there are no higher order lambdas in the file.

134- 149	mole(i,j),j=2,nas	calculated molality for each species
151- 169		table of final log activities
153	names(i),i=2,nas	column labels of species names
154- 169	tloga(i,j),j=2,nas	calculated log activity for each species
171- 189		table of calculated log activity coefficients
173	names(i),i=2,nas	column labels of species names
174- 189	(tloga(i,j)- log10(mole(i,j)), j=2,nas	calculated log activity coefficients for each species
191		notation; system at equilibrium
192- 278		standard chemical potential, $\beta^{(0)}$, and C_{MX}
280	fnorm	norm of the solution vector
283	info	exit parameter
286 - 291	ipar1(i), ipar2(i), ipar3(i), parv(i)	table of approximate solutions


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11.0 APPENDICES

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Note

The numbers to the left of each line in Appendices A through K are not actually present in the files and screen displays; they are used solely to reference the lines in this guide

Note

The sample files and displays provided in Appendices A through K are examples *only*. They *are not* necessarily representative of files used to support the 1996 WIPP PA regulatory calculation.





Appendix A - Example for Calculating Thermodynamic Parameters from Apparent Stability Constants

NONLIN was not originally designed to fit apparent stability constant data. However, because of the flexibility of thermodynamics, apparent stability constant data can be rewritten to look like a system of solubility data, and these data can then be fitted in the usual way with NONLIN. This section describes and illustrates this process for the 1:1 americium acetate complex.

The complexation of Am(III) with acetate ion proceeds according to the reaction

$$Am^{3+} + Ac^{-} \leftrightarrow AmAc^{2+}$$
 (A-1)

with the corresponding equilibrium expression

$$\beta^{\circ} = \frac{\gamma_{AmAc^{2+}}}{\gamma_{Am^{3+}}\gamma_{Ac^{-}}} \frac{m_{AmAc^{2+}}}{m_{Am^{3+}}m_{Ac^{-}}}$$
(A-2)

οг

$$\beta^{app} = \beta^{\circ} \frac{\gamma_{Am^{3+}} \gamma_{Ac^{-}}}{\gamma_{AmAc^{2+}}} = \frac{m_{AmAc^{2+}}}{m_{Am^{3+}} m_{Ac^{-}}}$$
(A-3)

where β° is the thermodynamic stability constant and β^{app} is the apparent stability constant. We can define a fictitious solid AmAc/Am/Ac(s) based on reaction A-1, giving

AmAc/Am/Ac(s)
$$\leftrightarrow$$
 AmAc²⁺ - Am³⁺ - Ac⁻

which has the corresponding solubility product expression

$$K_{sp} = \frac{\gamma_{AmAc^{2+}}}{\gamma_{Am^{3+}}\gamma_{Ac^{-}}} \frac{m_{AmAc^{2+}}}{m_{Am^{3+}}m_{Ac^{-}}}$$
(A-5)

Note that the solubility expression in Equation A-5 is identical to that for the stability constant in Equation A-2. For this reason, by declaring the fictitious solid in Equation A-4, we can fit apparent stability constant data as if it were solubility data.

At equilibrium, the change in Gibbs free energy of reaction A-4 is zero by definition. Using this fact, we can rearrange the condition for equilibrium of Equation A-4 to the expression

$$\begin{bmatrix} \begin{pmatrix} \mu^{\circ} \\ \overline{RT} \end{pmatrix}_{A m A c^{2+}} - \begin{pmatrix} \mu^{\circ} \\ \overline{RT} \end{pmatrix}_{A m A c/A m/A c(s)} \end{bmatrix} + \ln \left(\gamma_{A m A c^{2+}} m_{A m A c^{2+}} \right) \\ = \left(\frac{\mu}{RT} \right)_{A m^{3+}} + \left(\frac{\mu}{RT} \right)_{A c^{-}}$$
(A-6)

In Equation A-6 we will generally know the quantities on the right hand side of the equation, i.e., the dimensionless standard chemical potentials and the appropriate activity coefficient parameters for the uncomplexed species; all unknown quantities are on the left hand side. Thus, this method can be used to fit both the standard chemical potential of the aqueous complex, in this case AmAc²⁺, and the activity coefficient parameters that contribute to $\gamma_{AmAc^{2+}}$. This method fits the standard chemical potential for the linear combination shown in square brackets in Equation A-6. Because we are not interested in the value for $\left(\frac{\mu^{\circ}}{RT}\right)_{AmAc/Am/Ac(s)}$ we can specify that $\left(\frac{\mu^{\circ}}{RT}\right)_{AmAc/Am/Ac(s)} = 0$ for the calculation and fit a value for $\left(\frac{\mu^{\circ}}{RT}\right)_{AmAc^{2+}}$ directly. Alternatively, we can arbitrarily assign a value $\left(\frac{\mu^{\circ}}{RT}\right)_{AmAc^{2+}} = 0$ and fit the linear combination in the brackets above, which will yield a fitted value equal to $-\left(\frac{\mu^{\circ}}{RT}\right)_{AmAc^{2+}}$.

An additional subtlety must be addressed in fitting apparent stability constant data. These data provide information on the molality quotients of the various species in solution, which in the illustration are Am^{3+} , Ac^{-} , and $AmAc^{2+}$. In order to fit these apparent stability constant values, the individual concentrations of the species Am^{3+} , Ac^{-} , and $AmAc^{2+}$ must be constrained to be constant throughout the computer run. This can be accomplished by adding "constraint" elements, called "CE" for short, to the species in question. Consider the following table of stoichiometries.

	0 (charge)	95 (Am(III))	89 (Acetate)	71 (CE#1)	72 (CE#2)	73 (CE#3)
Am3+	3	1	0	0	1	0
Ac-	-1	0	1	1	0	0
AmAc2+	2	1	1	0	0	1
AmAc/Am/Ac(s)	0	0	0	-1	-1	1

One can see by inspection that the linear combination of the stoichiometries as specified in Equation A-1 holds. By declaring the stoichiometries of the species in this way, the molality values, as specified in the INPUT file, are constrained to remain constant throughout the fitting run. This means that the input values of $m_{Am^{3+}}$, $m_{Ac^{-}}$, and $m_{AmAc^{2+}}$ will remain the same throughout the run.

The final step is specifying input concentrations $m_{Am^{3+}}$, $m_{Ac^{-}}$, and $m_{AmAc^{2+}}$ that correspond to the apparent stability constant data. A simple way to accomplish this would be to arbitrarily assign values to $m_{Am^{3+}}$ and $m_{Ac^{-}}$ and then calculate the values for $m_{AmAc^{2+}}$ from the apparent stability constant data and Equation A-3.

The required NONLIN files for this example are given below. This problem calculates the dimensionless standard chemical potential of the fictitious solid AmAc/Am/Ac(s) (which is equal to the dimensionless standard chemical potential of AmAc²⁺) and the ion interaction parameters $\beta_{AmAc^{2+}-Cl^{-}}^{(0)}$, $\beta_{AmAc^{2+}-Cl^{-}}^{(1)}$, $\beta_{AmAc^{2+}-Cl^{-}}^{(1)}$, $\beta_{AmAc^{2+}-Cl^{-}}^{(1)}$, $\beta_{AmAc^{2+}-Cl^{-}}^{(1)}$, $\beta_{AmAc^{2+}-Cl^{-}}^{(1)}$, $\beta_{AmAc^{2+}-Cl^{-}}^{(1)}$, Figure A-1 is the GMIN file. Figure A-2 is the INPUT file, giving the parameters to be fitted and the initial estimates for those parameter values on lines 1 to 4, terminated with the -1 on line 5. Line 6 indicates that there are six data

points of solubility type data, and lines 7 through 12 give the species concentrations. Data input is terminated with the -1 on line 13.

The COMP file is given in Figure A-3. Note that the fictitious solid phase AmAc/Am/Ac(s) is included (line 34) and that the stoichiometries of Am³⁺, Ac⁻, and AmAc²⁺ (lines 16, 22, and 19, respectively) have been modified by the addition of constraint elements as discussed above.

The BINARYP file is given in Figure A-4. The default value of ion interaction parameters is zero if they are not explicitly included in the BINARYP, TERNARYP, or LAMBDA files.

The results of the NONLIN run are given in the OUTPUT file of Figure A-5. The following are some points to note here: lines 9 to 33 echo print the input species names and IDs and the specified stoichiometries, as read from COMP; lines 44 to 65 echo print the ion interaction parameters read from BINARYP, TERNARYP, and LAMBDA; lines 71-82 echo print the input molalities read from INPUT; lines 84-95 print the estimates of parameter values in each fitting iteration (and the initial set, line 84, are the values given in lines 1 to 4 of the INPUT file); and lines 99 to 103 present the best-fit parameter values along with specification of what those parameters are (in human, not computer, symbology). Finally, note that the "equilibrated" molalities, i.e., lines 165 to 173, are identical to the input molalities because of the constraint elements that were added.

To compare the input values to the model-calculated values, perform the following steps:

- Remove the fictitious elements from the COMP file. 1.
- 2. Add the newly regressed parameters to the data base and run NONLIN without fitting any parameters. (Note that in this sample problem the fictitious elements 71, 72, and 73 have been removed from the COMP file. See lines 17, 20, 23, and 34 in Figure A-3 and compare with corresponding line numbers in Appendix F.)

- Add the newly regressed standard chemical potential, as shown on line 20 in Appendix F.
- 4.
- Add the Pitzer parameters to the BINARYP file (see line 21 in Figure A-4). Note that C^{ϕ} is calculated using Equation 4-12 (on page 10); i.e.,

$$C^{\phi}_{AmAc^{2*}Cl^{-}} = C_{AmAc^{2*}Cl^{-}} \cdot 2 \cdot \left| Z_{AmAc^{2*}} Z_{Cl^{-}} \right|^{1/2}$$
(A-7)

substituting in the values provided at the end of Figure A-5, one gets

$$C^{\phi}_{AmAc^{2*}Cl^{-}} = -3.5943059 \times 10^{-2} \cdot 2 \cdot |2 \cdot 1|^{1/2}$$

= -1.02 × 10⁻¹ (A-8)

5. Run NONLIN without fitting any parameters, using the GMIN file in Figure A-6, the input file shown in Figure A-7, and the COMP database file shown in Figure A-8 (the same binary database file is used as before; see Figure A-4). The final output is shown in Figure A-9.

Figure A-10 contrasts the β_{app} calculated using Equation A-3 from the input molalitities (lines 75 to 80 in Figure A-9) with the β_{app} line using the curve-fitted final molalities (lines 101 to 106 in Figure A-9).

Note that in this sample problem NONLIN reports an abnormal termination condition because there is no solid phase to equilibrate with. This outcome is logical because NONLIN equilibrated the aqueous phase and then realized there was no solid phase (i/e., no AmAc/Am/Ac(s)) present.

The problem could be run by treating the solid phase as if it existed by adding the following species to the COMP file: AmAc/Am/Ac(s). The resulting GMIN file is shown in Figure A-11. The COMP database and output files are shown in Figures A-12 and A-13, respectively. WHEN the above species is added, NONLIN terminates normally. However, this calculation really has no

meaning. The new solid species AmAc/Am/Ac(s) is a solid with no chemical element in it, which can be thought of as an "empty" or "virtual" solid that solely satisfies NONLIN's need for a solid phase to equilibrate with.

	8	see Table	e 7-1	for	explanation	of this	listing.	
0 0	0 0							
0 0	0 0							
001080	0.0000	0000	1	0	Н2О			
011000	0.0000	0000	2	1	Na+			
001000	0.0000	0000	3	2	H+			
095001	0.0000	0000	4	3	Am+++F			A
095891	0.0000	0000	5	4	AmAc++F			and second and a
000170	0.0000	0000	6	1	C1-			
000891	0.0000	0000	7	2	Ac-F			
000000								
195890	0.0000	0000	8	AmA	c/Am/Ac(s)		۰ ب	See /
-1								and the second se
-1							· - 98.5	1.17 M
		Cimera A 1	Sar	mnla	Input File: AN	A ACET	CMINE	







·····	See Tabl	e 7-4 for ex	planation of this listing.	
001080H20	0	-95.6635	1 2.0 8 1.0	
001000H+	1	000.000	1 1.0	
011000Na+	1	-105.651	11 1.0	
019000K+	1	-113.957	19 1.0	
0000800н-	-1	-63.435	1 1.0 8 1.0	
000161HSO4-	-1	-304.942	16 1.0 8 4.0 1 1.0	
000170C1-	-1	-52.9550	17 1.0	
017080C104-	-1	-73.81	17 1.0 8 4.0	
000050B(OH)3(aq)	0	-390.810	5 1.0 8 3.0 1 3.0	
-				
090000Th++++	4	-284.227	90 1.0	
093080Np(V)02+	1	-369.109	93 1.0 8 2.0	
095000Am+++	3	-241.694	95 1.0	
095001Am+++F	3	-241.694	95 1.072 1.0	
095890AmAc++	2	-395.358	95 1.089 1.0	
095891AmAc++F	2	999.999	95 1.089 1.073 1.0	
000890Ac-	-1	-147.347	89 1.0	
000891Ac-F	-1	-147.347	89 1.071 1.0	
0009900x=	-2	-272.2	99 1.0	·
001990HOx-	-1	-281.94	99 1.0 1 1.0	- [*] ****
001991H2Ox(aq)	0	-284.99	99 1.0 1 2.0	· · · · · · · · · · · · · · · · · · ·
093890NpO2Ac(aq)	0	-519.800	93 1.0 8 2.089 1.0	i i a
101990H2Ox.2H2O(s) O	999.999	99 1.0 1 6.0 8 2.0	
111990Na2Ox(s)	0	999.999	99 1.011 2.0	
			.	
195890AmAc/Am/Ac	(s) 0	0.000	73 1.071-1.072-1.0	
199002Na+/NpO2+E	X	999.999	93-1.011 1.0 8-2.0	
199003Na+/Th++++	EX	999.999	90-1.011 4.0	
			17 1 1 1	
IIII/U Hali	te	-154.990	1/1,111.	
1191/2 Sylvi	te	-164.840	19 1. 1/ 1.	
1				
-1				
	Figure A	-3 Listing of	AM ACET COMP DAT	
	1	- D. Misung VI		and the second sec



			See	Table 7-	<u>5 for explanati</u>	on of this listing.
	•					
1	011000	000170	.0765	.2664	.000 .00127	Na+ - Cl-
2	011000	000161	.0454	.398	.000 .0000	Na+ - HSO4-
3	011000	000080	.0864	.253	.000 .0044	Na+ - OH-
4	011000	017080	.0554	0.2755	.00000118	Na+ - ClO4-
5	011000	001990	0307	.000	.000 .000	Na+ - HOx-
ĉ	011000	000990	.0028	1.661	.000 .027	Na+ - Ox=
7	011000	000890	.1426	.22	.00000629	Na+ - Ac-
ê.	011000	000891	.1426	.22	.00000629	Na+ - Ac-F
9	019000	000170	.04835	.2122	.00000084	K+ - Cl-
10	019000	000161	0003	.1735	.000 .000	K+ – HSO4–
11	019000	000080	.1298	.320	.000 .0041	К+ - ОН-
12	001000	000170	.1775	.2945	.000 .0008	H+ - Cl-
13	001000	000161	.2065	.5556	.000 .000	H+ - HSO4-
14	001000	017080	.1747	0.2931	.000 .00819	H+ - ClO4-
15	090000	000170	1.092	13.7	-160112	Th++++ - Cl- Roy et al. 1992
16	090000	017080	1.186	27.3	.0000566'	Th++++ - ClO4- GRC Extr Data
17	093080	000170	.1415	.281	.000 .000	NpO2+ - C1- NFRK95
18	093080	017080	.257	.180	.000 .0081	NpO2+ - C1O4- NFRK95
19	095000	000170	.6117	5.403	.0000284	Am+++ - Cl-
80	095001	000170	.6117	5.403	.0000284	Am+++F - Cl-
21	095890	000170	.2270	2.154	.000102	AmAc++ - Cl-
22	000000					
23						
24	cation	anion	beta0	betal	beta2 cphi	
25					-	

Figure A-4. Sample listing of AM_ACET_BINARYP.DAT



See Table 9-1 for explanation of this listing.

	-	Бу А.К	. Felmy							
INPUT GMIN OUTPUT	file name file name file name	is U1: is U1: is U1:	SCBABB.N SCBABB.N SCBABB.N	ONLIN. ONLIN.	USERGUID USERGUID USERGUID	E AM_ACET E AM_ACET E AM_ACET	.IN;1 .GMIN; .OUT;1	1		
	AQUEOUS SP	ECIES				-				
				~	•					
10	NAME	0 000	NEES BRORDBRORD	2	uurt	< 5				
11000020	,	0,0000		1	105 (8					
100084		0,000		, .	-105.63	30				
95001Am-	++F	0.0000	000000000	3	-241 69	34				
95891Am/	c++F	0.0000	00000000	2.	999.99	99				
17001	-	0.000	000000000	-1.	-52.9	55				
891Ac	-F	0.000	000000000	-1.	-147.3	47				
	JULID PRASE			_	_					
ID 195890AmA	NAMĒ .c/Am/Ac(s	M 0.00000	OLE5 0000000	2 0.	uOrt 0.0(00				
	CONSTRAINT	EOUATIO	NS							
	0	1	8	11	95	72	89	73	17	71
н20	0.0	2.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	٥.
Na+	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	ο.
H+	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0=0	0.0	0.
Am+++F	3.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	ο.
AmAc++F	2.0	0.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0	ο.
C1-	-1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.
AC-1 AmAc/Am/A	-1.0 c(s 0.0	0.0	0.0	0.0	0.0	-1.0	0.0 1.0	0.0	0.0	1. -1
Closed			COMP						***	
closed if	aput riles G	min and	COME							
COMP	file name	15 Ul:	[SCBABB.N	ONLIN.	USÉRGUII	DE) AM_ACET	COMP.	DAT; 1		
BINARYP	file name	is U1:	SCBABB.NO	ONLIN.	USERGUII	E AM_ACET	BINA	RYP.DAT; 1	L	
TERNARYP	file name	is U1:[SCBABB.NO	NLIN.I	NPUTFIL	ES] TERNAR	YP.DAT	;1		
LAMEDA	file name	is U1:[SCBABB.NC	NLIN.	INPUTFIL	ESILAMBDA	. DAT ; 1			
n	on-ideai ele	ctrotyte	paramete	25						
5	ingle electr	olyte pa	rameters	• •		0.00000				
Nat			0.07650	0.2	10040	0.00000	-0.0	0127		
Na+	C1-		0 17750	0.2	9450	0.00000	- 0.0	0025		
H+	Ac-F		0.00000	0.0	0000	0.00000	0.0	00000		
	C1-		0.61170	5.4	0300	0.00000	-0.0	2840		
Am+++F	Ac-F		0.00000	0.0	0000	0.00000	0.0	0000		
AmAc++F	C1-		0.00000	0.0	0000	0.00000	0.0	0000		
AmAc++F	Ac-F		0.00000	0.0	0000	0.00000	0.0	00000		
	•	rolure r								
t	ernary elect	TOTANC H	arameters							
t	ernary elect	201900 P	arameters	C1-	_	Ac-F				
t Na+	ernary elect H+	101300 6	0.03600	C1- -0.	- 00400	Ac-F 0.00000)			
t Na+ Na+	ernary elect H+ Am+++F	1043 <i>0</i> 0 P	0.03600 0.00000	C1- -0. 0.	- 00400 00000	Ac-F 0.00000 0.00000)			
t Na+ Na+ Na+	H+ Am+++F AmAc++F	201300 P	0.03600 0.00000 0.00000	c1- -0. 0. 0.	- 00400 00000 00000	Ac-F 0.00000 0.00000 0.00000)))			
t Na+ Na+ H+	H+ Am+++P AmAc++F Am+++F	2049***	0.03600 0.00000 0.00000 0.00000	c1- -0. 0. 0.	- 00400 00000 00000 00000	Ac-F 0.00000 0.00000 0.00000) 1 0			
t Na+ Na+ H+ H+	H+ Am+++P AmAc++F AmAc+F AmAc+F	20 4 9×4	0.03600 0.00000 0.00000 0.00000 0.00000	C1- 0. 0. 0.	- 00400 00000 00000 00000	Ac-F 0.00000 0.00000 0.00000 0.00000				
t Na+ Na+ H+ H+ Am+++F	H+ Am+++F AmAc++F AmAc++F AmAc++F AmAc++F	204980 P	0.03600 0.00000 0.00000 0.00000 0.00000 0.00000	C1- -0. 0. 0. 0.	- 00400 00000 00000 00000 00000 00000	Ac-F 0.00000 0.00000 0.00000 0.00000 0.00000	0 0 0 0 0			
t Na+ Na+ H+ H+ Am+++F Cl-	H+ Am++++F AmAc++F AmAc++F AmAc++F AmAc++F Ac-F		0.03600 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 /	C1- -0. 0. 0. 0. 0. Na 0.	- 00400 00000 00000 00000 00000 00000	Ac-F 0.00000 0.00000 0.00000 0.00000 0.00000 H+ 0.0000	0 0 0 0 0 0	Am+++F 0.00000	A	mAc++)
t Na+ Na+ H+ Am+++F Cl- TOTAL NUM NUMBER OF INDEPENDE	H+ Am+++F AmAc++F AmAc++F AmAc++F AmAc++F Ac-F MBER OF SFEC COMPONENTS NT CONSTRAIN	165 - 1 175 - 1	0.03600 0.00000 0.00000 0.00000 0.00000 0.00000 , -0.09000 8 0 7	C1- -0. 0. 0. 0. 0. Na	- 00400 00000 00000 00000 00000 00000	AC-F 0.0000 0.0000 0.0000 0.0000 0.0000 H+ 0.0000	0 0 0 0 0 0	Am+++F 0.00060	A 0	mAc++:
t Na+ Na+ H+ Am+++F Cl- TOTAL NUM NUMBER OF INDEPENDE	H+ Am+++F AmAc++F AmAc++F AmAc++F AmAc++F Ac-F BER OF SPEC COMPONENTS NT CONSTRAIN SOLUBILITY	IES - 1 ITS - 1 DATA	0.03600 0.00000 0.00000 0.00000 0.00000 0.00000 -0.00000 -0.09000 8 0 7	C1- -0. 0. 0. 0. 0. Na 0.	00400 00000 00000 00000 00000 00000 00000	Ac-F 0.0000 0.0000 0.0000 0.0000 0.0000 H+ 0.0000	0 0 0 0 0	Am+++F 0.00060	A 0	mAc++ .0000
t Na+ Na+ H+ Am+++F Cl- TOTAL NUM NUMBER OF INDEPENDE	H+ Am+++F AmAc++F AmAc++F AmAc++F AmAc++F Ac-F MBER OF SFEC COMPONENTS NT CONSTRAIN SOLUBILITY input mola:	IES - 1 TS - 1 ITS - DATA Lities	0.03600 0.00000 0.00000 0.00000 0.00000 0.00000 , -0.09000 8 0 7	C1- -0. 0. 0. 0. 0. Na	- 00400 00000 00000 00000 00000 00000 00000	AC-F 0.00000 0.00000 0.00000 0.00000 H+ 0.00000	0 0 0 0 0	Am+++F 0.00000	A O	mAc++
t Na+ Na+ H+ Am++F Cl- TOTAL NUM NUMBER OF INDEPENDE	H+ Am+++F AmAc++F AmAc++F AmAc++F AmAc++F Ac-F BBER OF SPEC COMPONENTS INT CONSTRAIN SOLUBILITY input molai	IES - 1 ITS - DATA Lities	0.03600 0.00000 0.00000 0.00000 0.00000 0.00000 , -0.09000 8 0 7	C10. 0. 0. 0. 0. 0. Na 0.	- 00400 00000 00000 00000 00000 00000 00000	Ac-F 0.00001 0.00001 0.00001 0.00001 H+ 0.0000		λπ+++F 0.00000	A 0	måc++ -0000
t Na+ Na+ H+ Am+++F Cl- TOTAL NUM NUMBER OF INDEPENDE	H+ Am+++F AmAc++F AmAc++F AmAc++F AmAc++F Ac-F BER OF SPEC COMPONENTS NT CONSTRAIN SOLUBILITY input mola: H+	IES - 1 ITS - 1 DATA Lities	0.03600 0.00000 0.00000 0.00000 0.00000 0.00000 (-0.09000 8 0 7	C1- -0. 0. 0. 0. Na 0.	- 00400 00000 00000 00000 00000 00000 00000 0000	Ac-F 0.00000 0.00000 0.00000 0.00000 H+ 0.00000	0	Am+++F 0.00000 Ac-F	A O	mAc++
t Na+ Na+ H+ Am+++F Cl- TOTAL NUM NUMBER OF INDEPENDE Na+ 3.0000	H+ Am+++F AmAc++F AmAc++F AmAc++F AmAc++F Ac-F COMPONENTS NT CONSTRAIN SOLUBILITY input mola. H+ E-01 1.422	IES = 1 ITS = DATA Lities	0.03600 0.00000 0.00000 0.00000 0.00000 -0.00000 -0.09000 8 0 7 7	C1- -0. 0. 0. 0. Na 0.	- 00400 00000 00000 00000 00000 ++ 01029 Ac++F 426E-07	Ac-F 0.00000 0.00000 0.00000 0.00000 H+ 0.00000 H+ C1- 3.000E	~01	Am+++F 0.00000 Ac-F 1.010E-	A 0	
t Na+ Na+ H+ Am+++F Cl- TOTAL NUM NUMBER OF INDEPENDE NA+ 3.0000 1.0000 2.0000	H+ Am+++F AmAc++F AmAc++F AmAc++F AmAc++F AmAc++F Ac-F MBER OF SPEC COMPONENTS NT CONSTRAIN SOLUBILITY input mola: E+01 1.42 E+00 1.442	IES - 1 ITS - DATA Lities VE-05 SE-05	0.03600 0.00000 0.00000 0.00000 0.00000 -0.09000 4 -0.09000 8 0 7 7 Am+++F 1.010E-06 1.021E-06	C1- -0. 0. 0. 0. 0. Na 0.	- 00400 00000 00000 00000 00000 00000 + 01029 Ac++F 426E-07 304E-07	Ac-F 0.00000 0.00000 0.00000 H+ 0.00000 H+ 0.00000	~01 +00	Am+++F 0.00000 Ac-F 1.010E-(1.021E-(1.021E-(0 0 02 02	māc++;
t Na+ Na+ H+ Am+++F Cl- TOTAL NUM NUMBER OF INDEPENDE NUMBER OF INDEPENDE 3.000 1.000 2.000 3.000	H+ Am+++F AmAc++F AmAc++F AmAc++F AmAc++F Ac-F HBER OF SPEC COMPONENTS INT CONSTRAIN SOLUBILITY input molai H+ E-01 1.422 E+00 1.442 E+00 1.442	IES - 1 ITS - 1 DATA Lities 22-05 52-05	Americal and the form of the f	C1C. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.	- 00400 00000 00000 00000 00000 01029 Ac++F 426E-07 304E-07 856E-07 706E-07	Ac-F 0.00000 0.00000 0.00000 0.00000 H+ 0.00000 C1- 3.0000 1.0000 2.0000 2.0000	~01 +00 +00	Am+++F 0.00000 Ac-F 1.010E-(1.021E-(1.039E-(1.039E-(1.039E-(0 0 0 0 2 0 2 0 2	
t Na+ Na+ H+ Am+++F Cl- TOTAL NUM NUMBER OF INDEPENDE NA+ 3.0000 1.0000 2.0000 3.0000 4.0000	H+ Am+++F AmAc++F AmAc++F AmAc++F AmAc++F AmAc++F AmAc++F AmAc++F Ac-F BEER OF SPEC * COMPONENTS NT CONSTRAIN SOLUBILITY input mola: H+ E-01 E+00 E+00 E+00 E+00 1.442 E+00 SOLUBILITY	IES - 1 ITS - 1 DATA Lities IE-05 SE-05 SE-05 SE-05	0.03600 0.00000 0.00000 0.00000 0.00000 (-0.09000 (-0.09000 8 0 7 7 7 8 1.010E-06 1.021E-06 1.039E-06 1.054E-06	C10. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0	- 00400 00000 00000 00000 00000 01029 Ac++F 425E-07 304E-07 855E-07 706E-07 240E-07	Ac-F 0.0000 0.0000 0.0000 0.0000 H+ 0.0000 E1 3.000E 1.000E 2.000E 3.000E	~01 +00 +00	Am+++F 0.00000 1.010E-(1.012E-(1.039E- 1.054E-(1.071E-(0 02 02 02 02 02 02 02	.mAC++1 .00001





Figure A-5. Sample Output File: AM_ACET.OUT (1 of 3)

83 94

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90 91

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-3.0000E+02 1.0000E-01 1.0000E-01 1.0000E-01 L2 NORM OF THE RESIDUALS 2.3449283E+02 -3.9536E+02 2.2701E+01 2.1540E+00 -3.5943E-02 L2 NORM OF THE RESIDUALS 1.4263862E-01 -3.9536E+02 2.2701E-01 2.1540E+00 -3.5943E-02 L2 NORM OF THE RESIDUALS 1.4263862E-01 ADJUSTED PARAMETERS ~3.9535830E+02 uOrt (AmAc++F 1 C1-C1-AmAc++F 2.2700551E-01 ь0 (b1 (AmAc++F) 2.1540417E+00 AmAc++F c1--3.5943059E-02 Cmx (DATA SET(1) diff input calc AVERAGE DEVIATION = 4.7759E-02 STANDARD DEVIATION = 5.82328-02 FINAL MOLALITIES Am+++F AmAc++F ¢1-Ac-F Na-3.000E-01 1.427E-05 1.000E+00 1.442E-05 3.000E-01 5 426E+07 1.0106-06 1.010E-02 1.021E-06 3.304E-07 1.000E+00 1.021E-02 2.000E+00 2.000E+00 1.465E-05 1.0398-06 2.856E-07 1.039E-02 3 0005+00 1.486E-05 1.0548-06 4.706E-07 3.000E+00 1.054E-02 1.513E-05 1.071E-06 7.240E-07 4.000E+00 1.071E-02 4.000E+00 1.538E-05 1.089E-06 1.725E-06 5.000E+00 1.089£-02 5.000E+00 FINAL LOG ACTIVITIES Am+++F AmAc++F C1-Ac-F H+
 a+
 AmAr+F
 AmArC+F
 CL AC-F

 -6.728E-01
 -4.958E+00
 -7.403E+00
 -6.823E+00
 -6.758E+01
 -2.160E+00

 -1.827E-01
 -4.901E+00
 -7.718E+00
 -7.167E+00
 -1.853E-01
 -2.207E+00

 1.261E-01
 -4.771E+00
 -7.834E+00
 -7.338E+00
 1.237E-01
 -2.212E+00

 3.310E-01
 -4.625E+00
 -7.836E+00
 -7.244E+00
 3.287E-01
 -2.194E+00

 4.960E-01
 -4.315E+00
 -7.755E+00
 -7.215E+00
 6.385E-01
 -2.166E+00
 Calculated Log Activity Coefficients . AmAc++F H+ Am+++F C1-Ac-F Na+ -0.1529 -0.1130 -0.5573 -0.1500 -0.0602 -1.7272 -0.1853 -0.1827-1.8505 -0.7936 -0.1773 -0.1749 0.0630 -0.9171 -0.1461 0.2022 -1.8589 -0.1485 0.3484 -1.8043 -0.1083 -0.1060-1.7082 -1.2750 -0.0604 -0.0582 0.4981 SOLID PHASE NOW IN EQUILIBRIUM DATA SET (1) input calc diff 0.00000000000000000000E+000 0.000000000000000E+000 0.0000000000000000E+000 AVERAGE DEVIATION - 0.0000E+00 STANDARD DEVIATION = 0.0000E+00





Figure A-5. Sample Output File: AM_ACET.OUT (2 of 3)

+0.1643

-0.2161

-0.2290

-0.2168

-0.1901

-0.1529

165	FINAL	MOLALIT	IES					
166						-		
167	Na+		H+	Am+++F	AmAc++F	C1-	AC-F	-
168	3.1	000E-01	1.427E-05	1.0105-06	5.426E-07	3.000E-01	1.0102-0	2
169	1.0	000E+00	1.442E-05	1.021E-06	3.304E-07	1.080E+00	1.021E-0	2
170	2.0	000E+00	1.465E-05	1.039E-06	2.856E-07	2.000E+00	1.039E~0	2
171	3.0	D00E+00	1.489E-05	1.054E-06	4.706E-07	3.000E+00	1.054E-0	2
172	4.1	000£+00	1.513E-05	1.071E-06	7.240E-07	4.000E+00	1.071E-0	2
173	5.0	000E+00	1.538E-05	1.089E-06	1.725E-06	5.000E+00	1.089E-0	2
174								
175	FINAL	LOG AC	TIVITIES					
176								
177	Na+		H+	Am+++F	AmAc++F	C1-	Ac-F	
179	-6.1	728E-01	-4.958E+00	-7.403E+00	-6.823E+00	-6.758E-01	-2.160E+0	0
179	-1.4	827£-01	-4.901E+00	-7.718E+00	-7.167E+00	-1.853E-01	-2.207E+0	0
180	1.	261E-01	-4.771E+00	-7.834E+00	~7.338E+00	1.237E-01	-2.212E+0	0
181	з.	310E-01	-4.625E+00	-7.836E+00	-7.244E+00	3.287E-01	-2.194E+0	0
182	4.	960E-01	-4.472E+00	-7.775E+00	~7.215E+00	4.936E-01	-2.160E+0	0
183	6.	408E-01	-4.315E+00	-7.671E+00	~7.038E+00	6.385E-01	-2.116E+0	0
184								
185	Calcu	lated L	og Activit	y Coefficier	ts			
186								
187	Na+		H +	Am+++ E	ARAC++F	C1-	Ac-F	
188		-0.1500	-0.113	30 -1.40	0.5	5573 -0	.1529	-0.1643
189		-0.1827	-0.060	2 -1.72	272 -0.6	5858 - 0	.1853	~0.2161
190		-0.1749	0.06	30 -1.85	505 -0.1	7936 -0	.1773	-0.2290
191		-0.1461	0.20	22 -1.85	589 ~0.9	-0	.1485	-0.2168
192		-0.1060	0.348	34 -1.80	043 -1.0	750 -0	.1083 .	-0.1901
193		-0.0582	0.498	31 -1.70	082 -1.2	750 -0	.0604	-0.1529
194								
195		FINAL	L2 NORM OF	THE RESIDUA	LS 1.426386	52E-01		
196								
197								
199		EXIT PA	RAMETER		3			
199					-			
200								
201		FINAL	APPROXIMATE	SOLUTION				
202		1 11412						
202								
204		0 0 5	-3 95358309	+02				
205		1 4 1	2 2700551	-01				
206		2 4 1	2 15404175	2+00				
207		4 4 1	2.104041/E	2-02				
6. C I			-3.32430331	· ••				

Figure A-5. Sample Output File: AM_ACET.OUT (3 of 3)





NC Us <u>Ar</u>	ONLIN er's M opendiz	l, Versi ianual (A - I	on 2.0 Example for	Calculating Therm	odyna	mic	Parameters fr	om Constants		WPO # 30740 January 31, 1996 Page 51
1	0	0	0	0						
2	0									
3	001	080	0.00	000000	1	0	H2O			
4	01]	000	0.00	000000	2	1	Na+			
5	001	000	0.00	000000	3	2	H+			
6	095	5000	0.00	000000	4	3	Am+++			
7	095	5890	0.00	000000	5	4	AmAc++			
9	000	0170	0.00	000000	6	1	C1-			
9	000	890	0.00	000000	7	2	Ac-			
10 -	. 000	0000								
11	-1									
12	-1									
13										
			Figu	ire A-6. Samp	le In	put	File: AM	_ACET_POST_	_ABN.GI	MIN
1	-1									
2		6	-1							
3	0	0	.30	1.4273e-5		1.0	010e-6	5.426e-7	.3	1.010e-2
	0	0	1.0	1.4422e-5		1.(021e-6	3.304e-7	1	1.021e-2
2	U	-		1.11460.0						
۲ ۲	0	Ō	2.0	1.4648e-5		1.0	039e-6	2.856e-7	2	1.039e-2
∠ 5 6	0 0 0	0	2.0	1.4648e-5 1.4883e-5		1.0	039e-6 054e-6	2.856e-7 4.706e-7	2 3	1.039e-2 1.054e-2
د ج 6 7	0 0 0	0 0 0	2.0 3.0 4.0	1.4648e-5 1.4883e-5 1.5127e-5		1.0 1.0 1.0	039e-6 054e-6 071e-6	2.856e-7 4.706e-7 7.240e-7	2 3 4	1.039e-2 1.054e-2 1.071e-2
∠ 5 6 7 €	0 0 0 0	0 0 0 0	2.0 3.0 4.0 5.0	1.4648e-5 1.4883e-5 1.5127e-5 1.5378e-5		1.0 1.0 1.0	039e-6 054e-6 071e-6 089e-6	2.856e-7 4.706e-7 7.240e-7 1.725e-6	2 3 4 5	1.039e-2 1.054e-2 1.071e-2 1.089e-2

Figure A-7. Sample Input File: AM_ACET_POST.IN

.

N U A	ONLIN, Version 2.0 ser's Manual ppendix A - Example for Calcu	lating T	hermodynamic Parameters from Constants
1	001080H20	0	-95.6635 1 2.0 8 1.0
2			
3	001000H+	1	000.000 1 1.0
4	011000Na+	1	-105.651 11 1.0
5	019000K+	1	-113.957 19 1.0
е 7	0000800H-	-1	-63,435 1 1.0 8 1.0
0	0001618504-	-1	-304.942 16 1.0 8 4.0 1 1.0
5	00017001-	-1	-52.9550 17 1.0
9 10	0170800104-	- 1	-73 81 17 1 0 8 4 0
10	01/0000104	-	,3.01 1, 1.0 0 4.0
12	000050B(OH)3(aq)	0	-390.810 5 1.0 8 3.0 1 3.0
13 14	09000075++++	4	-284.227 90 1.0
16	093080Np(V)02+	1	-369,109,93,1,0,8,2,0
10	09500000	4	-241 694 95 1 0
10	095000 Amt + + F	2	-241 694 95 1 072 1 0
17	095001All() () 1	5	241.034 93 1.072 1.0
19	095890AmAc++	2	-395.358 95 1.089 1.0
20	095891AmAc++F	2	999,999 95 1.089 1.073 1.0
21			
22	000890Ac-	-1	-147.347 89 1.0
23	000891Ac-F	-1	-147.347 89 1.071 1.0
24			
25	0009900x=	-2	-272.2 99 1.0
26	001990HOx-	-1	-281.94 99 1.0 1 1.0
27	001991H2Ox(aq)	0	-284.99 99 1.0 1 2.0
28			
29	093890NpO2Ac(aq)	0	-519.800 93 1.0 8 2.089 1.0
80			
31	101990H2Ox.2H2O(s)	0	999.999 99 1.0 1 6.0 8 2.0
2	111990Na2Ox(s)	0	999.999 99 1.011 2.0
2			
34	195890AmAc/Am/Ac(s)) ()	0.000 73 1.071-1.072-1.0
35	1000000 - (12 00		
36	199002Na+/NpO2+EX		999.999 93-1.011 1.0 8-2.0
37	199003Na+/Th+++EX		999.999 90-1.011 4.0
88			
39	IIII/O Halite		-154.990 1/ 1. 11 1.
40	119172 Sylvite		-164.840 19 1. 17 1.
¥1			
42	-1		



Figure A-8. Sample Input File: AM_ACET_COMP_POST_ABN.DAT



WPO # 30740 January 31, 1996 Page 52

INPUT	file name i	s U1:[SCBABB NO] s U1:[SCBABB NO]	NLIN.USERGUI NLIN.USERGUI	DE] AM_ACET_	POST ABN.GMIN;	
OUTPUT	file name i	s U1:[SCBABB.NO	NLIN.USERGUI	DE] AM_ACET_	POST_ABN.OUT:1	
	AQUEOUS SPEC	CIES				
ID	NAME	MOLES	Z uOrt	· ~ 3		
1080H20	о ,	0.00000000000000	U95.6 1 -105.6	103 151		
1000Na-	•	0.0000000000000000	1. 0.0	00		
95000Am	+++	0.0000000000000	3241.6	94		
95890Am	Ac++	0.0000000000000	2395.3	58		
170C1	-	0.0000000000000	-132.5	22		
890AC	SOLID PHASES	5.0000000000000000000000000000000000000	-1. 14/.5			
ID	NAME	MOLES	Z uOrt			
	CONSTRAINT I	EQUATIONS		00	17	
1120	0	2 0 1 0	0.0 0.0 TT 32	69 0.0	0.0	
п20 Na+	1.0	0.0 0.0	1.0 0.0	ŏ.ŏ	0.0	
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3.000E+0	1.488E-05 1.054E-06 4.706	E-07 3.000E+00 1.054E-02	
4.000E+0	1.513E-05 1.0/1E-06 /.240	E=07 4.000E+00 1.071E=02 E=06 5.000E+00 1.080E=03	
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-1.827E-01	-4.901E+00 -7.715E+00 -7.178E+00	-1.853E-01 -2.207E+00	
1.261E-01	-4.771E+00 -7.842E+00 -7.311E+00	1.237E-01 -2.212E+00	
3.310E-01	-4.625E+00 -7.824E+00 -7.274E+00	3.287E-01 -2.194E+00	
4.960E-01	-4.472E+00 -7.785E+00 -7.202E+00	4.938E-01 -2.160E+00	
6.408E-01	-4.315E+00 -7.669E+00 -7.042E+00	6.385E-U1 -2.116E+UU	
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134

Figure A-9. Sample Output File: AM_ACET_POST_ABN.OUT (2 of 2)

input calc diff **** SINGULAR MATRIX IN DECOMP, ZERO DIVIDE IN SOLVE



Figure A-10. Apparent stability constant for AmAc in NaCl media: comparison of the model with data.



1	0	0	0	0				
2	0							
3	0010	080	Ο.	00000	000	1	L C	H2O
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5	0010	000	Ο.	00000	000	3	3 2	H+
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7	0958	390	Ο.	00000	000	5	5 4	AmAc++
8	0001	L70	Ο.	00000	000	e	5 1	C1-
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10	0000	000						
11	1958	391	0.	000000	300			
12	-1							
13	-1						、	

Figure A-11. Sample Input File: AM_ACET_POST_NORM.GMIN.





001080H20	Ο	-95,6635	٦	2.0.8	1.0
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001000H+	1	000.000	1	1.0	
011000Na+	1	-105.651	11	1.0	
019000K+	1	-113.957	19	1.0	
0000800н-	-1	-63.435	1	1.0 8	1.0
000161HSO4-	-1	-304.942	16	1.0 8	4.0 1 1.0
000170Cl-	-1	-52.9550	17	1.0	
017080C104-	-1	-73.81	17	1.0 8	4.0
000050B (OH) 3 (aq) 0	-390.810	5	1.0 8	3.0 1 3.0
090000Th++++	4	-284.227	90	1.0	
093080Np(V)02+	1	-369.109	93	1.0 8	2.0
095000Am+++	3	-241.694	95	1.0	
095001Am+++F	3	-241.694	95	1.072	1.0
0958900m2c++	2	-395 358	95	1 089	1 0
095891AmAc++F	2	999.990	95	1.089	1 073 1 0
000001AMBRET (1	2		20	1.000	1.070 1.0
000890Ac-	-1	-147.347	89	1.0	
000891Ac-F	-1	-147.347	89	1.071	1.0
0009900x≠	-2	-272.2	99	1.0	
001990HOx-	-1	-281.94	99	1.0 1	1.0
001991H2Ox (aq)	0	-284.99	99	1.0 1	2.0
093890NpO2Ac (aq) 0	-519.800	93	1.0 8	2.089 1.0
101990H20x 2H20	(s) ()		99	1 0 1	60820
111990 Na 20 x (s)	0	999 999	99	1.011	2 0
x225501122011(0)	*			_ / V 1 1	2.0
195890AmAc/Am/A	c(s) 0	0.000	73	1.071	-1.072-1.0
195891AmAc/Am/A	c(s) 0	0.000	89	0.095	0.0
199002Na+/NpO2+3	EX	999.999	93-	1.011	1.0 8-2.0
199003Na+/Th+++	+EX	999.999	90-	1.011	4.0
111170 Hal	ite	-154.990	17	1. 11	1.
119172 Svlv	ite	-164.840	19	1. 17	1.



Figure A-12. Sample Input File: AM_ACET_COMP_POST_NORM.DAT



WPO # 30740 January 31, 1996 Page 57

NONLIN V	/2.0							
NONLIN	vas developed	by A.R.	Felmy		Aw .			
INPUT Gmin	file name file name	is Ul:	SCBABE . N		RGUIDE	AM_ACET	_POST.IN;1	
OUTPUT	file name	is U1:{	SCBABB.N	ONLIN.U	SERGUIDE	AM_ACET	_POST_NORM.OUT;	
	AQUEOUS SPE	CIES						
ID	NAME	MO	LES	zι	Ort			
1080H20	0	0.00000	0000000	Ċ.	-95.663			
11000Na-	+	0.00000	0000000	1	-105.651			
1000H+		0.00000	0000000	1.	0.000			
95890Am	Ac++	0.00000	00000000	2	-395.358			
170Cl	-	0.00000	0000000	-1.	-52.955			
890Ac	- SOLID PHASE	0.00000 S	00000000	-1	-147.347			
ID 195891Am	NAME Ac/Am/Ac(s	MO:000000	LES 000000	2 u 0.	0rt 0.000			
	CONSTRAINT	EQUATION						
	0	1	8	11	95	89	17	
H2O	D.0	2.0	1.0	0.0	0.0	0.0	0.0	
Na+	1.0	0.0	0.0	1.0	0.0	0.0	0.0	
л+ Ат+++	1.0 3 0	0 0 1.0	0.0	0.0	0.0	0.0	0.0	
AmAc++	2.0	0.0	0.0	0.0	1.0	1.0	0.0	
C1-	-1.0	0.0	D.0	0.0	0.0	0.0	1.0	
Ac-	-1.0	0.0	0.0	0.0	0.0	1.0	0.0	
1012107 1417 11	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Closed in	nput files G	MIN and (COMP					
COMP	file name	is U1:[SCBABB.N	ONLIN.US	ERGUIDE	AM_ACET	COMP_POST_NORM	S.A.C
BINARYP	file name	is U1:[5	CBABB.NC	ONLIN.US	ERGUIDE]	AM_ACET	BINARYP.DAT:1	
TERNARYP	file name	is 01:[S	CBABB.NO	NLIN.IN	PUTFILES] TERNARY	P.DAT;1	f.
BREBUK	IIIC Name	12 01.(3	CDABE.NO	MLIN.IN.	FOILTERS	J LAMBUA.	DAT;1	- L.
n	on-ideal elec	trolyte	paramete.	rs				14
5	ingle electro	lyte para	ameters					A.
ia+	C1-	t	0.07650	0.266	40 0	0.00000	0.00127	
1a+ 1+	Ac-	(J.14260	0.220	000 C	00000	-0.00629	
+	Ac+	í.	0.00000	0.294	100 0		0.00080	
m+++	C1-	Č	.61170	5.403	00 0	.00000	-0.02840	
m+++	Ac-	٥	.00000	0.000	00 0	.00000	0.00000	
mAc++	C1-	0	.22700	2.154	00 0	0.00000	-0.10200	
	AL-	U		0.000	00 0		0.0000	
t	ernary electr	olyte pai	rameters					
		_		C1-		Ac-		
a+	H+ Am+++	0	03600	-0.00	400	0.00000		
a+	AmAc++	0	.00000	0.00	000	0,00000		
+	Am+++	0	.00000	0.00	000	0.00000		
(+	AmAc++	0	.00000	0.00	000	0.00000		
.m+++	АлАс++	0	.00000	0.00	000	0.00000		
1-	Ac-	-0	09000	Na+	029	H+	Am+++	AmAc++
-		-0		0.01	527	5-00000	0.00000	0.0000
TOTAL NUM NUMBER OF	BER OF SPECI COMPONENTS	ES = 8 = 7						
INDEPENDE	NT CONSTRAINT	rs = 6						
	SOLUBILITY I	DATA						
	input molal:	ities						
Na+ 3 0001	H+ 2-01 14271	An נ-05 ו-2	0106-04	AmAc+	+ 67-07	C1- 3 000E-1	Ac-	
1.000	2+00 1.442	E-05 1	021E-06	3.30	4E-07	1.000E+0	00 1.021E+02	
2.000	+00 1.4655	E-05 1	039E-06	2.85	6E-07	2.000E+	00 1.039E-02	
3.000	+00 1.488	E-05 1.	054E-06	4.70	6E-07	3.000E+0	00 1.0545-02	
4.0005	5+00 1.5139 2+00 1.5139	E-05 1.	071E-06	7.24	DE-07	4.000E+0	00 1.071E-02	
5.000E	s+00 1.538E	1. co-us	.0896-06	1.72	D£i≁016	5.000E+0	UU 1.089E-02	



1 S	ૼૼૼૼૼૼૻ૽ૼ૱
~	, 1

Figure A-13. Sample Output File: AM_ACET_POST_NORM.OUT (1 of 3)

ADJUSTED PARAMETERS

DATA SET	(1)						
INDUE	calc	di	££				
0.00000	1000000000	6+000	0 000000	3000000000	+000		
n 0000000	000000000000000000000000000000000000000	£+000	0.000000	000000000E	+000		
0.000000		GTU000	0.000000	00000000000	+000		
0.000000		G-000	0.000000	00000000000	+000		
0.000000			0.000000	00000000000	+000		
0.000000		E+000	0.000000	00000000000	+000		
0.000000	0000000000	E+000	0.000000	0000000000	+000		
AVERAGE	DEVIATION	-	0.0000E+00				
STANDARD	DEVIATION	4 -	0.0000E+00				
FINAL MOL	ALITIES						
Na+	H+		Am+++	AmAc++	c1-	Ac	-
3.000E-	01 1.427	E-05	1.008E-06	5.449E-0	7 3.000	E-01 1.010	E-02
1.000E+	00 1.442	£-05	1.030E-06	3.219E-0	7 1.000	E+00 1.021	E-02
2 000E+	00 1.465	£-05	1.020E-06	3.043E~0	7 2.000	E+00 1.039	E-02
3 000E+	00 1.488	£-05	1.084E-06	4.404E-0	7 3,000	E+00 1.054	E-02
4 000E+	00 1 513	8-05	1 0455+06	7.496E-0	7 4.000	E+00 1.071	E-02
5 000E+	00 1.538	E-05	1.093E-06	1.721E-0	6 5.000	E+00 1.089	E-02
FINAL LUG	ACTIVITI	55					
Na+	H+		Am+++	AmAc++	c1-	Ac	
-6.728E-	01 -4.958	£+00	~7.404E+00	-6.821E+0	0 -6.758	E-01 -2.160	E+00 -
-1.827E-	01 -4.901	E+00	-7.715E+00	-7.178E+0	0 -1.853	E-01 -2.207	E+00
1.261E-	-01 -4.771	E+D0	-7.842E+D0	-7.311E+0	0 1.237	E-01 -2.212	£+00
3 310E-	01 -4.625	2+00	-7.824E+00	-7.274E+0	0 3.287	E-01 -2.194	E+00
4 9605-	-01 -4 472	£+00	-7 7858-00	-7.202E+0	1 4 938	E-01 -2.160	F+00
4 408E-	01 -4 315	£+00	-7.6698+00	-7.042E+0	0 6.385	E-01 -2.116	E+00
o-1-distor	t too Act		Coofficier				
Calcutated	I LOG ACC	1.10	COELIICIEI			_	
Na+	H+		Am+++	AmAc++	C1-	AC	-0 1643
-0.1		0.113	-1.40			-0.1963	-0.2161
-0.1	827 -	0.060.	2 -1.7.	<i>212</i> •••	.0039	-0.1853	-0.2101
-0.1	749	0.063	0 -1.8	505 -0	-/941	-0.1773	-0.2290
-0.1	461	0.202	2 -1.8	589 -0	9181	-0.1485	-0.2168
-0.1	060	0.348	4 -1.8	043 -1	.0767	-0.1083	-0.1901
-0.0	582	0.498	1 ~1.7	082 -1	.2776	~0.0604	-0.1529
SOLID PHA:	SE NOW IN	EQUI	LIBRIUM				
DATA SET	(1)						
input	calc	di:	ff				
projected	hessian	indef	inite				
	0000000000	E+000	0 000000	000000000	+000		
	hereian	indef	(nite				
a anagaa	nessian	10001	0 000000	00000000	+000		
0.000000		indof.	inite				
0,000000	10000000000	E+000	0.000000	000000000E	+000		
projected	hessian	indef	inite				
0.000000	000000000	E+000	0.000000	000000000E	+000		
projected	hessian	indef	inite				
0.00000	10000000000	E+000	0.000000	000000000000	+000		
projected	hessian	indef	inite 0 noocoo	00000000	+000		
0.000000		5+000	0.00000	00000000			
AVERAGE	DEVIATION	=	0.0000E+00				
			,				



Figure A-13. Sample Output File: AM_ACET_POST_NORM.OUT (2 of 3)



52	FINAL MOLALITI	£S					
54	Nat H	+	Am+++	AmAc++	cl-	Ac-	
55	3 0006-01	1.427E-05	1.008E-06	5.449E-07	3.0006-01	1.010E-02	
56	1 00000000	1.442E-05	1.030E-06	3.219E-07	1.0005+00	1.021E-02	
57	2 000E+00	1.465E-05	1.020E-06	3.043E-07	2.0002+00	1.039E-02	
52	3 000E+00	1.488E-05	1.084E-06	4.404E-07	3.0002+00	1,054E-02	
50	4 00000+00	1.513E-05	1.045E-06	7.496E-07	4.000£+00	1.071E-02	
60	5.0000+00	1.5382-05	1.093E-06	1.721E-06	5.000£+00	1.089E-02	
161	510002						
182	FINAL LOG ACT	IVITIES					
(C)	No. 4	+	&m+++	AmAc++	C1-	Ac-	
20		4 958E+00	-7.404E+00	-6.821E+00	-6.758£-01	-2.160E+00	
100	-1 9275-01	-4 9015+00	-7.715E+00	-7.178E+00	-1.8538-01	-2.207E+00	
100 160	1 2618=01	-4.771E+00	-7.842E+00	-7.311E+00	1.237E-01	-2.212E+00	
24	2 2015-01	-4 6258+00	-7.824E+00	+7.274E+00	3.287E-01	-2.194E+00	
120	4 9605-01	-4.472E+00	-7.785E+00	-7.202E+00	4.938E-01	-2.160E+00	
105	5 408F+01	-4.315E+00	-7.669E+00	-7.042E+00	6.385E-01	-2.116E+00	
171	0.4002 **						
	Calculated Lo	a Activity	Coefficier	its			
172							
172	Na+ H	*	Am+++	AmAc++	C1-	Ac-	
175	-0.1500	-0.1130	-1.40)77 -0.	5573 -0.	.1529 -	-0.1643
176	-0.1827	-0.0602	-1.72	272 -0.	6859 -0.	. 1853 -	-0.2161
177	-0.1749	0.0630) -1.8	505 -0.	7941 -0.	.1773 -	-0.2290
179	-0.1461	0.2023	2 -1.8	589 -0.	9181 -0.	.1485	-0.2168
179	-0.1060	0.3484	-1.8	043 -1.	0767 -0.	.1083 -	-0.1901
180	-0.0582	0.4981	-1.7	082 -1.	2776 -0.	.0604 -	-0.1529
131							
182	FINAL L	2 NORM OF 1	THE RESIDUA	LS 0.00000	00E+00		
163							
184							
185	EXIT PAR	AMETER		I	0		
196							
187							
198	FINAL A	PPROXIMATE	SOLUTION				DODLEOTE (2 - 52)
	Fic	mre A-13	Sampl	e Output	File: AM	I ACET	POST_NORM.OUT (3 of 3)
	1 18		. Samp	e corper			





1-

Appendix B - Sample Input File: EXTR_00.GMIN

		See Table	7-1 for explanation of this listing.
1	0 0	0 0	
2	0		
3	001080	0.00000000	H2O
4	011000	0.0000000	Na+
5	090000	0.0000000	Th++++
e	001000	0.0000000	H+
?	000080	0.0000000	OH-
8	017080	0.0000000	C104-
9	000000		
10	199003	0.0000000	Th++++/Na+ extracted
11	-1		
12	-1		

Appendix C - Sample Input File: EXTR_07_EXACT.IN

		Se	e Table	7-3 for ex	planation of th	is listing.	
1 2	000007 -12 010202	20.65	uo[Th++++ b(0) Th++	/Na+ extracte +/ClO4-	ed]	See key ir Figure A-	1.
3	-1		cpni /n++	+/0104-			
<u>د</u>	-1 -1						
5 6	1.00E-05	0.000	0.307	2.12E-05	1.00E-07	1.00E-07	0.307
7	1.00E-05	0.000	0.307	2.12E-05	1.00E-07	1.00E-07	0.307
e	1.00E-05	0.000	1.035	5.94E-05	1.00E-07	1.00E-07	1.035
9	1.00E-05	0.000	1.035	5.81E-05	1.00E-07	1.00E-07	1.035
10	1.00E-05	0.000	2.129	1.69E-04	1.00E-07	1.00E-07	2.129
11	1.00E-05	0.000	2.129	1.69E-04	1.00E-07	1.00E-07	2.129
12	1.00E-05	0.000	3.322	3.15E-04	1.00E-07	1.00E-07	3.322
13	1.00E-05	0.000	3.322	3.39E-04	1.00E-07	1.00E-07	3.322
14	1.00E-05	0.000	4.657	9.45E-04	1.00E-07	1.00E-07	4.657
15	1.00E-05	0.000	4.657	9.45E-04	1.00E-07	1.00E-07	4.657
16	1.00E-05	0.000	6.176	1.26E-03	1.00E-07	1.00E-07	6.176
17	1.00E-05	0.000	6.176	1.45E-03	1.00E-07	1.00E-07	6.176
18	1.00E-05	0.000	9.929	1.93E-03	1.00E-07	1.00E-07	9.929
19	1.00E-05	0.000	9.929	2.19E-03	1.00E-07	1.00E-07	9.929
20	1.00E-05	0.000	14.916	2.33E-03	1.00E-07	1.00E-07	14.916
21	1.00E-05	0.000	14.916	2.29E-03	1.00E-07	1.00E-07	14.916
22	- 1						
23	-1						
24							
25	mORG	рH	mNa+	mTh++++	mH+	mOH-	mC104-



Appendix D - Sample Input File: SOLUB_00.GMIN

See Table 7-1 for explanation of this listing.

	0 0	0 0	
1	0 0	0 0	
2	0		
3	001080	0.00000000	H2O
ź	001000	0,00000000	H+
5	000080	0.00000000	OH-
6	000161	0.00000000	HSO4-
7	001991	0.00000000	H2Ox (aq)
ę	000000		
9	101990	.000000000	H2Ox.2H2O(s)
10	-1		
11	-1		

Appendix E - Sample Input File: SOLUB_01.IN

	·····		See Ta	ble 7-3 for e	xplanation of	f this li	sting.	
1	000006 -1	-1	0.0	u0 H2C2O4.	2H2O(s))		See key in Figure A-1.	
З	07	-1		-				
4	0.0	0.0	1.168	8.56E-15	1.168	0.875		
5	0.0	0.0	1.965	5.09E-15	1,965	0.653		· · · · · ·
6	0.0	0.0	2.927	3.42E-15	2.927	0.534		à
7	0.0	0.0	4.450	2.25E-15	4.450	0.476		· ·
S	0.0	0.0	6.660	1.50E-15	6,660	0.432		
Đ	0.0	0.0	9.548	1.05E-15	9.548	0.574		2
10	0.0	0.0	13.941	7.17E-16	13.941	1.268		, C
11	-1							· `
12	-1							
13								
14								
15	0.0	рH	mH+	mOH-	mHSO4-	mH2O	x	



Appendix F - Listing of COMP.DAT

$\begin{array}{cccccccccccccccccccccccccccccccccccc$	ng.
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
9 $000170C1$ 1 -52.9550 17 1.0 10 $017080C104$ 1 -73.81 17 1.0 8 4.0 11 12 $000050B(OH)3(aq)$ 0 -390.810 5 1.0 8 3.0 1 3.0 13 14 $090000Th$ ++++ 4 -284.227 90 1.0 15 $093080Np(V)02$ + 1 -369.109 93 1.0 8 2.0 16 $095000Am$ +++ 3 -241.694 95 1.0 17 $095001Am$ +++F 3 -241.694 95 1.072 1.0 19 19 $095890AmAc$ ++ 2 999.999 95 1.089 1.0 20 $095891AmAc$ ++F 2 999.999 95 1.089 1.0 21 22 $000890Ac$ 1 -147.347 89 1.0 22 $000890Ac$ 1 -147.347 89 1.0	
10 $017080C104 -1$ $-73.81 \ 17 \ 1.0 \ 8 \ 4.0$ 11 12 $000050B(OH) \ 3(aq)$ 0 $-390.810 \ 5 \ 1.0 \ 8 \ 3.0 \ 1 \ 3.0$ 13 14 $090000Th + + + +$ 4 $-284.227 \ 90 \ 1.0$ 15 $093080Np(V)02 +$ $1 \ -369.109 \ 93 \ 1.0 \ 8 \ 2.0$ 16 $095000Am + +$ $3 \ -241.694 \ 95 \ 1.0$ 17 $095001Am + +F$ $3 \ -241.694 \ 95 \ 1.072 \ 1.0$ 18 $99500Am + +F$ $3 \ -241.694 \ 95 \ 1.072 \ 1.0$ 19 $095890AmAc + +$ $2 \ 999.999 \ 95 \ 1.089 \ 1.0$ 20 $095891AmAc + +F$ $2 \ 999.999 \ 95 \ 1.089 \ 1.073 \ 1.0$ 21 $2000890Ac -1 \ -147.347 \ 89 \ 1.0$	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
14 090000Th++++ 4 -284.227 90 1.0 15 093080Np(V)02+ 1 -369.109 93 1.0 8 2.0 15 095000Am+++ 3 -241.694 95 1.0 17 095001Am+++F 3 -241.694 95 1.072 1.0 18	
15 093080Np(V)02+ 1 -369.109 93 1.0 8 2.0 16 095000Am+++ 3 -241.694 95 1.0 17 17 095001Am+++F 3 -241.694 95 1.072 1.0 18 19 095890AmAc++ 2 999.999 95 1.089 1.0 20 095891AmAc++F 2 999.999 95 1.089 1.073 1.0 21 22 000890Ac- -1 -147.347 89 1.0	
16 095000Am+++ 3 -241.694 95 1.0 17 095001Am+++F 3 -241.694 95 1.072 1.0 19 095890AmAc++ 2 999.999 95 1.089 1.0 20 095891AmAc++F 2 999.999 95 1.089 1.0 21 22 000890Ac- -1 -147.347 89 1.0	
17 095001Am+++F 3 -241.694 95 1.072 1.0 19 095890AmAc++ 2 999.999 95 1.089 1.0 20 095891AmAc++F 2 999.999 95 1.089 1.0 21 22 000890Ac- -1 -147.347 89 1.0	
19 095890AmAc++ 2 999.999 95 1.089 1.0 19 095891AmAc++ 2 999.999 95 1.089 1.0 21 22 000890Ac- -1 -147.347 89 1.0	
19 095890AmAc++ 2 999.999 95 1.089 1.0 20 095891AmAc++F 2 999.999 95 1.089 1.073 1.0 21 22 000890Ac- -1 -147.347 89 1.0 22 000890Ac- -1 -147.347 89 1.0	
20 095891AmAc++F 2 999.999 95 1.089 1.073 1.0 21 22 000890Ac- -1 -147.347 89 1.0 22 000890Ac- -1 -147.347 89 1.0	
21 22 000890Ac1 -147.347 89 1.0 22 000890Ac1 147.347 89 1.0	
22 000890Ac1 -147.347 89 1.0	
23 UUU891AC+F +1 =14/.34/ 89 1.0/1 1.0	
24	
-25 0009900x = -2 -272.2 99 1.0	
26 001990HOX1 -281.94 99 1.0 1 1.0	
27 001991H2Ox(aq) 0 -284.99 99 1.0 1 2.0	
28	
29 093890NpO2Ac(aq) 0 -519.800 93 1.0 8 2.089 1.0	
$\frac{1}{2}$ 1019900207(c) 0 999 99 101 20	
\sim 195890 $amac/am/ac(s)$ 0 000 73 1.071-1 072-1 0	
₩ 199002Na+/NmO2+FX 999 999 93-1.011 1.0 8-2 0	
77 199003Na+/7D++++EX 999 90-1-011 4.0	
∞ ∞ 111170 Halite ~154 990 17 1, 11 1.	
← 119172 Sulvite −164.840 19 1. 17 1.	
42 -1	
43	



Appendix G - Listing of BINARYP.DAT

See Table 7-5 for explanation of this listing.

1	011000	000170	.0765	.2664	.000 .00127	Na+ - Cl-	
2	011000	000161	.0454	.398	.000. 000.	Nat - HSO4-	
Э	011000	000080	.0864	.253	.000 .0044	Na+ - OH-	
4	011000	017080	.0554	0.2755	.00000118	Na+ - ClO4-	
5	011000	001990	0307	.000	.000 .000	Na+ - HOx-	
6	011000	000990	.0028	1.661	.000 .027	Na+ - Ox=	
7	011000	000890	.1426	.22	.00000629	Na+ - Ac-	
3	011000	000891	.1426	.22	.00000629	Na+ - Ac-F	
9	019000	000170	.04835	.2122	.00000084	K+ - Cl-	
10	019000	000161	0003	.1735	.000 .000	K+ - HSO4-	
11	019000	000080	.1298	.320	.000 .0041	K+ - OH-	
12	001000	000170	.1775	.2945	.000 .0008	H+ - Cl-	
13	001000	000161	.2065	.5556	.000 .000	H+ - HSO4-	
14	001000	017080	.1747	0.2931	.000 .00819	H+ - ClO4-	
15	090000	000170	1.092	13.7	-160112	Th++++ - Cl- Roy et al. 1992	
18	090000	017080	1.186	27.3	.0000566	Th++++ - ClO4- GRC Extr Data	
17	093080	000170	.1415	.281	.000 .000	NpO2+ - Cl- NFRK95	
18	093080	017080	.257	.180	.000 .0081	Np02+ - C104- NFRK95	
19	095000	000170	.6117	5.403	.0000284	Am+++ - Cl-	
20	095001	000170	.6117	5.403	.0000284	Am+++F - Cl-	
21	000000						
22							Ż
23	cation	anion	beta0	betal	beta2 cphi	l.	1



Appendix H - Listing of TERNARYP.DAT

See Table 7-6 for explanation of this listing.

1 2 3 4 5 6 7 8 9 10	011000 011000 019000 000170 000170 000170 000170 000080 017080 090000	019000 001000 00161 000080 000890 000891 017080 000890 000890	012 .036 .005 006 05 090 090 0320 0.064	000170 000170 000170 011000 011000 011000 011000 011000	0018 004 011 006 006 .01029 .01029 0072	000161 000160 001000 019000	0129 .197 .0130 006	017080 000161	0160 0265
10	090000	001000	.600						
11	090000	011000	.420						
12	000000								
13									





Appendix I - Listing of LAMBDA.DAT

- ----

See Table 7-7 for explanation of this listing.

.000 000170 -.0102 -.14 000050 001000 1

- 000050 019000 2
- 000000 3



Appendix J - Sample Output File: EXTR_07_EXACT.OUT

See Table 9-1 for explanation of this listing.

1	NONLIN	V2.0								
2 3 4	NONLIN	was deve	elope	d by A.R	. Felmy					
7 5 8 7	INPUT GMIN OUTPUT	file file file	name name name	is U1:[is U1:[is U1:[SCBABB.NO SCBABB.NO SCBABB.NO	NLIN. NLIN.	USERGUII USERGUII USERGUII	DE] EXTR_07_ DE] EXTR_00. DE] EXTR_07_	EXACT.IN;1 GMIN;1 EXACT.OUT;1	
9		AQUEO	US SP	ECIES						
10	ID	NAME	E	M	OLES	z	uOrt			
12	1080H	20		0.0000	00000000	0.	-95.6	63		
13	11000Na	а+ Баан		0.0000	00000000	⊥. ∧	-105.6	151		
15	1000H-	117777 1		0.0000	000000000	1.	-204.2	100		
16	800	н-		0.0000	00000000	-1.	-63.4	.35		
17	17080C	104-		0.0000	00000000	-1.	-73.8	10		
18		SOLID	PHAS	ES						
19 20	TD	NAME	2	M	OLES	7.	110 2 7			
21	199003Na	a+/Th+++	+EX	0.00000	00000000	ō.	999.9	99		
22										
23		CONST	RAINT	EQUATIO	NS					
24			0	1	8	11	90	17		
25 26	HZQ Nat		1 0	2.0	1.0	1 0	0.0	0.0		
27	Tb++++		4.0	0.0	0.0	0.0	1.0	0.0		
22	H+		1.0	1.0	0.0	0.0	0.0	0.0		• .
29	OH-		-1.0	1.0	1.0	0.0	0.0	0.0		
30	C104-		-1.0	0.0	4.0	0.0	0.0	1.0	i	
31	Na+/Th++	⊦++EX	0.0	0.0	0.0	4.0	-1.0	0.0	•	•
32		.	1 /		COND					
33	Closed	input fi	Lies (SMIN and	COMP					and the second
36	COMP	file	name	is UD-13	CBABB NO	NLTN .	NPUTETI	ESI COMP DA	ጥ • ጓ	and a set
36	BINARYP	file	name	is U1:[S	CBABB . NO	NLIN.	INPUTFII	ES] BINARYP	.DAT:2	1 17 - 18 - 19 - 19 - 19 - 19 - 19 - 19 - 19
37	TERNARY	P file	name	is Ul:[S	CBABB . NO	NLIN.	INPUTFII	ES] TERNARY	P.DAT;1	
38	LAMBDA	file	name	is U1:[S	CBABB.NO	NLIN.J	INPUTFII	ES] LAMBDA.	DAT;1	
39										
40	n	ion-idea	l eie	ctroiyte	paramete	ers				
41	e	ingle e	lectr	olvte na	rameters					A DESCRIPTION OF THE OWNER OWNER OF THE OWNER OWNER OF THE OWNER
43	Na+	0H-		01]00 PH	0.08640	0.2	25300	0.00000	0.00440	
44	Na+	C104	! -		0.05540	0.2	27550	0.00000	-0.00118	
45	Th++++	OH-			0.00000	0.0	0000	0.00000	0.00000	
46	Th++++	C104	i —		1.18600	27.3	30000	0.00000	-0.05660	
47	H+	OH-			0.00000	0.0	00000	0.00000	0.00000	
48	H+	C104	1 -		0.17470	0.2	29310	0.00000	0.00819	
49 60	+	OTNOTIV (alect	rolyte o	aramotors					- we
51	-	ernary .		rorace b	arametere					
52						OH	i-	C104-		
50	Na+	Th++	+++		0.42000	Ο.	00000	0.00000		
54	Na+	H+			0.03600	0.	.00000	-0.01600		
55	Th++++	H+			0.60000	0.	00000	0.00000		
5ê								m b		
57	04-	C10	-	_	0 03200	Na O	00000	0 00000	n nonor	
эс 59	Un-	CT04		-	0.05200	υ.		0.00000	0.00000	,
60	TOTAL NU	UMBER OF	SPEC	CIES = '	7					
61	NUMBER C	OF COMPO	NENTS	; = (6					
62	INDEPENI	DENT CON	ISTRAI	NTS = 3	5					
63					D N G T					
64 94		SOLVE	NT EX	TRACTION	DATA					
C D										

60	input molalities	
67	-	
69		
80		
C9		
11.1 No.	3.070E-01 2.120E-05 1.000E-07 1.000E-07 3.070E-01	
1	3.070E-01 2.120E-05 1.000E-07 1.000E-07 3.070E-01	
72	1.035E+00 5.940E-05 1.000E-07 1.000E-07 1.035E+00	
73	1.035E+00 5.810E-05 1.000E-07 1.000E-07 1.035E+00	
74	2.129E+00 1.690E-04 1.000E-07 1.000E-07 2.129E+00	
75	2.129E+00 1.690E-04 1.000E-07 1.000E-07 2.129E+00	
76	3.322E+00 3.150E-04 1.000E-07 1.000E-07 3.322E+00	
77	3.322E+00 3.390E-04 1.000E-07 1.000E-07 3.322E+00	
78	4.657E+00 9.450E-04 1.000E-07 1.000E-07 4.657E+00	
79	4.657E+00 9.450E-04 1.000E-07 1.000E-07 4.657E+00	
80	6.176E+00 1.260E-03 1.000E-07 1.000E-07 6.176E+00	
61 01	6.176F+00 1 $450F-03$ 1 $000F-07$ 1 $000F-07$ 6 $176F+00$	
01 00		
62	9.9292700 1.9302-03 1.0002-07 1.0002-07 9.9292700	
9 3	9.9292+00 2.1902-03 1.0002-07 1.0002-07 9.9292+00	
64	1.492E+01 2.330E-03 1.000E-07 1.000E-07 1.492E+01	
£ 5	1.492E+01 2.290E-03 1.000E-07 1.000E-07 1.492E+01	
8ĉ		
87	-1.2065E+02 1.1860E+00 -1.4100E-02	
68	L2 NORM OF THE RESIDUALS 2.3701936E+01	
<u>89</u>		
90		
91		
3) 20	-1 20655+02 7 66505-01 -1 41345-02	
~	$1.2003 \pm 10^{2} \text{ MOD MOR THE DESTRIATE 5 $967175E_01}$	
30	E2 NORM OF THE RESIDERES 5.000/17/5E-01	
94		
95		
96		
97	-1.2065E+02 7.6650E-01 -1.4134E-02	
98	L2 NORM OF THE RESIDUALS 5.8867175E-01	
39		
100		
101		
102	ADTICTED PARAMETERS	
100	Nat/ThittEY1 _1 20653755102	
103	uOrt (Na+/Th+++EX) -1.2065375E+02	
103	uOrt(Na+/Th+++EX) -1.2065375E+02 b0(Th++++ Cl04-) 7.6649537E-01	
103 104 105	u0rt(Na+/Th+++EX) -1.2065375E+02 b0(Th++++ Cl04-) 7.6649537E-01 cmx(Th++++ Cl04-) -1.4134295E-02	
103 104 105 106	u0rt (Na+/Th+++EX) -1.2065375E+02 b0 (Th++++ Cl04- 7.6649537E-01 cmx (Th++++ Cl04- -1.4134295E-02	
103 104 105 106 107	u0rt(Na+/Th+++EX) -1.2065375E+02 b0(Th++++ Cl04-) cmx(Th++++ Cl04-) DATA SET(1)	
102 103 104 105 106 107 108	u0rt(Na+/Th+++EX) -1.2065375E+02 b0(Th++++ Cl04-) 7.6649537E-01 cmx(Th++++ Cl04-) -1.4134295E-02 DATA SET(1)	
102 103 104 105 106 107 108 109	uOrt(Na+/Th++++EX) -1.2065375E+02 b0(Th++++ ClO4-) 7.6649537E-01 cmx(Th++++ ClO4-) -1.4134295E-02 DATA SET(1) input calc diff	
103 104 105 106 107 108 109 110	uOrt(Na+/Th+++EX) -1.2065375E+02 b0(Th++++ ClO4-) 7.6649537E-01 cmx(Th++++ ClO4-) -1.4134295E-02 DATA SET(1) input calc diff 1.00000000000000000000000000000000000	
103 104 105 106 107 108 109 110 111	UOTt(Na+/Th+++EX) -1.2065375E+02 b0(Th++++ Cl04-) 7.6649537E-01 cmx(Th++++ Cl04-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000000E-005 0.101481694490094 1.00000000000000E-005 0.101481694490094	
103 104 105 106 107 108 109 110 111 111	UOTt (Na+/Th+++EX) -1.2065375E+02 b0 (Th++++ Cl04-) 7.6649537E-01 cmx (Th++++ Cl04-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000000000000000000000000000	
102 103 104 105 106 107 108 109 110 111 111 112 113	UOTT (Na+/Th++++EX) -1.2065375E+02 b0 (Th++++ Cl04-) 7.6649537E-01 cmx (Th++++ Cl04-) -1.4134295E-02 DATA SET (1) input calc diff 1.00000000000000E-005 0.101481694490094 1.00000000000000E-005 -0.220537193518512 1.00000000000000E-005 -0.242559039934136	
103 104 105 106 107 108 109 110 111 111 112 113 114	Nocontep Friderities u0rt(Na+/Th+++EX) b0(Th+++ cmx(Th+++ Cl04-) -1.4134295E-02 DATA SET(1) Input calc diff 1.00000000000000E-005 0.101481694490094 1.00000000000000E-005 -0.220537193518512 1.00000000000000E-005 -0.242559039934136 1.0000000000000E-005 6.301298267648374E-002	
102 103 104 105 106 107 108 109 110 111 111 112 113 114	u0rt(Na+/Th+++EX) -1.2065375E+02 b0(Th+++ Cl04-) 7.6649537E-01 cmx(Th+++ Cl04-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000000000000000000000000000	
102 103 104 105 106 107 108 109 110 111 111 112 113 114 115	u0rt(Na+/Th++++EX) -1.2065375E+02 b0(Th++++ Cl04-) 7.6649537E-01 cmx(Th++++ Cl04-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000000000000000000000000000	
102 103 104 105 106 107 108 109 110 111 111 112 113 114 115 116	u0rt(Na+/Th++++EX) -1.2065375E+02 b0(Th++++ Cl04-) 7.6649537E-01 cmx(Th++++ Cl04-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000000000000000000000000000	
102 103 104 105 106 107 108 109 110 111 111 112 113 114 115 116 117	u0rt(Na+/Th++++EX) -1.2065375E+02 b0(Th++++ Cl04-) 7.6649537E-01 cmx(Th++++ Cl04-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000000000000000000000000000	
102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118	Notified Finite u0rt(Na+/Th++++EX) -1.2065375E+02 b0(Th++++ Cl04- > 7.6649537E-01 cmx(Th++++ Cl04-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000000000000000000000000000	
102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119	u0rt(Na+/Th++++EX) -1.2065375E+02 b0(Th++++ Cl04-) 7.6649537E-01 cmx(Th++++ Cl04-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000000000000000000000000000	
102 103 104 105 106 107 108 109 110 111 111 112 113 114 115 116 117 119 119 120	u0rt(Na+/Th++++EX) -1.2065375E+02 b0(Th++++ Cl04-) 7.6649537E-01 cmx(Th++++ Cl04-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000000000000000000000000000	
102 103 104 105 106 107 108 109 110 111 111 112 113 114 115 116 117 119 1120 120 121	u0rt(Na+/Th++++EX) -1.2065375E+02 b0(Th++++ Cl04-) 7.6649537E-01 cmx(Th++++ Cl04-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000000000000000000000000000	
102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122	u0rt(Na+/Th++++EX) -1.2065375E+02 b0(Th++++ Cl04-) 7.6649537E-01 cmx(Th++++ Cl04-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000000000000000000000000000	
102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 123	u0rt(Na+/Th++++EX) -1.2065375E+02 b0(Th++++ Cl04-) 7.6649537E-01 cmx(Th++++ Cl04-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000000000000000000000000000	
102 103 104 105 106 107 108 109 110 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124	u0rt(Na+/Th++++EX) -1.2065375E+02 b0(Th++++ Cl04- > 7.6649537E-01 cmx(Th++++ Cl04-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000000000000000000000000000	
102 103 104 105 106 107 108 109 110 111 111 112 113 114 115 116 117 119 120 121 122 123 124 125	u0rt(Na+/Th++++EX) -1.2065375E+02 b0(Th++++ Cl04-) 7.6649537E-01 cmx(Th++++ Cl04-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000000000000000000000000000	
102 103 104 105 106 107 108 109 110 111 111 112 113 114 115 116 117 119 120 121 122 123 124 125 125	u0rt(Na+/Th++++EX) -1.2065375E+02 b0(Th++++ Cl04-) 7.6649537E-01 cmx(Th++++ Cl04-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000000000000000000000000000	
102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 119 120 121 122 123 124 125 126	u0rt(Na+/Th++++EX) -1.2065375E+02 b0(Th++++ Cl04-) 7.66649537E-01 cmx(Th++++ Cl04-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000000000000000000000000000	
102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 119 120 121 122 123 124 125 126 127	u0rt(Na+/Th++++EX) -1.2065375E+02 b0(Th++++ Cl04-) 7.6649537E-01 cmx(Th++++ Cl04-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000000000000000000000000000	
102 103 104 105 106 107 108 109 110 111 111 112 113 114 115 116 117 119 120 121 122 123 124 125 126 127 128	u0rt(Na+/Th++++EX) -1.2065375E+02 b0(Th++++ Cl04-) 7.6649537E-01 cmx(Th++++ Cl04-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000000000000000000000000000	
102 103 104 105 106 107 108 109 110 111 111 112 113 114 115 116 117 119 120 121 122 123 124 125 126 127 128 129	u0rt (Na+/Th+++EX) -1.2065375E+02 b0 (Th++++ Cl04-) 7.6649537E-01 cmx (Th++++ Cl04-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000000000000000000000000000	
102 103 104 105 106 107 108 109 110 111 111 112 113 114 115 116 117 119 120 121 122 123 124 125 126 127 128 129 130	<pre>ND000000000000000000000000000000000000</pre>	
102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 127 129 130 131	<pre>November FARMETERS uOrt (</pre>	
102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 119 120 121 122 124 125 126 127 129 130 131 132	<pre>Notice Final Fields u0rt (</pre>	
102 103 104 105 106 107 108 109 110 111 111 112 113 114 115 116 117 119 120 121 122 124 125 126 127 128 129 131 132 133	u0rt(Na+/Th++++EX) -1.2065375E+02 b0(Th++++ ClO4-) 7.6649537E-01 cmx(Th++++ ClO4-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000000000000000000000000000	
102 103 104 105 106 107 108 109 110 111 111 112 113 114 115 116 117 119 120 121 122 123 124 125 129 130 131 132 133 134	uOrt(Na+/Th++++EX) -1.2065375E+02 b0(Th++++ Cl04-) 7.6649537E-01 cmx(Th++++ Cl04-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000000000000000000000000000	
102 103 104 105 106 107 108 109 110 111 111 112 113 114 115 116 117 119 120 121 122 123 124 125 129 130 131 132 3 134 135	uOrt(Na+/Th+++EX) -1.2065375E+02 b0(Th++++ ClO4-) 7.6649537E-01 cmx(Th++++ ClO4-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000E-005 0.101481694490094) .000000000000000000000000000000000000	
102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 119 120 121 122 123 124 125 127 129 130 131 132 134 135 136	uOrt(Na+/Th+++EX) -1.2065375E+02 b0(Th++++ ClO4-) 7.6649537E-01 cmx(Th++++ ClO4-) -1.4134295E-02 DATA SET(1) input calc diff 1.000000000000000000000000000000000000	

137	1.035E+00	5.8106-05	1.346E-07	1.346E-0/	1.035E+00
138	2.129E+00	1.690E-04	1.157E-07	1.157E-07	2.129E+00
139	2.129E+00	1.690E-04	1.157E-07	1.157E-07	2.129E+00
1/0	3 3225+00	3 1505-04	9 3265-08	9 326E-08	3 3225+00
140	3.3222+00	0.1000-04	2.326 <u>5</u> -00	9.3200-00	3.3225+00
141	3.322E+00	3.3908-04	9.32/E-08	9.327E-08	3.322E+00
142	4.657E+00	9.450E-04	7.150E-08	7.150E-08	4.657E+00
143	4 657E+00	9.450E-04	7.150E - 08	7.150E-08	4.657E+00
	6 1765-00	1 2605-02	5 1015 00	E 101E-00	6 1765:00
يعفرا	0.1/05+00	1.2006-03	5.191E-00	5.1916-00	0.1765+00
145	6.176E+00	1.450E-03	5.194E-08	5.194E~08	6.176E+00
146	9,929E+00	1.930E-03	2.303E-08	2.303E-08	9.929E+00
1.17	9 9295+00	2 1905-03	2 303E-08	2 303E-08	9 929E+00
()	1 4000-00	2.2000 03	2.00000 00	0.0070.00	1 4035101
148	1.4926+01	2.3306-03	8.00/E-09	8.00/E-09	1.4926+01
149	1.492E+01	2.290E-03	8.007E-09	8.007E-09	1.492E+01
150					
151	ETNAT TOC N	CTTVTTTCC			
121	LINYP DOG Y				
152					
153	Nat	Th++++	H+	OH-	C104~
164	-6 693E-01	-5.330E+00	-6.977E+00	-7.024E+00	-6.689E-01
104	6.0000 01	- E 2202+00	6 9775.00	-7 0245+00	-6 6905-01
156	-0.693E-01	-2.3305+00	-0.97/E+00	-/.0246+00	-0.0092-01
156	-1.884E-01	-3.547E+00	-6.933E+00	-7.078E+00	-1.879E-01
157	-1.884E-01	-3.556E+00	-6.933E+00	-7.078E+00	-1.879£-01
160	1 1025-01	-2 2295+00	-6 8755+00	-7 153E+00	1 1126-01
108	1.1025-01	-2.2296+00	-0.0735700	-1.1335+00	1.1126-01
159	1.102E-01	-2.229E+00	-6.8/5E+00 ·	-/.153E+00	1.1126-01
160	3.088E-01	-1.509E+00	-6.820E+00 ·	-7.227E+00	3.102E-01
161	3 0875-01	-1 478E+00	-6.820E+00	-7 227E+00	3.1036-01
101	1 2202 01	1.100000	6.7600.00	7.2272700	5.105D 01
162	4./19E-01	-/.0386-01	-0.709E+00	-/.3U2E+00	4.7546-01
163	4.719E-01	-7.038E-01	-6.769E+00 ·	-7.302E+00	4.754E-01
164	6.210E-01	-2.366E-01	-6.724E+00 ·	-7.376E+00	6.247E-01
165	6 207E-01	-1 7958-01	-6 7248+00	-7 376F+00	6 2515-01
100	0.2072-01	-1.7935-01	-0.7242+00	-7.370E+00	0.2310-01
186	9.022E-01	8.118E-01	-6.669E+00 ·	-7.511E+00	9.062E-01
167	9.019E-01	8.633E-01	-6.669E+00 ·	-7.511E+00	9.065E-01
168	1 172E+00	2.017E+00	-6.719E+00	-7.581E+00	1.176E+00
	1 1725:00	2 0106+00	-6 7100.00	-7 6915+00	1 1758+00
(Det	1.1/28+00	2.0105-00	-0.7195+00	-/.5016+00	1.1/36+00
170					
171	Calculated I	Log Activity	Coefficient	ts	
172					
172	N - 1		7 7 ±	011-	C104-
172 173	Na+	Th++++	H+	он-	C104-
172 173 174	Na+ -0.1564	Th++++ 4 -0.656	H+ 55 -0.112	он- 29 -0.	ClO4- 1593 -0.1561
172 173 174 175	Na+ -0.1564 -0.1564	Th++++ 4 -0.656 4 -0.656	H+ 55 -0.112 55 -0.112	он- 29 -0. 29 -0.	ClO4- 1593 -0.1561 1593 -0.1561
172 173 174 175	Na+ -0.1564 -0.1564	Th++++ 4 -0.656 4 -0.656	H+ 55 -0.112 55 -0.112	OH- 29 -0. 29 -0.	C104- 1593 -0.1561 1593 -0.1561 2074 -0.2028
172 173 174 175 176	Na+ -0.1564 -0.2034	Th++++ 4 -0.656 9 -0.656 4 0.679	H+ 55 -0.112 55 -0.112 97 -0.06	OH- 29 -0. 29 -0. 22 -0.	C104- 1593 -0.1561 1593 -0.1561 2074 -0.2028
172 173 174 175 176 177	Na+ -0.1564 -0.1564 -0.2034 -0.2034	Th++++ 4 -0.656 4 -0.656 4 0.679 4 0.679	H+ 55 -0.112 55 -0.112 97 -0.062 97 -0.062	OH- 29 -0. 29 -0. 22 -0. 22 -0.	Cl04- 1593 -0.1561 1593 -0.1561 2074 -0.2028 2074 -0.2028
172 173 174 175 176 177 178	Na+ -0.1564 -0.2034 -0.2034 -0.2180	Th++++ 4 -0.656 4 -0.656 4 0.679 4 0.679 0 1.543	H+ 55 -0.112 55 -0.112 97 -0.062 97 -0.062 90 0.062	OH- 29 -0. 29 -0. 22 -0. 22 -0. 22 -0. 22 -0.	Cl04- 1593 -0.1561 1593 -0.1561 2074 -0.2028 2074 -0.2028 2164 -0.2170
172 173 174 175 176 177 178 179	Na+ -0.1564 -0.2034 -0.2034 -0.2180 -0.2180	Th++++ 4 -0.656 4 -0.656 4 0.679 4 0.679 0 1.543	H+ 55 -0.112 55 -0.112 57 -0.062 57 -0.062 50 0.062 50 0.062	OH- 29 -0. 29 -0. 22 -0. 22 -0. 22 -0. 22 -0.	C104- 1593 -0.1561 1593 -0.1561 2074 -0.2028 2074 -0.2028 2164 -0.2170 2164 -0.2170
172 173 174 175 176 177 178 179	Na+ -0.1564 -0.2034 -0.2034 -0.2180 -0.2180	Th++++ 4 -0.656 4 -0.656 4 0.679 4 0.679 0 1.543 0 1.543	H+ 55 -0.112 55 -0.112 57 -0.062 57 -0.062 50 0.062 50 0.062 50 0.062	OH- 29 -0. 29 -0. 22 -0. 22 -0. 22 -0. 22 -0. 22 -0.	C104- 1593 -0.1561 1593 -0.1561 2074 -0.2028 2074 -0.2028 2164 -0.2170 2164 -0.2170
172 173 174 175 176 177 178 179 180	Na+ -0.1564 -0.2034 -0.2034 -0.2180 -0.2180 -0.2180 -0.2120	Th++++ 4 -0.656 4 -0.656 4 0.679 4 0.679 0 1.543 0 1.543 5 1.992	H+ 55 -0.112 55 -0.112 57 -0.062 57 -0.062 50 0.062 50 0.062 57 0.210	OH- 29 -0. 29 -0. 22 -0. 22 -0. 22 -0. 22 -0. 22 -0. 22 -0.	Cl04- 1593 -0.1561 1593 -0.2028 2074 -0.2028 2164 -0.2170 2164 -0.2170 1970 -0.2112
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172 173 174 175 176 177 178 179 180 181 182	Na+ -0.1564 -0.2034 -0.2034 -0.2180 -0.2180 -0.2180 -0.2126 -0.2127 -0.1962	Th++++ 4 -0.656 4 -0.656 4 0.679 4 0.679 0 1.543 0 1.543 0 1.543 6 1.992 7 1.992 2 2.320	H+ 55 -0.112 55 -0.112 57 -0.062 57 -0.062 50 0.062 50 0.062 57 0.210 57 0.210 57 0.370 50 0.370	OH- 29 -0. 29 -0. 22 -0. 22 -0. 22 -0. 22 -0. 22 -0. 0. 5 -0. 69 -0.	C104- 1593 -0.1561 1593 -0.2028 2074 -0.2028 2164 -0.2170 2164 -0.2170 1970 -0.2112 1971 -0.2111 1560 -0.1927
172 173 174 175 176 177 178 179 180 181 192 183	Na+ -0.1564 -0.2034 -0.2034 -0.2180 -0.2180 -0.2126 -0.2127 -0.2127 -0.1962	Th++++ 4 -0.656 4 -0.656 4 0.679 5 1.543 5 1.992 7 1.991 2 2.320 2 2.320	H+ 55 -0.112 55 -0.112 57 -0.062 57 -0.062 50 0.062 50 0.062 50 0.210 59 0.210 59 0.210 57 0.370 57 0.370	OH- 29 -0. 22 -0. 22 -0. 22 -0. 22 -0. 22 -0. 05 -0. 05 -0. 69 -0.	Cl04- 1593 -0.1561 2074 -0.2028 2074 -0.2028 2164 -0.2170 2164 -0.2170 1970 -0.2112 1971 -0.2111 1560 -0.1927
172 173 174 175 176 177 178 179 180 181 182 182	Na+ -0.1564 -0.2034 -0.2034 -0.2180 -0.2180 -0.2126 -0.2127 -0.1962 -0.1962 -0.1962	Th++++ 4 -0.656 4 -0.656 4 0.679 4 0.679 5 1.543 5 1.992 7 1.991 2 2.320 2 2.320	H+ 55 -0.112 55 -0.112 57 -0.062 57 -0.062 50 0.062 50 0.062	OH- 29 -0. 22 -0. 22 -0. 22 -0. 22 -0. 22 -0. 05 -0. 05 -0. 69 -0. 69 -0.	Cl04- 1593 -0.1561 1593 -0.2028 2074 -0.2028 2074 -0.2170 2164 -0.2170 2164 -0.2170 1970 -0.2112 1971 -0.2111 1560 -0.1927 1560 -0.1927 1560 -0.1927
172 173 174 175 176 177 178 179 180 181 182 183 184	Na+ -0.1564 -0.2034 -0.2034 -0.2180 -0.2180 -0.2120 -0.2127 -0.1962 -0.1962 -0.1962	Th++++ 4 -0.656 4 0.679 4 0.679 5 1.543 5 1.992 7 1.991 2 2.320 7 2.663	H+ 55 -0.112 55 -0.112 57 -0.062 57 -0.062 50 0.062 50 0.062 50 0.062 57 0.210 57 0.210 57 0.376 50 0.566 50 0.566	OH- 29 -0. 29 -0. 22 -0. 22 -0. 22 -0. 22 -0. 22 -0. 05 -0. 05 -0. 69 -0. 11 -0.	C104- 1593 -0.1561 1593 -0.2028 2074 -0.2028 2164 -0.2170 2164 -0.2170 1970 -0.2112 1971 -0.2111 1560 -0.1927 1560 -0.1927 0912 -0.1660
172 173 174 175 176 177 178 179 180 181 182 183 184 185	Na+ -0.1564 -0.2034 -0.2034 -0.2180 -0.2180 -0.2127 -0.2127 -0.1962 -0.1962 -0.1962 -0.1962 -0.1962	Th++++ 4 -0.656 4 0.679 4 0.679 5 1.543 5 1.992 7 1.991 2 2.320 2 2.659	H+ 55 -0.112 55 -0.112 57 -0.062 50 0.062 50 0.062 50 0.062 50 0.062 50 0.062 50 0.062 50 0.062 50 0.216 50 0.216 50 0.216 50 0.256 50 0.566 50 0.566	OH- 29 -0. 29 -0. 22 -0. 22 -0. 22 -0. 22 -0. 22 -0. 5 -0. 5 -0. 69 -0. 11 -0. 09 -0.	C104- 1593 -0.1561 1593 -0.2028 2074 -0.2028 2164 -0.2170 2164 -0.2170 1970 -0.2112 1971 -0.2111 1560 -0.1927 1560 -0.1927 0912 -0.1660 0914 -0.1657
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172 173 174 175 176 177 178 180 181 182 183 184 185 186 187 198 188 189 191 192 193 194 195 196 196 197 198 199 200 201 202 203 203	Na+ -0.1564 -0.2034 -0.2034 -0.2180 -0.2180 -0.2127 -0.1962 -0.1962 -0.1962 -0.1962 -0.1962 -0.1967 -0.1962 -0.1967 -0.1962 -0.0956 -0.0017 -0.0046 SOLVENT EXTH uOrt (b0 (cmx (DATA SET (1 input of 1.00000000 1.00000000 1.00000000 1.00000000	Th++++ 4 -0.656 4 0.679 4 0.679 4 0.679 5 1.992 7 1.991 2 2.320 7 2.663 0 2.659 8 3.526 0 3.522 7 4.649 5 4.650 RACTION SYST Th++ Th+- 1) calc dis 0000000E-005 0000000E-005 0000000E-005 0000000E-005 000000E-005 0000000E-005 0000000E-005 00000E-005 000000E-005 000000E-005 00000E-005 00000E-005 00000E-005 00000E-005 00000E-005 00000E-005 0000E-005 0000E-005 0000E-005 0000E-005 0000E-005 00000E-005 00000E-005 000E-005 000E-005 0	H+ 55 -0.112 55 -0.112 57 -0.062 57 -0.062 50 0.062 50 0.062 50 0.062 50 0.210 50 0.200 50 0.2000 50 0.2000 50 0.2000 50 0.2000 50 0.2000 50 0.2000 50	OH- 29 -0. 29 -0. 22 -0. 22 -0. 22 -0. 22 -0. 22 -0. 22 -0. 5 -0. 69 -0. 69 -0. 11 -0. 87 0. 86 0. 81 0. ATED ATED //Th+++EX) 4-) 00000000E+ 0000000E+ 0000000E+	Cl04- 1593 -0.1561 2074 -0.2028 2074 -0.2028 2164 -0.2170 2164 -0.2170 1970 -0.2112 1971 -0.2111 1560 -0.1927 1560 -0.1927 0912 -0.1660 0914 -0.1657 1267 -0.0907 1266 -0.0904 5156 0.0019 5156 0.0019 5156 0.0018 -1.2065375E+02 7.6649537E-01 -1.4134295E-02 000 000 000 000 000 000 000
172 173 174 175 176 177 180 181 182 183 184 185 186 187 198 188 186 187 198 188 186 190 191 192 194 195 196 196 196 200 201 202 203 204	Na+ -0.1564 -0.2034 -0.2034 -0.2034 -0.2126 -0.2126 -0.2127 -0.1962 -0.1962 -0.1962 -0.1962 -0.1962 -0.1962 -0.1962 -0.1962 -0.1962 -0.0956 -0.0017 -0.0016 SOLVENT EXTH uOrt (b0 (cmx (DATA SET (] input co 1.00000000 1.00000000 1.00000000 1.00000000	Th++++ 4 -0.656 4 0.679 4 0.679 5 1.543 5 1.992 7 2.659 8 3.526 7 2.659 8 3.526 7 2.659 8 3.526 7 4.649 5 4.650 RACTION SYST Th++ Th+- 1) calc di 0000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 0000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 0000000E-005 000000E-005 0000000E-005 0000000E-005 0000000E-005 0000000E-005 0000000E-005 0000000E-005 0000000E-005 0000000E-005 0000000E-005 0000000E-005 0000000E-005 0000000E-005 0000000E-005 0000000E-005 0000000E-005 000000E-005 0000000E-005 0000000E-005 0000000E-005 0000000E-005 0000000E-005 0000000E-005 0000000E-005 0000000E-005 0000000E-005 0000000E-005 0000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 00000E-005 000000E-005 00000E-005 00000E-005 00000E-005 00000E-005 00000E-005 00000E-005 00000E-005 00000E-005 00000E-005 0000E-005 00000E-005 00000E-005 000E	H+ 55 -0.112 55 -0.112 57 -0.062 57 -0.062 50 0.062 50 0.062 57 0.210 57 0.370 50 0.562 59 0.968 59 0.968 59 0.968 59 1.378 50 EQUILIBRA Na+ +++ Cloc 50 0.0000000 50.00000000 50.0000000 50.0000000 50.0000000 50.0000000 50.00000000 50.00000000 50.00000000 50.00000000 50.0000000 50.00000000 50.0000000 50.0000000 50.0000000 50.0000000 50.0000000 50.0000000 50.0000000 50.0000000 50.00000000 50.0000000 50.00000000 50.0000000000	OH- 29 -0. 29 -0. 22 -0. 22 -0. 22 -0. 22 -0. 22 -0. 22 -0. 22 -0. 5 -0. 69 -0. 69 -0. 11 -0. 87 0. 86 0. 81 0. ATED -/Th++++EX) 4-) 4-) 00000000E+ 0000000E+ 0000000E+ 0000000E+	ClO4- 1593 -0.1561 1593 -0.1561 2074 -0.2028 2074 -0.2028 2164 -0.2170 2164 -0.2170 1970 -0.2112 1971 -0.2111 1560 -0.1927 1560 -0.1927 0912 -0.1660 0914 -0.1657 1267 -0.0907 1266 -0.0904 5156 0.0019 5156 0.0019 5156 0.0018 -1.2065375E+02 7.6649537E-01 -1.4134295E-02 000 000 000 000 000 000 000
172 173 174 175 176 177 178 180 181 182 183 184 185 186 187 198 188 189 190 191 192 193 194 195 196 197 196 199 200 201 202 203 204 205 206	Na+ -0.1564 -0.2034 -0.2034 -0.2034 -0.2180 -0.2180 -0.2126 -0.2127 -0.1962 -0.1962 -0.1962 -0.1962 -0.0946 -0.0950 -0.0017 -0.0016 SOLVENT EXTH uOrt (b0 (cmx (DATA SET (1) input c 1.00000000 1.00000000 1.00000000 1.00000000	Th++++ 4 -0.656 4 0.679 4 0.679 0 1.543 5 1.992 7 2.662 8 3.526 7 2.665 8 3.526 7 2.655 8 3.526 7 4.649 5 4.650 RACTION SYST Th++ Th+- 1) calc di 0000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 0000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 00000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 000000E-005 00000E-005 00000E-005 00000E-005 00000E-005 00000E-005 00000E-005 0000E-005 0000E-005 0000E-005 0000E-005 0000E-005 0000E-005 0000E-005 0000E-005 0000E-	H+ 55 -0.112 55 -0.112 57 -0.062 57 -0.062 50 0.062 50 0.062 50 0.216 50 0.2000 50 0.20000 50 0.20000 50 0.20000000000000000000000000000000000	OH- 29 -0. 29 -0. 22 -0. 22 -0. 22 -0. 22 -0. 22 -0. 22 -0. 22 -0. 59 -0. 69 -0. 11 -0. 09 -0. 86 0. 80 0. 81 0. ATED -/Th++++EX) 4-) 00000000E+ 00000000E+ 0000000E+ 0000000E+ 0000000E+ 0000000E+ 0000000E+ 0000000E+ 0000000E+ 0000000E+ 0000000E+ 0000000E+ 0000000E+ 0000000E+ 00000000E+ 0000000E+ 0000000E+ 0000000E+ 0000000E+ 0000000E+ 0000000E+ 0000000E+ 0000000E+ 0000000E+ 0000000E+ 0000000E+ 0000000E+ 0000000E+ 000000000E+ 000000000E+ 0000000000	ClO4- 1593 -0.1561 1593 -0.2028 2074 -0.2028 2164 -0.2170 2164 -0.2170 1970 -0.2112 1971 -0.2111 1560 -0.1927 1560 -0.1927 0912 -0.1660 0914 -0.1657 1267 -0.0907 1266 -0.0904 5156 0.0019 5156 0.0019 5156 0.0018 -1.2065375E+02 7.6649537E-01 -1.4134295E-02 000 000 000 000 000 000 000





208	1.000000000000000	005 0.000000	000000005+000	
209	1.000000000000000000	005 0.000000	000000000E+000	
210	1.0000000000000000E-	005 0.000000	000000000E+000	
211	-30000000000000000	005 0.000000	nnnnnnnn e +nnn	
212	1 000000000000000000	005 0 000000	000000000000000000000000000000000000000	
212	1.00000000000000000		000000000000000000000000000000000000000	
213	1.00000000000000000	005 0.000000	000000000000000000000000000000000000000	
214	1.00000000000000000E-	005 0.000000	000000000E+000	
215				
216	AVERAGE DEVIATION	= 0.0000E+00		
217				
217	CONSIDE STUDETON	- 0.00000.00		
218	STANDARD DEVIATION	= 0,0000E+00		
219				
220	FINAL MOLALITIES			
221				
222	Nat Th+++	H+	08-	C104~
0000	3 0705-01 1 9165-	05 1 3675-07	1 3675-07 3	0708-01
22.3	3.070E-01 1.910E-	05 1.3075-07	1.3076-07 3	0705-01
224	3.070E-01 1.916E-	05 1.367E-07	1.36/E-0/ 3	.070E-01
225	1,035E+00 7.409E-	05 1.346E-07	1.346E-07 1	.035E+00
226	1.035E+00 7.409E-	05 1.346E-07	1.346E-07 1	.035E+00
227	2 129E+00 1 586E-	04 1.157E-07	1 157E-07 2	1296+00
200	2 1295+00 1 5865-	04 1 1575-07	1 1575-07 2	1205+00
225	2.129E+00 1.386E-	04 1.13/5-0/	1.1576-07 2	-1295+00
229	3.322E+00 3.514E-	04 9-328E-08	9.328E-08 3	.3226+00
230	3.322E+00 3.516E-	04 9.328E-08	9.328E-08 3	.322E+00
231	4,658E+00 7.374E-	04 7.145E-08	7.145E-08 4	.657E+00
232	4 658E+00 7 374E-	04 7.145E-08	7 1455-08 4	.657£+00
	6 126E:00 1 332E-		5 1025-00 6	1765+00
2.30	6.176E+00 1.332E-	05 5.1925-08	5.1922-08 0	1705700
234	6.176E+00 1.336E-	03 5.192E-08	5.192E-08 6	.1/6E+00
225	9.927E+00 2.443E-	03 2.305E-08	2.305E-08 9	.929E+00
236	9.928E+00 2.449E-	03 2.304E-08	2.304E-08 9	.9298+00
227	1 492E+01 2.190E-	03 8,006E-09	8.006E-09 1	4926+01
220	1 4025+01 2 1005-	03 8 0065-09	8 006E-09 1	4925-01
230	1.4926+01 2.1906-	02 010002-03	8.000E-09 I	. 4526401
2.9				
240	FINAL LOG ACTIVITIES			
241				
242	Na+ Th++++	H+	ОН~	C104-
249	-6 603E-01 -5 374E+	00 -6 9775+00	-7 024E+00 -6	6905-01
240	-0.093E-01 -3.374E+	00 -0.9775+00	-7.0248+00 -0	.0905-01
244	-6.693E-01 -5.3/4E+	00 -6.97/E+00	-7.0242+00 -6	.0906-01
245	-1.885E-01 -3.451E+	00 -6.933E+00	-7.078E+00 -1	.878E-01
248	-1.885E-01 -3.451E+	00 -6.933E+00	-7.078E+00 -1	.878E-01
267	1.102E-01 -2.256E+	00 -6.875E+00	-7.153E+00 1	.112E-01
2/9	1 1025+01 -2 2565+	00 -6 8755+00	-7 1538+00 1	1125-01
240	2 0070 01 1 46004		7 1075-00 7	1025.01
269	3.08/E-01 -1.462E+	00 -6.820E+00	-1.227E+00 3	.1036-01
250	3.087E-01 -1.462E+	00 -6.820E+00	-7.227E+00 3	.103E-01
251	4.724E-01 -8.077E-	01 -6.769E+00	-7.302E+00 4	.750E-01
252	4.724E-01 -8.077E-	01 -6.769E+00	-7.302E+00 4	.750E-01
253	6 209E+01 -2 136E-	01 - 6 724E + 00	-7 376E+00 6	2495-01
254			7 3765:00 6	2405.01
274	6.209E-01 -2.135E-	01 -6.7245+00	-/.3/62+00 6	.249E-01
255	9.016E-01 9.094E-	01 -6.669E+00	-7.511E+00 9	.067E-01
256	9.016E-01 9.095E-	01 -6.669E+00	-7.511E+00 9	.067E-01
257	1.172E+00 1.991E+	00 -6.719E+00	-7.581E+00 1	.175E+00
258	7 172E+00 1 991E+	00 - 6 719E + 00	-7 581E+00 1	1755+00
050	1.1720.00 1.9915.	00 01/201100	7.501 <u>B</u> .00 1	.1,00,00
209				
260	Calculated Log Activ	ity Coefficie	nts	
261				
262	Na+ Th++++	H+	OH-	C104-
253	-0.1564 -0.1	6565 -0 1	-0.159	3 -0 1561
264	-0 1564 -0	6565 =0.11		3 _0 1641
204	-0.1384 -0.4			5 -0.1561
ഷാ	-0.2034 0.	-0.0 191 -0.0	623 -0.207	-0.2027
266	-0.2034 0.1	6792 -0.0	623 -0.207	5 -0.2027
267	-0.2180 1.	5433 0.0	622 -0.216	3 -0.2170
262	-0.2180 1.	5433 0.04	622 -0.216	3 -0.2170
269	-0 2127 1	9918 0.2	104 -0.107	1 _0 0111
~~~				
210	-0.212/ 1.1	5510 0.2	104 -0.19/	-0.2111
271	-0.1958 2.3	3246 0.3	772 -0.155	7 -0.1931
272	-0.1958 2-	3246 0.3	772 -0.155	7 -0.1931
273	-0.1698 2.	6620 0.5	611 -0.091	3 -0.1659
274	-0.1698 2	6609 0.5	610 -0.001	3 -0 1658
375		5215 0.01		
210		U210 U.91	004 U.126	-0.0902
276	-0.0952 3.	5∠U5 0.9	684 0,126	4 -0.0902
277	-0.0016 4.0	6508 1.3	781 0.515	7 0.0017
278	-0.0016 4.0	6509 1.3	781 0.515	7 0.0017




279 280 281	FINAL L2 NORM OF THE RESIDUALS	5.8867175E-01
292 283 284	EXIT PARAMETER	3
285 286 297	FINAL APPROXIMATE SOLUTION	
287 288 289	0 0 7 -1.2065375E+02 1 2 2 7.6649537E-01	
291	4 2 2 ~1.4134295E-02	

.



Appendix K - Sample Output File: SOLUB_01.OUT

See Table 9-1 for explanation of this listing.

```
NONLIN V2.0
 1
 2
       NONLIN was developed by A.R. Felmy
 3
 4
                  file name is U1: [SCBABB.NONLIN.USERGUIDE] SOLUB 01.IN; 1
 5
       INPUT
                  file name is U1:[SCBABB.NONLIN.USERGUIDE] SOLUB 00.GMIN;1
 6
       GMIN
 7
       OUTPUT
                 file name is U1:[SCBABB.NONLIN.USERGUIDE] SOLUB 01.OUT;1
 8
                 AQUEOUS SPECIES
9
tO
          ID
                   NAME
                                    MOLES
                                                     uOrt
11
                                                 Z
         1080H20
                               0.0000000000000
                                                      -95.663
                                                 Ο.
12
13
         1000H+
                              0.000000000000
                                                1.
                                                        0.000
           800H-
                               0.000000000000
                                                -1.
                                                       -63.435
14
          161HSO4-
                               0.000000000000
15
                                                -1.
                                                      -304.942
                              0.000000000000
         1991H2Ox(aq)
                                                 0.
                                                     -284.990
16
                 SOLID PHASES
17
18
          ĪÐ
                   NAME
                                    MOLES
                                                     uOrt
                                                 Z
19
       101990H2Ox.2H2O(s)
                              0.000000000000
                                                      999.999
20
                                                 Ο.
21
                 CONSTRAINT EQUATIONS
22
23
                         0
                                 1
                                         8
                                                16
                                                        99
                         0.0
       H20
                                2.0
                                        1.0
                                                0.0
                                                        0.0
24
25
       H+
                        1.0
                                1.0
                                        0.0
                                                0.0
                                                        0.0
       OH-
                        -1.0
                                1.0
                                        1.0
                                                0.0
                                                        0.0
26
       HSO4-
                        -1.0
                                                1.0
                                                        0.0
                                        4.0
27
                                1.0
22
       H20x (aq)
                        0.0
                                2.0
                                        0.0
                                                0.0
                                                        1.0
       H2Ox.2H2O(s)
                        0.0
                                        2.0
                                                0.0
                                                        1.0
29
                                6.0
30
31
       Closed input files GMIN and COMP
32
32
       COMP
                 file name is U1:[SCBABB.NONLIN.INPUTFILES]COMP.DAT;3
       BINARYP file name is U1:[SCBABB.NONLIN.INPUTFILES] BINARYP.DAT;2
34
       TERNARYP file name is U1:[SCBABB.NONLIN.INPUTFILES] TERNARYP.DAT;1
35
       LAMBDA
                 file name is U1:[SCBABB.NONLIN.INPUTFILES] LAMBDA.DAT;1
36
37
æ
              non-ideal electrolyte parameters
39
40
              single electrolyte parameters
41
                   OH-
                                     0.00000
                                                 0.00000
                                                             0.00000
                                                                         0.00000
     H+
                                                 0.55560
42
     H+
                   8504-
                                     0.20650
                                                             0.00000
                                                                         0.00000
43
              ternary electrolyte parameters
44
45
                                                  H+
48
                                                  0.00000
                                     0.00000
     OH-
                   HSO4-
47
48
              neutral ion parameters
49
50
                  H2Ox (aq)
51
     H+
                         0.0000
                        0.0000
52
     OH-
     HSO4-
                         0.0000
53
                        0.0000
54
     H2Ox(aq)
55
56
               higher order lambdas
57
58
                               OH-
                                            HSO4-
                                     0.00000
                                                 0.00000
59
     H2Ox(aq)
                   H+
60
61
       TOTAL NUMBER OF SPECIES =
                                     6
62
      NUMBER OF COMPONENTS
                                     5
63
       INDEPENDENT CONSTRAINTS =
                                     4
64
                 SOLUBILITY DATA
65
```

H+

input molalities

 H+
 OH HSO4 H2Ox(aq)

 1.168E+00
 8.560E-15
 1.168E+00
 8.750E-01

 1.965E+00
 5.090E-15
 1.965E+00
 6.530E-01

135

136

H+

66 67

68 69

> 2.927E+00 3.420E-15 2.927E+00 5.340E-01 4.450E+00 2.250E-15 4.450E+00 4.760E-01 6.660E+00 1.500E-15 6.660E+00 4.320E-01 9.548E+00 1.050E-15 9.548E+00 5.740E-01 1.394E+01 7.170E-16 1.394E+01 1.268E+00 -1.0000E+01 L2 NORM OF THE RESIDUALS 1.2378927E+03 -4.7788E+02 L2 NORM OF THE RESIDUALS 2.7255679E+00 -4.7788E+02 L2 NORM OF THE RESIDUALS 2.7255679E+00 ADJUSTED PARAMETERS H2Ox.2H2O(s)) -4.7787833E+02 uOrt( DATA SET( 1) input calc diff 0.000000000000000E+000 -0.611447612394127 0.0000000000000000E+000 1.87975307818427 AVERAGE DEVIATION = 8.8417E-01 STANDARD DEVIATION = 1.0302E+00 FINAL MOLALITIES OH-HSO4-H2Ox(aq) 1.168E+00 1.845E-14 1.168E+00 8.750E-01 1.965E+00 9.859E-15 1.965E+00 6.530E-01 2.927E+00 5.247E-15 2.927E+00 5.340E-01 4.450E+00 7.000E-15 4.450E+00 4.760E-01 6.660E+00 7.000E-15 6.660E+00 4.320E-01 9.548E+00 7.000E-15 9.548E+00 5.740E-01 1.394E+01 7.000E-15 1.394E+01 1.268E+00 FINAL LOG ACTIVITIES OH-HSO4-H2Ox (aq) H+ 7.007E-02 -1.409E+01 7.007E-02 -5.799E-02 3.985E-01 -1.444E+01 3.985E-01 -1.851E-01 7.056E-01 -1.477E+01 7.056E-01 -2.725E-01 
>
>  1.114E+00
>  -1.471E+01
>  1.114E+00
>  -3.224E-01
>
>
>  1.636E+00
>  -1.477E+01
>  1.636E+00
>  -3.645E-01
>
>
>  2.265E+00
>  -1.482E+01
>  2.265E+00
>  -2.411E-01
>
>
>  3.168E+00
>  -1.487E+01
>  3.168E+00
>  1.031E-01
>
>  Calculated Log Activity Coefficients

> > HSO4-

H2Ox(aq)

OH-



137	0.0026 -0.3603 0.0026 0.0000
138	0.1051 -0.4330 0.1051 0.0000
139	0.2392 -0.4922 0.2392 0.0000
140	0.4657 -0.5552 0.4657 0.0000
141	0.8128 -0.6145 0.8128 D.0000
142	1.2849 -0.6654 1.2849 0.0000
143	2.0238 -0.7168 2.0238 0.0000
16.	
145	SOLID PHASE NOW IN EQUILIBRIUM
146	
147	DATA SET( 1)
14-	
149	input calc diff
150	0.000000000000000E+000 0.0000000000000E+000
151	0.000000000000000E+000 0.0000000000000E+000
152	0,000000000000000000000000000000000000
153	0,0000000000000000000000000000000000000
154	0,000000000000000000000000000000000000
150	0.00000000000000E+000 0.0000000000000E+000
100	0,000000000000000000000000000000000000
157	AMERACE DEVIATION = $0.0000E+00$
150	AVENUED DEVINITION = 0:00000700
180	STANDARD DEVIATION = $0.0000E\pm00$
161	
182	FINAL MOLALITIES
162	
164	H+ OH- HSO4- H2Ox (ag)
165	1.168E+00 1.777E-14 1.168E+00 2.280E-01
166	1.965E+00 9.589E-15 1.965E+00 2.506E-01
167	2.927E+00 7.000E-15 2.927E+00 2.857E-01
168	4.450E+00 7.000E-15 4.450E+00 3.691E-01
160	6.660E+00 7.000E-15 6.660E+00 5.992E-01
170	9.548E+00 7.000E-15 9.548E+00 1.353E+00
171	1.394E+01 7.000E-15 1.394E+01 5.061E+00
172	
173	FINAL LOG ACTIVITIES
174	
175	H+ OH- HSO4- H2Ox (aq)
176	8.371E-02 -1.410E+01 8.371E-02 -6.319E-01
177	4.087E-01 -1.445E+01 4.087E-01 -5.947E-01
178	7.133E-01 -1.464E+01 7.133E-01 -5.402E-01
179	1.118E+00 -1.4/1E+01 1.118E+00 -4.312E-01
180	1.62/E+00 -1.4//E+01 1.62/E+00 -2.250E-01
181	2.210E+00 -1.483E+01 2.210E+00 1.194E=01
102	2.828E+00 -1.49IE+01 2.828E+00 6.488E-01
163	Colculated Log Activity Coofficients
185	calculated bog Activity Coelectence
196	$H^+$ OH- $HSO4 H2Ox(ag)$
187	0.0163 -0.3532 0.0163 0.0102
198	0.1153 -0.4288 0.1153 0.0063
189	0.2469 -0.4897 0.2469 0.0039
190	0.4700 -0.5541 0.4700 0.0017
191	0.8038 -0.6163 0.8038 -0.0026
192	1.2296 -0.6736 1.2296 -0.0120
193	1.6841 -0.7552 1.6841 -0.0556
194	
195	FINAL L2 NORM OF THE RESIDUALS 2.7255679E+00
196	
197	
198	EXIT PARAMETER 3
199	
200	
201	FINAL APPROXIMATE SOLUTION
202	
203	
2.H	0 0 0 -4.//8/8332+02





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## Appendix L - Review Forms

This Appendix contains the review forms for the NONLIN User's Manual.





**NOTE:** Copies of the User's Manual Reviewer's Forms are available in the Sandia WIPP Central Files.



