530220

Sandia National Laboratories
Waste Isolation Pilot Plant

Calculation of the Quantities of MgO Required for Consumption of CO_2 for the WIPP Compliance Recertification Application

BOE 1.3.5.4.3

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1 ABBREVIATIONS, ACRONYMS, AND INITIALISMS

Table 1 defines the abbreviations, acronyms, and initialisms used in this report.

Table 1. Abbreviations, Acronyms, and Initialisms.

Abbreviation, Acronym, or Initialism	Definition
AMWTP	Advanced Mixed Waste Treatment Project
BRAGFLO	Brine and Gas Flow, a WIPP PA code
brucite	$Mg(OH)_2$
C	carbon
CCA	(WIPP) Compliance Certification Application
CH	contact-handled (transuranic waste)
CPR	cellulosics, plastics, and rubbers
CO_2	carbon dioxide
CRA	(WIPP) Compliance Recertification Application
DOE	(U.S.) Department of Energy
EPA	(U.S.) Environmental Protection Agency
ERDA-6	Energy Research and Development Administration (WIPP Well) 6, a synthetic brine representative of fluids in Castile brine reservoirs
g	gram(s)
GWB	Generic Weep Brine, a synthetic brine representative of intergranular Salado brines
H, H^+	hydrogen, hydrogen ion
hydromagnesite	$Mg_4(CO_3)_3(OH)_2 \cdot 3H_2O$ or $Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$
ID	identification
IN-BN-510	the AMWTP supercompacted waste stream
kg	kilogram(s)
m^3	cubic meter(s)
MgO	magnesium oxide, used to refer to the WIPP engineered barrier, which includes periclase as the primary constituent and ~5-10 wt % impurities
mol	mole(s)
N	nitrogen
NO_3^-	nitrate ion, nitrate
O	oxygen
PA	performance assessment

Table 1. Abbreviations, Acronyms, and Initialisms (cont.).

Abbreviation, Acronym, or Initialism	Definition
periclase	pure, crystalline MgO, the primary constituent of the WIPP engineered barrier
RH	remote-handled (transuranic waste)
S	sulfur
SNL	Sandia National Laboratories
SO_4^{2-}	sulfate ion, sulfate
TRU	transuranic
TWBIR	*Transuranic Waste Baseline Inventory Report* (to be published by Los Alamos national Laboratory)
WIPP	(U.S. DOE) Waste Isolation Pilot Plant

2 INTRODUCTION

This analysis report documents a series of calculations that determine the amount of MgO required to consume the maximum quantity of CO_2 that could be generated from the possible microbial degradation of cellulosics, plastics, and rubbers (CPR) in the Waste Isolation Pilot Plant (WIPP). CPR are present in contact handled (CH) and remote-handled (RH) transuranic waste to be deposited in the WIPP. Similar calculations were previously performed by Peterson (1996) using the CPR inventory reported by U.S. DOE (1996a). The calculations described herein used the inventory updates by Crawford (2003) and Leigh and Crawford (2003) for the U.S. Department of Energy's (DOE's) first WIPP Compliance Recertification Application (CRA).

This work was carried out under the task entitled "Chemical Conditions in the Repository" in Table 2 of Hansen et al. (2003).

Microorganisms in the WIPP would degrade CPR sequentially by the following reaction pathways (Brush, 1990; Brush 1995; Wang and Brush, 1996; Francis et al., 1997):

$$C_6H_{10}O_5 + 4.8H^+ + 4.8NO_3^- \rightarrow 7.4H_2O + 6CO_2 + 2.4N_2; \quad (1)$$

$$C_6H_{10}O_5 + 6H^+ + 3SO_4^{2-} \rightarrow 5H_2O + 6CO_2 + 3H_2S; \quad (2)$$

$$C_6H_{10}O_5 + H_2O \rightarrow 3CH_4 + 3CO_2. \quad (3)$$

Microbial degradation of CPR according to Reaction 1 (denitrification) and Reaction 2 (sulfate reduction) generate 1.00 mol of CO_2 per mol of organic C; Reaction 3 (methanogenesis) yields 0.500 mol of CO_2 per mol of organic C. For the CCA, Wang and Brush (1996) calculated that Reaction 3 will account for over 95% of the (possible) microbial gas generation in the WIPP. They concluded that methanogenesis would be much more important than denitrification and sulfate reduction because the quantity of CPR greatly exceeded those of NO_3^- and SO_4^{2-} at the time of the CCA (U.S. DOE, 1996a). Based on a total quantity of 77,640 metric tons of MgO to be emplaced in the repository in supersacks and minisacks (U.S. DOE, 1996b, Chapter 3) and an effective CO_2 yield consistent with the quantities of CPR, NO_3^-, and SO_4^{2-} estimated by U.S. DOE (1996a), the MgO safety factor (the total quantity of MgO to be emplaced divided by the quantity of CO_2 that could be produced by complete degradation of CPR) was 3.73 at the time of the CCA Brush et al. (2002). The U.S. Environmental Protection Agency (EPA), however, calculated an MgO safety factor of 1.95 at the time of the CCA by assuming that microbial degradation of 1.00 mol of organic C would yield 1.00 ml of CO_2 (Brush et al., 2002).

In July 2000, the DOE proposed the elimination of the MgO minisacks to reduce the risk of injury associated with manual emplacement of the minisacks, and to further reduce exposure to radiation. The EPA approved this change in January 2001 (Marcinowski, 2001). Elimination of the minisacks has resulted in a 15% reduction in the total mass of MgO to be emplaced in the repository (from 77,640 to about 66,000 metric tons), and has reduced the safety factor from 3.73 to 3.23 assuming the proportions of CPR degraded by Reactions 1, 2, and 3 calculated by Brush and Wang (1996), or from 1.95 to 1.67 assuming that microbial degradation of 1.00 mol of organic C produces 1.00 mol of CO_2 (Brush et al. 2002).

Since then, the DOE has not requested and the EPA has not approved any further reductions in the MgO safety factor.

3 CALCULATIONS

All calculations were done using the Microsoft EXCEL 2000 spreadsheet program running Windows 2000. Spreadsheets are entitled "MgOsafetyfactorEPA.XLS," "MgOsafetyfactorSNL.XLS," and "MgOsafetyfactorAMWTP.XLS." The first spreadsheet calculates the MgO safety factor by assuming that microbial degradation of 1.00 mol of organic C generates 1.00 mol of CO_2; the second file assumes 1.00 mol of C yields about 0.500 mol of CO_2; and the third file assumes one panel of the repository is filled entirely with the supercompacted waste stream from the Advanced Mixed Waste Treatment Project (AMWTP) at the Idaho National Engineering and Environmental Laboratory, *Transuranic Waste Baseline Inventory Report* (TWBIR) code ID IN-BN-510.

The EXCEL file MgOsafetyfactorEPA.XLS is divided into four sheets (Appendix A). The sheet tabs are labeled "Moles of MgO Dissolved in Brine,"

"CH CPR," "RH CPR," and "Safety Factor." The sheet Moles of MgO Dissolved in Brine displays calculations of how many moles of MgO dissolve in WIPP brines in equilibrium with brucite ($Mg(OH)_2$) and hydromagnesite ($Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$), the expected hydration and carbonation products of periclase (MgO). The second and third sheets (CH CPR and RH CPR) calculate the maximum moles of CO_2 that could be produced from CH and RH CPR present in the updated TWBIR (Crawford, 2003). The sheet Safety Factor displays the MgO safety factor assuming that microbial degradation of 1.00 mol of organic C produces 1.00 mol of CO_2.

The EXCEL file MgOsafetyfactorSNL.XLS is divided into four sheets (Appendix B). Each sheet has the same tab titles as the previous file. The first, third, and fourth sheets show the same calculations described above. The second sheet (CH CPR) differs by the addition of NO_3^- and SO_4^{2-} present in the CH waste reported in the updated waste baseline inventory report (Leigh and Crawford, 2003). These calculations were performed assuming that microbial degradation would be dominated by methanogenesis (Reaction (3)), by which 1.00 mol of organic C generates 0.500 mol of CO_2.

The EXCEL file MgOsafetyfactorAMWTP.XLS is divided into five sheets (Appendix C). The sheet tabs are labeled "Moles of MgO Dissolved in Brine," "AMWTP CPR," "Safety Factor," "PA Panel Calcs," and "PA Safety Factors." The first three sheets follow identical calculations as the previous two files. The difference is that only the waste stream IN-BN-510 (Gross, 2002) is being considered for these calculations, and we assume that microbial degradation of 1.00 mol of C produces 0.500 mol of CO_2. The fourth sheet (PA Panel Calcs) repeats the calculations of AMWTP CPR, except now the CPR is scaled for one panel instead of for the entire repository. The final sheet (PA Safety Factors) first calculates the safety factor for one panel assuming 1.00 mol of C yields 0.500 mol of CO_2. The lower half of the sheet displays a table that gives safety factors as a function of the IN-BN-510:MgO volumetric ratio, to be used for calculations with the PA code Brine and Gas Flow (BRAGFLO).

These MgO safety factor calculations follow those of Peterson (1996). The first two spreadsheets (MgOsafetyfactorEPA.XLS and MgOsafetyfactorSNL.XLS) are identical, the exception being that the first file assumes that microbial degradation of 1.00 mol of organic C will generate 1.00 mol of CO_2, whereas the second file assumes that 1.00 mol of C yields about 0.500 mol of CO_2.

The first sheet in both files calculates the number of moles of MgO that would dissolve in GWB and ERDA-6. (GWB is a synthetic brine representative of intergranular Salado-Formation brines at or near the stratigraphic horizon of the WIPP; ERDA-6 is an synthetic typical of fluids from brine reservoirs in the underlying Castile Fm.) This is critical to the calculations because in the event of a borehole intrusion, MgO would be lost by dissolution and transport up the borehole, thus reducing the amount available to consume CO_2. Therefore, additional MgO must be added to the final calculated amount in order to account for this possibility. To begin with, the initial and final concentrations of MgO were determined in both GWB and ERDA-6 from EQ3NR calculations

performed by Yongliang Xiong. (These input files are contained in Appendix D.) The results are presented in Table 1.

Table 1. Concentrations of MgO in WIPP Brines Calculated by EQ3NR.

Brine	Initial Conc mol/L	Final Conc in equil with MgO, mol/Kg	Molality to molarity ratio	Final Conc mol/L
GWB	1.000	7.900E-01	1.146	6.893E-01
ERDA-6	0.019	1.004E-01	1.137	8.834E-02

Note that the final MgO concentration of GWB is less than the initial concentration. Therefore, GWB will be excluded from further calculations. The total moles of MgO dissolved in ERDA-6 was determined by the following steps:
(1) The volume of brine to be chemically controlled was assumed to be 1.46×10^5 m^3, the maximum brine flow up the borehole at the upper disturbed-rock-zone S3 scenario (E1 at 1000+ yrs) determined by the computer model BRAGFLO.
(2) The total moles of MgO dissolved in ERDA-6 were obtained by taking the product of the change in concentration (mol/L) x the volume of brine (m^3) x 1000 L/m^3.

The total moles of MgO dissolved in ERDA-6 is 1.01×10^7.

The second sheet in both files determines the maximum moles of CO_2 that could be produced from microbial activity of CPR from CH waste. The updated waste baseline inventory report provides the average densities or CPR per drum of CH waste. Table 2 presents the results.

A molecular weight of 162 g/mol was used by Wang and Brush (1996) for all cellulosics. The average concentration (density) of CPR in the waste in kg/m^3 is provided by Crawford (2003). Brush and Wang (1996) converted the masses of plastics and rubbers to equivalent masses of cellulosics based on the relative quantities of C contained in these materials. They determined that $Q = 1.7\ P + R$. In this equation, Q, P, and R are the masses of cellulosics, plastics, and rubbers in kg (see Wang and Brush, 1996, for more detail). The total volume of CH waste in the repository is from the PA parameter database. Thus the total moles of CO_2 that could be produced from possible microbial activity of CPR from the CH waste is 1.4×10^9.

Table 2. Total Moles of CO_2 That Could Be Produced by Microbial Degradation of CPR.

	Formula wt (g/mol)	Avg density (kg/m3)	Cellulosic equvialent (kg/m3)	CH waste volume m3	weight kg	Total moles of C	Total moles of CO_2
Cellulosics	162	75	75				
Rubber	162	19	19				
Plastics	162	55	94				
Container plastic	162	21	36				
Total Cellulosics			223	1.7E+05	3.8E+07	1.4E+09	1.4E+09

In the second file (MgOsafetyfactorsSNL), the second half of the second sheet (CH CPR) calculates the effects of including the total amount of NO_3^- and SO_4^{2-} in the updated inventory, and the effects of these components on the proportions of CPR degraded by denitrification, sulfate reduction, and methanogenesis (see Reactions 1, 2, and 3 above).

The masses of NO_3^- and SO_4^{2-} are listed in Table 3. To determine the percentages of the total moles of CO_2 produced by Reactions 1, 2, and 3, the total moles of NO_3^- and SO_4^{2-} are divided by the total moles of CO_2 produced from the CPR multiplied by the stoichiometric ratio of C to NO_3^- or SO_4^{2-}, which is finally multiplied by 100. The moles left over are produced by methanogenesis. Thus the molar percentages of cellulosics degraded by denitrification is 3.84%, that degraded by sulfate reduction is 0.86%, and that by methanogenesis is 95.3%.

Table 3. Masses of NO_3^- and SO_4^{2-} in the CH Waste (from Crawford, 2003).

	kg	g	Formula wt. g/mol	Moles
Nitrate	2.66E+06	2.66E+09	62.01	4.29E+07
Sulfate	5.76E+05	5.76E+08	96.06	6.00E+06

The final moles of CO_2 that could be produced from the CPR is equal to (0.0384 + 0.0086 + 0.953/2) x total moles of organic carbon (C) (1.4×10^9).

The third sheet lists the CPR inventory for RH waste and the total moles of CO_2 that could be produced due to possible microbial activity. See Table 4 for results.

Table 4. Total Moles of CO_2 That Could Be Produced by Microbial Activity of RH-Waste CPR.

	Formula wt (g/mol)	Avg density (kg/m3)	Cellulosic equvialent (kg/m3)	volume m3	weight kg	Total moles of C	Total moles of CO_2
Cellulosics	162	6.1	6.1				
Rubber	162	3.6	3.6				
Plastics	162	7.0	12				
Total Cellulosics			22	7.1E+03	1.5E+05	5.7E+06	5.7E+06

The final sheets in both files show how the safety factors were determined. A different safety factor was determined for each file based on the previously stated assumptions of CO_2 yields. The safety factors were determined by dividing the total moles of MgO to be emplaced with the total possible moles of CO_2 that cellulosics could produce. The total moles of MgO to be emplaced was determined from the total MgO mass (66,000 tons reported in EPA, 1996) divided by the molecular weight of MgO. However, the final result was then multiplied by 0.846 because only 84.6% of the bulk MgO is hydrating in laboratory experiments. The percentage was obtained by taking the last eight data points from an inundated MgO hydration experiment being run at 90 °C in deionized water, along with the last 16 data points from humid MgO hydration experiment run at 80 °C in 95% relative humidity (Snider, 2002).The safety factor assuming that microbial degradation of 1.00 mol of organic C produces 1.00 mol of CO_2 is 0.98 ; the safety factor assuming that methanogenesis is a dominant biodegradation pathway is 1.85.

The third EXCEL spreadsheet file (MgOsafetyfactorsAMWTP.XLS) differed from the previous two files only by assuming that one panel is filled entirely with IN-BN-510 waste. In the second sheet (AMWTP CPR), the AMWTP cellulosics were used and the results are listed in Table 5 below. The safety factor assuming that microbial degradation of 1.00 mol of organic C generates 1.00 mol of CO_2 is 0.18 .

Table 5. Total Moles of CO_2 That Could Be Produced by Microbial Activity in AMWTP Waste.

	Formula wt (g/mol)	Avg density (kg/m3)	Cellulosic equvialent (kg/m3)	CH waste volume m3	weight kg	Total moles of C	Total moles of CO_2
Cellulosics	162	517	517				
Rubber	162	136.5	136.5				
Plastics	162	349.4	594.0				
Total Cellulosics			1247	1.69E+05	2.11E+08	7.81E+09	7.81E+09

The last two sheets in the file labeled PA Panel Calcs and PA Safety Factors are included at the request of PA personnel for use in BRAGFLO. The PA Panel Calcs sheet is identical to the previous sheet (AMWTP CPR), except that we are now considering how much CO_2 could be produced in one panel filled with AMWTP waste, in which 1.00 mol of C yields 0.500 mol of CO_2. The volume has been multiplied by 0.1044 (the proportion of the WIPP disposal inventory in one waste panel, obtained from the PA database), and the initial total moles of CO_2 has been divided by 2. Table 6 shows the results.

Table 6. Total Moles of CO_2 Produced per AMWTP Panel (1.00 mol C yields 0.500 mol CO_2).

	Formula wt (g/mol)	Avg density (kg/m3)	Cellulosic equvialent (kg/m3)	volume per panel m3	weight kg	Total moles of C	1 to 1 Total moles of CO_2	1 to 1/2 Total moles of CO_2
Cellulosics	162	517	517					
Rubber	162	136.5	136.5					
Plastics	162	349.4	594.0					
Total Cellulosics			1247	1.76E+04	2.20E+07	8.15E+08	8.15E+08	4.08E+08

There is no NO_3^- or SO_4^{2-} present in the AMWTP waste. All microbial degradation is assumed to be methanogenic, and the safety factor is 0.35.

The lower half of the last sheet (PA Safety Factors) displays a table of data to be used in BRAGFLO. The table is based on 1.00 m^3 of IN-BN-510 waste. As this waste is removed, MgO is emplaced in the resulting void volume. The safety factor is then obtained for each waste:MgO ratio. The table is presented in the following manner:

1. Columns B and C are the volumetric proportions of IN-BN-510 waste and MgO. Each row adds up to 1.00 m^3.

2 Columns D and F represent the number of moles of either IN-BN-510 waste or MgO present in each volume. For the initial moles of CPR in 1 m^3 of In-Bn-510 waste was obtained from the total moles present in one repository panel and scaled down accordingly. The corresponding moles of MgO, as the waste volume decreases and the

MgO volume increases, is calculated by taking the total volume available in the repository if no waste were present and multiplying it by the density of MgO present in a supersack (1.41×10^6 g/m^3), which is divided by the molecular weight of MgO (40.3 g/mol). The value found is then multiplied by the volume of MgO added.
3. Column E displays how many moles of MgO are already planned to be emplaced in one panel of the repository (the current design-basis quantity of MgO).
4. The total moles of MgO, column G, is calculated by adding column E and F.
5. Column H is the moles of MgO required to consume the total amount of CO_2 produced from CPR. This number was previously attained in the calculations and as scaled accordingly to changing volumes of waste.
6. The safety factors are listed in Column I.

4 CONCLUSIONS

MgO safety factors have been recalculated using revised quantities of CPR (Crawford, 2003) and NO_3^- and SO_4^{2-} (Leigh and Crawford, 2003) for the WIPP CRA PA.

The MgO safety factors for the entire repository with homogeneously distributed IN-BN-510 are now 0.98 (assuming that microbial degradation of 1.00 mol of organic C generates 1.00 mol of CO_2) and 1.85 (assuming that 1.00 mol of C yields 0.500 mol of CO_2). These values are significantly lower than the value approved by Marcinowski (2001), 1.67 (equivalent to a value of 3.23 assuming that 1.00 mol of C yields 0.500 mol of CO_2). This decrease is mainly the result of the high concentrations of CPR in the supercompacted AMWTP waste stream constituting IN-BN-510.

The MgO safety factors for one waste panel filled entirely with IN-BN-510 waste are 0.18 (assuming that 1.00 mol of C yields 1.00 mol of CO_2) and 0.35 (assuming that 1.00 mol of C yields 0.500 mol of CO_2).

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APPENDIX A: EXCEL SPREADSHEET MgOsafetyfactorEPA

MgO safety factor EPA

Shelt Moles of MgO dissolved in brine

GWB **Moles of MgO dissolved in brines**

Initial and final concs by EQ3 done by Youngliang Xiong

Concentration of Mg in brine

Molality to molarity ratio factor 1.146

	Initial Conc Mol/L	Final Conc in equil with MgO, mol/Kg	Final Conc mol/L
Mg	1.000	7.8996E-01	6.89E-01

GWB ends up with less Mg++ in solution and will be neglected for further calcs

Molality to molarity ratio factor 1.137

ERDA-6 Calculated by EQ3

	Initial Conc Mol/L	Final Conc in equil with MgO, mol/Kg	Final Conc mol/L	Volume m3 *	Moles of MgO dissolved
Mg	0.019	1.0044E-01	8.83E-02	1.46E+05	1.01E+07

* Max brine flow up the bore hole at the upper DRZ S3 scenario (E1 @ 1000+ yrs) in Bragflow

MgO safety factor EPA
Sheet CH CPR

Letter 2003, Waste Material Parameter Disposal Inventory **Average drum of CH waste**

	Formula Wt (g/mol)	Avg Density (Kg/m3)	Cellulosic equvialent	volume m3	weight kg	Total moles of C	Total moles of CO2
Cellulosics	162	75	75				
Rubber	162	19	19				
Plastics	162	55	93.5				
Container plastic	162	21	35.7				
Total Cellulosics			223.2	1.7E+05	3.8E+07	1.4E+09	1.4E+09

Wang and Brush (1996)

P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulosics, based on carbon equivalence: Q=1.7P+R

162 g/mol was used for all cellulosics

Assume 1 mole of C = 1 mole fo CO2

PA parameter data base
Total volume of CH waste 1.69E+05

MgOsafetyfactorEPA
Sheet RH CPR

Letter 2003, Waste Material Parameter Disposal Inventory **Average drum of CH waste**

	Formula Wt (g/mol)	Avg Density (Kg/m3)	Cellulosic equvialent	volume m3	weight kg	Total moles of C	Total moles of CO2
Cellulosics	162	6.1	6.1				
Rubber	162	3.6	3.6				
Plastics	162	7	11.9				
Total Cellulosics			21.6	7.1E+03	1.5E+05	5.7E+06	5.7E+06

Wang and Brush (1996)

P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulosics, based on carbon equivalence: Q=1.7P+R

162 g/mol was used for all cellulosics

Assume 1 mole of C = 1 mole fo CO2

PA parameter data base
Total volume of RH waste 7.08E+03

MgO Safety factor EPA

Sheet Safety Factor

Total MgO required for dissolving in brine and reacting with CO2 generated by microbial activity.

	Moles	Volume m3
Mg dissolved	1.01E+07	
Max CO2 generated	1.40E+09	
Max CO2 (RH)	5.66E+06	
Total MgO required	1.41E+09	

Total MgO currently being emplaced in WIPP

2001 MgO minisack elimination report.

Tons	kg	g	moles	85% react
66000	66000000	6.60E+10	1.64E+09	1.39E+09

Safety Factor with new inventory data assuming one mole of C produces one mole CO2

Safety Factor	9.81E-01

APPENDIX B: EXCEL SPREADSHEET MgOsafetyfactorSNL

MgO Safety Factor SNL

Sheet Moles of MgO dissolved in brine

GWB **Moles of MgO dissolved in brines**

Initial and final concs by EQ3 done by Youngliang Xiong

Concentration of Mg in brine

	Initial Conc Mol/L	Final Conc in equil with MgO, mol/Kg	Final Conc mol/L
Mg	1.000	7.8996E-01	0.6893194

Molality to molarity ratio factor 1.146

GWB ends up with less Mg++ in solution and will be neglected for further calcs

Castile Calculated by EQ3

Molality to molarity ratio factor 1.137

	Initial Conc Mol/L	Final Conc in equil with MgO, mol/Kg	Final Conc mol/L	Volume m3 *	Moles of MgO dissolved
Mg	0.019	1.0044E-01	8.8338E-02	1.46E+05	1.01E+07

* Max brine flow up the bore hole at the upper DRZ S3 scenario (E1 @ 1000+ yrs) in BRAGFLO

MgO safety factor SNL
Sheet CH CPR

Letter 2003, Waste Material Parameter Disposal Inventory **Average drum of CH waste**

	Formula Wt (g/mol)	Avg Density (Kg/m3)	Cellulosic equvialent	volume m3	weight kg	Total moles of C	Total moles of CO2
Cellulosics	162	75	75				
Rubber	162	19	19				
Plastics	162	55	93.5				
Container plastic	162	21	35.7				
Total Cellulosics			223.2	1.7E+05	3.8E+07	1.4E+09	1.4E+09

Wang and Brush (1996)

P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulosics, based on carbon equivalence: Q=1.7P+R

162 g/mol was used for all cellulosics

PA parameter data base
Total volume of CH waste 1.69E+05

Moles of Nitrate and Sulfate Initially Present in the Waste

*from "Final Estimate of Oxyanion Mass in TRU Waste for Disposal in WIPP for the Compliance Recertification".

	kg*	g	fw	moles
Nitrate (NO3)	2.66E+06	2.66E+09	62.01	4.29E+07
Sulfate (SO4)	5.76E+05	5.76E+08	96.06	6.00E+06

	fraction %
Molar fraction of cellulosics biodegraded via denitrification	3.84
Molar fraction of cellulosics biodegraded via sulfate reduction	0.86
Molar fraction of cellulosics from methanogenisis	95.30

	moles
Total CO2 production for the repository	7.3E+08

MgO safety factor SNL
RH CPR

Letter 2003, Waste Material Parameter Disposal Inventory **Average drum of CH waste**

	Formula Wt (g/mol)	Avg Density (Kg/m3)	Cellulosic equvialent	volume m3	weight kg	Total moles of C	Total moles of CO2
Cellulosics	162	6.1	6.1				
Rubber	162	3.6	3.6				
Plastics	162	7	11.9				
Total Cellulosics			21.6	7.1E+03	1.5E+05	5.7E+06	5.7E+06

Wang and Brush (1996)

P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulosics, based on carbon equivalence: $Q=1.7P+R$

162 g/mol was used for all cellulosics

PA parameter data base
Total volume of RH waste 7.08E+03

MgOsafetyfactorSNL

Sheet Safety Factor

Total MgO required for dissolving in brine and reacting with CO2 generated by microbial activity.

	Moles	Volume m3
Mg dissolved	1.01E+07	
Max CO2 generated	7.31E+08	
Mas CO2 (RH)	5.66E+06	
Total MgO required	7.47E+08	1.88E+04

Total MgO currently being emplaced in WIPP

Tons	Kg	g	moles	85% react
66000	66000000	6.60E+10	1.64E+09	1.39E+09

Safety Factor with new inventory data assuming one mole of C produces one mole CO2

Safety Factor	1.85E+00

APPENDIX C: EXCEL SPREADSHEET MgOsafetyfactorAMWTP

MgO Safety factor AMWTP

Sheet Moles of MgO dissolved in brine

GWB **Moles of MgO dissolved in brines**

Initial and final concs by EQ3 done by Youngliang Xiong

Concentration of Mg in brine

	Initial Conc Mol/L	Final Conc in equil with MgO, mol/Kg	Final Conc mol/L
Mg	1.000	7.8996E-01	6.89E-01

Molality to molarity ratio factor 1.146

GWB ends up with less Mg++ in solution and will be neglected for further calcs

Molality to molarity ratio factor 1.137

Castile Calculated by EQ3

	Initial Conc Mol/L	Final Conc in equil with MgO, mol/Kg	Final Conc mol/L	Volume m3 *	Moles of MgO dissolved
Mg	0.019	1.0044E-01	8.83E-02	145824	1.01E+07

* Max brine flow up the bore hole at the upper DRZ S3 scenario (E1 @ 1000+ yrs) in Bragflow

MgO safety factor, AMWTP

Sheet AMWTP CPR

Report: Assessment of Impacts on Long-Term Performance from Supercompacted Wastes Produced by the AMWTP
by M. B. Gross

	Formula wt (g/mol)	Avg Density (kg/m3)	Cellulosic equvialent	volume m3	weight kg	Total moles of C	Total moles of CO_2
Cellulosics	162	517	517				
Rubber	162	136.5	136.5				
Plastics	162	349.4	594.0				
Total Cellulosics			1247	1.69E+05	2.11E+08	7.81E+09	7.81E+09

Wang and Brush (1996)

P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulosics, based on carbon equivalence: Q=1.7P+R

162 g/mol was used for all cellulosics

Assume 1 mole of C = 1 mole fo CO2

*PA parameter database
Total volume of CH waste 1.69E+05

MgO safety factor AMWTP
Sheet Safety Factor

Total MgO required for dissolving in brine and reacting with CO2 generated by microbial activity.

	Moles	Volume m3
Mg dissolved	1.01E+07	
Max CO2 generated	7.81E+09	
Total MgO required	7.82E+09	

Total MgO currently being emplaced in WIPP

Tons	kg	g	moles	moles *0.85
66000	66000000	6.60E+10	1.64E+09	1.39E+09

Safety Factor with new inventory data assuming one mole of C produces one mole CO2

Safety Factor	1.77E-01

MgO Safety factor AMWTP
Sheet PA panel Calcs

Report: Assessment of Impacts on Long-Term Performance from Supercompacted Wastes Produced by the AMWTP
by M. B. Gross

PER ONE PA PANEL

	Formula Wt (g/mol)	Avg Density (Kg/m3)	Cellulosic equvialent	volume per panel m3*	weight kg	Total moles of C	1 to 1 Total moles of CO2	1 to 1/2 Total moles of CO2
Cellulosics	162	517	517					
Rubber	162	136.5	136.5					
Plastics	162	349.4	593.98					
Total Cellulosics			1247.48	1.8E+04	2.2E+07	8.2E+08	8.2E+08	4.08E+08

Wang and Brush (1996)

P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulosics, based on carbon equivalence: Q=1.7P+R

162 g/mol was used for all cellulosics

Assume 1 mole of C = 1 mole fo CO2 Assume 1 mole of C = 1/2 mole of CO2

*PA parameter database
Total volume of CH waste 1.69E+05

MgO Safetyfactors AMWTP

Sheet PA safety factors

Total MgO required for dissolving in brine and reacting with CO2 generated by microbial activity.
Asumes one mole of C = 1/2 mole of CO2

PER ONE PA PANEL

	Moles	Volume m3
Mg dissolved	1.06E+06	
Max CO2 generated	4.08E+08	
Total MgO required	4.09E+08	

	Tons	kg	g	moles	moles *85%
Total MgO currently being emplaced in WIPP	66000	66000000	6.60E+10	1.64E+09	1.39E+09
Total MgO for one PA panel	6890.4	6890400	6.89E+09	1.71E+08	1.45E+08

Safety Factor assuming one pannel filled with AMWTP waste

Safety Factor 3.54E-01

Data for following table calculations

Given				
cellulosic density	1247.48	kg/m3		
Super sack volume	47.6	ft3	1.35E+00	m3
MgO mass per sack	4200	lb	1.91E+06	g
Super sack density	1.41E+06	g/m3		
panel CH volume	1.76E+04	m3		

Sheet PA safety factors (cont.)

Table

AMWTP m3	MgO addition m3	AMWTP moles	Currently emplaced MgO mol	MgO addition moles	Total MgO moles	Required MgO moles	Safety Factor
1	0	4.08E+08	1.45E+08	0.00E+00	1.45E+08	4.09E+08	3.54E-01
0.99	0.01	4.04E+08	1.45E+08	6.19E+06	1.51E+08	4.05E+08	3.73E-01
0.98	0.02	3.99E+08	1.45E+08	1.24E+07	1.57E+08	4.00E+08	3.92E-01
0.97	0.03	3.95E+08	1.45E+08	1.86E+07	1.63E+08	3.96E+08	4.12E-01
0.96	0.04	3.91E+08	1.45E+08	2.48E+07	1.69E+08	3.92E+08	4.32E-01
0.95	0.05	3.87E+08	1.45E+08	3.09E+07	1.76E+08	3.88E+08	4.52E-01
0.94	0.06	3.83E+08	1.45E+08	3.71E+07	1.82E+08	3.84E+08	4.73E-01
0.93	0.07	3.79E+08	1.45E+08	4.33E+07	1.88E+08	3.80E+08	4.95E-01
0.92	0.08	3.75E+08	1.45E+08	4.95E+07	1.94E+08	3.76E+08	5.16E-01
0.91	0.09	3.71E+08	1.45E+08	5.57E+07	2.00E+08	3.72E+08	5.39E-01
0.9	0.1	3.67E+08	1.45E+08	6.19E+07	2.07E+08	3.68E+08	5.62E-01
0.89	0.11	3.63E+08	1.45E+08	6.81E+07	2.13E+08	3.64E+08	5.85E-01
0.88	0.12	3.59E+08	1.45E+08	7.43E+07	2.19E+08	3.60E+08	6.09E-01
0.87	0.13	3.55E+08	1.45E+08	8.04E+07	2.25E+08	3.56E+08	6.33E-01
0.86	0.14	3.51E+08	1.45E+08	8.66E+07	2.31E+08	3.51E+08	6.58E-01
0.85	0.15	3.46E+08	1.45E+08	9.28E+07	2.37E+08	3.47E+08	6.84E-01
0.84	0.16	3.42E+08	1.45E+08	9.90E+07	2.44E+08	3.43E+08	7.10E-01
0.83	0.17	3.38E+08	1.45E+08	1.05E+08	2.50E+08	3.39E+08	7.37E-01
0.82	0.18	3.34E+08	1.45E+08	1.11E+08	2.56E+08	3.35E+08	7.64E-01
0.81	0.19	3.30E+08	1.45E+08	1.18E+08	2.62E+08	3.31E+08	7.92E-01
0.8	0.2	3.26E+08	1.45E+08	1.24E+08	2.68E+08	3.27E+08	8.21E-01
0.79	0.21	3.22E+08	1.45E+08	1.30E+08	2.75E+08	3.23E+08	8.51E-01
0.78	0.22	3.18E+08	1.45E+08	1.36E+08	2.81E+08	3.19E+08	8.81E-01
0.77	0.23	3.14E+08	1.45E+08	1.42E+08	2.87E+08	3.15E+08	9.12E-01
0.76	0.24	3.10E+08	1.45E+08	1.49E+08	2.93E+08	3.11E+08	9.44E-01
0.75	0.25	3.06E+08	1.45E+08	1.55E+08	2.99E+08	3.06E+08	9.77E-01
0.74	0.26	3.02E+08	1.45E+08	1.61E+08	3.06E+08	3.02E+08	1.01E+00
0.73	0.27	2.98E+08	1.45E+08	1.67E+08	3.12E+08	2.98E+08	1.04E+00
0.72	0.28	2.93E+08	1.45E+08	1.73E+08	3.18E+08	2.94E+08	1.08E+00
0.71	0.29	2.89E+08	1.45E+08	1.79E+08	3.24E+08	2.90E+08	1.12E+00
0.7	0.3	2.85E+08	1.45E+08	1.86E+08	3.30E+08	2.86E+08	1.15E+00
0.69	0.31	2.81E+08	1.45E+08	1.92E+08	3.36E+08	2.82E+08	1.19E+00

Sheet PA Safety factors (cont)

AMWTP m3	MgO addition m3	AMWTP moles	Currently emplaced MgO mol	MgO addition moles	Total MgO moles	Required MgO moles	Safety Factor
0.68	0.32	2.77E+08	1.45E+08	1.98E+08	3.43E+08	2.78E+08	1.23E+00
0.67	0.33	2.73E+08	1.45E+08	2.04E+08	3.49E+08	2.74E+08	1.27E+00
0.66	0.34	2.69E+08	1.45E+08	2.10E+08	3.55E+08	2.70E+08	1.32E+00
0.65	0.35	2.65E+08	1.45E+08	2.17E+08	3.61E+08	2.66E+08	1.36E+00
0.64	0.36	2.61E+08	1.45E+08	2.23E+08	3.67E+08	2.62E+08	1.40E+00
0.63	0.37	2.57E+08	1.45E+08	2.29E+08	3.74E+08	2.57E+08	1.45E+00
0.62	0.38	2.53E+08	1.45E+08	2.35E+08	3.80E+08	2.53E+08	1.50E+00
0.61	0.39	2.49E+08	1.45E+08	2.41E+08	3.86E+08	2.49E+08	1.55E+00
0.6	0.4	2.45E+08	1.45E+08	2.48E+08	3.92E+08	2.45E+08	1.60E+00
0.59	0.41	2.40E+08	1.45E+08	2.54E+08	3.98E+08	2.41E+08	1.65E+00
0.58	0.42	2.36E+08	1.45E+08	2.60E+08	4.05E+08	2.37E+08	1.71E+00
0.57	0.43	2.32E+08	1.45E+08	2.66E+08	4.11E+08	2.33E+08	1.76E+00
0.56	0.44	2.28E+08	1.45E+08	2.72E+08	4.17E+08	2.29E+08	1.82E+00
0.55	0.45	2.24E+08	1.45E+08	2.78E+08	4.23E+08	2.25E+08	1.88E+00
0.54	0.46	2.20E+08	1.45E+08	2.85E+08	4.29E+08	2.21E+08	1.95E+00
0.53	0.47	2.16E+08	1.45E+08	2.91E+08	4.35E+08	2.17E+08	2.01E+00
0.52	0.48	2.12E+08	1.45E+08	2.97E+08	4.42E+08	2.12E+08	2.08E+00
0.51	0.49	2.08E+08	1.45E+08	3.03E+08	4.48E+08	2.08E+08	2.15E+00
0.5	0.5	2.04E+08	1.45E+08	3.09E+08	4.54E+08	2.04E+08	2.22E+00
0.49	0.51	2.00E+08	1.45E+08	3.16E+08	4.60E+08	2.00E+08	2.30E+00
0.48	0.52	1.96E+08	1.45E+08	3.22E+08	4.66E+08	1.96E+08	2.38E+00
0.47	0.53	1.92E+08	1.45E+08	3.28E+08	4.73E+08	1.92E+08	2.46E+00
0.46	0.54	1.87E+08	1.45E+08	3.34E+08	4.79E+08	1.88E+08	2.55E+00
0.45	0.55	1.83E+08	1.45E+08	3.40E+08	4.85E+08	1.84E+08	2.64E+00
0.46	0.56	1.87E+08	1.45E+08	3.47E+08	4.91E+08	1.88E+08	2.61E+00
0.43	0.57	1.75E+08	1.45E+08	3.53E+08	4.97E+08	1.76E+08	2.83E+00
0.42	0.58	1.71E+08	1.45E+08	3.59E+08	5.04E+08	1.72E+08	2.93E+00
0.41	0.59	1.67E+08	1.45E+08	3.65E+08	5.10E+08	1.68E+08	3.04E+00
0.4	0.6	1.63E+08	1.45E+08	3.71E+08	5.16E+08	1.63E+08	3.16E+00
0.39	0.61	1.59E+08	1.45E+08	3.77E+08	5.22E+08	1.59E+08	3.28E+00
0.38	0.62	1.55E+08	1.45E+08	3.84E+08	5.28E+08	1.55E+08	3.40E+00
0.37	0.63	1.51E+08	1.45E+08	3.90E+08	5.34E+08	1.51E+08	3.53E+00
0.36	0.64	1.47E+08	1.45E+08	3.96E+08	5.41E+08	1.47E+08	3.68E+00
0.35	0.65	1.43E+08	1.45E+08	4.02E+08	5.47E+08	1.43E+08	3.82E+00

Sheet PA safety factors (cont.)

AMWTP m3	MgO addition m3	AMWTP moles	Currently emplaced MgO mol	MgO addition moles	Total MgO moles	Required MgO moles	Safety Factor
0.34	0.66	1.39E+08	1.45E+08	4.08E+08	5.53E+08	1.39E+08	3.98E+00
0.33	0.67	1.35E+08	1.45E+08	4.15E+08	5.59E+08	1.35E+08	4.15E+00
0.32	0.68	1.30E+08	1.45E+08	4.21E+08	5.65E+08	1.31E+08	4.32E+00
0.31	0.69	1.26E+08	1.45E+08	4.27E+08	5.72E+08	1.27E+08	4.51E+00
0.3	0.7	1.22E+08	1.45E+08	4.33E+08	5.78E+08	1.23E+08	4.71E+00
0.29	0.71	1.18E+08	1.45E+08	4.39E+08	5.84E+08	1.19E+08	4.93E+00
0.28	0.72	1.14E+08	1.45E+08	4.46E+08	5.90E+08	1.14E+08	5.16E+00
0.27	0.73	1.10E+08	1.45E+08	4.52E+08	5.96E+08	1.10E+08	5.41E+00
0.26	0.74	1.06E+08	1.45E+08	4.58E+08	6.03E+08	1.06E+08	5.67E+00
0.25	0.75	1.02E+08	1.45E+08	4.64E+08	6.09E+08	1.02E+08	5.96E+00
0.24	0.76	9.78E+07	1.45E+08	4.70E+08	6.15E+08	9.81E+07	6.27E+00
0.23	0.77	9.37E+07	1.45E+08	4.76E+08	6.21E+08	9.40E+07	6.61E+00
0.22	0.78	8.97E+07	1.45E+08	4.83E+08	6.27E+08	8.99E+07	6.98E+00
0.21	0.79	8.56E+07	1.45E+08	4.89E+08	6.33E+08	8.58E+07	7.38E+00
0.2	0.8	8.15E+07	1.45E+08	4.95E+08	6.40E+08	8.17E+07	7.83E+00
0.19	0.81	7.74E+07	1.45E+08	5.01E+08	6.46E+08	7.76E+07	8.32E+00
0.18	0.82	7.34E+07	1.45E+08	5.07E+08	6.52E+08	7.36E+07	8.86E+00
0.17	0.83	6.93E+07	1.45E+08	5.14E+08	6.58E+08	6.95E+07	9.48E+00
0.16	0.84	6.52E+07	1.45E+08	5.20E+08	6.64E+08	6.54E+07	1.02E+01
0.15	0.85	6.11E+07	1.45E+08	5.26E+08	6.71E+08	6.13E+07	1.09E+01
0.14	0.86	5.71E+07	1.45E+08	5.32E+08	6.77E+08	5.72E+07	1.18E+01
0.13	0.87	5.30E+07	1.45E+08	5.38E+08	6.83E+08	5.31E+07	1.29E+01
0.12	0.88	4.89E+07	1.45E+08	5.45E+08	6.89E+08	4.90E+07	1.41E+01
0.11	0.89	4.48E+07	1.45E+08	5.51E+08	6.95E+08	4.50E+07	1.55E+01
0.1	0.9	4.08E+07	1.45E+08	5.57E+08	7.02E+08	4.09E+07	1.72E+01
0.09	0.91	3.67E+07	1.45E+08	5.63E+08	7.08E+08	3.68E+07	1.92E+01
0.08	0.92	3.26E+07	1.45E+08	5.69E+08	7.14E+08	3.27E+07	2.18E+01
0.07	0.93	2.85E+07	1.45E+08	5.75E+08	7.20E+08	2.86E+07	2.52E+01
0.06	0.94	2.45E+07	1.45E+08	5.82E+08	7.26E+08	2.45E+07	2.96E+01
0.05	0.95	2.04E+07	1.45E+08	5.88E+08	7.33E+08	2.04E+07	3.58E+01
0.04	0.96	1.63E+07	1.45E+08	5.94E+08	7.39E+08	1.63E+07	4.52E+01
0.03	0.97	1.22E+07	1.45E+08	6.00E+08	7.45E+08	1.23E+07	6.08E+01
0.02	0.98	8.15E+06	1.45E+08	6.06E+08	7.51E+08	8.17E+06	9.19E+01
0.01	0.99	4.08E+06	1.45E+08	6.13E+08	7.57E+08	4.09E+06	1.85E+02

Sheet PA safety factors (cont.)

AMWTP m3	MgO addition m3	AMWTP moles	Currently emplaced MgO mol	MgO addition moles	Total MgO moles	Required MgO moles	Safety Factor*
0	1	0.00E+00	1.45E+08	6.19E+08	7.63E+08	0.00E+00	∞

APPENDIX D: EQ3 OUTPUT FILES

EQ3/6, Version 7.2c (EQ3/6-V7-REL-V7.2c-PC)
EQ3NR Speciation-Solubility Code (EQ3/6-V7-EQ3NR-EXE-R141-P6)
Supported by the EQLIB library (EQ3/6-V7-EQLIB-LIB-R172-P6)

Run 09:57:10 08May2003

--- Reading the input file ---

EQ3NR input file name= ER_prs3.3i
Description= "ERDA brine"
Version level= 7.2
Created 05/08/03 Creator= Yongliang Xiong
This input file is modified from c:\eq3_6v7.2\xiong\erda\eq3_6_Fe\ERDA_PRS.3i.
Revised 05/08/03 Revisor= Yongliang Xiong

ERDA brine, after Popielak et al. (1983).

Purpose: to generate a pick-up file for reaction path calculations involving a very concentrated brine, using Pitzer's equations to calculate the activity coefficients of the aqueous species.

This problem is addressed using the thermodynamic data base of Harvie, Moller, and Weare (1984) modified by E. Giambalvo, named hmp.

The print option switch IOPR6 is set to 1 to direct the code to print a table of mean ionic properties.

Because Br- in not part of the Harvie-Moller-Weare model, the reported 0.027 M Br- is ignored on this input file.

References

Brush, L.H., 1990, Test plan for laboratory and modeling studies of repository and radionuclide chemistry for the waste isolation pilot plant. SAND90-0266.

Harvie, C. E., Moller, N., and Weare, J. H., 1984, The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25C: Geochimica et Cosmochimica Acta, v. 48, p. 723-751.

Popielak, R.S., Beauheim, R.L., Black, S.R., Coons, W.E., Ellingson, C.T, and Olsen, R.L., 1983, Brine reserviors in the Castile

Formation, Waste Isolation Pilot Plant project, southwestern New Mexico. TME 3153. Carlsbad, NM. US Department of Energy WIPP Project Office.

Temperature (C)	25.00	Density(gm/cm3)	1.2160
Total Dissolved Salts	330000	mg/kg | *mg/l	not used

Electrical Balancing on	H+	code selects	not performed

SPECIES	BASIS SWITCH/CONSTRAINT	CONC/ETC	UNITS OR TYPE
Na+		4.870	Molarity
K+		0.097	Molarity
Mg++	Brucite	0.000	Mineral
Ca++		0.012	Molarity
Cl-		4.800	Molarity
HCO3-		1.60E-02	Molarity
SO4--		0.170	Molarity
H+		9.00	pH

Input Solid Solutions

none

SUPPRESSED SPECIES (suppress,replace,augmentk,augmentg)			value
Magnesite	mineral	Suppress	0.0
Dolomite	mineral	Suppress	0.0

OPTIONS

- SOLID SOLUTIONS -
  - * ignore solid solutions
    process hypothetical solid solutions
    process input and hypothetical solid solutions
- LOADING OF SPECIES INTO MEMORY -
  - * does nothing
    lists species loaded into memory
- ECHO DATABASE INFORMATION -
  - * does nothing
    lists all reactions
    lists reactions and log K values
    lists reactions, log K values and polynomial coef.
- LIST OF AQUEOUS SPECIES (ordering) -
  - * in order of decreasing concentration
    in same order as input file
- LIST OF AQUEOUS SPECIES (concentration limit) -
  - * all species
    only species > 10**-20 molal
    only species > 10**-12 molal
    not printed
- LIST OF AQUEOUS SPECIES (by element) -
  - * print major species
    print all species
    don't print
- MINERAL SATURATION STATES -

```
|   * print if affinity > -10 kcals                                          |
|     print all                                                              |
|     don't print                                                            |
| - pH SCALE CONVENTION -                                                    |
|   * modified NBS                                                           |
|     internal                                                               |
|     rational                                                               |
| - ACTIVITY COEFFICIENT OPTIONS -                                           |
|     use B-dot equation                                                     |
|     Davies' equation                                                       |
|   * Pitzer's equations                                                     |
| - AUTO BASIS SWITCHING -                                                   |
|   * off                                                                    |
|     on                                                                     |
| - PITZER DATABASE INFORMATION -                                            |
|   * print only warnings                                                    |
|     print species in model and number of Pitzer coefficients               |
|     print species in model and names of Pitzer coefficients                |
| - PICKUP FILE -                                                            |
|   * write pickup file                                                      |
|     don't write pickup file                                                |
| - LIST MEAN IONIC PROPERTIES -                                             |
|     don't print                                                            |
|   * print                                                                  |
| - LIST AQUEOUS SPECIES, ION SIZES, AND HYDRATION NUMBERS -                 |
|   * print                                                                  |
|     don't print                                                            |
| - CONVERGENCE CRITERIA -                                                   |
|   * test both residual functions and correction terms                      |
|     test only residual functions                                           |
|----------------------------------------------------------------------------|
|DEBUGGING SWITCHES (0 = off, 1,2 = on                                       |
|----------------------------------------------------------------------------|
|0  generic debugging information                                           |2
|0  print details of pre-Newton-Raphson iteration                           |2
|0  print details of Newton-Raphson iteration                               |
|0  print details of stoichiometric factors                                 |2
|0  print details of stoichiometric factors calculation                     |
|0  write reactions on RLIST                                                |
|0  list stoichiometric concentrations of master species                    |
|0  request iteration variables to be killed                                |
|----------------------------------------------------------------------------|
|DEVELOPMENT OPTIONS  (used for code development)                            |
|----------------------------------------------------------------------------|
| none                                                                       |
|----------------------------------------------------------------------------|
|TOLERANCES                    (desired values)        (defaults)            |
|----------------------------------------------------------------------------|
|      residual functions  |                        |1.0e-10  tolbt        |
|        correction terms  |                        |1.0e-10  toldl        |
|        saturation state  |                        |0.5      tolsat       |
|number of N-R iterations  |                        |30       itermx       |
|----------------------------------------------------------------------------|
```

--- The input file has been successfully read ---

--- Reading the data1 file ---

```
--- The data1 file has been successfully read ---

The species Magnesite                has been user-suppressed

The species Dolomite                 has been user-suppressed

                    --- Pitzer Coefficient Summary ---




eeee   qqq   33333  n   n  rrrr
e     q   q      3  nn  n  r   r
eeee  q   q    33   n n n  rrrr
e     q q q      3  n  nn  r  r
eeee   qqq   3333   n   n  r   r
          q


EQ3NR, version 7.2c (R141    )
 supported by EQLIB, version 7.2c (R172    )


|EQ3NR input file name= ER_prs3.3i                                          |
|Description= "ERDA brine"                                                  |
|Version level= 7.2                                                         |
|Created 05/08/03    Creator= Yongliang Xiong                               |
|This input file is modified from c:\eq3_6v7.2\xiong\erda\eq3_6_Fe\          |
|  ERDA_PRS.3i.                                                             |
|Revised 05/08/03    Revisor= Yongliang Xiong                               |
|                                                                           |
|  ERDA brine, after Popielak et al. (1983).                                |
|                                                                           |
|  Purpose: to generate a pick-up file for reaction path calculations       |
|involving a very concentrated brine, using Pitzer's equations to           |
|calculate the activity coefficients of the aqueous species.                |
|                                                                           |
|  This problem is addressed using the thermodynamic data base of           |
|Harvie, Moller, and Weare (1984) modified by E. Giambalvo, named hmp.      |
|                                                                           |
|  The print option switch IOPR6 is set to 1 to direct the code to          |
|print a table of mean ionic properties.                                    |
|                                                                           |
|  Because Br- in not part of the Harvie-Moller-Weare model, the            |
|reported 0.027 M Br- is ignored on this input file.                        |
|                                                                           |
|                                                                           |
|                              References                                   |
|                                                                           |
|Brush, L.H., 1990, Test plan for laboratory and modeling studies of        |
|  repository and radionuclide chemistry for the waste isolation pilot      |
```

| plant. SAND90-0266.
|
|Harvie, C. E., Moller, N., and Weare, J. H., 1984, The prediction
| of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-
| OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25C:
| Geochimica et Cosmochimica Acta, v. 48, p. 723-751.
|
|Popielak, R.S., Beauheim, R.L., Black, S.R., Coons, W.E., Ellingson,
| C.T, and Olsen, R.L., 1983, Brine reserviors in the Castile
| Formation, Waste Isolation Pilot Plant project, southwestern New
| Mexico. TME 3153. Carlsbad, NM. US Department of Energy WIPP
| Project Office.

data0.hmw.V8.R6
CII: GEMBOCHS.V2-EQ8-data0.hmw.V8.R6
THERMODYNAMIC DATABASE
generated by GEMBOCHS.V2-Jewel.src.R5 02-dec-1996 11:27:50
Output package: eq3
Data set: hmw
+---

The activity coefficients of aqueous solute species
and the activity of water are calculated according to the
Pitzer equations

E-lambda flag= on

Temperature= 25.00 degrees Celsius
pressure= 1.0132 bars

9 elements are in the data base
110 elements can be loaded into memory
9 elements are active in this problem

17 aqueous species are in the data base
17 aqueous species were loaded into memory
2500 aqueous species can be loaded into memory
16 aqueous species are active in this problem

7 aqueous reactions are in the data base
7 aqueous reactions were loaded into memory
2389 aqueous reactions can be loaded into memory

57 minerals are in the data base
57 minerals were loaded into memory
1500 minerals can be loaded into memory
55 minerals are active in this problem

0 solid solutions are in the data base
50 solid solutions can be loaded into memory

3 gases are in the data base

```
  3 gases were loaded into memory
200 gases can be loaded into memory
  3 gases are active in this problem
```

```
iopt1  =  0 (redox option switch)
iopt2  =  0 (automatic basis switching switch)
iopt3  =  0 (interfacing output control switch)
iopt4  =  0 (turn-on solid solutions switch)
iopt5  =  0 (not used)
iopt6  =  0 (conv. test criteria switch)
iopt7  =  0 (0/1 version 7/post-version 7 pickup file)
iopt8  =  0 (not used)
iopt9  =  0 (not used)
iopt10 =  0 (not used)
```

```
iopg1  =  1 (act. coeff. choice)
iopg2  =  0 (pH scale convention switch)
iopg3  =  0 (not used)
iopg4  =  0 (not used)
iopg5  =  0 (not used)
iopg6  =  0 (not used)
iopg7  =  0 (not used)
iopg8  =  0 (not used)
iopg9  =  0 (not used)
iopg10 =  0 (not used)
```

```
iopr1  =  0 (list loading of species)
iopr2  =  0 (list reactions and log K values)
iopr3  =  0 (aqueous species print order control)
iopr4  =  0 (aqueous species print cut-off control)
iopr5  =  0 (mass balance percentages print control)
iopr6  =  1 (mean ionic act coeff print control)
iopr7  =  0 (mineral affinity print control)
iopr8  =  0 (ion size and hydr. no. print control)
iopr9  =  0 (Pitzer coefficients tabulation)
iopr10 =  0 (print concbs array)
iopr11 =  0 (not used)
iopr12 =  0 (not used)
iopr13 =  0 (not used)
iopr14 =  0 (not used)
iopr15 =  0 (not used)
iopr16 =  0 (not used)
iopr17 =  0 (not used)
iopr18 =  0 (not used)
iopr19 =  0 (not used)
iopr20 =  0 (not used)
```

```
iodb1  =  0 (print info. messages switch)
iodb2  =  0 (print pre-Newton-Raphson optimizations switch)
iodb3  =  0 (request iteration variables to kill)
```

```
iodb4  =  0 (print Newton-Raphson iterations switch)
iodb5  =  0 (list stoichiometric equivalences)
iodb6  =  0 (controls iodb5 level of detail)
iodb7  =  0 (write reactions on file rlist switch)
iodb8  =  0 (not used)
iodb9  =  0 (not used)
iodb10 =  0 (not used)
```

The default redox state is constrained by log fO2 = -999.0000 (log bars)

```
Solution density =  1.21600 g/mL

Total dissolved salts =       0.00 mg/kg solution
Total dissolved salts =  330000.00 mg/L
```

```
Tolbt  =  0.10000E-05 (convergence tolerance on residual functions)
Toldl  =  0.10000E-05 (convergence tolerance on correction terms)
Tolsat =  0.50000E+00 (phase saturation tolerance, does not affect
                       convergence)
```

--- Input Constraints ---

Species	Csp	Jflag	Input Type/Co-species
Na+	4.8700E+00	1	Total conc, molar
K+	9.7000E-02	1	Total conc, molar
Mg++	0.0000E+00	19	Mineral equilibrium
			Brucite
	1.000 Brucite		
	+ 2.000 H+		
	==		
	2.000 H2O		
	+ 1.000 Mg++		
Ca++	1.2000E-02	1	Total conc, molar
Cl-	4.8000E+00	1	Total conc, molar
HCO3-	1.6000E-02	1	Total conc, molar
SO4--	1.7000E-01	1	Total conc, molar
H+	-9.0000E+00	16	Log activity

Electrical balance will be achieved by adjusting
the concentration of "H+ ". Any other specified
constraint will be overridden.

--- Inactive Aqueous Species ---

--- Modified Input Constraints ---

```
   Species                      Csp       Jflag   Input Type/Co-species

Ca++                        1.3544E-02     0    Total conc, molal
Cl-                         5.4176E+00     0    Total conc, molal
H+                         -9.0000E+00    16    Log activity
HCO3-                       1.8059E-02     0    Total conc, molal
K+                          1.0948E-01     0    Total conc, molal
Mg++                        0.0000E+00    19    Mineral equilibrium
                                                   Brucite

                      1.000  Brucite
                  +   2.000  H+
                         ==
                      2.000  H2O
                  +   1.000  Mg++
Na+                         5.4966E+00     0    Total conc, molal
SO4--                       1.9187E-01     0    Total conc, molal


--- Optimization ended within requested limits ---


iter=   0
       del(                 )=  0.00000E+00, delfnc=  0.00000E+00
      beta(conc    HCO3-    )=  2.91230E-02, betfnc=  0.00000E+00
        bbig=  2.91230E-02, ubbig= HCO3-
        bneg= -2.88675E-12, ubneg= SO4--
        bgamx= -4.29816E-02, ubgamx= CO3--
        bsigmm= -1.18836E-02
        bxi=  1.50641E-03
        btfcnr=  0.00000E+00

iter=   1
      Gammas are fixed
       del(conc    Mg++     )=  3.28856E-01, delfnc=  0.00000E+00
      beta(conc    HCO3-    )=  5.40259E-02, betfnc= -8.55095E-01
        bbig=  5.40259E-02, ubbig= HCO3-
        bneg=  0.00000E+00, ubneg= none
        bgamx= -9.50775E-02, ubgamx= CO3--
        bsigmm=  5.23226E-03
        bxi=  1.88139E-02
        btfcnr= -8.55095E-01

iter=   2
      Gammas are fixed
       del(conc    Mg++     )= -7.34920E-02, delfnc=  7.76522E-01
      beta(conc    HCO3-    )=  3.76521E-03, betfnc=  9.30307E-01
        bbig=  3.76521E-03, ubbig= HCO3-
        bneg=  0.00000E+00, ubneg= none
        bgamx= -7.85996E-02, ubgamx= CO3--
        bsigmm= -1.59407E-03
        bxi= -5.52470E-03
        btfcnr=  9.30307E-01
```

```
iter=   3
      Gammas are fixed
       del(conc    Mg++     )= -6.80512E-03, delfnc=  9.07403E-01
      beta(conc    HCO3-    )=  2.85346E-05, betfnc=  9.92422E-01
        bbig=  2.85346E-05, ubbig= HCO3-
        bneg=  0.00000E+00, ubneg= none
        bgamx= -7.72124E-02, ubgamx= CO3--
        bsigmm= -1.33333E-04
        bxi= -4.65093E-04
        btfcnr=  9.92422E-01

iter=   4
      Gammas are fixed
       del(conc    Mg++     )= -5.24871E-05, delfnc=  9.92287E-01
      beta(conc    H2O      )=  2.55519E-09, betfnc=  9.99910E-01
        bbig=  1.68950E-09, ubbig= HCO3-
        bneg=  0.00000E+00, ubneg= none
        bgamx= -7.72018E-02, ubgamx= CO3--
        bsigmm= -1.02053E-06
        bxi= -3.56068E-06
        btfcnr=  9.99910E-01

iter=   5
      Gamma relaxation factor=  0.20000
       del(conc    Mg++     )= -3.07645E-09, delfnc=  9.99941E-01
      beta(conc    Mg++     )=  3.78205E-03, betfnc= -1.48015E+06
        bbig=  0.00000E+00, ubbig= none
        bneg= -2.05637E-03, ubneg= HCO3-
        bgamx= -7.72018E-02, ubgamx= CO3--
        bsigmm= -5.97091E-11
        bxi= -2.08236E-10
        btfcnr=  9.99874E-01

iter=   6
      Gamma relaxation factor=  0.30000
       del(conc    H+       )= -1.80090E-03, delfnc= -5.85382E+05
      beta(conc    Mg++     )=  4.54444E-03, betfnc= -2.01580E-01
        bbig=  0.00000E+00, ubbig= none
        bneg= -2.40321E-03, ubneg= HCO3-
        bgamx= -6.18076E-02, ubgamx= CO3--
        bsigmm=  4.12655E-06
        bxi=  3.09866E-05
        btfcnr=  9.98979E-01

iter=   7
      Gamma relaxation factor=  0.40000
       del(conc    H+       )= -2.16296E-03, delfnc= -2.01043E-01
      beta(conc    Mg++     )=  4.25115E-03, betfnc=  6.45371E-02
        bbig=  0.00000E+00, ubbig= none
        bneg= -2.18528E-03, ubneg= HCO3-
        bgamx= -4.33212E-02, ubgamx= CO3--
        bsigmm=  5.00285E-06
        bxi=  3.76165E-05
        btfcnr=  9.98810E-01

iter=   8
      Gamma relaxation factor=  0.50000
```

```
 del(conc    H+      )= -2.02214E-03, delfnc=  6.51051E-02
beta(conc    Mg++    )=  3.19982E-03, betfnc=  2.47306E-01
  bbig=  0.00000E+00, ubbig= none
  bneg= -1.60770E-03, ubneg= HCO3-
  bgamx= -2.60457E-02, ubgamx= CO3--
  bsigmm=  4.72708E-06
  bxi=  3.55808E-05
  btfcnr=  9.98921E-01

iter=   9
Gamma relaxation factor=  0.60000
 del(conc    H+      )= -1.52123E-03, delfnc=  2.47714E-01
beta(conc    Mg++    )=  1.93034E-03, betfnc=  3.96734E-01
  bbig=  0.00000E+00, ubbig= none
  bneg= -9.57270E-04, ubneg= HCO3-
  bgamx= -1.30630E-02, ubgamx= CO3--
  bsigmm=  3.59028E-06
  bxi=  2.70460E-05
  btfcnr=  9.99207E-01

iter=  10
Gamma relaxation factor=  0.70000
 del(conc    H+      )= -9.17324E-04, delfnc=  3.96984E-01
beta(conc    Mg++    )=  9.08241E-04, betfnc=  5.29492E-01
  bbig=  0.00000E+00, ubbig= none
  bneg= -4.49277E-04, ubneg= HCO3-
  bgamx= -5.24965E-03, ubgamx= CO3--
  bsigmm=  2.18209E-06
  bxi=  1.64426E-05
  btfcnr=  9.99529E-01

iter=  11
Gamma relaxation factor=  0.80000
 del(conc    H+      )= -4.31479E-04, delfnc=  5.29633E-01
beta(conc    Mg++    )=  3.15408E-04, betfnc=  6.52726E-01
  bbig=  0.00000E+00, ubbig= none
  bneg= -1.57103E-04, ubneg= HCO3-
  bgamx= -1.58647E-03, ubgamx= CO3--
  bsigmm=  1.03320E-06
  bxi=  7.78307E-06
  btfcnr=  9.99779E-01

iter=  12
Gamma relaxation factor=  0.90000
 del(conc    H+      )= -1.49805E-04, delfnc=  6.52810E-01
beta(conc    Mg++    )=  7.25424E-05, betfnc=  7.70005E-01
  bbig=  0.00000E+00, ubbig= none
  bneg= -3.67378E-05, ubneg= HCO3-
  bgamx= -3.21335E-04, ubgamx= CO3--
  bsigmm=  3.61110E-07
  bxi=  2.71815E-06
  btfcnr=  9.99923E-01

iter=  13
 del(conc    H+      )= -3.44458E-05, delfnc=  7.70063E-01
beta(conc    Mg++    )=  8.46569E-06, betfnc=  8.83300E-01
  bbig=  0.00000E+00, ubbig= none
```

```
      bneg= -4.44670E-06, ubneg= HCO3-
      bgamx= -3.30706E-05, ubgamx= CO3--
      bsigmm=  8.37736E-08
      bxi=  6.29851E-07
      btfcnr=  9.99922E-01

iter=  14
     del(conc    H+      )= -4.01858E-06, delfnc=  8.83336E-01
    beta(conc    Mg++    )=  4.79668E-08, betfnc=  9.94334E-01
      bbig=  0.00000E+00, ubbig= none
      bneg= -4.31666E-08, ubneg= HCO3-
      bgamx= -1.11152E-07, ubgamx= CO3--
      bsigmm=  9.94329E-09
      bxi=  7.46118E-08
      btfcnr=  9.99920E-01

iter=  15
     del(conc    H+      )= -2.29577E-08, delfnc=  9.94287E-01
    beta(conc    Mg++    )=  3.44968E-10, betfnc=  9.92808E-01
      bbig=  0.00000E+00, ubbig= none
      bneg= -3.19756E-10, ubneg= HCO3-
      bgamx= -8.29519E-10, ubgamx= CO3--
      bsigmm=  7.47189E-11
      bxi=  5.46612E-10
      btfcnr=  9.99886E-01

Hybrid Newton-Raphson iteration converged in  15 steps.
```

--- Summary of the Aqueous Solution ---

--- Elemental Composition of the Aqueous Solution ---

Element	mg/L	mg/kg	Moles/kg
O	0.79851E+06	0.65667E+06	0.5633061742E+02
Ca	480.94	395.51	0.1354401806E-01
Cl	0.17017E+06	0.13994E+06	0.5417607223E+01
H	99146.	81534.	0.1110213025E+03
C	192.18	158.04	0.1805869074E-01
K	3792.5	3118.9	0.1094808126E+00
Mg	2162.9	1778.7	0.1004402237E+00
Na	0.11196E+06	92073.	0.5496613995E+01
S	5451.2	4482.9	0.1918735892E+00

--- Elemental Composition as Strict Basis Species ---

Species	mg/L	mg/kg	Moles/kg
H2O	0.89912E+06	0.73941E+06	0.5633061742E+02
Ca++	480.94	395.51	0.1354401806E-01

Cl-	0.17017E+06	0.13994E+06	0.5417607223E+01
H+	99146.	81534.	0.1110213025E+03
HCO3-	976.27	802.86	0.1805869074E-01
K+	3792.5	3118.9	0.1094808126E+00
Mg++	2162.9	1778.7	0.1004402237E+00
Na+	0.11196E+06	92073.	0.5496613995E+01
SO4--	16331.	13430.	0.1918735892E+00

--- Equivalent Composition of the Aqueous Solution ---

--- Original Basis ---

Species	Moles/kg H2O
H2O	0.5633061742E+02
Ca++	0.1354401806E-01
Cl-	0.5417607223E+01
H+	0.1110213025E+03
HCO3-	0.1805869074E-01
K+	0.1094808126E+00
Mg++	0.1004402237E+00
Na+	0.5496613995E+01
SO4--	0.1918735892E+00

--- Current Basis (cte) ---

Species	Moles/kg H2O
H2O	0.5633061742E+02
Ca++	0.1354401806E-01
Cl-	0.5417607223E+01
H+	0.1110213025E+03
HCO3-	0.1805869074E-01
K+	0.1094808126E+00
Mg++	0.1004402237E+00
Na+	0.5496613995E+01
SO4--	0.1918735892E+00

Single ion activities and activity coefficients are here defined
with respect to the modified NBS pH scale

	pH	Eh	pe
modified NBS pH scale	8.8569	-14.0660	-2.3778E+02
rational pH scale	9.6700	-14.1141	-2.3859E+02

pHCl = 8.3913

Activity of water = 0.77709
Log activity of water = -0.10953

```
          True osmotic coefficient=    1.23477
Stoichiometric osmotic coefficient=    1.23364

          Sum of true molalities=   11.3372627463177
Sum of stoichiometric molalities=   11.3476195529924

          True ionic strength=    6.1115711780028
Stoichiometric ionic strength=    6.1325965229200
```

--- Electrical Balance Totals ---

	equiv/kg H2O
Sigma(mz) cations =	0.5812819185E+01
Sigma(mz) anions =	-0.5812819185E+01
Total charge =	0.1162563837E+02
Mean charge =	0.5812819185E+01
Charge imbalance =	-0.9555911618E-11

Total charge = sigma(mz) cations + abs (sigma(mz) anions)
Mean charge = 1/2 total charge

The electrical imbalance is

-0.822E-10 per cent of the total charge
-0.164E-09 per cent of the mean charge
-0.164E-09 per cent of sigma(mz) cations
-0.164E-09 per cent of abs (sigma(mz) anions)

--- Electrical Balancing on H+ ---

	Log activity
input	-9.0000
final	-8.8569
adj	0.14307

--- Activity Ratios of Ions -----

Log (act(Ca++	) / act(H+)xx 2) =	16.2339
Log (act(Cl-	) x act(H+)xx 1) =	-8.3913
Log (act(HCO3-	) x act(H+)xx 1) =	-11.9560
Log (act(K+	) / act(H+)xx 1) =	7.8320
Log (act(Mg++	) / act(H+)xx 2) =	17.3281
Log (act(Na+	) / act(H+)xx 1) =	9.8076
Log (act(SO4--	) x act(H+)xx 2) =	-20.6545

--- Distribution of Aqueous Species ---

Species	Molality	Log molality	Log gamma	Log activity

Na+	5.4966E+00	0.7401	0.2105	0.9506
Cl-	5.4176E+00	0.7338	-0.2682	0.4656
SO4--	1.9187E-01	-0.7170	-2.2236	-2.9406
K+	1.0948E-01	-0.9607	-0.0643	-1.0250
Mg++	9.0801E-02	-1.0419	0.6561	-0.3858
Ca++	1.2314E-02	-1.9096	0.4296	-1.4800
MgCO3(aq)	9.1455E-03	-2.0388	0.0000	-2.0388
HCO3-	3.9194E-03	-2.4068	-0.6923	-3.0991
CO3--	3.7629E-03	-2.4245	-2.1569	-4.5814
CaCO3(aq)	1.2299E-03	-2.9101	0.0000	-2.9101
MgOH+	4.9337E-04	-3.3068	-0.1407	-3.4475
OH-	1.9564E-05	-4.7085	-0.5407	-5.2493
CO2(aq)	9.9902E-07	-6.0004	0.4913	-5.5091
HSO4-	4.7160E-10	-9.3264	-0.4925	-9.8190
H+	2.1380E-10	-9.6700	0.8131	-8.8569

--- Mean Stoichiometric Ionic Properties ---

Species	Species	Log a(+/-)	a(+/-)	Log gamma(+/-)	gamma(+/-)
Ca++	Cl-	-0.1829	6.5631E-01	-0.0493	8.9259E-01
Ca++	HCO3-	-2.5594	2.7581E-03	-0.7744	1.6810E-01
Ca++	SO4--	-2.2103	6.1619E-03	-0.9177	1.2087E-01
H+	Cl-	-4.1956	6.3731E-05	-5.4347	3.6749E-06
H+	HCO3-	-5.9780	1.0519E-06	-5.9786	1.0506E-06
H+	SO4--	-6.8848	1.3037E-07	-7.8088	1.5532E-08
K+	Cl-	-0.2797	5.2522E-01	-0.1662	6.8197E-01
K+	HCO3-	-2.0620	8.6689E-03	-0.7100	1.9496E-01
K+	SO4--	-1.6635	2.1701E-02	-0.7841	1.6441E-01
Mg++	Cl-	0.1818	1.5199E+00	0.0253	1.0600E+00
Mg++	HCO3-	-2.1947	6.3873E-03	-0.6998	1.9963E-01
Mg++	SO4--	-1.6632	2.1716E-02	-0.8057	1.5643E-01
Na+	Cl-	0.7081	5.1066E+00	-0.0288	9.3580E-01
Na+	HCO3-	-1.0742	8.4287E-02	-0.5726	2.6753E-01
Na+	SO4--	-0.3465	4.5035E-01	-0.6009	2.5069E-01

Stoichiometric quantities are consistent with the
cte mass balance lumpings, except that
1. effective cte(H+) = cte(H+) - conc(H2O)
2. effective cte(OH-) = cte(H2O) - conc(H2O)

--- Mean Ionic Properties ---

Species	Species	Log a(+/-)	a(+/-)	Log gamma(+/-)	gamma(+/-)
Ca++	Cl-	-0.1829	6.5631E-01	-0.0356	9.2137E-01
Ca++	HCO3-	-2.5594	2.7581E-03	-0.3183	4.8046E-01
Ca++	SO4--	-2.2103	6.1619E-03	-0.8970	1.2677E-01
H+	Cl-	-4.1956	6.3731E-05	0.2724	1.8726E+00
H+	HCO3-	-5.9780	1.0519E-06	0.0604	1.1491E+00
H+	SO4--	-6.8848	1.3037E-07	-0.1992	6.3215E-01
K+	Cl-	-0.2797	5.2522E-01	-0.1662	6.8197E-01
K+	HCO3-	-2.0620	8.6689E-03	-0.3783	4.1849E-01
K+	SO4--	-1.6635	2.1701E-02	-0.7841	1.6441E-01

Mg++	Cl-	0.1818	1.5199E+00	0.0399	1.0963E+00
Mg++	HCO3-	-2.1947	6.3873E-03	-0.2429	5.7166E-01
Mg++	SO4--	-1.6632	2.1716E-02	-0.7838	1.6452E-01
Na+	Cl-	0.7081	5.1066E+00	-0.0288	9.3580E-01
Na+	HCO3-	-1.0742	8.4287E-02	-0.2409	5.7425E-01
Na+	SO4--	-0.3465	4.5035E-01	-0.6009	2.5069E-01

--- Major Aqueous Species Contributing to Mass Balances ---

Aqueous species accounting for 99% or more of Ca++

Species	Factor	Molality	Per Cent
Ca++	1.00	1.2314E-02	90.92
CaCO3(aq)	1.00	1.2299E-03	9.08
Total		1.3544E-02	100.00

Aqueous species accounting for 99% or more of Cl-

Species	Factor	Molality	Per Cent
Cl-	1.00	5.4176E+00	100.00
Total		5.4176E+00	100.00

Aqueous species accounting for 99% or more of HCO3-

Species	Factor	Molality	Per Cent
MgCO3(aq)	1.00	9.1455E-03	50.64
HCO3-	1.00	3.9194E-03	21.70
CO3--	1.00	3.7629E-03	20.84
CaCO3(aq)	1.00	1.2299E-03	6.81
Total		1.8059E-02	99.99

Aqueous species accounting for 99% or more of K+

Species	Factor	Molality	Per Cent
K+	1.00	1.0948E-01	100.00
Total		1.0948E-01	100.00

Aqueous species accounting for 99% or more of Mg++

Species	Factor	Molality	Per Cent
Mg++	1.00	9.0801E-02	90.40
MgCO3(aq)	1.00	9.1455E-03	9.11

Total		1.0044E-01	99.51

Aqueous species accounting for 99% or more of Na+

Species	Factor	Molality	Per Cent
Na+	1.00	5.4966E+00	100.00
Total		5.4966E+00	100.00

Aqueous species accounting for 99% or more of SO4--

Species	Factor	Molality	Per Cent
SO4--	1.00	1.9187E-01	100.00
Total		1.9187E-01	100.00

--- Summary of Aqueous Redox Reactions ---

Couple	Eh, volts	pe-	Log fO2	Ah, kcal
DEFAULT	-14.066	-0.2378E+03	-999.000	-324.394

--- Summary of Aqueous Non-equilibrium Non-redox Neactions ---

Reaction	Log Q/K	Aff, kcal	State

None

--- Summary of Pure Mineral Saturation States ---

(Minerals with affinities .lt. -10 kcal are not listed)

Mineral	Log Q/K	Aff, kcal	State
Anhydrite	-0.0585	-0.0798	satd
Antarcticite	-5.3494	-7.2982	
Aphthitalite	-4.2028	-5.7338	
Aragonite	2.1581	2.9442	ssatd
Arcanite	-3.2142	-4.3851	
Bischofite	-4.5671	-6.2308	
Bloedite	-2.4570	-3.3521	
Brucite	0.0000	0.0000	satd
Burkeite	-3.9867	-5.4391	
CaCl2:4H2O	-6.7039	-9.1460	
Calcite	2.3449	3.1991	ssatd
Carnallite	-5.0014	-6.8234	
Epsomite	-2.2120	-3.0178	

Gaylussite	0.1317	0.1797	satd
Glauberite	-0.2154	-0.2939	satd
Gypsum	-0.0591	-0.0807	satd
Halite	-0.1541	-0.2103	satd
Hexahydrite	-2.3485	-3.2040	
Hydromagne5424	5.9060	8.0575	ssatd
Hydromagne4323	4.0860	5.5745	ssatd
KNaCO3:6H2O	-5.1970	-7.0901	
Kainite	-4.0217	-5.4868	
Kalicinite	-4.4055	-6.0103	
Kieserite	-3.3133	-4.5202	
Leonite	-4.7761	-6.5159	
Mirabilite	-0.9068	-1.2372	
Na2CO3:7H2O	-2.9867	-4.0747	
Na4Ca(SO4)3:2H2O	-1.0461	-1.4271	
Nahcolite	-1.7455	-2.3813	
Natron	-2.9507	-4.0256	
Nesquehonite	-0.1288	-0.1757	satd
Oxychloride-Mg	-0.5316	-0.7252	
Periclase	-4.1169	-5.6166	
Picromerite	-4.6464	-6.3391	
Pirssonite	0.2825	0.3854	satd
Polyhalite	-3.6331	-4.9565	
Portlandite	-6.7886	-9.2616	
Sylvite	-1.4592	-1.9908	
Syngenite	-2.0722	-2.8271	
Thenardite	-0.7519	-1.0258	
Thermonatrite	-3.2715	-4.4633	
Trona	-4.0033	-5.4616	

8 approx. saturated pure minerals
0 approx. saturated input solid solutions
0 saturated hypothetical solid solutions

4 supersaturated pure minerals
0 supersatd. input solid solutions
0 supersatd. hypothetical solid solutions

--- Summary of Gases ---

Gas	Fugacity	Log fugacity
CO2(g)	9.3925E-05	-4.0272
H2(g)	1.0000+282	457.8444
O2(g)	0.0000E+00	-999.0000

--- Reading the input file ---

--- No further input found ---

Start time = 09:57:10 08May2003
End time = 09:57:10 08May2003

```
          Run time =  0.600E-01 seconds

Normal exit
```

EQ3/6, Version 7.2c (EQ3/6-V7-REL-V7.2c-PC)
EQ3NR Speciation-Solubility Code (EQ3/6-V7-EQ3NR-EXE-R141-P6)
Supported by the EQLIB library (EQ3/6-V7-EQLIB-LIB-R172-P6)

Run 09:53:09 08May2003

--- Reading the input file ---

EQ3NR input file name= gwb_acs2.3i
Description= "GWB brine"
Version level= 7.2
Created 05/08/03 Creator= Yongliang Xiong
This input file is modified from c:\eq3_6v7.2\xiong\gwblb\gwb_lb.3i

GWB brine, after A.C. Snider (2003). The pH is calculated from the assumption that the brine is charge balance.
Total dissolved salts (TDS) are the average value of SB-1, SB-2 and SB-3 of L.H. Brush (1990, Table 2.1). Total carbonate concentration expressed as HCO3- is based on total inorganic carbon (TIC) for SB-1 from L.H. Brush (1990, Table 2.1).

Purpose: to generate a pick-up file for reaction path calculations involving a very concentrated brine, using Pitzer's equations to calculate the activity coefficients of the aqueous species.

This problem is addressed using the thermodynamic data base of Harvie, Moller, and Weare (1984) modified by E. Giambalvo, named hmp.

The print option switch IOPR6 is set to 1 to direct the code to print a table of mean ionic properties.

Because Br- in not part of the Harvie-Moller-Weare model, the reported 0.027 M Br- is ignored on this input file.

References

Brush, L.H., 1990, Test plan for laboratory and modeling studies of repository and radionuclide chemistry for the waste isolation pilot plant. SAND90-0266.

Harvie, C. E., Moller, N., and Weare, J. H., 1984, The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25C: Geochimica et Cosmochimica Acta, v. 48, p. 723-751.

Snider, A.C., 2003. Verification of the definition of the generic weep brine and the development of a recipe for this brine. Unpublished report, April 8, 2003. Carlsbad, NM. Sandia National Laboratories. ERMS527505.

Temperature (C)	25.00	Density(gm/cm3)	1.2
Total Dissolved Salts		mg/kg | mg/l	*not used
Electrical Balancing on	H+	code selects	not performed

SPECIES	BASIS SWITCH/CONSTRAINT	CONC/ETC	UNITS OR TYPE
Na+		3.480	Molarity
K+		0.458	Molarity
Mg++	Brucite	0.000	Mineral
Ca++		0.014	Molarity
Cl-		5.510	Molarity
HCO3-		3.70E-04	Molarity
SO4--		0.175	Molarity
H+		9.00000	pH

Input Solid Solutions

none

SUPPRESSED SPECIES	(suppress,replace,augmentk,augmentg)	value
Magnesite	mineral	Suppress | 0.0
Dolomite	mineral	Suppress | 0.0

OPTIONS

- SOLID SOLUTIONS -
  - * ignore solid solutions
    process hypothetical solid solutions
    process input and hypothetical solid solutions
- LOADING OF SPECIES INTO MEMORY -
  - * does nothing
    lists species loaded into memory
- ECHO DATABASE INFORMATION -
  - * does nothing
    lists all reactions
    lists reactions and log K values
    lists reactions, log K values and polynomial coef.
- LIST OF AQUEOUS SPECIES (ordering) -
  - * in order of decreasing concentration
    in same order as input file
- LIST OF AQUEOUS SPECIES (concentration limit) -
  - * all species
    only species > 10**-20 molal
    only species > 10**-12 molal
    not printed
- LIST OF AQUEOUS SPECIES (by element) -
  - * print major species

```
|     print all species                                                    |
|     don't print                                                          |
| - MINERAL SATURATION STATES -                                            |
|   * print if affinity > -10 kcals                                        |
|     print all                                                            |
|     don't print                                                          |
| - pH SCALE CONVENTION -                                                  |
|   * modified NBS                                                         |
|     internal                                                             |
|     rational                                                             |
| - ACTIVITY COEFFICIENT OPTIONS -                                         |
|     use B-dot equation                                                   |
|     Davies' equation                                                     |
|   * Pitzer's equations                                                   |
| - AUTO BASIS SWITCHING -                                                 |
|   * off                                                                  |
|     on                                                                   |
| - PITZER DATABASE INFORMATION -                                          |
|   * print only warnings                                                  |
|     print species in model and number of Pitzer coefficients             |
|     print species in model and names of Pitzer coefficients              |
| - PICKUP FILE -                                                          |
|   * write pickup file                                                    |
|     don't write pickup file                                              |
| - LIST MEAN IONIC PROPERTIES -                                           |
|     don't print                                                          |
|   * print                                                                |
| - LIST AQUEOUS SPECIES, ION SIZES, AND HYDRATION NUMBERS -               |
|   * print                                                                |
|     don't print                                                          |
| - CONVERGENCE CRITERIA -                                                 |
|   * test both residual functions and correction terms                    |
|     test only residual functions                                         |
|--------------------------------------------------------------------------|
|DEBUGGING SWITCHES (0 = off, 1,2 = on                                     |
|--------------------------------------------------------------------------|
|0  generic debugging information                                          |2
|0  print details of pre-Newton-Raphson iteration                          |2
|0  print details of Newton-Raphson iteration                              |
|0  print details of stoichiometric factors                                |2
|0  print details of stoichiometric factors calculation                    |
|0  write reactions on RLIST                                               |
|0  list stoichiometric concentrations of master species                   |
|0  request iteration variables to be killed                               |
|--------------------------------------------------------------------------|
|DEVELOPMENT OPTIONS  (used for code development)                           |
|--------------------------------------------------------------------------|
| none                                                                     |
|--------------------------------------------------------------------------|
|TOLERANCES                    (desired values)        (defaults)          |
|--------------------------------------------------------------------------|
|      residual functions  |                          |1.0e-10  tolbt     |
|        correction terms  |                          |1.0e-10  toldl     |
|        saturation state  |                          |0.5      tolsat    |
|number of N-R iterations  |                          |30       itermx    |
|--------------------------------------------------------------------------|
```

```
--- The input file has been successfully read ---

--- Reading the data1 file ---

--- The data1 file has been successfully read ---

The species Magnesite                has been user-suppressed

The species Dolomite                 has been user-suppressed

                    --- Pitzer Coefficient Summary ---
```

```
eeee   qqq   33333  n   n  rrrr
e     q   q      3  nn  n  r   r
eeee  q   q    33   n n n  rrrr
e     q q q      3  n  nn  r  r
eeee   qqq   3333   n   n  r   r
          q
```

```
EQ3NR, version 7.2c (R141    )
 supported by EQLIB, version 7.2c (R172    )
```

```
|EQ3NR input file name= gwb_acs2.3i                                          |
|Description= "GWB brine"                                                    |
|Version level= 7.2                                                          |
|Created 05/08/03    Creator= Yongliang Xiong                                |
|This input file is modified from c:\eq3_6v7.2\xiong\gwb1b\gwb_1b.3i          |
|                                                                            |
|  GWB brine, after A.C. Snider (2003). The pH is calculated from the        |
|assumption that the brine is charge balance.                                |
|Total dissolved salts (TDS) are the average value of                        |
|SB-1, SB-2 and SB-3 of L.H. Brush (1990, Table 2.1).  Total carbonate       |
|concentration expressed as HCO3- is based on total inorganic carbon         |
|(TIC) for SB-1 from L.H. Brush (1990, Table 2.1).                           |
|                                                                            |
|  Purpose: to generate a pick-up file for reaction path calculations        |
|involving a very concentrated brine, using Pitzer's equations to           |
|calculate the activity coefficients of the aqueous species.                 |
|                                                                            |
|  This problem is addressed using the thermodynamic data base of            |
|Harvie, Moller, and Weare (1984) modified by E. Giambalvo, named hmp.       |
|                                                                            |
|  The print option switch IOPR6 is set to 1 to direct the code to           |
|print a table of mean ionic properties.                                     |
|                                                                            |
|  Because Br- in not part of the Harvie-Moller-Weare model, the             |
|reported 0.027 M Br- is ignored on this input file.                         |
```

References

Brush, L.H., 1990, Test plan for laboratory and modeling studies of repository and radionuclide chemistry for the waste isolation pilot plant. SAND90-0266.

Harvie, C. E., Moller, N., and Weare, J. H., 1984, The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25C: Geochimica et Cosmochimica Acta, v. 48, p. 723-751.

Snider, A.C., 2003. Verification of the definition of the generic weep brine and the development of a recipe for this brine. Unpublished report, April 8, 2003. Carlsbad, NM. Sandia National Laboratories. ERMS527505.

data0.hmw.V8.R6
CII: GEMBOCHS.V2-EQ8-data0.hmw.V8.R6
THERMODYNAMIC DATABASE
generated by GEMBOCHS.V2-Jewel.src.R5 02-dec-1996 11:27:50
Output package: eq3
Data set: hmw

The activity coefficients of aqueous solute species
and the activity of water are calculated according to the
Pitzer equations

E-lambda flag= on

Temperature= 25.00 degrees Celsius
pressure= 1.0132 bars

9 elements are in the data base
110 elements can be loaded into memory
9 elements are active in this problem

17 aqueous species are in the data base
17 aqueous species were loaded into memory
2500 aqueous species can be loaded into memory
16 aqueous species are active in this problem

7 aqueous reactions are in the data base
7 aqueous reactions were loaded into memory
2389 aqueous reactions can be loaded into memory

57 minerals are in the data base
57 minerals were loaded into memory
1500 minerals can be loaded into memory

```
 55 minerals are active in this problem

  0 solid solutions are in the data base
 50 solid solutions can be loaded into memory

  3 gases are in the data base
  3 gases were loaded into memory
200 gases can be loaded into memory
  3 gases are in the active in this problem



iopt1  =  0 (redox option switch)
iopt2  =  0 (automatic basis switching switch)
iopt3  =  0 (interfacing output control switch)
iopt4  =  0 (turn-on solid solutions switch)
iopt5  =  0 (not used)
iopt6  =  0 (conv. test criteria switch)
iopt7  =  0 (0/1 version 7/post-version 7 pickup file)
iopt8  =  0 (not used)
iopt9  =  0 (not used)
iopt10 =  0 (not used)


     iopg1  =  1 (act. coeff. choice)
     iopg2  =  0 (pH scale convention switch)
     iopg3  =  0 (not used)
     iopg4  =  0 (not used)
     iopg5  =  0 (not used)
     iopg6  =  0 (not used)
     iopg7  =  0 (not used)
     iopg8  =  0 (not used)
     iopg9  =  0 (not used)
     iopg10 =  0 (not used)


          iopr1  =  0 (list loading of species)
          iopr2  =  0 (list reactions and log K values)
          iopr3  =  0 (aqueous species print order control)
          iopr4  =  0 (aqueous species print cut-off control)
          iopr5  =  0 (mass balance percentages print control)
          iopr6  =  1 (mean ionic act coeff print control)
          iopr7  =  0 (mineral affinity print control)
          iopr8  =  0 (ion size and hydr. no. print control)
          iopr9  =  0 (Pitzer coefficients tabulation)
          iopr10 =  0 (print concbs array)
          iopr11 =  0 (not used)
          iopr12 =  0 (not used)
          iopr13 =  0 (not used)
          iopr14 =  0 (not used)
          iopr15 =  0 (not used)
          iopr16 =  0 (not used)
          iopr17 =  0 (not used)
          iopr18 =  0 (not used)
          iopr19 =  0 (not used)
```

```
iopr20 =  0 (not used)

     iodb1  =  0 (print info. messages switch)
     iodb2  =  0 (print pre-Newton-Raphson optimizations switch)
     iodb3  =  0 (request iteration variables to kill)
     iodb4  =  0 (print Newton-Raphson iterations switch)
     iodb5  =  0 (list stoichiometric equivalences)
     iodb6  =  0 (controls iodb5 level of detail)
     iodb7  =  0 (write reactions on file rlist switch)
     iodb8  =  0 (not used)
     iodb9  =  0 (not used)
     iodb10 =  0 (not used)

The default redox state is constrained by log fO2 = -999.0000 (log bars)

     Solution density =  1.20000 g/mL

     Total dissolved salts =       0.00 mg/kg solution
     Total dissolved salts =       0.00 mg/L

   Tolbt  =  0.10000E-05 (convergence tolerance on residual functions)
   Toldl  =  0.10000E-05 (convergence tolerance on correction terms)
   Tolsat =  0.50000E+00 (phase saturation tolerance, does not affect
                          convergence)

                    --- Input Constraints ---

   Species                  Csp      Jflag   Input Type/Co-species

Na+                     3.4800E+00    1    Total conc, molar
K+                      4.5800E-01    1    Total conc, molar
Mg++                    0.0000E+00   19    Mineral equilibrium
                                            Brucite

                  1.000  Brucite
                + 2.000  H+
                     ==
                  2.000  H2O
                + 1.000  Mg++
Ca++                 1.4000E-02    1    Total conc, molar
Cl-                  5.5100E+00    1    Total conc, molar
HCO3-                3.7000E-04    1    Total conc, molar
SO4--                1.7500E-01    1    Total conc, molar
H+                  -9.0000E+00   16    Log activity

Electrical balance will be achieved by adjusting
  the concentration of "H+                    ". Any other specified
  constraint will be overridden.
```

--- Inactive Aqueous Species ---

--- Modified Input Constraints ---

Species	Csp	Jflag	Input Type/Co-species
Ca++	1.1667E-02	0	Total conc, molal
Cl-	4.5917E+00	0	Total conc, molal
H+	-9.0000E+00	16	Log activity
HCO3-	3.0833E-04	0	Total conc, molal
K+	3.8167E-01	0	Total conc, molal
Mg++	0.0000E+00	19	Mineral equilibrium
			Brucite
	1.000 Brucite		
	+ 2.000 H+		
	==		
	2.000 H2O		
	+ 1.000 Mg++		
Na+	2.9000E+00	0	Total conc, molal
SO4--	1.4583E-01	0	Total conc, molal

--- Optimization ended within requested limits ---

```
iter=   0
       del(                )=  0.00000E+00, delfnc=  0.00000E+00
      beta(conc    H+      )= -1.60808E-01, betfnc=  0.00000E+00
        bbig=  1.86307E-02, ubbig= HCO3-
        bneg= -4.84997E-03, ubneg= Ca++
        bgamx=  8.67153E-02, ubgamx= Mg++
        bsigmm= -1.19931E-03
        bxi= -4.34171E-03
        btfcnr=  0.00000E+00

iter=   1
      Gammas are fixed
       del(conc    Mg++    )=  2.60427E+00, delfnc=  0.00000E+00
      Relaxation factor=  0.76797
      Relaxed del(conc    Mg++    )=  2.00000E+00
      beta(conc    HCO3-   )=  2.28767E+00, betfnc= -1.32261E+01
        bbig=  2.28767E+00, ubbig= HCO3-
        bneg=  0.00000E+00, ubneg= none
        bgamx= -1.00637E+01, ubgamx= CO3--
        bsigmm=  1.36991E+00
        bxi=  4.98238E+00
        btfcnr= -1.32261E+01

iter=   2
      Gammas are fixed
       del(conc    Mg++    )= -4.03907E-01, delfnc=  8.44906E-01
```

```
      Relaxation factor=  0.50000
      Relaxed del(conc    Mg++    )= -2.01953E-01
      beta(conc    HCO3-   )=  1.32555E+00, betfnc=  4.20568E-01
        bbig=  1.32555E+00, ubbig= HCO3-
        bneg=  0.00000E+00, ubneg= none
        bgamx= -5.65503E+00, ubgamx= CO3--
        bsigmm=  2.36925E-01
        bxi=  1.74059E+00
        btfcnr=  4.20568E-01

iter=   3
      Gammas are fixed
       del(conc    Mg++    )= -3.85906E-01, delfnc=  4.45671E-02
      Relaxation factor=  0.50000
      Relaxed del(conc    Mg++    )= -1.92953E-01
      beta(conc    HCO3-   )=  7.52595E-01, betfnc=  4.32240E-01
        bbig=  7.52595E-01, ubbig= HCO3-
        bneg=  0.00000E+00, ubneg= none
        bgamx= -3.51246E+00, ubgamx= CO3--
        bsigmm= -1.68035E-01
        bxi=  3.23081E-01
        btfcnr=  4.32240E-01

iter=   4
      Gammas are fixed
       del(conc    Mg++    )= -3.58826E-01, delfnc=  7.01714E-02
      Relaxation factor=  0.50000
      Relaxed del(conc    Mg++    )= -1.79413E-01
      beta(conc    HCO3-   )=  4.17451E-01, betfnc=  4.45318E-01
        bbig=  4.17451E-01, ubbig= HCO3-
        bneg=  0.00000E+00, ubneg= none
        bgamx= -2.43459E+00, ubgamx= CO3--
        bsigmm= -1.22195E-01
        bxi= -2.30448E-01
        btfcnr=  4.45318E-01

iter=   5
      Gamma relaxation factor=  0.50000
       del(conc    Mg++    )= -3.20211E-01, delfnc=  1.07617E-01
      beta(conc    HCO3-   )= -2.54502E-01, betfnc=  3.90343E-01
        bbig=  0.00000E+00, ubbig= none
        bneg= -2.54502E-01, ubneg= HCO3-
        bgamx= -1.24720E+00, ubgamx= CO3--
        bsigmm= -1.41962E-01
        bxi= -3.05367E-01
        btfcnr=  7.19506E-01

iter=   6
      Gamma relaxation factor=  0.60000
       del(conc    H+      )= -1.99645E-01, delfnc=  3.76520E-01
      beta(conc    HCO3-   )=  5.08688E-02, betfnc=  8.00124E-01
        bbig=  5.08688E-02, ubbig= HCO3-
        bneg= -1.21277E-10, ubneg= SO4--
        bgamx= -6.29282E-01, ubgamx= CO3--
        bsigmm= -5.50756E-02
        bxi= -1.46326E-01
        btfcnr=  7.90064E-01
```

```
iter=   7
      Gamma relaxation factor=  0.70000
       del(conc    Mg++    )= -5.99318E-02, delfnc=  6.99808E-01
      beta(conc    HCO3-   )=  6.23405E-02, betfnc= -2.25516E-01
        bbig=  6.23405E-02, ubbig= HCO3-
        bneg= -1.67235E-10, ubneg= SO4--
        bgamx= -3.47476E-01, ubgamx= CO3--
        bsigmm= -1.31850E-02
        bxi= -3.87821E-02
        btfcnr=  9.61526E-01

iter=   8
      Gamma relaxation factor=  0.80000
       del(conc    HCO3-   )= -1.77538E-02, delfnc=  7.03767E-01
      beta(conc    HCO3-   )=  5.01584E-02, betfnc=  1.95413E-01
        bbig=  5.01584E-02, ubbig= HCO3-
        bneg= -4.79285E-11, ubneg= SO4--
        bgamx= -1.63868E-01, ubgamx= CO3--
        bsigmm= -9.36086E-04
        bxi= -2.82805E-03
        btfcnr=  9.70760E-01

iter=   9
      Gamma relaxation factor=  0.90000
       del(conc    HCO3-   )= -1.78134E-02, delfnc= -3.36132E-03
      beta(conc    HCO3-   )=  1.33137E-02, betfnc=  7.34568E-01
        bbig=  1.33137E-02, ubbig= HCO3-
        bneg= -1.06726E-11, ubneg= SO4--
        bgamx= -3.27396E-02, ubgamx= CO3--
        bsigmm= -3.54026E-06
        bxi= -9.08052E-06
        btfcnr=  9.76429E-01

iter=  10
       del(conc    HCO3-   )= -5.04500E-03, delfnc=  7.16787E-01
      beta(conc    HCO3-   )=  1.46028E-03, betfnc=  8.90317E-01
        bbig=  1.46028E-03, ubbig= HCO3-
        bneg= -1.20075E-12, ubneg= SO4--
        bgamx= -3.27543E-03, ubgamx= CO3--
        bsigmm=  3.11571E-07
        bxi=  1.49989E-06
        btfcnr=  9.93447E-01

iter=  11
       del(conc    HCO3-   )= -5.60248E-04, delfnc=  8.88950E-01
      beta(conc    HCO3-   )=  8.27900E-07, betfnc=  9.99433E-01
        bbig=  8.27900E-07, ubbig= HCO3-
        bneg= -7.61296E-16, ubneg= SO4--
        bgamx= -1.70189E-07, ubgamx= CO3--
        bsigmm=  3.68843E-08
        bxi=  1.72861E-07
        btfcnr=  9.99270E-01

iter=  12
       del(conc    HCO3-   )= -4.10172E-07, delfnc=  9.99268E-01
      beta(conc    H2O     )= -6.76131E-12, betfnc=  9.99992E-01
```

bbig= 0.00000E+00, ubbig= none
bneg= -3.70199E-12, ubneg= HCO3-
bgamx= -1.97459E-11, ubgamx= Ca++
bsigmm= -3.27858E-11
bxi= -9.95106E-12
btfcnr= 9.99992E-01

Hybrid Newton-Raphson iteration converged in 12 steps.

--- Summary of the Aqueous Solution ---

--- Elemental Composition of the Aqueous Solution ---

Element	mg/L	mg/kg	Moles/kg
O	0.10770E+07	0.89747E+06	0.5609370155E+02
Ca	561.09	467.58	0.1166666667E-01
Cl	0.19534E+06	0.16279E+06	0.4591666667E+01
H	0.13428E+06	0.11190E+06	0.1110179167E+03
C	4.4441	3.7034	0.3083333333E-03
K	17907.	14923.	0.3816666667E+00
Mg	23040.	19200.	0.7899598874E+00
Na	80004.	66670.	0.2900000000E+01
S	5611.6	4676.3	0.1458333333E+00

--- Elemental Composition as Strict Basis Species ---

Species	mg/L	mg/kg	Moles/kg
H2O	0.12127E+07	0.10105E+07	0.5609370155E+02
Ca++	561.09	467.58	0.1166666667E-01
Cl-	0.19534E+06	0.16279E+06	0.4591666667E+01
H+	0.13428E+06	0.11190E+06	0.1110179167E+03
HCO3-	22.576	18.814	0.3083333333E-03
K+	17907.	14923.	0.3816666667E+00
Mg++	23040.	19200.	0.7899598874E+00
Na+	80004.	66670.	0.2900000000E+01
SO4--	16811.	14009.	0.1458333333E+00

--- Equivalent Composition of the Aqueous Solution ---

--- Original Basis ---

Species	Moles/kg H2O
H2O	0.5609370155E+02
Ca++	0.1166666667E-01
Cl-	0.4591666667E+01
H+	0.1110179167E+03

HCO3-	0.3083333333E-03
K+	0.3816666667E+00
Mg++	0.7899598874E+00
Na+	0.2900000000E+01
SO4--	0.1458333333E+00

--- Current Basis (cte) ---

Species	Moles/kg H2O
H2O	0.5609370155E+02
Ca++	0.1166666667E-01
Cl-	0.4591666667E+01
H+	0.1110179167E+03
HCO3-	0.3083333333E-03
K+	0.3816666667E+00
Mg++	0.7899598874E+00
Na+	0.2900000000E+01
SO4--	0.1458333333E+00

Single ion activities and activity coefficients are here defined with respect to the modified NBS pH scale

	pH	Eh	pe
modified NBS pH scale	8.4544	-14.0428	-2.3738E+02
rational pH scale	9.1470	-14.0838	-2.3808E+02

pHCl = 8.0592

Activity of water = 0.81644
Log activity of water = -0.08807

True osmotic coefficient= 1.27618
Stoichiometric osmotic coefficient= 1.27615

Sum of true molalities= 8.8208894686547
Sum of stoichiometric molalities= 8.8211015877852

True ionic strength= 5.8297573041189
Stoichiometric ionic strength= 5.8317406250520

--- Electrical Balance Totals ---

	equiv/kg H2O
Sigma(mz) cations =	0.4883473617E+01
Sigma(mz) anions =	-0.4883473617E+01
Total charge =	0.9766947235E+01
Mean charge =	0.4883473617E+01

Charge imbalance = -0.1421085472E-13

Total charge = sigma(mz) cations + abs (sigma(mz) anions)
Mean charge = 1/2 total charge

The electrical imbalance is

-0.145E-12 per cent of the total charge
-0.291E-12 per cent of the mean charge
-0.291E-12 per cent of sigma(mz) cations
-0.291E-12 per cent of abs (sigma(mz) anions)

--- Electrical Balancing on H+ ---

Log activity

input	-9.0000
final	-8.4544
adj	0.54562

--- Activity Ratios of Ions -----

Log (act(Ca++	) / act(H+)xx 2) =	15.2494
Log (act(Cl-	) x act(H+)xx 1) =	-8.0592
Log (act(HCO3-	) x act(H+)xx 1) =	-13.5271
Log (act(K+	) / act(H+)xx 1) =	7.9747
Log (act(Mg++	) / act(H+)xx 2) =	17.2851
Log (act(Na+	) / act(H+)xx 1) =	9.1100
Log (act(SO4--	) x act(H+)xx 2) =	-19.9643

--- Distribution of Aqueous Species ---

Species	Molality	Log molality	Log gamma	Log activity
Cl-	4.5917E+00	0.6620	-0.2668	0.3952
Na+	2.9000E+00	0.4624	0.1932	0.6556
Mg++	7.8874E-01	-0.1031	0.4795	0.3764
K+	3.8167E-01	-0.4183	-0.0613	-0.4797
SO4--	1.4583E-01	-0.8361	-2.2194	-3.0555
Ca++	1.1663E-02	-1.9332	0.2738	-1.6594
MgOH+	9.9438E-04	-3.0024	-0.0640	-3.0664
MgCO3(aq)	2.2247E-04	-3.6527	0.0000	-3.6527
CO3--	4.4070E-05	-4.3559	-2.6017	-6.9575
HCO3-	3.8343E-05	-4.4163	-0.6564	-5.0727
OH-	1.3802E-05	-4.8600	-0.7703	-5.6304
CaCO3(aq)	3.4224E-06	-5.4657	0.0000	-5.4657
CO2(aq)	3.2361E-08	-7.4900	0.3884	-7.1016
H+	7.1287E-10	-9.1470	0.6926	-8.4544
HSO4-	6.0520E-10	-9.2181	-0.3132	-9.5313

--- Mean Stoichiometric Ionic Properties ---

Species	Species	Log a(+/-)	a(+/-)	Log gamma(+/-)	gamma(+/-)
Ca++	Cl-	-0.2897	5.1324E-01	-0.0866	8.1914E-01
Ca++	HCO3-	-3.9349	1.1617E-04	-0.9499	1.1222E-01
Ca++	SO4--	-2.3574	4.3909E-03	-0.9728	1.0645E-01
H+	Cl-	-4.0296	9.3409E-05	-5.2328	5.8508E-06
H+	HCO3-	-6.7635	1.7237E-07	-5.8802	1.3175E-06
H+	SO4--	-6.6548	2.2143E-07	-7.5390	2.8909E-08
K+	Cl-	-0.0423	9.0729E-01	-0.1641	6.8536E-01
K+	HCO3-	-2.7762	1.6742E-03	-0.8115	1.5434E-01
K+	SO4--	-1.3383	4.5890E-02	-0.7807	1.6569E-01
Mg++	Cl-	0.3889	2.4485E+00	-0.0183	9.5877E-01
Mg++	HCO3-	-3.2563	5.5419E-04	-0.8816	1.3135E-01
Mg++	SO4--	-1.3396	4.5754E-02	-0.8703	1.3480E-01
Na+	Cl-	0.5254	3.3527E+00	-0.0368	9.1877E-01
Na+	HCO3-	-2.2085	6.1867E-03	-0.6842	2.0690E-01
Na+	SO4--	-0.5814	2.6216E-01	-0.6110	2.4492E-01

Stoichiometric quantities are consistent with the
cte mass balance lumpings, except that
1. effective cte(H+) = cte(H+) - conc(H2O)
2. effective cte(OH-) = cte(H2O) - conc(H2O)

--- Mean Ionic Properties ---

Species	Species	Log a(+/-)	a(+/-)	Log gamma(+/-)	gamma(+/-)
Ca++	Cl-	-0.2897	5.1324E-01	-0.0866	8.1922E-01
Ca++	HCO3-	-3.9349	1.1617E-04	-0.3463	4.5049E-01
Ca++	SO4--	-2.3574	4.3909E-03	-0.9728	1.0647E-01
H+	Cl-	-4.0296	9.3409E-05	0.2129	1.6327E+00
H+	HCO3-	-6.7635	1.7237E-07	0.0181	1.0426E+00
H+	SO4--	-6.6548	2.2143E-07	-0.2781	5.2716E-01
K+	Cl-	-0.0423	9.0729E-01	-0.1641	6.8536E-01
K+	HCO3-	-2.7762	1.6742E-03	-0.3589	4.3766E-01
K+	SO4--	-1.3383	4.5890E-02	-0.7807	1.6569E-01
Mg++	Cl-	0.3889	2.4485E+00	-0.0181	9.5927E-01
Mg++	HCO3-	-3.2563	5.5419E-04	-0.2778	5.2750E-01
Mg++	SO4--	-1.3396	4.5754E-02	-0.8700	1.3491E-01
Na+	Cl-	0.5254	3.3527E+00	-0.0368	9.1877E-01
Na+	HCO3-	-2.2085	6.1867E-03	-0.2316	5.8671E-01
Na+	SO4--	-0.5814	2.6216E-01	-0.6110	2.4492E-01

--- Major Aqueous Species Contributing to Mass Balances ---

Aqueous species accounting for 99% or more of Ca++

Species	Factor	Molality	Per Cent
Ca++	1.00	1.1663E-02	99.97
Total		1.1667E-02	99.97

Aqueous species accounting for 99% or more of Cl-

Species	Factor	Molality	Per Cent
Cl-	1.00	4.5917E+00	100.00
Total		4.5917E+00	100.00

Aqueous species accounting for 99% or more of HCO3-

Species	Factor	Molality	Per Cent
MgCO3(aq)	1.00	2.2247E-04	72.15
CO3--	1.00	4.4070E-05	14.29
HCO3-	1.00	3.8343E-05	12.44
CaCO3(aq)	1.00	3.4224E-06	1.11
Total		3.0833E-04	99.99

Aqueous species accounting for 99% or more of K+

Species	Factor	Molality	Per Cent
K+	1.00	3.8167E-01	100.00
Total		3.8167E-01	100.00

Aqueous species accounting for 99% or more of Mg++

Species	Factor	Molality	Per Cent
Mg++	1.00	7.8874E-01	99.85
Total		7.8996E-01	99.85

Aqueous species accounting for 99% or more of Na+

Species	Factor	Molality	Per Cent
Na+	1.00	2.9000E+00	100.00
Total		2.9000E+00	100.00

Aqueous species accounting for 99% or more of SO4--

Species	Factor	Molality	Per Cent
SO4--	1.00	1.4583E-01	100.00
Total		1.4583E-01	100.00

--- Summary of Aqueous Redox Reactions ---

Couple	Eh, volts	pe-	Log fO2	Ah, kcal
DEFAULT	-14.043	-0.2374E+03	-999.000	-323.860

--- Summary of Aqueous Non-equilibrium Non-redox Neactions ---

Reaction	Log Q/K	Aff, kcal	State
None			

--- Summary of Pure Mineral Saturation States ---

(Minerals with affinities .lt. -10 kcal are not listed)

Mineral	Log Q/K	Aff, kcal	State
Anhydrite	-0.3528	-0.4813	satd
Antarcticite	-5.5411	-7.5596	
Aphthitalite	-3.0917	-4.2180	
Aragonite	-0.3975	-0.5423	
Arcanite	-2.2386	-3.0540	
Bischofite	-3.8172	-5.2077	
Bloedite	-2.4288	-3.3136	
Brucite	0.0000	0.0000	satd
CaCl2:4H2O	-6.9384	-9.4660	
Calcite	-0.2107	-0.2874	satd
Carnallite	-3.7767	-5.1524	
Epsomite	-1.4146	-1.9299	
Gaylussite	-5.2827	-7.2071	
Glauberite	-1.2147	-1.6572	
Gypsum	-0.3105	-0.4237	satd
Halite	-0.5196	-0.7089	
Hexahydrite	-1.5725	-2.1453	
Hydromagne5424	-0.4639	-0.6329	
Hydromagne4323	-0.6914	-0.9433	
KNaCO3:6H2O	-7.1941	-9.8148	
Kainite	-2.8353	-3.8681	
Kalicinite	-5.8338	-7.9589	
Kieserite	-2.6445	-3.6079	
Leonite	-3.0673	-4.1847	
Mirabilite	-1.3972	-1.9062	
Na2CO3:7H2O	-5.8027	-7.9165	
Na4Ca(SO4)3:2H2O	-2.7073	-3.6935	
Nahcolite	-4.0141	-5.4763	
Natron	-5.7023	-7.7796	
Nesquehonite	-1.6784	-2.2898	
Oxychloride-Mg	-0.1351	-0.1844	satd
Periclase	-4.1383	-5.6459	
Picromerite	-2.8947	-3.9493	
Pirssonite	-5.1963	-7.0892	

Polyhalite	-2.5558	-3.4869
Sylvite	-0.9844	-1.3430
Syngenite	-1.3694	-1.8683
Thenardite	-1.4568	-1.9875
Thermonatrite	-6.2162	-8.4807

5 approx. saturated pure minerals
0 approx. saturated input solid solutions
0 saturated hypothetical solid solutions

0 supersaturated pure minerals
0 supersatd. input solid solutions
0 supersatd. hypothetical solid solutions

--- Summary of Gases ---

Gas	Fugacity	Log fugacity
CO2(g)	2.4004E-06	-5.6197
H2(g)	1.0000+282	457.8658
O2(g)	0.0000E+00	-999.0000

--- Reading the input file ---

--- No further input found ---

Start time = 09:53:09 08May2003
End time = 09:53:09 08May2003

Run time = 0.700E-01 seconds

Normal exit