Geochemical Analysis of the Sealing System

Technical Report to
Work Package 9.1.2

Preliminary Safety Case of the
Gorleben Site (VSG)

GRS - 308

Gesellschaft für Anlagen-
und Reaktorsicherheit
(GRS) mbH

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Mingliang Xie
Horst-Jürgen Herbert

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Preliminary remark – changed objective of the VSG project (as at: December 2012)

The Preliminary Safety Case of the Gorleben Site (VSG) is a research project of Gesellschaft für Anlagen- und Reaktorsicherheit (GRS). GRS has taken over the scientific and organisational management of the project that is funded by the Federal Ministry and deals with the major part of the work packages itself.

Original Objectives

In its original concept, the VSG project pursued three major objectives. The first objective was to prepare a systematic summary of the state of knowledge relating to Gorleben. On this basis, a preliminary suitability prognosis was to be made as a second objective. This prognosis was to provide an answer to the question of how and, if so, under what conditions a repository for heat-generating radioactive waste could be operated at the Gorleben site. The preliminary character of such a prognosis follows inevitably i.a. from the circumstance that a final statement on suitability is only possible following a complete underground exploration, which is not the case at Gorleben. Finally, the third objective of the VSG was to identify any further need for research and development, i.e. the site-specific and site-independent issues that remain to be clarified.

Adapted objectives

When the project was already underway, broad political consensus was reached that the site for a future repository for heat-generating radioactive waste should be found by way of comparing different sites within the framework of a multistage selection procedure. It follows from this fundamental decision that the question of the suitability of a site can in future only be answered by comparing it with other sites. „Suitable“ in this sense will be the site that fulfils various fundamental and comparative criteria and which, regarding safety, therefore shows itself to be the best site compared to others. As these criteria have not yet been defined to this date, it is not possible to make a preliminary prognosis as part of the VSG of the suitability of the Gorleben site as understood in this way.

Against this background, GRS – by mutual agreement with the Federal Environment Ministry (BMU) as sponsor of the VSG – adapted the objectives of the project to the changed boundary conditions. While the systematic summary of the state of knowledge relating to Gorleben and the identification of the future need for research and development remained as objectives of the VSG, the changes concerned the following points:

- The originally intended provisional prognosis of the suitability of the Gorleben site will no longer be pursued. What will be examined will be whether the repository concepts developed in the VSG project in combination with the geological barrier at the Gorleben site or with respect to a comparable site regarding the geological situation are suitable from today‘s point of view to fulfil the requirements of the BMU‘s Safety Criteria.
- The objectives of the project so far will be supplemented by an analysis of the question of which methodological approaches of the VSG may reasonably be used in a future site selection procedure for a comparison of repository sites. Irrespective of the concrete structuring of the future site selection procedure, it is already foreseeable today that during the course of such a procedure, it will be necessary again and again to systematically summarise and assess the state of knowledge regarding the different sites up to a certain step of the procedure.
- Moreover, the project is to examine beyond the original objectives which of the technical concepts developed as part of the VSG for the emplacement of the radioactive waste and for closing the repository mine may be transferred to repository systems at sites with different geological conditions.

Adapted project planning

Due to the decision of May 2011 to phase out nuclear power, the prognosis of the total amount of heat-generating radioactive waste has changed considerably compared with what was assumed at the start of the project in the summer of 2010. This led to the fact that a considerable part of the concept developments and model calculations performed until May 2011 had to be carried out again with the new data and that some sub-reports that had already been complete had to be replaced by revised versions. This additional effort and the above-mentioned supplements regarding the objectives of the VSG meant that it was not possible to conclude the project – as originally intended – at the end of 2012 but at the end of March 2013 instead.

Project partners

Since specialist knowledge from different disciplines is needed for working on the VSG, various partners are involved in the project apart from GRS. Among these are: Dr. Bruno Baltes, the Federal Institute for Geosciences and Natural Resources (Bundesanstalt für Geowissenschaften und Rohstoffe - BGR), DBE TECHNOLOGY GmbH, the Institute of Mineral and Waste Processing, Waste Disposal and Geomechanics (Institut für Aufbereitung, Deponietechnik und Geomechanik) of Clausthal University of Technology (TU Clausthal), the Institute for Rock Mechanics (Institut für Gebirgsmechanik GmbH - IfG), the Institute for Safety Technology (Institut für Sicherheitstechnologie - ISTec), the Karlsruhe Institute of Technology/Institute for Nuclear Waste Disposal (Karlsruher Institut für Technologie/Institut für Nukleare Entsorgung - KIT/INE), international nuclear safety engineering GmbH (nse; several institutes of RWTH Aachen) as well as the Institute for Atmospheric and Environmental Sciences (Institut für Atmosphäre und Umwelt - IAU) of Frankfurt University.

Work packages

The overview of the work packages (WP) of the Preliminary Safety Case of the Gorleben Site (VSG) comprises the following:

- WP 1: Project co-ordination
- WP 2: Geoscientific site characterisation and long-term prediction
- WP 3: Waste specification and volume
- WP 4: Safety and demonstration concept
- WP 5: Repository concept
- WP 6: Repository design and optimisation
- WP 7: Catalogue of FEPs
- WP 8: Development of scenarios
- WP 9: Integrity analyses
- WP 10: Analysis of release scenarios
- WP 11: Assessment of human intrusion
- WP 12: Assessment of operational safety
- WP 13: Assessment of the results
- WP 14: Recommendations

Keywords:
Gas Entry Pressure, Mont Terri Rock Laboratory, Permeability, Sand/Bentonite Mixture, Self-sealing Barriers, Swelling Pressure

Short summary

As part of the Preliminary Safety Analysis of the Gorleben Site (VSG), several sealing materials (e. g. bentonite, rock salt, standard concrete, salt concrete, sorel concrete) are supposed to be applied at different construction levels to ensure the isolation of nuclear waste. To evaluate the long-term chemical stability of these materials in case of solution intrusion, geochemical simulations were undertaken and discussed in this report.

Table of content

1 Introduction

The geochemical reaction simulation of ground water and brines with sealing materials for a proposed repository at the Gorleben site is a task under the framework of the VSG project. The calculations presented in this report are aimed to provide a preliminary evaluation of the geochemical stability of three potential engineering barrier materials foreseen in the shaft sealing system in case of groundwater and brine intrusion. The long-term stability of these materials is a key issue for the sealing function of the shaft seals. This is governed by many factors such as geotechnical, hydraulic and geochemical processes. In order to better understand the potential effect of geochemical processes on the long-term properties of these sealing materials, geochemical simulations of the potential interactions between groundwater and brine and shaft sealing materials were performed.

2 Task definition

2.1 Scenarios and processes

The selection of appropriate building materials for a construction must meet the applicable loading conditions, comprising mechanical impacts and the environmental conditions that the materials will be exposed to. The selection comprise the specification of the material type and can define mixtures in terms of its constituents and their proportions. In the case of the shaft construction interactions of the materials with solutions are regarded, which are characterized by very different ionic contents and dissolved salts. First of all, the chemical reactions of the shaft lining with non-saline rain water must be considered. In the vicinity of the salt-Table NaCl-dominated solutions, stored in the anhydrite cap rock, are most important. All solutions in the salt formation (rock salt) are NaCl-saturated and characterized by $MgCl_2$ contents. These solutions are classified and named according to multicomponent oceanic salt systems, whereby the hexary system considers the cations Na^+, K^+, Mg^{2+}, and Ca^{2+}, as well as the anions Cl^- and SO_4^{2-}. Halite and anhydrite are the main minerals of rock salt. In the case of a sufficient amount of polyhalite an IP9-solution may occur, which is in equilibrium with halite, anhydrite, glauberite, syngenite, and polyhalite. Due to reactions with potash seams an IP21-solution may develop, which is equilibrated to the minerals halite, sylvite, kieserite, and anhydrite. According to the representative solutions, four serials are distinguished; the rain water, Gipshut, IP9, and IP21 serial.

Rain water and Gipshut solution react with the standard concrete of the shaft lining. Regarding to the chemical evolution of the solutions flowing downwards and the requirements on durability three sealing materials were selected. Thus, the topmost or first element consists of bentonite, a clay dominated by Ca-montmorillonite. In addition to the bentonite, a high chemical stability in NaCl-dominated solutions is known for salt concrete, which are the potential building material of the second seal. In the lower part of the shaft $MgCl_2$-solutions can not be excluded. A sealing element of sorel concrete is arranged, as sorel concrete mixtures are the classical building material of seals in the field of potash mining, and is characterized by a high stability in $MgCl_2$-solutions.

In addition to the sealing elements, the construction of the shaft sealing comprise abutments of basalt gravel and sorel concrete at the disposal level, which can be assumed to be chemical stable. In addition, parts of the shaft will be backfilled with bischofite ($MgCl_2 \cdot 6\ H_2O$). The high dissolution rate of this mineral leads to an increase of the $MgCl_2$ content of the solution prior to its contact with the sorel concrete.

2.2 Materials and solutions

2.2.1 Solid materials

Solid materials considered for the geochemical simulations are:

Rock salt and minig waste salt (Haldensalz)

Rock salt is the host rock, while Haldensalz serves as aggregate to salt concrete and sorel concrete. Haldensalz in Gorleben are the debris of the tunnel excavation. Therefore, they both are treated as the same material. The chemical composition of Haldensalz in Gorleben (96 w% halite, 3 w% anhydrite, <1 w% clay, <0.5 w% other salt minerals such as polyhalite, carnallite and kieserite) was analyzed by /GIE 1989/. As the amount of clay and other minerals amounts no more than 1 w%, additionally, no detailed data for their mineral compositions, only halite and anhydrite (amounts to 99 w%) were taken into consideration for the simulation.

Standard concrete

Standard concrete is the shaft lining and the foundation of the shaft lining. standard concrete locates in a depth of 340 m with a thickness of 5 m (Fig. 2.1 in section 2.4). It serves as foundation to support the shaft lining above it. There are three potential concrete types to be used – B35, B45 and B55 concrete according to /LIN 2012/. B45 is selected as representative concrete for the simulations (Tab. 2.1). The cement CEM III/A is a type of blast furnace slag cement (Hochofenzement). Its averaged chemical composition is listed in Tab. 2.2 /LIN 2012/. In the simulations, Ti, Mn, P and Fe were not considered. Sand and gravel as concrete additives were assumed to be chemically stable and thus treated as inert fractions and not included by the calculation of standard concrete chemical composition (Tab. 2.2).

The simulations of the reactions with standard concrete consider the chemical composition of a CEM III/A cement according to Tab. 2.2. The aggregate (sand, gravel) were assumed to be chemically stable.

Tab. 2.1 Recipes of standard concretes in kg /LIN 2012/

	B45
CEM III	420
Water	200
Sand/gravel	1710
Total	2330
W/C-ratio*	0.48

* W/C ratio – weight ratio of water/cement

Tab. 2.2 Chemical composition of CEM III in weight percent /LIN 2012/

	Blast furnace cement	
Component	**DIN**	**Calculation**
SiO_2	28.690	28.690
TiO_2	0.523	-
Al_2O_3	7.315	7.315
Mn_2O_3	0.171	-
Fe_2O_3	1.154	-
P_2O_5	0.048	-
CaO ges.	50.643	50.643
MgO	5.510	5.510
SO_3	1.927	1.927
Na_2O	0.314	0.314
K_2O	0.632	0.632
H_2O	2.195	2.195
CO_2	0.879	0.879
Total	100.00	98.11

Salt concrete and sorel concrete: salt concrete type Asse (salt concrete Type Asse), which is simply called salt concrete in this report and sorel concrete A1, which is simply called sorel concrete in this report.

The concrete sealing materials include sorel concrete and salt concrete. Sorel concrete is obtained by mixing MgO, crushed rock salt as aggregate and $MgCl_2$-solution. The binder of sorel concrete is Oxychloride-Mg, which is quite stable in saline solution with higher Mg^{2+} concentration /VOI 2008/, /NIE 2009/. But if the Mg^{2+} concentration in saline solution is very low, the binder Mg-Oxychloride will not be stable any more.

A recipe of sorel concrete is listed in Tab. 2.3. In the calculation, the chemical composition of Haldensalz was used for rock salt, while that of Magnesium oxide product is in

Tab. 2.4, and that of $MgCl_2$ solution is listed in Tab. 2.5. The porosity is about 20 % and bulk dry density 1850 kg/m^3 /ENG 2011/.

Tab. 2.3 Recipe of sorel concrete /ENG 2011/

	Weight %	**kg/m^3**
Magnesium oxide	11.3	218.0
Rock salt	63.7	1237.0
$MgCl_2$-solution	25.0	485.0
Total	100.0	1940.0

Tab. 2.4 Chemical composition of the Magnesium oxide product in w% /ENG 2011/

	Original	**Calculation**
MgO	97.0	97.0
CaO	1.8	1.8
SO_3	0.1	0.1
Fe	0.2	n.c.
Total	99.1	98.9

n.c. – not considered

Tab. 2.5 Chemical composition of the $MgCl_2$ solution in w% /ENG 2011/

	Concentration range	**Averaged concentration**
$MgCl_2$	28.6 – 31.6	30.1
$MgSO_4$	2.3 – 2.5	2.4
$CaSO_4$	0.07 – 0.1	0.1
KCl	0.1 – 0.11	0.1
NaCl	0.3 – 0.36	0.3
H_2O	-	67.0

Salt concrete is a mixture of 18.32 w% cement (CEM III/B) with 71.65 w% rock salt and 10.03 w% saturated NaCl solution (Tab. 2.6). The Na^+ and Cl^- concentration of the saturated NaCl solution is calculated using EQ3/6 with 6.1048 mol/kg·H_2O. The chemical composition of Haldensalz was used for rock salt, while that of cement CEM III/B is listed in Tab. 2.7.

Tab. 2.6 Recipe of salt concrete /ENG 2011/

	Weight %	kg/m^3
Cement (CEM III/B)	18.32	380.0
Rock salt	71.65	1486.0
Saturated NaCl-solution	10.03	208.0
Total	100.00	2074.0

Tab. 2.7 Chemical composition of the CEM III/B in w% /ENG 2011/

	Concentration range	Averaged concentration
SiO_2	29.7 – 33.6	31.7
Al_2O_3	8.1 – 11.8	9.9
MgO	3.86 – 8.55	6.38
CaO	44.8 – 48.7	46.3
SO_3	≤ 4	3.0
Fe_2O_3	0.87 – 1.25	1.02
Cl	≤ 0.1	n.c.
Na_2O	0.27 – 0.50	0.38
K_2O	0.57 – 0.85	0.67

n.c. – not considered

Ca-bentonite (calcigel)

The clayey sealing material calcigel contains 63 – 70 w% alkaline earth montmorillonite together with quartz (12 – 15 w%), illite (4 – 7 w%), and other minor minerals such as chlorite, calcite, dolomite and K-Feldspar /ENG 2011/. In the calculation, calcigel is assumed to be stable and only the ionic exchange was considered in the geochemical simulation. The calcigel will be highly compacted with dry density of 1600 – 1700 kg/m^3, porosity 27 – 34 %. Averaged values of dry density (1650 kg/m^3) and porosity (30 %) were used for the calculation. The cation exchange capacity (CEC) is 62 meq/100 g for the calcigel /MUE 1983/. The exchangeable ions are Na^+ (1.8 meq/100 g), K^+ (1.8 meq/100 g), Mg^{2+} (22.4 meq/100 g) and Ca^{2+} (37.6 meq/100 g) /MUE 1983/. Cation Ca^{2+} is the main fraction in 37.6 meq/100 g followed by Mg^{2+} in 22.4 meq/100 g.

Bischofite product

The Bischofite product is provided for example by DEUSA International GmbH (see Appendix I). This material as Mg provider is supposed to be used close to the sorel concrete, in order to ensure a minimum Mg^{2+} concentration (0.5 M for saturated NaCl solution) of the solution before entering the sorel concrete /VOI 2008/, /NIE 2009/. The mineral compositions of Bischofite product are: 47.2 w% of Magnesium chloride (as a mixture of $MgCl_2$:$6H_2O$ and $MgCl_2$:$4H_2O$) (without H_2O), 0.2 w% $MgSO_4$, 0.1 w% $CaSO_4$, 0.4 w% KCl and 0.7 w% NaCl, which amounts to 48.4 w%. Assuming the rest are all H_2O as crystal water, the mixture ratio of $MgCl_2$:$6H_2O$ and $MgCl_2$:$4H_2O$ is calculated as 85 w% to 15 w%.

Steel embedded in the concrete lining or as support structures in shaft are not included in the simulations. This is owing to the facts:

- Iron is not the basic composition of cement phases;
- It is believed that iron has no major impact on the reactions as calculated here.

Based on the data mentioned above, the chemical compositions of all solid materials except bentonite are listed in Tab. 2.8, which are used for the geochemical calculations.

Tab. 2.8 Chemical composition of solid phases in [mol/kg]

Element	Haldensalz	Standard concrete#	Salt concrete	Sorel concrete	Bischofite Product
Na	16.426	0.014	12.346	10.565	0.120
K	0.000	0.019	0.026	0.003	0.054
Ca	0.220	1.250	1.685	0.180	0.007
Mg	0.000	0.189	0.292	3.571	4.974
Cl	16.426	0.000	12.253	12.161	10.088
S	0.220	0.033	0.228	0.195	0.024
Si	0.000	0.661	0.975	0.000	0.000
Al	0.000	0.199	0.359	0.000	0.000
O	0.881	10.488	9.348	12.907	28.353
H	0.000	14.517	8.275	18.734	56.514
C	0.000	0.028	0.000	0.000	0.000

- The fraction of sand and gravel not included

2.2.2 Solutions

The solutions potentially to enter the shafts are rain water (RW), cap rock solution (Gipshut-Solution, GS), IP9 and IP21 solutions. GS is present in high amounts at the top of the salt formation in the cap rock. The origin of this solution is the interaction of groundwater with the salt formation. GS is normally saturated with respect to halite and anhydrite. IP9 solution is a hypothetical solution which is saturated with respect to halite, anhydrite and polyhalite /HER 2000/. Polyhalite is a Mg bearing sulfate which is often present in rock salt. The important difference between GS and IP9 is the Mg content. As standard concrete and salt concrete are sensible against Mg in the attacking fluids IP9 solution with up to 1.04 mol Mg/kg water was included in this study. IP21 is a solution often encountered in salt formations in the vicinity of potash beds. Outcrops of potash beds are present in the deeper parts of the shaft profile. IP21 solution is saturaded with respect to the minerals halite, polyhalite, sylvite, carnallite and kainite and contains 4.21 mol Mg/kg water /HER 2000/. The chemical compositions of the IP9 and IP21 solutions were calculated with the database in Appendix II and are listed in Tab. 2.11.

Rain water was taken from /DUR 2010/ and calculated using EQ3/6 in equilibrium with CO_2 (partial pressure 0.31 mbar, which represents the average value in the air). This value is increasing with the global warming process and the CO_2 partial pressure in soil can be much higher (APP 2005), which are however for the current calculations not considered (as they are assumed negligible).

The chemical compositions of several Gipshut-solutions were provided by Mr. Hans Klinge (BGR) through email communications /KLI 2011/. One of the analytic solutions with the highest concentration of Mg^{2+} was selected for the Gipshut-solution, because Mg^{2+} is the critical element for salt concrete corrosion /HAG 2009/. The original chemical composition of Gipshut-solution is in Tab. 2.9.

Tab. 2.9 Chemical composition of a Gipshut-solution (in mg/L) /KLI 2011/

Element	Concentration	Element	Concentration	Element	Concentration
K	1410	Al	0.32	B	11.6
Na	114000	Cl	181000	SiO_2	33
Mg	1370	SO_4	4950	NH_4	0
Ca	1410	HCO_3	128.1	NO_2	0
Fe	14.4	NO_3	-0.05*	TOC/DOC	0
Mn	1.2	PO_4	0	S_{ANION}	5210.55
Li	0.2	F	275	S_{CATION}	5178.36
Sr	13.9	Br	64.2	TDI	10388.91
Ba	0.02	I	0.32	pH	6.3

*-negative value means the concentration of the component is below the measurement limit.

Only main elements (Na, K, Ca, Mg, Cl and S) have been considered in the EQ3/6 calculations. The Cl^- concentration was adjusted for charge balance. The chemical composition of Gipshut-solution as input data for the calculation is given in Tab. 2.10 in mg/L and in Tab. 2.11 in mol/kg·H_2O.

Tab. 2.10 Chemical composition of the Gipshut-solution for the EQ3/6 geochemical simulation

Species	Concentration	Unit
Na^+	114000	mg/L
K^+	1410	mg/L
Ca^{++}	1410	mg/L
Mg^{++}	1370	mg/L
Cl^-	179844.6	mg/L
$SO4^{--}$	4950	mg/L
$HCO3^-$	128.1	mg/L
SiO2(aq)	33	mg/L
Al^{+++}	0.32	mg/L
pH	6.3	-

The chemical compositions of IP9- and IP21-solutions were calculated using EQ3/6 with the database described in section 3.

Tab. 2.11 Chemical compositions of liquids used in the geochemical modeling

Composition	Concentration [mol/kg H_2O]			
	Rain water	**Gipshut-solution**	**IP9**	**IP21**
Na+	$8.07{\cdot}10^{-05}$	4.96	4.18	$4.80{\cdot}10^{-01}$
K+	$1.90{\cdot}10^{-06}$	$3.61{\cdot}10^{-02}$	$9.19{\cdot}10^{-01}$	$5.68{\cdot}10^{-01}$
Ca++	$1.98{\cdot}10^{-04}$	$3.52{\cdot}10^{-02}$	$5.88{\cdot}10^{-03}$	$6.35{\cdot}10^{-04}$
Mg++	n.e.	$5.64{\cdot}10^{-02}$	1.04	4.21
Cl^-	$8.07{\cdot}10^{-05}$	5.07	6.39	8.84
SO_4^{--}	$1.98{\cdot}10^{-04}$	$5.15{\cdot}10^{-02}$	$4.00{\cdot}10^{-01}$	$3.16{\cdot}10^{-01}$
SiO_2(aq)	n.e.	$5.49{\cdot}10^{-04}$	n.e.	n.e.
Al^{+++}	n.e.	$1.19{\cdot}10^{-05}$	n.e.	n.e.
HCO_3^-	$3.19{\cdot}10^{-06}$	$2.10{\cdot}10^{-03}$	n.e.	n.e.
pH	5.81	6.3	6.9	5.5

n.e. – not existing

It is important to note that some of the chemical composition data (especially based on chemical analysis) may result in charge imbalance, which may cause problems in geochemical modelling. The elemental total concentration values of O (for standard concrete) and Cl (for salt concrete and sorel concrete) were thus adjusted accordingly.

The fluid density values in section 5 were calculated by the method described in Krumgalz et al. /KRU 1994/, /KRU 1995/.

2.3 General assumptions

The general assumptions for all geochemical calculations are:

1. In the cases of rain water intrusion, rain water flows downwards through the upper part of the shaft without significant geochemical changes until it reaches the first concrete foundation made of standard concrete;
2. Significant geochemical reactions for concrete corrosion were assumed to occur in the shaft from the first concrete foundation on;
3. In the case of Gipshut-solution series, only Gipshut-solution fills the pore in the layer just above the first concrete foundation of the shaft. The mixing of rain water with Gipshut-solution was not considered.
4. IP9 serial was considered as a worst case. This solution occurs if the rock salt which reacts with rain water contains polyhalite and this Mg-mineral can reach satu-

ration in the solution. It is assumed that if such a solution can occur, it can react only with salt concrete.

5. It is assumed that solutions entering and penetrating the layers and sealing materials within the shaft come from the top of the first concrete foundation. An exception is the solution IP21 which is considered to occur only in the deeper parts of the shafts where only sorel concrete exists.
6. The temperature and pressure conditions were assumed to be constant (25 °C and 1 bar) for all geochemical simulations;
7. All geochemical calculations refer to a state of thermodynamic equilibrium, kinetic reactions are not considered;
8. Rain water is in thermodynamic equilibrium with CO_2 in the atmosphere. In all other calculations, gas phases are eliminated;
9. For the reference calculations with cement binders (e. g. standard concrete and salt concrete), it was assumed that only certain solid phases can appear. This implies that only kerolite for M-S-H (Magnesium-Silicate-Hydrate) phases was considered, other phases like talc, chrysotile, and sepiolite were thus suppressed /HAG 2009/. For the the C-S-H (Calcium-Silicate-Hydrate) phases, only the model phases according to Glasser in /REV 1997/ were allowed. Tobermorite and jennite were suppressed even though they are thermodynamically stable but strongly kinetically depended /HAG 2009/.
10. For the geochemical simulation of bentonite with solutions, only the ionic exchange process was considered; Dissolution/precipitation processes of solid components in bentonite were not considered.
11. Sand and gravels as additives in standard concrete were assumed to be inert.

2.4 Main tasks

The main tasks can be defined in four serials according to several scenarios (Fig. 2.1, Fig. 2.2, Tab. 2.12):

1. **Rain water serial**: Rain water flows through the standard concrete, resulting a solution at the time leaving the standard concrete, which is named corrosion solution R1 (Fig. 2.1); R1 reacts with rock salt, which is the additive in the layer just above the bentonite layer, and by the end results in a solution R2; For this calculation,

chemical composition of Haldensalz (Tab. 2.8) was used for rock salt. It is important to note that the solution R1 remained dilute with very low total concentration. Therefore, R1 tends to react with any salt materials it encounters. The chemical composition of the target solution should be comparable to the measured (6.1) chemical composition of the in situ Gipshut-solution. We have to concentrate on the most critical elements for concrete corrosion. As Mg^{2+} is the most critical component responsible for salt concrete corrosion, a solution with the highest concentration of Mg^{2+} with 0.056 M of Gipshut-solution was selected as reference value for calculating the amount of salt to be added in the system. This procedure is here called the Gipshut-solution oriented calculation (Tab. 2.12). Solution R2 flows further through bentonite and results the solution R3 due to ionic exchange; When solution R3 reaches the layer of salt concrete, it flows further downwards through the salt concrete, producing the corrosion solution R4; R4 reacts with Bischofite within the layers between salt concrete and sorel concrete, resulting solution R5; By the end R5 reacts with sorel concrete and results in the corrosion solution R6 (see Fig. 2.1 and Tab. 2.12).

2. **Gipshut serial**: Analog to the rain water serial case, similar corrosion solutions was produced by replacing the starting solution of Gipshut-solution (GL) with rain water. GL flows through the standard concrete, resulting in a corrosion solution G1 (Fig. 2.2 and Tab. 2.12); G1 reacts with rock salt (Spiegelsalz), resulting in a solution G2; Similar to the R2, G2 was also simulated according to the Gipshut-solution oriented calculation principle. Solution G2 flows further through bentonite and resulting the solution G3 through ionic exchange; When solution G3 reaches the layer of salt concrete, it flows further downwards through the salt concrete, producing the corrosion solution G4; G4 reacts with Bischofite product within the layers between salt concrete and sorel concrete, resulting solution G5; By the end G5 reacts with sorel concrete and results in G6 (see Fig. 2.2 and Tab. 2.12).

3. **IP9 serial**: This serial is regarded as a worst case scenario. Solution IP9 flows through salt concrete, producing the solution H4; H4 reacts with Bischofite product within the layers between salt concrete and sorel concrete and results in solution H5; By the end H5 reacts with sorel concrete and results in H6 (Tab. 2.12).

4. **IP21 serial**: This represents another scenario. IP21 flows through sorel concrete and results in I6 (Tab. 2.12).

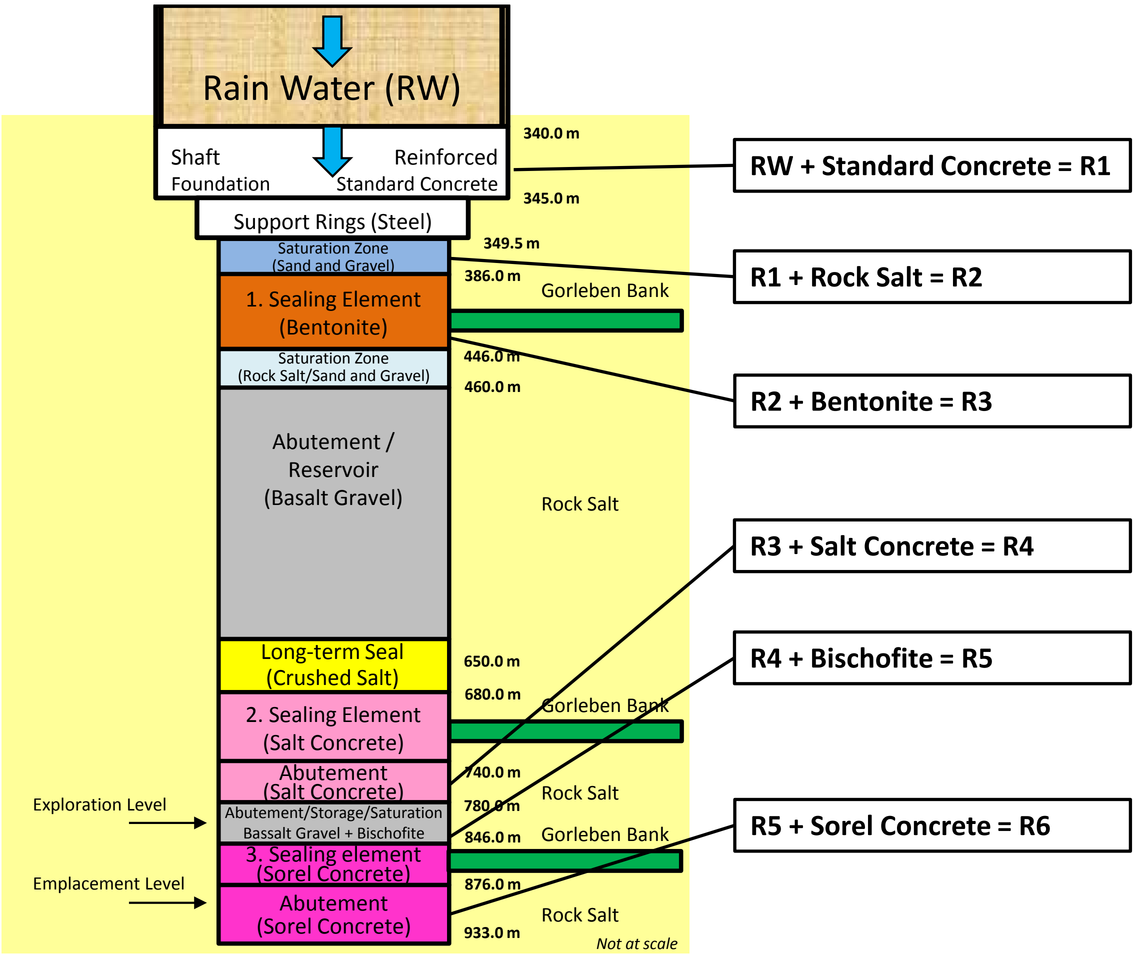

Fig. 2.1 Concrete corrosion cases I: Rain water serial (based on /MUE 2012/

Tab. 2.12 Corrosion solutions produced by the reactions between solutions and solid phases in shaft

Horizontal	Condition	Solutions			
		Rain water	Gipshut Solution	IP9	IP21
standard concrete	zi = 4 #	R1	G1		
Salzspiegel	Gipshutlsg.-oriented	R2	G2		
Bentonite	Equil. ionic exchange	R3	G3		
salt concrete	zi = 4	R4	G4	H4	
Bischofite	$[Mg^{2+}]$> 0.5 M	R5	G5	H5	
sorel concrete	zi = 4	R6	G6	H6	I6

zi – is the parameter representing the ratio of solid/water in kg/kg (see section 3).

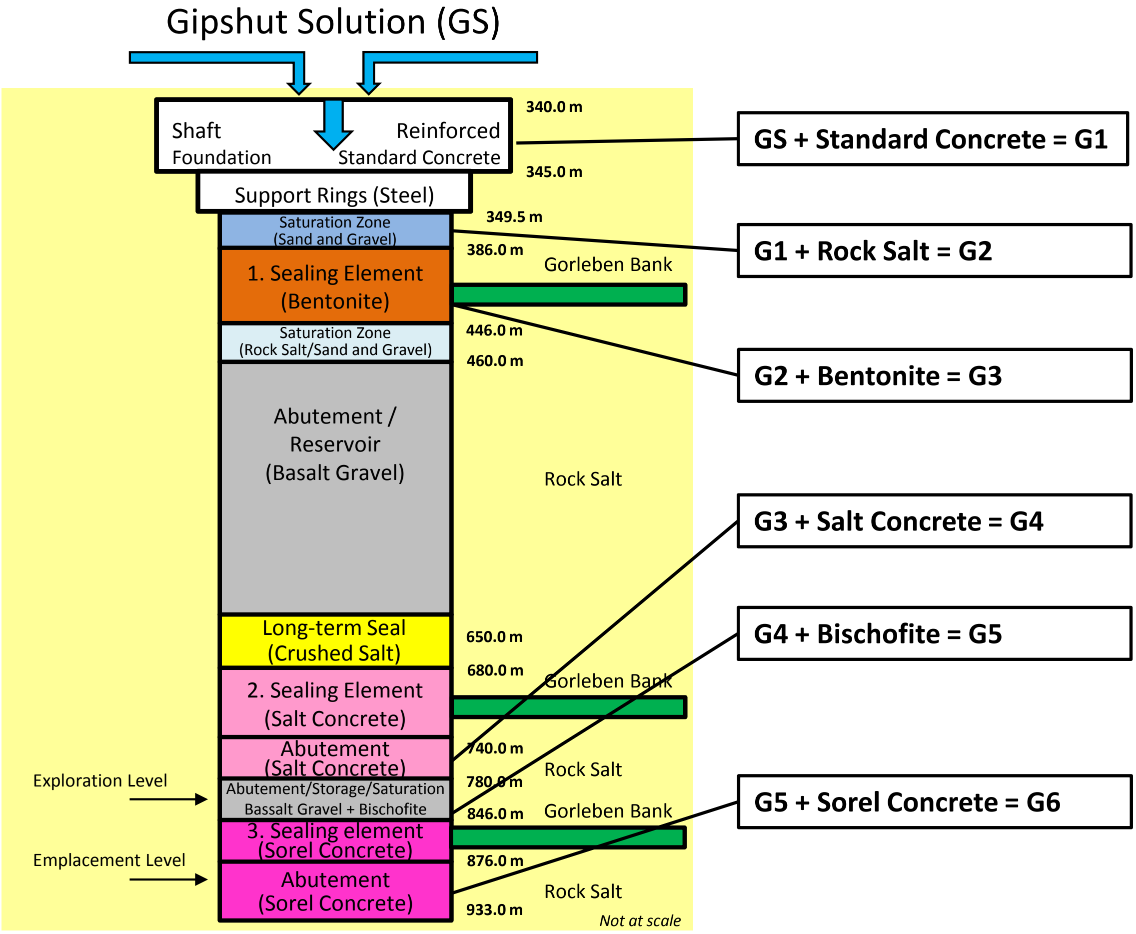

Fig. 2.2 Concrete corrosion cases: Gipshut-solution serial (based on /MUE 2012/

It is important to note that the amount of the solutions reached the sorel concrete in the above scenarios is largely dependent on the material properties and thickness of each layer especially the sealing materials in the shaft. It is important to note that the amount of solutions penetrating the shaft will be limited owing to the engineering barrier materials. The amount of IP9 and IP21 is supposed to be much less.

3 Geochemical simulators and databases

Two geochemical simulators were used for the geochemical simulations – EQ3/6 and PHREEQC. Both codes are based on equilibrium constants and widely used for the geochemical simulations in the fields of environmental engineering and geoscience. PHREEQC is public domain software /PAR 1999/, EQ3/6 has to be purchased at the Lawrence Livermore National Laboratories. In the current work, PHREEQC was applied for simulating the ionic exchange process of bentonite when solutions penetrate. For this reaction the NAGRA-PSI database was used (Appendix III). The thermodynamic data for the ionic exchange in the reaction with bentonite was based on Curti and Wersin /CUR 2002/ and given directly in the input files. All other geochemical calculations were simulated with EQ3/6 version 8.0a as well as EQ3/6 version 8.0 (Case I6, see section 5.4). A graphic user interface (GUI)-tool EQBlitz developed by Dr. Hagemann (GRS) was applied for automatically generating of input files and post processing of the output files for EQ3/6 calculations /HAG 2009/.

The EQ3/6 version 8.0a is an upgrade of the EQ3/6 version 8.0 /WOL 2003/. Pitzer model was selected for all EQ3/6 calculations. The database used was developed by /HAG 2009/ for the calculations. This database has been upgraded with data from the special geochemical database in the data format of EQ3/6 v7.2 /HAG 2009/, which was generated, verified and applied for the concrete corrosion calculation for salt cement /MEY 2003/, /HAG 2009/. The solid phases considered in the database for the modeling are listed in Tab. 3.1. However, some tracer elements like N, Fe, Mn, Br, I, Ti, P etc were not included in the database. It is considered that these tracer elements don’t influence the modeling results. Therefore, in the calculations, NO_3^- was substituted by Cl^- with the same mol amount. The other elements Fe, Mn, Ti, P, I, Br etc. were not included in the geochemical simulations in this project.

Tab. 3.1 Phases considered for the modeling /HAG 2009/

Phase	Chemical formula	Reaction equation	log K
Afwill	$CaSi_2O_5 \cdot 3H_2O$	1 Afwill + 2 H^+ <=> 1 Ca^{2+} + 4 H_2O + 2 SiO_2(aq)	46.9
Alunite	$KAl_3(OH)_6(SO_4)_2$	1 Alunit + 6 H^+ <=> 1 K^+ + 2 SO_4^{2-} + 3 Al^{3+} + 6 H_2O	-2.912
Anhydrite	$CaSO_4$	1 Anhydrite <=> 1 Ca^{2+} + 1 SO_4^{2-}	-4.3621
Antarcticite	$CaCl_2 \cdot 6H_2O$	1 Antarcticite <=> 1 Ca^{2+} + 2 Cl^- + 6 H_2O	4.1436
Aphthitalite	$NaK_3(SO_4)_2$	1 Aphthitalite <=> 1 Na^+ + 2 SO_4^{2-} + 3 K^+	-3.8027
Arcanite	K_2SO_4	1 Arcanite <=> 1 SO_4^{2-} + 2 K^+	-1.7763
Bischofite	$MgCl_2 \cdot 6H_2O$	1 Bischofite <=> 1 Mg^{2+} + 2 Cl^- + 6 H_2O	4.4554
Bloedite	$Na_2Mg(SO_4)_2 \cdot 4H_2O$	1 Bloedite <=> 1 Mg^{2+} + 2 Na^+ + 2 SO_4^{2-} + 4 H_2O	-2.3469
Brucite	$Mg(OH)_2$	1 Brucite + 2 H^+ <=> 1 Mg^{2+} + 2 H_2O	17.109
$Ca_2Cl_2 \cdot (OH)_2 \cdot H_2O$	$Ca_2Cl_2 \cdot (OH)_2 \cdot H_2O$	1 $Ca_2Cl_2(OH)_2 \cdot H_2O$ + 2 H^+ <=> 2 Ca^{2+} + 2 Cl^- + 3 H_2O	26.5313
$Ca_4Cl_2 \cdot (OH)_6 \cdot 13 H_2O$	$Ca_4Cl_2 \cdot (OH)_6 \cdot 13H_2O$	1 $Ca_4Cl_2(OH)_6 \cdot 13H_2O$ + 6 H^+ <=> 2 Cl^- + 4Ca^{2+} + 19 H_2O	68.7343
$CaCl_2 \cdot 4H_2O$	$CaCl_2 \cdot 4H_2O$	1 $CaCl_2 \cdot 4H_2O$ <=> 1 Ca^{2+} + 2 Cl^- + 4 H_2O	5.717
Carnallite	$KMgCl_3 \cdot 6H_2O$	1 Carnallite <=> 1 K^+ + 1 Mg^{2+} + 3 Cl^- + 6 H_2O	4.3304
Chabazite	$CaAl_2Si_4O_{12} \cdot 6H_2O$	1 Chabazite + 8 H^+ <=> 2 Al^{3+} + 10 H_2O + 1Ca^{2+} + 4 SiO_2(aq)	13.0
CSH(0.8)	$Ca_{0.8}SiO_{2.8} \cdot H_2O$	1 CSH(0.8) + 1.6 H^+ <=> 0.8 Ca^{2+} + 1 SiO_2(aq) + 1.8 H_2O	11.07
CSH(1.1)	$Ca_{1.1}SiO_{3.1} \cdot 3H_2O$	1 CSH(1.1) + 2.2 H^+ <=> 1.1 Ca^{2+} + 1 SiO_2(aq) + 4.1 H_2O	16.71
CSH(1.8)	$Ca_{1.8}SiO_{3.8} \cdot 5H_2O$	1 CSH(1.8) + 3.6 H^+ <=> 1.8 Ca^{2+} + 1 SiO_2(aq) + 6.8 H_2O	32.54
Dicalcium-aluminathydrate	$Ca_2Al_2O_5 \cdot 8H_2O$	1 Dicalciumaluminathydrate + 10 H^+ <=> 2 Al^{3+} + 2 Ca^{2+} + 13 H_2O	59.67
Epsomite	$MgSO_4 \cdot 7H_2O$	1 Epsomite <=> 1 Mg^{2+} + 1 SO_4^{2-} + 7 H_2O	-1.8811
Ettringite	$Ca_6Al_2(SO_4)_3(OH)_{12} \cdot 26H_2O$	1 Ettringite + 12 H^+ <=> 2 Al^{3+} + 3 SO_4^{2-} + 6 Ca^{2+} + 38 H_2O	55.3527
Friedel's salt	$Ca_4Al_2Cl_2O_6 \cdot 10H_2O$	1 Friedel's salt + 12 H^+ <=> 2 Al^{3+} + 4 Ca^{2+} + 16 H_2O + 2 Cl^-	72.52 ± 1
Gehlenithydrate	$Ca_2Al_2SiO_7 \cdot 8H_2O$	1 Gehlenithydrate + 10 H^+ <=> + 2 Al^{3+} + 2 Ca^{2+} + 13 H_2O + 1 SiO_2(aq)	49.38
Gibbsite	$Al(OH)_3$	1 Gibbsite + 3 H^+ <=> 1 Al^{3+} + 3 H_2O	8.025 ± 1
Glauberite	$Na_2Ca(SO_4)_2$	1 Glauberite <=> 1 Ca^{2+} + 2 Na^+ + 2 SO_4^{2-}	-5.2445
Gypsum	$CaSO_4 \cdot 2H_2O$	1 Gypsum <=> 1 Ca^{2+} + 1 SO_4^{2-} + 2 H_2O	-4.5805
Halite	NaCl	1 Halite <=> + 1 Cl^- + 1 Na^+	1.5704
Halloysite	$Al_2Si_2O_7 \cdot 2H_2O$	1 Halloysite + 6 H^+ <=> 2 Al^{3+} + 5 H_2O + 2 SiO_2(aq)	15.1
Hexahydrite	MgSO4.6H2O	1 Hexahydrite <=> 1 Mg2+ + 1 SO42+-+ 6 H2O	-1.6351

Tab. 3.1 [continued] Phases considered for the modeling /HAG 2009/

Phase	Chemical formula	Reaction equation	log K
Hydrogarnet	$Ca_3Al_2O_6 \cdot 6H_2O$	1 Hydrogarnet + 12 H^+ <=> 2 Al^{3+} + 3 Ca^{2+} + 12 H_2O	80.55
Hydrotalcit	$Mg_4Al_2O_7 \cdot 10H_2O$	1 Hydrotalcit + 14 H^+ <=> 4 Mg^{2+} + 17 H_2O + 2 Al^{3+}	83.22 ± 2
Jennite	$Ca_9Si_6O_{21} \cdot 11H_2O$	1 Jennite + 18 H^+ <=> 6 SiO_2(aq) + 9 Ca^{2+} + 20 H_2O	150.81
$K_3H(SO_4)_2$	$K_3H(SO_4)_2$	1 $K_3H(SO_4)_2$ <=> 1 H^+ + 2 SO_4^{2-} + 3 K^+	-3.5425
Kainite	$KMgClSO_4 \cdot 3H_2O$	1 Kainite <=> 1 Cl^- + 1 K^+ + 1 Mg^{2+} + 1 SO_4^{2-} + 3 H_2O	-0.1926
Kaolinite	$Al_2Si_2O_7 \cdot H_2O$	1 Kaolinite + 6 H^+ <=> 2 SiO_2(aq) + 2 Al^{3+} + 4 H_2O	6.7
Kieserite	$MgSO_4 \cdot H_2O$	1 Kieserite <=> 1 H_2O + 1 Mg^{2+} + 1 SO_4^{2-}	-0.1227
Leonite	$K_2Mg(SO_4)_2 \cdot 4H_2O$	1 Leonite <=> 1 Mg^{2+} + 2 K^+ + 2 SO_4^{2-} + 4 H_2O	-3.979
Mercallite	$KHSO_4$	1 Mercallite <=> 1 H^+ + 1 K^+ + 1 SO_4^{2-}	-1.4015
$MgSO_4$	$MgSO_4$	1 $MgSO_4$ <=> 1 Mg^{2+} + 1 SO_4^{2-}	400
Mirabilite	$Na_2SO_4 \cdot 10H_2O$	1 Mirabilite <=> 1 SO_4^{2-} + 2 Na^+ + 10 H_2O	-1.2278
Misenite	$K_8H_6(SO_4)_7$	1 Misenite <=> 6 H^+ + 7 SO_4^{2-} + 8 K^+	-10.8062
Monosulfate	$Ca_4Al_2SO_4O_6 \cdot 12H_2O$	1 Monosulfate + 12 H^+ <=> 2 Al^{3+} + 4 Ca^{2+} + 18 H_2O + 1 SO_4^{2-}	71.36
Muscovite	$KAl_3Si_3O_{10}(OH)_2$	1 Muscovite + 10 H^+ <=> 1 K^+ + 3 Al^{3+} + 3 SiO_2(aq) + 6 H_2O	11.0217 ± 1
$Na_3H(SO_4)_2$	$Na_3H(SO_4)_2$	1 $Na_3H(SO_4)_2$ <=> 1 H^+ + 2 SO_4^{2-} + 3 Na^+	-0.8143
$Na_4Ca(SO_4)_3 \cdot 2H_2O$	$Na_4Ca(SO_4)_3 \cdot 2H_2O$	1 $Na_4Ca(SO_4)_3 \cdot 2H_2O$ <=> 1 Ca^{2+} + 2 H_2O + 3 SO_4^{2-} + 4 Na^+	-5.6723
Oxychloride-Mg	$Mg_2Cl(OH)_3 \cdot 4H_2O$	1 Oxychloride-Mg- + 3 H^+ <=> 1 Cl^- + 2 Mg^{2+} + 7 H_2O	26.0297 ± 0.5
Picromerit	$K_2Mg(SO_4)_2 \cdot 6H_2O$	1 Picromerite <=> + 1 Mg^{2+} + 2 K^+ + 2 SO_4^{2-} + 6 H_2O	-4.3277
Polyhalite	$K_2MgCa_2(SO_4)_4 \cdot 2H_2O$	1 Polyhalite <=> + 1 Mg^{2+} + 2 Ca^{2+} + 2 H_2O + 2 K^+ + 4 SO_4^{2-}	-13.7441
Portlandite	$Ca(OH)_2$	1 Portlandite + 2 H^+ <=> + 1 Ca^{2+} + 2 H_2O	22.8035
Quarz	SiO_2(aq)	1 Quarz <=> + 1 SiO_2(aq)	-4
Si-Hydrogarnet	$Ca_3Al_2SiO_8 \cdot 4H_2O$	1 Si-Hydrogarnet + 12 H^+ <=> + 2 Al^{3+} + 3 Ca^{2+} + 10 H_2O + 1 SiO_2(aq)	69.35
Silica (Kieselsäure)	SiO_2(am)	1 SiO_2(am) <=> + 1 SiO_2(aq)	-2.66
Sylvite	KCl	1 Sylvite <=> + 1 Cl^- + 1 K^+	0.8999
Syngenite	$K_2Ca(SO_4)_2 \cdot H_2O$	1 Syngenite <=> 1 Ca^{2+} + 1 H_2O + 2 K^+ + 2 SO_4^{2-}	-7.4484
Tricalciumaluhemisilik	$Ca_3Al_2Si_{0.5}O_7$	1 Tricalciumaluhemisilik + 12 H^+ <=> 2 Al^{3+} +3 Ca^{2+} +6 H_2O + 0.5 SiO_2(aq)	74.12

The procedure of the simulations with EQ3/6 can be described as the following: a solution containing 1 kg H_2O serves as the base pool and cement/concrete is gradually added into the pool. This is realized by defining a parameter zi – mass of solid to be added into the pool. If the initial pool contains exact 1 kg H_2O, zi is equivalent to the internal parameter Xi (the reaction progress value), and represents the ratio of solid to water. By a reference case assuming that one pore volume solution flows through each concrete (total porosity 20 %), the ratio is 4. The chemical composition of the solution at zi = 4 corresponds to an equilibrium solution resulted from the equilibration of 1 kg water in the initial solution with 4 kg of concrete. One kg H_2O correspondes roughly to an assumed total porosity of 20 % of the concrete. The entire corrosion/reaction path till zi = 4 for most cases has been calculated. This is for sure not an exact value. However, at current stage it is accurate enough for understanding the principle of concrete corrosion under different potential geochemical conditions.

The general idea of the geochemical simulations for each serial (see section 2.4 and section 5) is that solutions migrate from top downwards and sequentially through different layers of the shaft. The corresponding geochemical simulations were conducted sequentially by mixing the solution with solid materials and calculating the geochemical system at equilibrium. The resulted solution was used as input for the next calculation.

It is important to note that in some calculations with high pH values, the concentrations of some ions such as OH^-, $HSiO_3^-$ are relatively high. However, these components cannot be directly included for further calculations because they are not primary species as defined in EQ3/6. Fortunately, EQ6 can save such geochemical system as it is into a so called pickup file, which is actually a complete EQ6 input file /WOL 2003/. The pickup files for the last calculation (e. g. zi = 4) was saved and used for further calculations. However, the pickup file has to be modified: 1. adjusting the reaction progress Xi value for starting and ending according to the requirements of the following calculations; 2. replacing the solid phase composition part with the corresponding solid materials. The advantage of using pickup files lies in the conservation of geochemical conditions. However, the amount of free water within the solution described in the pickup file is normally not exact 1 kg any more, because water might be consumed or released through geochemical reactions, and/or adding solid material including free water. To maintain a solid/liquid ratio of 4, the amount of solid material to be added has been adjusted accordingly.

4 Theoretical background of concrete corrosion

Based on the previous experimental and modeling investigations /MEY 2002/, /MEY 2003/, /MEY 2008/, /HAG 2009/, the corrosion of such cemented materials considered in current project (like standard concrete, salt concrete, sorel concrete) in highly saline solutions is dominated by dissolution corrosion.

In order to evaluate the capacity of a solution to corrode a cemented material, a parameter *dissolution capacity* Ku (Umlösekapazität in [m^3/m^3]) was adopted /MEY 2008/:

$$Ku = \frac{V_c}{V_L} = \frac{m_c \cdot \rho_L}{m_L \cdot \rho_c} \tag{4.1}$$

In which V_c is the volume of the cemented material (without pore space) in [m^3], V_L is the minimum volume of solution (in [m^3]) needed to totally dissolve the binders within the cemented material. In the standard concrete and salt concrete, the binders refer to all C-S-H (Calcium-Silicate-Hydrate) phases (e. g. CSH(0.8), CSH(1.1) and CSH(1.8)). For sorel concrete the binder is the Mg-Oxychloride ($Mg_2Cl(OH)_3 \cdot 4H_2O$). m_L – the minimum mass of the solution (in [kg]) by which the binders of cemented material were totally dissolved, m_c – the corresponding mass of the cemented material (in [kg]), ρ_c – the bulk density of the cemented material in [kg/m^3] (without pore space), ρ_L – the density of the solution in [kg/m^3].

This parameter can be recalculated and simplified as Km in [kg/kg]:

$$Km = \frac{m_c}{m_L} \tag{4.2}$$

According to these definitions, Ku or Km describes the corrosion capacity of a solution against cemented material. The higher the values of Ku or Km, the easier is the dissolution and more corrosive is a solution against the cemented material.

5 Simulated results

5.1 Rain water serial

The simulations of rain water serial calculated the geochemical evolution of rain water penetrating through the shaft starting from the standard concrete foundation, three engineering barrier layers (bentonite, salt concrete and sorel concrete) and the layers between them. The simulated total elemental concentrations of the corrosion solutions for the rain water serial are listed in Tab. 5.1. Detailed descriptions of all simulations can be found in the following sections.

Tab. 5.1 The total elemental concentrations of the corrosion solutions for the rain water serial (in mol/kg·H_2O at zi = 4 for R1, R4 and R6, zi = 0.63 for R2, zi = 0.11 for R5)

	C	Ca	Cl	K	Mg	Na	S	Si	Al	pcH	ρ_L^*
R1	$2.43\cdot10^{-5}$	$2.93\cdot10^{-3}$	$6.09\cdot10^{-5}$	$5.69\cdot10^{-2}$	$4.13\cdot10^{-8}$	0.04	$1.35\cdot10^{-4}$	$2.20\cdot10^{-5}$	$1.56\cdot10^{-5}$	12.77	1.00
R2	$1.56\cdot10^{-5}$	$1.07\cdot10^{-2}$	6.07	$2.65\cdot10^{-1}$	$5.21\cdot10^{-2}$	6.09	$2.06\cdot10^{-1}$	$1.23\cdot10^{-8}$	$2.31\cdot10^{-6}$	9.84	1.22
R3	$3.56\cdot10^{-6}$	1.05	6.07	$8.27\cdot10^{-5}$	$5.32\cdot10^{-1}$	3.31	$2.06\cdot10^{-1}$	$7.69\cdot10^{-9}$	$6.77\cdot10^{-1}9$	8.48	1.23
R4	$3.63\cdot10^{-6}$	$4.38\cdot10^{-1}$	6.26	$1.07\cdot10^{-1}$	$4.41\cdot10^{-6}$	5.29	$5.04\cdot10^{-3}$	$1.27\cdot10^{-6}$	$6.01\cdot10^{-1}0$	12.09	1.21
R5	$3.43\cdot10^{-6}$	$4.13\cdot10^{-1}$	6.36	$1.07\cdot10^{-1}$	$5.26\cdot10^{-1}$	4.39	$5.01\cdot10^{-3}$	$7.55\cdot10^{-9}$	$5.69\cdot10^{-1}0$	9.32	1.21
R6	$3.16\cdot10^{-6}$	$9.22\cdot10^{-1}$	6.52	$1.13\cdot10^{-1}$	$3.67\cdot10^{-1}$	3.84	$2.57\cdot10^{-3}$	$6.31\cdot10^{-9}$	$1.16\cdot10^{-1}0$	9.42	1.22

*- ρ_L – solution density in kg/m^3

Tab. 5.2 Dissolution capacity of solutions against nomal concrete (R1), salt concrete (R4) and sorel concrete (R6) for the rain water serial

	m_c [kg/kg H_2O]	m_L [kg/kg H_2O]	ρ_L [kg/m^3]	ρ_c [kg/m^3]	Ku [m^3/m^3]	Km [kg/kg]	Corrosion evaluation
R1	0.0015	1.000	1000	2100	$7.12\cdot10^{-4}$	0.0015	very low
R4	0.54	1.370	1210	2100	0.225	0.394	medium
R6	$1.59\cdot10^{-7}$	1.37	1220	2100	$6.73\cdot10^{-8}$	$1.16\cdot10^{-7}$	non corrosive

5.1.1 Case R1

Rain water penetrates the standard concrete and results in the corrosion solution R1 (Tab. 5.1 and Tab. 5.2). For the simulation, the following conditions were applied:

1. Starting solution: Rain water in equilibrium with CO_2 (partial pressure 0.31 mbar) containing 1 kg H_2O

2. Solid phase: standard concrete (standard concrete in Tab. 2.8)
3. Temperature: 25 °C
4. Pressure: 1 atm
5. Database: data0-V8_extend.bfs
6. Suppressed solid phases are:
7. Trichlorid – Ca6Al2(Cl2)3O6:30H2O
8. Chrysotil – Mg3Si2O5(OH)4
9. Jennit – Ca9Si6O21:11H2O
10. Tobermorit – $Ca_5Si_6O_{17}$:$9H_2O$
11. nput files for EQ3/6: R1.3i, R1.6i
12. Output file for EQ3/6: R1.6o
13. Pickup file after EQ6 calculation by zi = 4: R1.6p
14. Results for all EQ3/6 titration calculations: R1.xls
15. The chemical compositions of species of solution R1 are listed in Tab. 5.3.

Tab. 5.3 Chemical composition of R1 in [mol/kg·H_2O]

Species	Concentration	Species	Concentration
Ca^{++}	$2,927\cdot10^{-03}$	$CaCO_3$(aq)	$5,559\cdot10^{-06}$
SO_4^{--}	$1,350\cdot10^{-04}$	SiO_2(aq)	$6,734\cdot10^{-09}$
Na^+	$4,294\cdot10^{-02}$	$MgOH^+$	$3,385\cdot10^{-08}$
Cl^-	$6,095\cdot10^{-05}$	$Al(OH)_3$	$1,484\cdot10^{-10}$
CO_2(aq)	$4,416\cdot10^{-15}$	$Al(OH)_2^+$	$1,262\cdot10^{-17}$
K^+	$5,686\cdot10^{-02}$	$H_3SiO_4^-$	$1,105\cdot10^{-05}$
H^+	$1,684\cdot10^{-13}$	$Al(OH)^{++}$	$9,212\cdot10^{-26}$
HCO_3^-	$2,228\cdot10^{-08}$	$MgCO_3$(aq)	$1,033\cdot10^{-11}$
HSO_4^-	$6,028\cdot10^{-16}$	$Al(OH)_4^-$	$1,556\cdot10^{-05}$
OH^-	$1,052\cdot10^{-01}$	Al^{+++}	$7,804\cdot10^{-33}$
Mg^{++}	$7,405\cdot10^{-09}$	$H_2SiO_4^{--}$	$1,099\cdot10^{-05}$
CO_3^{--}	$1,868\cdot10^{-05}$		

The main solid phases in the standard concrete are: CSH(1.1), CSH(1.8), brucite, entrigite and Tricalciumaluhemisilik (Fig. 5.1). The pH value (calculated as -LOG10[H^+]) increases from 5.81 to 12.77. The main species are OH^-, K^+, Na^+ and Ca^{2+} (Fig. 5.2). As the concentration of OH^- was relatively high and OH^- is not primary species. Therefore, pickup file R1.6p was used for the followed R2 calculation.

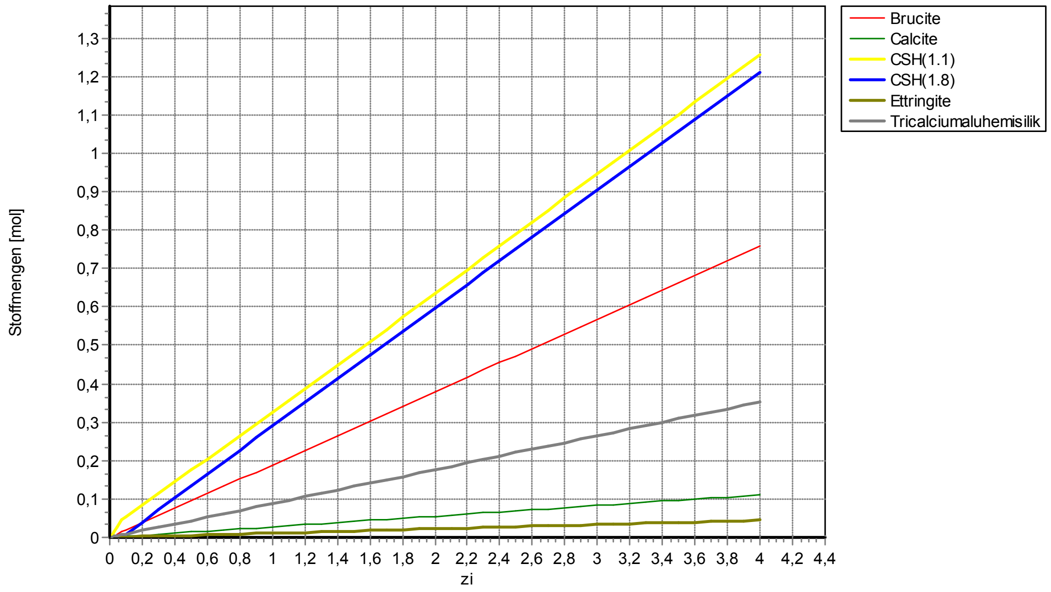

Fig. 5.1 Mineral composition evolution for case R1 by adding standard concrete into rain water

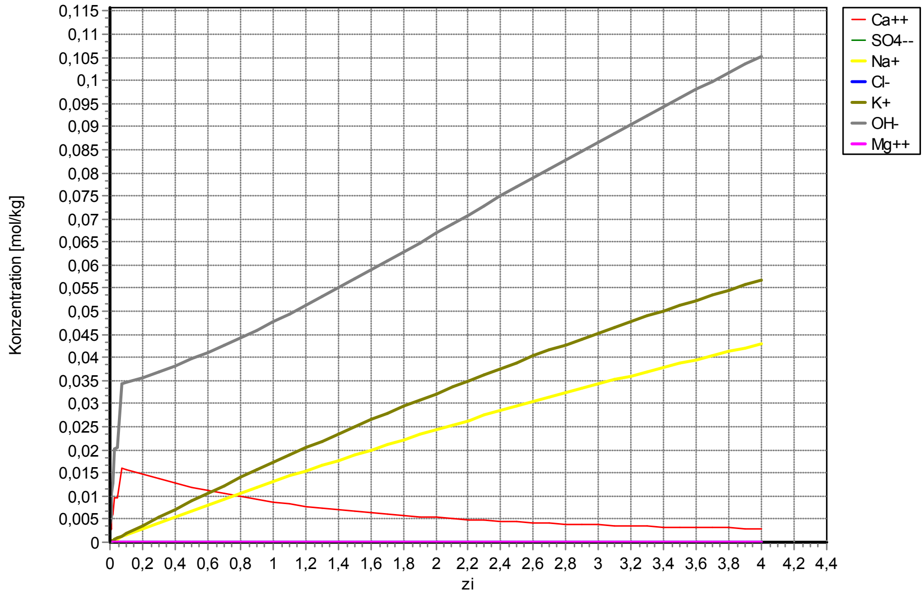

Fig. 5.2 Species evolution for case R1 by adding standard concrete into rain water

The CSH(1.1) phase was totally dissolved at zi = 0.0015 kg/kg·H_2O (Fig. 5.1). The corresponding values of dissolution capacity Km with 0.0015 kg/kg and Ku with $7.12 \cdot 10^{-3}$ m^3/m^3 are very low (Tab. 5.2). This indicates that the standard concrete is fairly stable against rain water.

Geochemical equilibrium calculations provide information about the amount of material that is in equilibrium with an amount of initial solution containing 1 kg of water. As further information the chemical composition of the resulting equilibrium solution at different z_i (solid/solution ratio) until the final equilibrium is reached. The final equilibrium is reached when the maximal amount of material dissolvable in 1 kg water is dissolved. The solution concentrations given in this report refer to the solid/liquid ratio of 4 which corresponds about to the equilibrium of a solution volume in the 20 % pores of the concrete.

5.1.2 Case R2

The corrosion solution R1 flows downwards and might be in contact with rock salt within the layer between the standard concrete foundation and the bentonite, or the host rock. The simulation was conducted according to the Gipshut-solution oriented method (section 2.4). The minimum zi needed to reach the reference Mg^{2+} concentration 0.05 M is about 0.63 (Fig. 5.3).

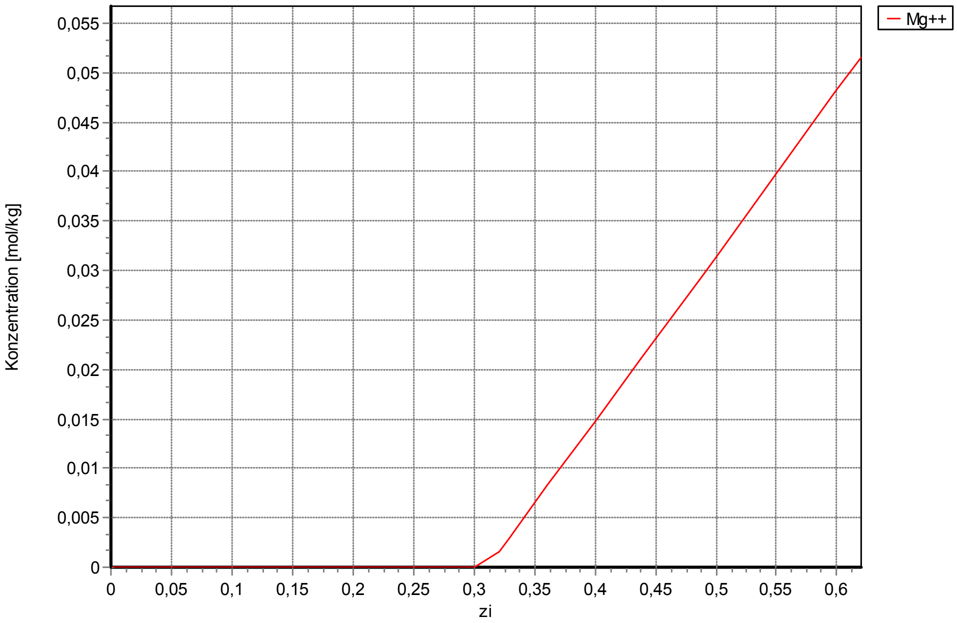

Fig. 5.3 The concentration evolution of Mg^{2+} by adding rock salt into R1

For the simulation, the following conditions were applied:

1. Solution: R1 (the pickup file R1.6p is used)
2. Solid phase: rock salt (Haldensalz in Tab. 2.8)
3. Temperature: 25 °C
4. Pressure: 1 atm
5. Database: data0-V8_extend.bfs
6. Suppressed solid phases are:
    - Trichlorid – $Ca_6Al_2(Cl_2)_3O_6:30H_2O$
    - Chrysotil – $Mg_3Si_2O_5(OH)_4$
    - Jennit – $Ca_9Si_6O_{21}:11H_2O$
    - Tobermorit – $Ca_5Si_6O_{17}:9H_2O$
    - Hydrotalcit – $Mg_4Al_2(OH)14:3H_2O$
    - Hydrotalcit-Semi-CO_3 – $Mg_4Al_2(OH)12CO_3:2H_2O$
7. Input files for EQ3/6 of the last reaction (zi = 0.62): R2pickup.3i, R2pickup.6i
8. Output file for EQ3/6: R2pickup.6o
9. Pickup file after EQ6 calculation by zi = 0.62: R2pickup.6p
10. Results for all EQ3/6 titration calculations can be found in file R2pickup.xls.
11. The concentration evolution of main species by adding rock salt into R1 is showed in Fig. 5.4. The chemical compositions of R2 at zi = 0.62 are listed in Tab. 5.1 (total elemental concentration) and Tab. 5.4 (species concentration).

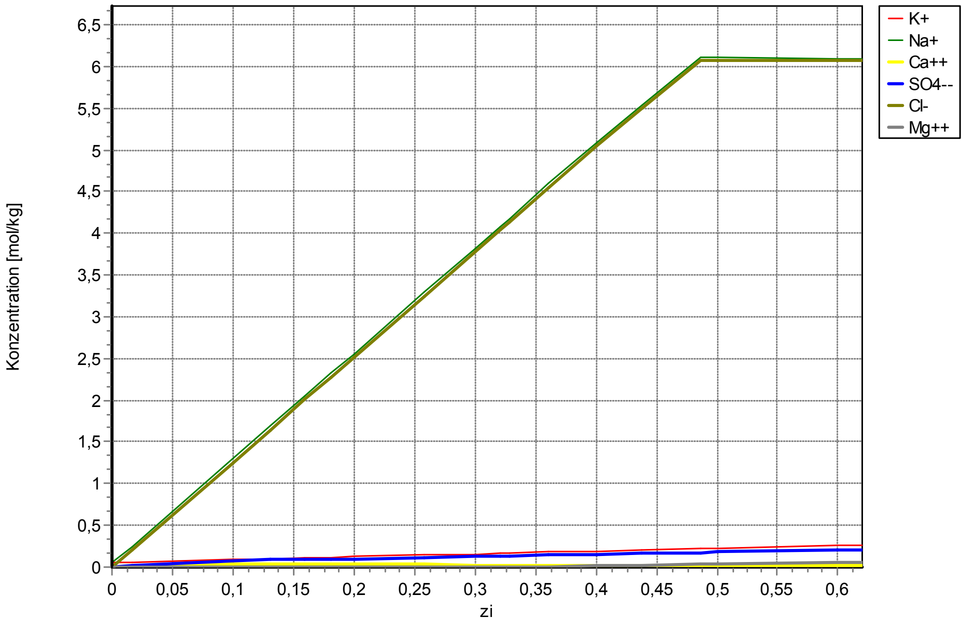

Fig. 5.4 The concentration evolution of main species by adding rock salt into R1

The simulated results showed that the pcH value of the corrosion solution decreased significantly from 12.77 to 9.84 by reacting with rock salt (Tab. 5.1). The reason was the precipitation of brucite ($Mg(OH)_2$). The Polyhalite ($K_2MgCa_2(SO_4)_4$:$2H_2O$) in rock salt was the Mg provider. Na^+, Cl^- concentration increased also significantly and reached its maximum by zi = 0.49 (halite saturated). That is to say that R1 solution with 1 kg H_2O can dissolve about 0.49 kg rock salt.

Tab. 5.4 Chemical composition of R2 in [mol/kg·H_2O]

Species	Concentration	Species	Concentration
OH-	$2,090\cdot10^{-05}$	HCO_3^-	$3,555\cdot10^{-06}$
K^+	$2,651\cdot10^{-01}$	Mg^{++}	$5,155\cdot10^{-02}$
Na^+	6,088	SiO_2(aq)	$7,688\cdot10^{-09}$
Ca^{++}	$1,069\cdot10^{-02}$	$Al(OH)_3$	$1,059\cdot10^{-07}$
SO_4^{--}	$2,056\cdot10^{-01}$	$MgCO_3$(aq)	$7,131\cdot10^{-06}$
Cl^-	6,067	H^+	$1,449\cdot10^{-10}$
CO_3^{--}	$3,487\cdot10^{-06}$	CO_2(aq)	$6,675\cdot10^{-10}$
$Al(OH)_4^-$	$2,207\cdot10^{-06}$	HSO_4^-	$4,284\cdot10^{-10}$
$H3SiO_4^-$	$4,564\cdot10^{-09}$	$Al(OH)_2^+$	$1,674\cdot10^{-10}$
$H2SiO_4^{--}$	$1,551\cdot10^{-11}$	$Al(OH)^{++}$	$2,984\cdot10^{-13}$
$CaCO_3$(aq)	$1,393\cdot10^{-06}$	Al^{+++}	$6,765\cdot10^{-19}$
$MgOH^+$	$4,971\cdot10^{-04}$		

5.1.3 Case R3

The corrosion solution of R2 flows downwards through the compacted bentonite. Through ionic exchange, Mg^{2+} and Ca^{2+} in bentonite are released from the calcigel and Na+ in the R2 solution is partially absorbed. This simulation was conducted with PHREEQC. The important ionic exchange equations and log_k values together with the amount of exchangeable ions in the calcigel were:

```
EXCHANGE_SPECIES
# Nagra NTB 02-09 Anhang D-1
 X- = X-
   log_k = 0.0
 X- + Na+ = NaX
   log_k = 0.0
 2X- + Ca+2 = CaX2
   log_k = 0.37
 X- + K+ = KX
   log_k = 4.0
 2X- + Mg+2 = MgX2
   log_k = 0.31
 2X- + Sr+2 = SrX2
   log_k = 0.37
 X- + H+ = HX
   log_k = 1.0

EXCHANGE 1
        #equilibrate 1
NaX      0.113008461 # in mol of exchangeable species/kg H₂O
KX       0.012556496
MgX2     0.703163757
CaX2     1.180310592
```

For the simulation, the following conditions were applied:

1. Solution: R2 as the following

```
SOLUTION 0  R2
pH         9.84
Na  6.0881 mol/kgw
K   0.26513 mol/kgw
Ca  0.010689 mol/kgw
Mg  0.051547 mol/kgw
Cl  6.0671 mol/kgw
S(6)0.20555 mol/kgw
C(4)3.5549E-06 mol/kgw
Si  7.6876E-09 mol/kgw
Al  6.765E-19 mol/kgw
```

2. Solid phase: Calcigel

3. Temperature: 25 °C

4. Pressure: 1 atm

5. Database: phreeqc_NAGRA_PSI.dat

6. Input files for PHREEQC calculation: R3

7. Output or result file of PHREEQC: R3.out

The results of the simulated solution R3 were:

```
-----------------------------Exchange composition---------------
---------------

X               3.893e+000 mol

                              Equiv-    Equivalent      Log
Species              Moles    alents      Fraction     Gamma

NaX              2.893e+000  2.893e+000  7.433e-001     0.000
KX               2.776e-001  2.776e-001  7.132e-002     0.000
MgX2             2.227e-001  4.454e-001  1.144e-001     0.000
CaX2             1.381e-001  2.763e-001  7.098e-002     0.000
HX               1.967e-008  1.967e-008  5.053e-009     0.000

-----------------------------Solution composition---------------
---------------

Elements           Molality       Moles

Al               6.765e-019  6.765e-019
C                3.555e-006  3.555e-006
Ca               1.053e+000  1.053e+000
Cl               6.067e+000  6.067e+000
K                8.271e-005  8.271e-005
Mg               5.320e-001  5.320e-001
Na               3.308e+000  3.308e+000
S                2.056e-001  2.056e-001
Si               7.688e-009  7.688e-009

pH  =   8.481
```

The elemental compositions of R3 are listed in Tab. 5.1. The results showed that pH decreases slightly. The concentration of Ca in the solution increased from 0.011 M to 1.05 M, Mg from 0.05 M to 0.53 M respectively, while Na decreased from 6.09 M to 3.31 M.

5.1.4 Case R4

The solution of R3 flows further downwards through the salt concrete and results the corrosion solution R4. For the simulation, the following conditions were applied:

1. Solution: R3 as the following for EQ3/6 (in [mol/kg H_2O])

```
Al+++      6.77E-19
HCO3-      3.56E-06
Ca++       1.053
Cl-        6.067
K+         8.27E-05
Mg++       0.532
Na+        3.308
SO4--      0.2056
SiO2(aq)   7.69E-09
pH         8.48
```

2. Solid phase: Salt concrete (chemical composition of salt concrete in Tab. 2.8)
3. Temperature: 25 °C
4. Pressure: 1 atm
5. Database: data0-V8_extend.bfs
6. Suppressed solid phases are:
    - Trichlorid – Ca6Al2(Cl2)3O6:30H2O
    - Chrysotil – $Mg_3Si_2O_5(OH)_4$
    - Jennit – $Ca_9Si_6O_{21}:11H_2O$
    - Tobermorit – $Ca_5Si_6O_{17}:9H_2O$
    - Hydrotalcit – $Mg_4Al_2(OH)_{14}:3H_2O$
    - Hydrotalcit-Semi-CO_3 – $Mg_4Al_2(OH)_{12}CO_3:2H_2O$
    - $Ca_5Si_5O_{14}(OH)_2:4H_2O$ – Ca5Si5O14(OH)2:4H_2O
    - Talcit – $Mg_3Si_4O11:H_2O$
7. Input files for EQ3/6 of the last reaction (zi = 4): R4.3i, R4.6i
8. Output file for EQ3/6: R4.6o
9. Pickup file after EQ6 calculation by zi = 4: R4.6p
10. Results for all EQ3/6 titration calculations can be found in file R4.xls.

11. The concentration evolution of main species by adding rock salt into R3 is showed in Fig. 5.5, while the mineral evolution in Fig. 5.6. The chemical compositions of R4 at zi = 4 are listed in Tab. 5.1 (total elemental concentration) and Tab. 5.5 (species concentration).

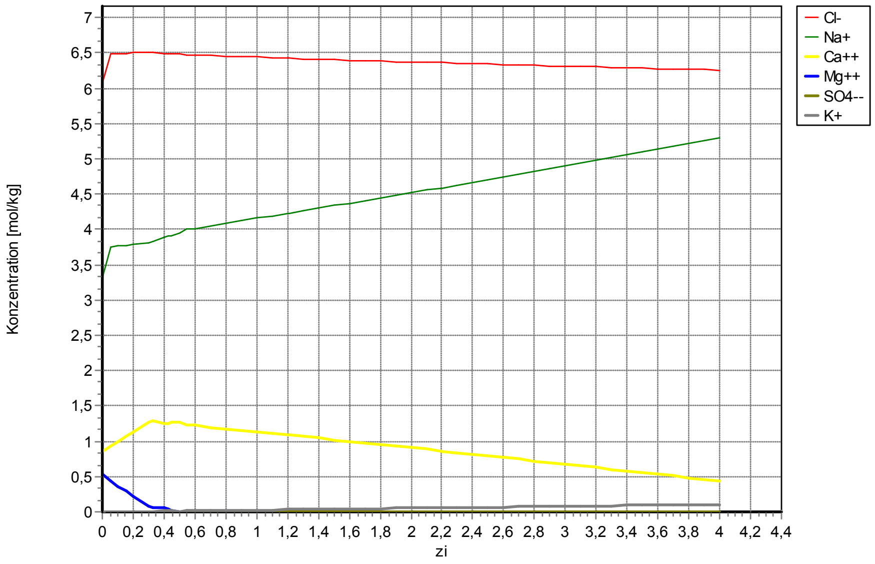

Fig. 5.5 The concentration evolution of main species by adding salt concrete into R3

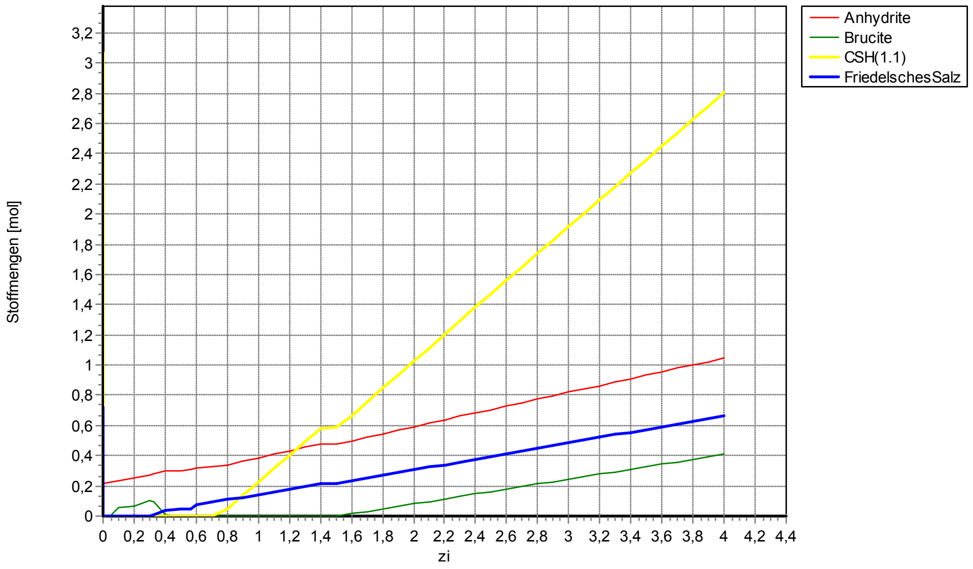

Fig. 5.6 The mineral composition evolution by adding salt concrete into R3

Tab. 5.5 Chemical composition of R4 in [mol/kg·H_2O]

Species	Concentration	Species	Concentration
Cl^-	6.26	SiO_2(aq)	$6.83 \cdot 10^{-09}$
Na^+	5.29	H^+	$8.17 \cdot 10^{-13}$
Ca^{++}	$4.38 \cdot 10^{-01}$	$H_3SiO_4^-$	$7.03 \cdot 10^{-07}$
Mg^{++}	$1.58 \cdot 10^{-06}$	CO_2(aq)	$1.17 \cdot 10^{-15}$
SO_4^{--}	$5.04 \cdot 10^{-03}$	HSO_4^-	$4.39 \cdot 10^{-14}$
$MgOH^+$	$2.83 \cdot 10^{-06}$	$H_2SiO_4^{--}$	$5.63 \cdot 10^{-07}$
K^+	$1.07 \cdot 10^{-01}$	$Al(OH)_4^-$	$6.01 \cdot 10^{-10}$
OH^-	$6.05 \cdot 10^{-03}$	$Al(OH)_3$	$1.91 \cdot 10^{-13}$
$CaCO_3$(aq)	$3.33 \cdot 10^{-06}$	$Al(OH)_2^+$	$1.73 \cdot 10^{-18}$
$MgCO_3$(aq)	$1.16 \cdot 10^{-11}$	$Al(OH)^{++}$	$1.47 \cdot 10^{-23}$
CO_3^{--}	$2.97 \cdot 10^{-07}$	Al^{+++}	$8.02 \cdot 10^{-32}$
HCO_3^-	$6.14 \cdot 10^{-10}$		

The simulated results showed that the pH value increased up to 12.1. The C-S-H phase CSH(1.1) was totally dissolved at zi = 0.54. The corresponding mass of solution is 1.37 kg, the density of salt concrete is 2100 kg/m^3, while the density of solution R4 is 1210 kg/m^3. The values of dissolution capacity are thus calculated with Ku 0.225 m^3/m^3 and Km 0.394 kg/kg (Tab. 5.2). The Mg^{2+} concentration was very low owing to brucite precipitation.

5.1.5 Case R5

The solution of R4 flows further downwards and reacts with bischofite which served as Mg-donator in the layer between salt concrete and the sorel concrete. Consequently, the resulting solution approaching the sorel concrete will have a minimal Mg^{2+} concentration of 0.5 M. The required minimal zi for the calculation was 0.11.

For the simulation with EQ3/6, the following conditions were applied:

1. Starting solution: R4 (the EQ6 pickup file (R4.6p) of the last reaction for R4 was used)
2. Solid phase: Bischofite product (chemical composition values in Tab. 2.8)
3. Temperature: 25 °C
4. Pressure: 1 atm
5. Database: data0-V8_extend.bfs

6. Suppressed solid phases are:
   - Trichlorid – $Ca_6Al_2(Cl_2)_3O_6{:}30H_2O$
   - Chrysotil – $Mg_3Si_2O_5(OH)_4$
   - Jennit – $Ca_9Si_6O_{21}{:}11H_2O$
   - Tobermorit – $Ca_5Si_6O_{17}{:}9H_2O$
7. Input files for EQ3/6 of the last reaction (zi = 0.11): R5pickup.3i, R5pickup.6i
8. Output file for EQ3/6: R5pickup.6o
9. Pickup file after EQ6 calculation by zi = 0.11: R5pickup.6p
10. Results for all EQ3/6 titration calculations can be found in file R5pickup.xls.

The concentration evolution of Mg^{2+} by adding Bischofite product into R4 is showed in Fig. 5.7. The chemical compositions of R5 at zi = 0.11 are listed in Tab. 5.1 (total elemental concentration) and Tab. 5.6 (species concentration).

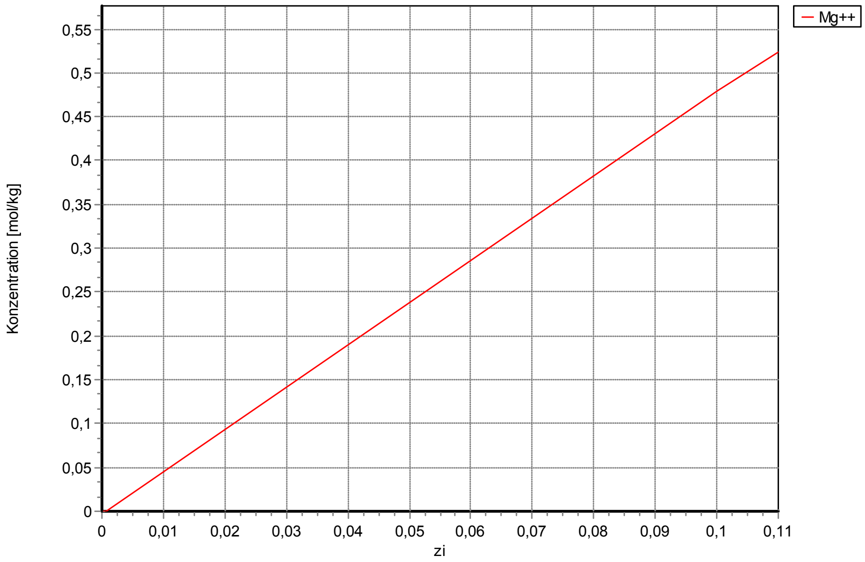

Fig. 5.7 The concentration evolution of Mg^{2+} by adding Bischofite product into corrosion solution R4

Tab. 5.6 Chemical composition of R5 in [mol/kg·H_2O]

Species	Concentration	Species	Concentration
Cl^-	6,36	SiO_2(aq)	$6,65\cdot10^{-09}$
Na^+	4,39	HCO_3-	$1,65\cdot10^{-07}$
Ca^{++}	$4,13\cdot10^{-01}$	$Al(OH)_4^-$	$4,43\cdot10^{-10}$
K^+	$1,07\cdot10^{-01}$	$MgCO_3$(aq)	$1,72\cdot10^{-06}$
OH^-	$1,31\cdot10^{-05}$	H^+	$4,81\cdot10^{-10}$
SO_4^{--}	$5,01\cdot10^{-03}$	$Al(OH)_3$	$1,24\cdot10^{-10}$
$CaCO_3$(aq)	$1,31\cdot10^{-06}$	HSO_4^-	$1,98\cdot10^{-11}$
$MgOH^+$	$1,67\cdot10^{-03}$	CO_2(aq)	$1,84\cdot10^{-10}$
Mg^{++}	$5,24\cdot10^{-01}$	$Al(OH)_2^+$	$7,01\cdot10^{-13}$
$H_3SiO_4^-$	$8,95\cdot10^{-10}$	$Al(OH)^{++}$	$3,18\cdot10^{-15}$
$H_2SiO_4^{--}$	$1,54\cdot10^{-12}$	Al^{+++}	$8,73\cdot10^{-21}$
CO_3^{--}	$2,37\cdot10^{-07}$		

The total amount of Bischofite product needed depends on the amount of R5 solutions reached the sorel concrete. It is to note that the concentration value of $MgOH^+$ was relatively high in R5. Therefore, pickup file was used for the followed geochemical simulation.

5.1.6 Case R6

The solution of R5 flows further through the last sealing material sorel concrete and results corrosion solution R6.

1. Starting solution: R5 (using the EQ6 pickup file R5pickup.6p of last reaction)
2. Solid phase: Sorel concrete (sorel concrete in Tab. 2.8)
3. Temperature: 25 °C
4. Pressure: 1 atm
5. Database: data0-V8_extend.bfs
6. Suppressed solid phases are:
    - Trichlorid – $Ca_6Al_2(Cl_2)_3O_6{:}30H_2O$
    - Chrysotil – $Mg_3Si_2O_5(OH)_4$
    - Jennit – $Ca_9Si_6O_{21}{:}11H_2O$
    - Tobermorit – $Ca_5Si_6O_{17}{:}9H_2O$

7. Input files for EQ3/6 of the last reaction (zi = 4): R6pickup.3i, R6pickup.6i

8. Output file for EQ3/6: R6pickup.6o

9. Pickup file after EQ6 calculation by zi = 4: R6pickup.6p

10. Results for all EQ3/6 titration calculations can be found in file R6pickup.xls.

11. The concentration evolution of main species by adding sorel concrete into R5 is showed in Fig. 5.8, while the mineral evolution in Fig. 5.9. The chemical compositions of R6 at zi = 4 are listed in Tab. 5.1 (total elemental concentration) and Tab. 5.7 (species concentration).

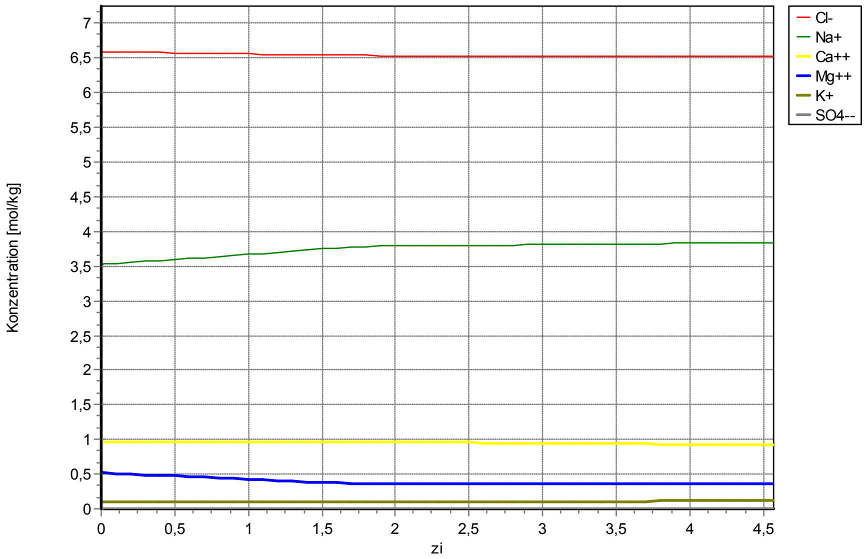

Fig. 5.8 Concentration evolution of main species with the addition of sorel concrete into solution R5

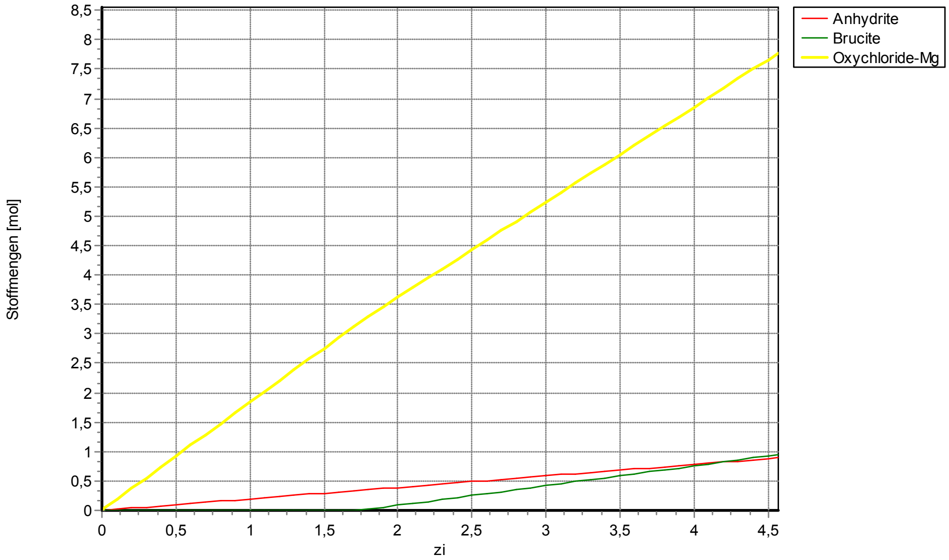

Fig. 5.9 Mineral composition evolution with the addition of sorel concrete into solution R5

Tab. 5.7 Chemical composition of R6 in [mol/kg·H_2O]

Species	Concentration	Species	Concentration
Cl^-	6.52	$SiO_2(aq)$	$5.36{\cdot}10^{-09}$
Na^+	3.84	$H_3SiO_4^-$	$9.46{\cdot}10^{-10}$
Ca^{++}	$9.22{\cdot}10^{-01}$	H^+	$3.83{\cdot}10^{-10}$
Mg^{++}	$3.65{\cdot}10^{-01}$	$CO_2(aq)$	$8.01{\cdot}10^{-11}$
K^+	$1.13{\cdot}10^{-01}$	$Al(OH)_4^-$	$9.32{\cdot}10^{-11}$
SO_4^{--}	$2.57{\cdot}10^{-03}$	$Al(OH)_3$	$2.23{\cdot}10^{-11}$
$MgOH^+$	$1.68{\cdot}10^{-03}$	HSO_4^-	$6.62{\cdot}10^{-12}$
OH^-	$2.60{\cdot}10^{-05}$	$H_2SiO_4^{--}$	$2.47{\cdot}10^{-12}$
$CaCO_3(aq)$	$2.04{\cdot}10^{-06}$	$Al(OH)_2^+$	$1.05{\cdot}10^{-13}$
$MgCO_3(aq)$	$8.26{\cdot}10^{-07}$	$Al(OH)^{++}$	$3.65{\cdot}10^{-16}$
CO_3^{--}	$2.35{\cdot}10^{-07}$	Al^{+++}	$6.54{\cdot}10^{-22}$
HCO_3^-	$5.35{\cdot}10^{-08}$		

The simulated results of the mineral composition evolution showed that the binder Mg-Oxychloride precipitated even from the beginning of adding sorel concrete into the R5 solution (zi approaching 0) with zi = $1.59{\cdot}10^{-7}$ kg/kg H_2O (Fig. 5.9). The amount of solution was 1.37 kg/kg H2O. The dissolution capacity Ku corresponds to $6.73{\cdot}10^{-8}$ m^3/m^3, while Km is $1.16{\cdot}10^{-7}$ kg/kg (Tab. 5.2). The solution R6 is thus not corrosive to sorel concrete.

5.2 Gipshut-solution serial

Analog to the rain water serial, the simulations of Gipshut-solution serial describes the geochemical evolution of Gipshut-solution penetrating through the shaft starting from the concrete foundation, three engineering barrier layers (bentonite, salt concrete and sorel concrete) and layers between them. The simulated total elemental concentrations of the corrosion solutions for the Gipshut-solution serial are listed in Tab. 5.8. Calculated values of dissolution capacity of solutions against concretes for the Gipshut-solution serial are listed in Tab. 5.9. Detailed descriptions of all simulations can be found in the following sections.

Tab. 5.8 The total elemental concentrations of the corrosion solutions for the Gipshut serial (in mol/kg·H_2O at z i= 4 for G1, G4 and G6, zi = 1.4 for G2 and zi = 0.11 for G5)

	C	Ca	Cl	K	Mg	Na	S	Si	Al	pcH	ρ_L*
G1	$9.60 \cdot 10^{-4}$	$5.12 \cdot 10^{-4}$	3.37	$8.70 \cdot 10^{-2}$	$1.78 \cdot 10^{-8}$	3.96	$1.46 \cdot 10^{-1}$	$1.04 \cdot 10^{-3}$	$2.59 \cdot 10^{-6}$	13.63	1.14
G2	$1.57 \cdot 10^{-5}$	$1.03 \cdot 10^{-2}$	6.21	$5.69 \cdot 10^{-1}$	$5.51 \cdot 10^{-2}$	5.95	$2.20 \cdot 10^{-1}$	$1.23 \cdot 10^{-8}$	$2.31 \cdot 10^{-6}$	9.84	1.22
G3	$3.65 \cdot 10^{-6}$	1.08	6.21	$2.30 \cdot 10^{-4}$	$5.63 \cdot 10^{-1}$	3.36	$2.20 \cdot 10^{-1}$	$1.26 \cdot 10^{-7}$	$8.17 \cdot 10^{-20}$	8.47	1.23
G4	$3.72 \cdot 10^{-6}$	$4.83 \cdot 10^{-1}$	6.27	$1.07 \cdot 10^{-1}$	$4.74 \cdot 10^{-6}$	5.21	$4.65 \cdot 10^{-3}$	$1.19 \cdot 10^{-6}$	$5.31 \cdot 10^{-10}$	12.07	1.22
G5	$3.52 \cdot 10^{-6}$	$4.55 \cdot 10^{-1}$	6.38	$1.07 \cdot 10^{-1}$	$5.25 \cdot 10^{-1}$	4.32	$4.60 \cdot 10^{-3}$	$7.52 \cdot 10^{-9}$	$5.02 \cdot 10^{-10}$	9.32	1.22
G6	$3.53 \cdot 10^{-6}$	$3.96 \cdot 10^{-1}$	6.35	$1.21 \cdot 10^{-1}$	$4.48 \cdot 10^{-1}$	4.55	$5.26 \cdot 10^{-3}$	$7.11 \cdot 10^{-9}$	$5.04 \cdot 10^{-10}$	9.37	1.22

*- ρ_L – solution density in kg/m^3

Tab. 5.9 Dissolution capacity of solutions against standard concrete (G1), salt concrete (G4) and sorel concrete (G6) in the Gipshut-solution serial

	m_c [kg/kg H_2O]	m_L [kg/kg H_2O]	ρ_L [kg/m^3]	ρ_c [kg/m^3]	Ku [m^3/m^3]	Km [kg/kg]	Corrosion evaluation
G1	0.0713	1.300	1140	2100	0.03	0.055	low
G4	0.572	1.372	1220	2100	0.24	0.417	medium
G6	$1.63 \cdot 10^{-07}$	1.411	1220	2100	$6.72 \cdot 10^{-8}$	$1.16 \cdot 10^{-07}$	non corosive

5.2.1 Case G1

Gipshut-solution penetrates the standard concrete (Normbeton) and resultes in the corrosion solution G1 (Tab. 5.8). For the simulation, the following conditions were applied:

1. Staring solution: Gipshut-solution containing 1 kg H_2O
2. Solid phase: standard concrete (standard concrete in Tab. 2.8)
3. Temperature: 25 °C
4. Pressure: 1 atm
5. Database: data0-V8_extend.bfs
6. Suppressed solid phases are:
    - Trichlorid – $Ca_6Al_2(Cl_2)_3O_6{:}30H_2O$
    - Chrysotil – $Mg_3Si_2O_5(OH)_4$
    - Jennit – $Ca_9Si_6O_{21}{:}11H_2O$
    - Tobermorit – $Ca_5Si_6O_{17}{:}9H_2O$
    - Kaolinit – $Al_2Si_2O_5(OH)_4$
    - $Ca_5Si_5O_{14}(OH)_2{:}4H_2O$ – $Ca_5Si_5O_{14}(OH)_2{:}4H_2O$
    - Talcit – $Mg_3Si_4O_{11}{:}H_2O$
    - Hydrotalcit – $Mg_4Al_2(OH)_{14}{:}3H_2O$
    - Hydrotalcit-Semi-CO_3 – $Mg_4Al_2(OH)_{12}CO_3{:}2H_2O$
7. Input file for EQ3/6: G1.3i, G1.6i
8. Output file for EQ3/6: G1.6o
9. Pickup file after EQ6 calculation by zi = 4: G1.6p
10. Results for all EQ3/6 titration calculations: G1.xls

The chemical compositions of G1 are listed in Tab. 5.10 (species concentration) and in Tab. 5.8 (total elemental concentration).

Tab. 5.10 Chemical composition of G1 in [mol/kg·H_2O] by zi = 4.0

Species	Concentration	Species	Concentration
Cl^-	3.37	$MgOH^+$	$1.71 \cdot 10^{-08}$
Na^+	3.96	H^+	$2.36 \cdot 10^{-14}$
Mg^{++}	$6.94 \cdot 10^{-10}$	HSO_4^-	$2.37 \cdot 10^{-14}$
SO_4^{--}	$1.46 \cdot 10^{-01}$	OH^-	$3.73 \cdot 10^{-01}$
K^+	$8.70 \cdot 10^{-02}$	$H_3SiO_4^-$	$3.01 \cdot 10^{-05}$
Ca^{++}	$5.06 \cdot 10^{-04}$	$Al(OH)_2^+$	$5.24 \cdot 10^{-19}$
HCO_3^-	$6.82 \cdot 10^{-08}$	$Al(OH)^{++}$	$2.90 \cdot 10^{-26}$
$CO_2(aq)$	$1.32 \cdot 10^{-15}$	$Al(OH)_3$	$7.05 \cdot 10^{-12}$
$SiO_2(aq)$	$3.33 \cdot 10^{-09}$	$Al(OH)_4^-$	$2.59 \cdot 10^{-06}$
$MgCO_3(aq)$	$7.83 \cdot 10^{-12}$	Al^{+++}	$8.29 \cdot 10^{-35}$
CO_3^{--}	$9.54 \cdot 10^{-04}$	$H_2SiO_4^{--}$	$1.01 \cdot 10^{-03}$
$CaCO_3(aq)$	$5.56 \cdot 10^{-06}$		

The simulated results showed that the concentration values of the main species Na^+ and Cl^- decreased with the addition of standard concrete (Fig. 5.10). This was mainly because that the water in the standard concrete was more than the need for hydration process. Therefore, the free water amount accumulated from 1 kg at zi = 0 to 1.27 kg at zi = 4. The concentration of Na+ decreased even though no precipitation of Na-minerals (Fig. 5.11). The precipitation of Friedelsches Salz ($Ca_4Al_2Cl_2O_6 \cdot 10H_2O$) strengthened the Cl^- concentration decrease. The main C-S-H binders of the standard concrete CSH(1.1) and CSH(1.8) could only be completely dissolved by zi≤0.0713. This can be interpreted that the Gipshut-solution with 1 kg of H_2O can totally dissolve the binders within 0.0713 kg standard concrete. The corresponding dissolution capacity Ku was 0.03 m^3/m^3, Km in 0.055 kg/kg (Tab. 5.9).

5.2.2 Case G2

The corrosion solution of G1 flows downwards and might be in contact with rock salt within the layer between the standard concrete foundation and the bentonite, or the host rock. The simulation was conducted according to the Gipshut-solution oriented method. The minimum zi needed to reach the reference Mg^{2+} concentration in 0.055 M is about 1.40 (Fig. 5.12).

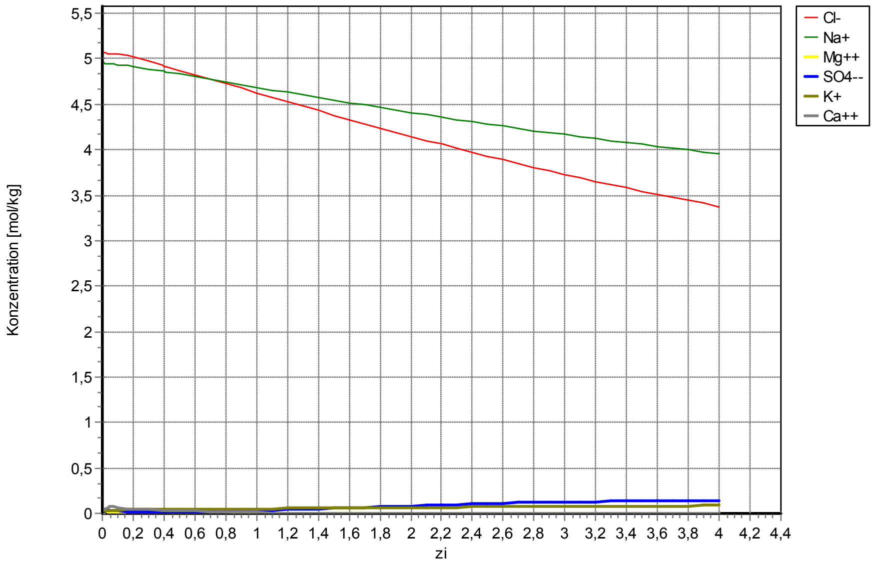

Fig. 5.10 Concentration evolution of main species with the addition of standard concrete into Gipshut-solution (GL)

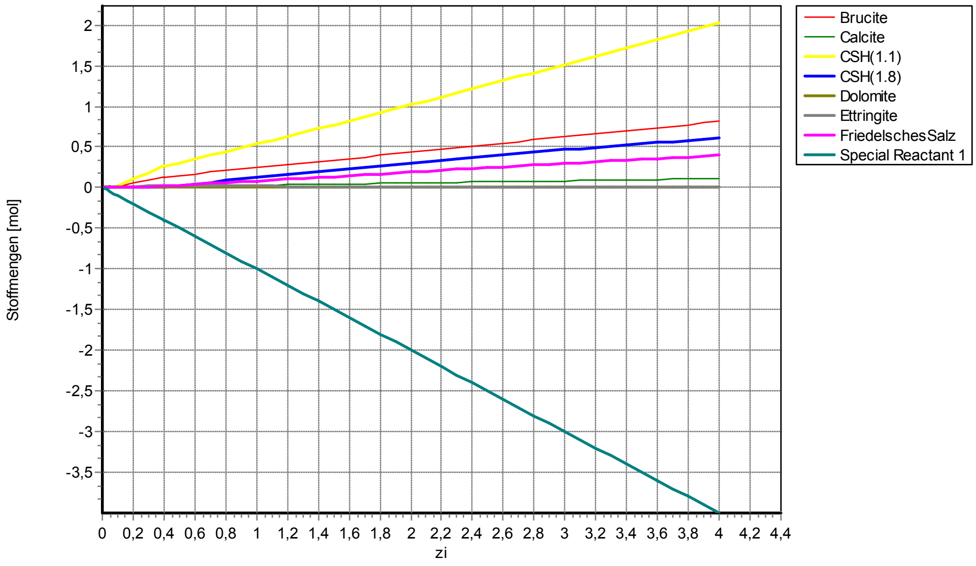

Fig. 5.11 Mineral composition evolution with the addition of standard concrete into Gipshut-solution (GL), Special Reactant represented the standard concrete

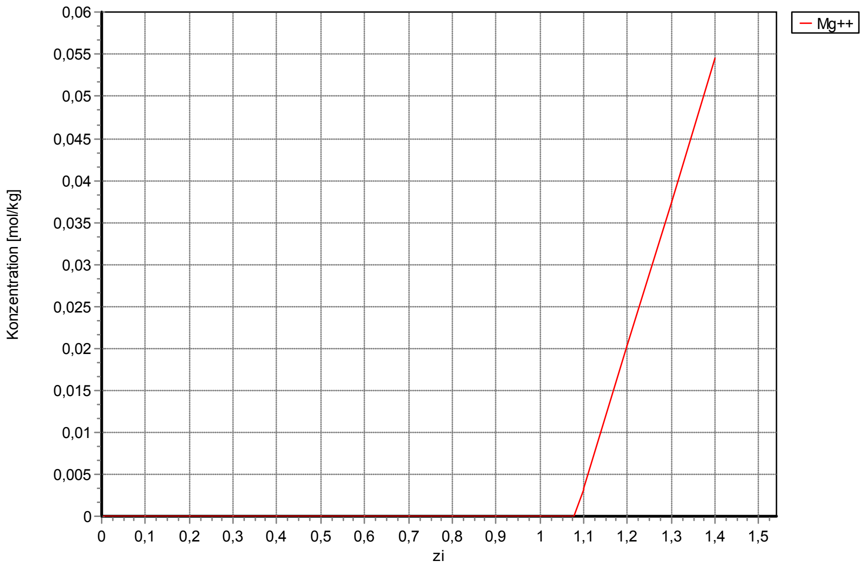

Fig. 5.12 Mg^{2+} concentration evolution by adding rock salt into dissolution solution G1

For the simulation, the following conditions were applied:

1. Solution: G1 (the pickup file G1.6p was used)
2. Solid phase: rock salt (Haldensalz in Tab. 2.8)
3. Temperature: 25 °C
4. Pressure: 1 atm
5. Database: data0-V8_extend.bfs
6. Suppressed solid phases are:
   - Trichlorid – $Ca_6Al_2(Cl_2)_3O_6:30H_2O$
   - Chrysotil – $Mg_3Si_2O_5(OH)_4$
   - Jennit – $Ca_9Si_6O_{21}:11H_2O$
   - Tobermorit – $Ca_5Si_6O_{17}:9H_2O$
7. Input files for EQ3/6 of the last reaction (zi = 1.40): G2pickup.3i, G2pickup.6i
8. Output file for EQ3/6: G2pickup.6o
9. Pickup file after EQ6 calculation by zi = 1.40: G2pickup.6p
10. Results for all EQ3/6 titration calculations can be found in file G2pickup.xls.

The concentration evolution of main species by adding rock salt into G1 is showed in Fig. 5.13. The chemical compositions of G2 at zi = 1.40 are listed in Tab. 5.8 (total elemental concentration) and Tab. 5.11 (species concentration).

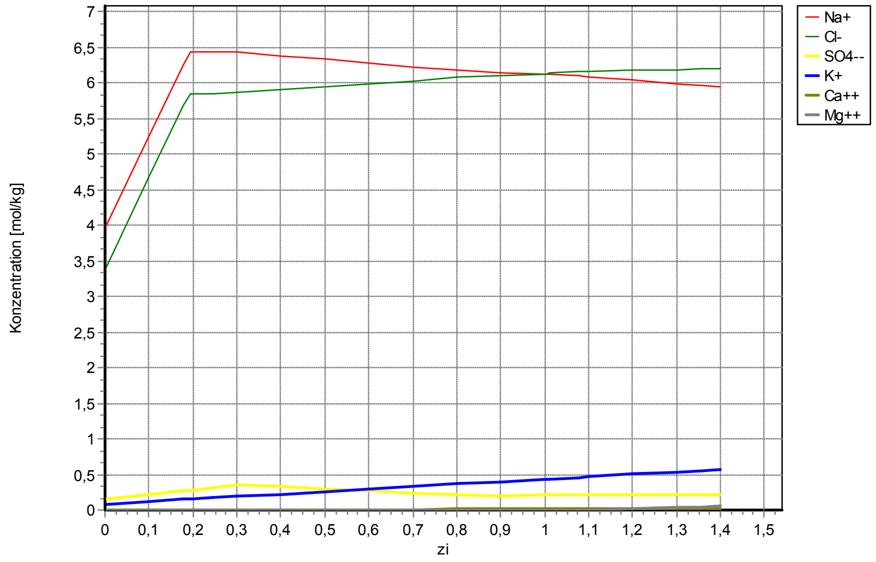

Fig. 5.13 Concentration evolution of main species with the addition of rock salt into the corrosion solution G1

Tab. 5.11 Chemical composition of G2 in [mol/kg·H_2O] by z_i = 1.40

Species	Concentration	Species	Concentration
Na^+	5.95	$MgOH^+$	$5.35\cdot10^{-04}$
Cl^-	6.21	$SiO_2(aq)$	$1.26\cdot10^{-07}$
OH^-	$1.96\cdot10^{-05}$	Mg^{++}	$5.46\cdot10^{-02}$
SO_4^{--}	$2.20\cdot10^{-01}$	$MgCO_3(aq)$	$7.51\cdot10^{-06}$
K^+	$5.69\cdot10^{-01}$	$Al(OH)_3$	$1.23\cdot10^{-08}$
$H_2SiO_4^{--}$	$2.44\cdot10^{-10}$	HSO_4^-	$4.72\cdot10^{-10}$
CO_3^{--}	$3.25\cdot10^{-06}$	H^+	$1.44\cdot10^{-10}$
Ca^{++}	$1.03\cdot10^{-02}$	$CO_2(aq)$	$6.95\cdot10^{-10}$
$H_3SiO_4^-$	$7.36\cdot10^{-08}$	$Al(OH)_2^+$	$2.03\cdot10^{-11}$
$CaCO_3(aq)$	$1.32\cdot10^{-06}$	$Al(OH)^{++}$	$3.87\cdot10^{-14}$
$Al(OH)_4^-$	$2.57\cdot10^{-07}$	Al^{+++}	$8.17\cdot10^{-20}$
HCO_3^-	$3.65\cdot10^{-06}$		

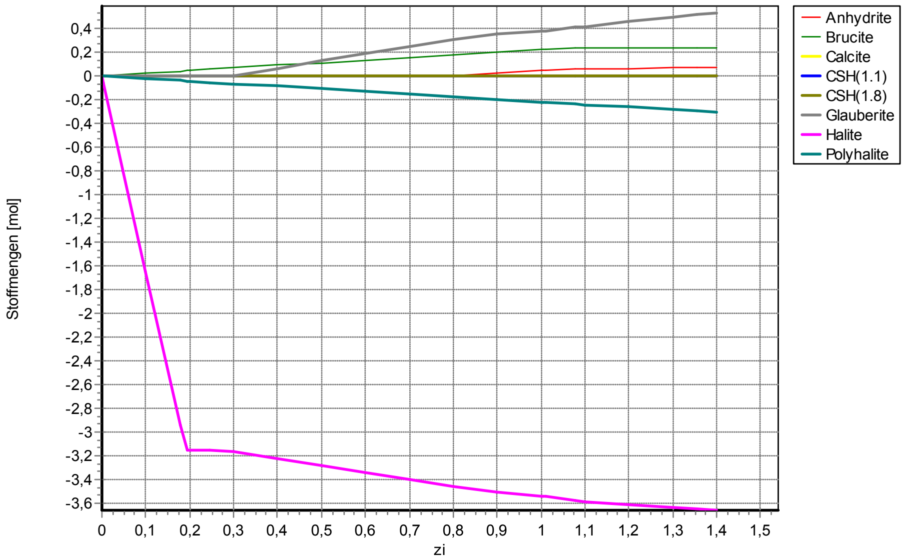

Fig. 5.14 Mineral composition evolution with the addition of adding rock salt into the solution G1

The simulated results showed that the pcH value of the corrosion solution decreased significantly from 13.63 to 9.84 by reacting with rock salt (Tab. 5.8). The reason was the precipitation of brucite ($Mg(OH)_2$). The Polyhalite ($K_2MgCa_2(SO_4)_4{:}2H_2O$) in rock salt was the Mg provider. Na^+, Cl^- concentration increased also significantly and reached its maximum by zi = 0.2 (halite saturated). In comparison with case R2 with the halite saturation at z i= 0.49, less halite is dissolved.

5.2.3 Case G3

The solution of G2 flows downwards through the compacted bentonite. Through ionic exchange, Mg^{2+} and Ca^{2+} in bentonite are released from the calcigel and Na^+ in the G2 solution is partially absorbed. The calculation was conducted with PHREEQC. The important ionic exchange equations and log_k values are the same as described in section 5.1.3. The amount of exchangeable ions in the calcigel was a little different owing to the small difference of the solution density values of R2 and G2:

```
EXCHANGE 1
        #equilibrate 1
NaX      0.113375248 # in mol of exchangeable species/kg H2O
KX       0.01263916
MgX2     0.70779323
CaX2     1.18808149
```

For the simulation, the following conditions were applied:

1. Solution: G2 as the following

```
SOLUTION 0  G2
units           mol/kgw
pH              9.84

Na   5.9471
K    0.56867
Ca   0.010287
Mg   0.054597
Cl   6.205
S(6) 0.21993
C(4) 3.6492E-06
Si   1.2588E-07
Al   8.1685E-20
```

2. Solid phase: Calcigel
3. Temperature: 25 °C
4. Pressure: 1 atm
5. Database: phreeqc_NAGRA_PSI.dat
6. Input files for PHREEQC calculation: G3
7. Output or result file of PHREEQC: G3.out

The results of the simulated solution G3 were:

```
--------------------Exchange composition--------------

X               4.032e+000 mol

                               Equiv-    Equivalent      Log
Species              Moles      alents      Fraction     Gamma

NaX               2.703e+000  2.703e+000  6.705e-001    -0.000
KX                6.948e-001  6.948e-001  1.723e-001    -0.000
MgX2              1.995e-001  3.990e-001  9.896e-002    -0.000
CaX2              1.173e-001  2.347e-001  5.821e-002    -0.000
HX                1.826e-008  1.826e-008  4.530e-009    -0.000

--------------------Solution composition---------------

Elements            Molality       Moles

Al                8.169e-020  8.169e-020
C                 3.649e-006  3.649e-006
Ca                1.081e+000  1.081e+000
Cl                6.205e+000  6.205e+000
```

```
K                2.299e-004  2.299e-004
Mg               5.629e-001  5.629e-001
Na               3.357e+000  3.357e+000
S                2.199e-001  2.199e-001
Si               1.259e-007  1.259e-007

pH  =   8.467
```

The elemental compositions of G3 are listed in Tab. 5.8. The results showed that pH decreases slightly. The concentration of Ca in the solution increases from 0.010 M to 1.08 M; the concentration of Mg changes from 0.055 M to 0.563 M respectively, while that of Na decreases from 5.95 M to 3.36 M.

5.2.4 Case G4

The solution of G3 flows further downwards through the salt concrete and resulted the corrosion solution G4. For the simulation with EQ3/6, the following conditions were applied:

1. Solution: G3 as the following for EQ3/6 (in [mol/kg H2O])

```
Al+++    8.17E-20
HCO3-    3.65E-06
Ca++     1.08E+00
Cl-      6.21E+00
K+       2.30E-04
Mg++     5.63E-01
Na+      3.36E+00
SO4--    2.20E-01
SiO2(aq) 1.26E-07
pH       8.47
```

2. Solid phase: Salt concrete (chemical composition of salt concrete in Tab. 2.8)
3. Temperature: 25 °C
4. Pressure: 1 atm
5. Database: data0-V8_extend.bfs
6. Suppressed solid phases are:
    - Trichlorid – $Ca_6Al_2(Cl_2)_3O_6:30H_2O$
    - Chrysotil – $Mg_3Si_2O_5(OH)_4$
    - Jennit – $Ca_9Si_6O_{21}:11H_2O$
    - Tobermorit – $Ca_5Si_6O_{17}:9H_2O$

- Hydrotalcit – $Mg_4Al_2(OH)_{14}:3H_2O$
- Hydrotalcit-Semi-CO3 – $Mg_4Al_2(OH)_{12}CO_3:2H_2O$
- Ca5Si5O14(OH)2:4H2O – $Ca_5Si_5O_{14}(OH)_2:4H_2O$
- Talcit – $Mg_3Si_4O_{11}:H_2O$

7. Input files for EQ3/6 of the last reaction (zi = 4): G4.3i, G4.6i
8. Output file for EQ3/6: G4.6o
9. Pickup file after EQ6 calculation by zi = 4: G4.6p
10. Results for all EQ3/6 titration calculations can be found in file G4.xls.
11. The concentration evolution of main species by adding rock salt into G3 is showed in Fig. 5.15, while the mineral evolution in Fig. 5.16. The chemical compositions of G4 at zi = 4 are listed in Tab. 5.8 (total elemental concentration) and Tab. 5.12 (species concentration).

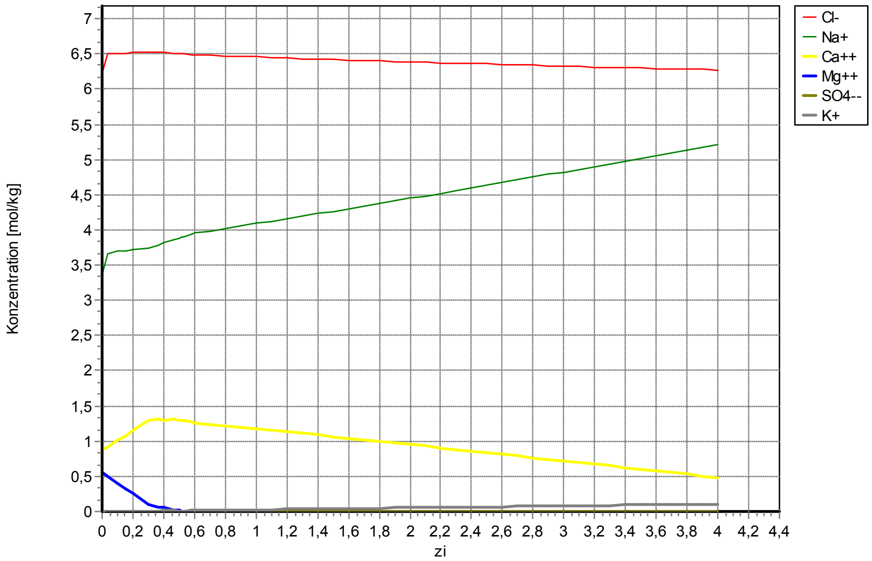

Fig. 5.15 The concentration evolution of main species by adding salt concrete into G3

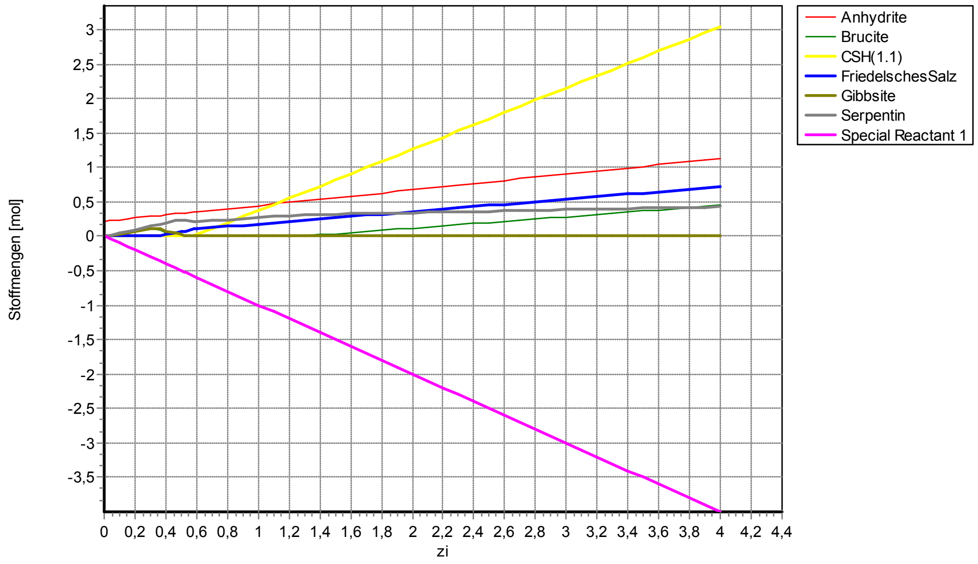

Fig. 5.16 The mineral composition evolution by adding salt concrete into G3

Tab. 5.12 Chemical composition of G4 in [mol/kg·H_2O]

Species	Concentration	Species	Concentration
Cl^-	6.27	SiO_2(aq)	$6.74 \cdot 10^{-09}$
Na^+	5.21	$H_3SiO_4^-$	$6.62 \cdot 10^{-07}$
Ca^{++}	$4.83 \cdot 10^{-01}$	H^+	$8.56 \cdot 10^{-13}$
Mg^{++}	$1.73 \cdot 10^{-06}$	CO_2(aq)	$1.20 \cdot 10^{-15}$
SO_4^{--}	$4.65 \cdot 10^{-03}$	HSO_4^-	$4.11 \cdot 10^{-14}$
$MgOH^+$	$3.01 \cdot 10^{-06}$	$H_2SiO_4^{--}$	$5.21 \cdot 10^{-07}$
K^+	$1.07 \cdot 10^{-01}$	$Al(OH)_4^-$	$5.31 \cdot 10^{-10}$
OH^-	$6.07 \cdot 10^{-03}$	$Al(OH)_3$	$1.79 \cdot 10^{-13}$
$CaCO_3$(aq)	$3.43 \cdot 10^{-06}$	$Al(OH)_2^+$	$1.71 \cdot 10^{-18}$
$MgCO_3$(aq)	$1.19 \cdot 10^{-11}$	$Al(OH)^{++}$	$1.51 \cdot 10^{-23}$
CO_3^{--}	$2.94 \cdot 10^{-07}$	Al^{+++}	$8.44 \cdot 10^{-32}$
HCO_3^-	$5.73 \cdot 10^{-10}$		

The simulated results showed that the pH value increased up to 12.1. The C-S-H phase CSH(1.1) was totally dissolved at zi = 0.572. The corresponding mass of solution was 1.372 kg, the density of salt concrete was 2100 kg/m^3, while the density of solution G4 was 1220 kg/m^3. Dissolution capacity Ku can be thus calculated with 0.24 m^3/m^3 (Tab. 5.23). The Mg^{2+} concentration was very low owing to brucite precipitation.

5.2.5 Case G5

The solution of G4 flows further downwards and reacts with bischofite which served as Mg-donator in the layer between salt concrete and the sorel concrete . Consequently, the resulted solution approached the sorel concrete had a minimal Mg^{2+} concentration of 0.5 M. The required minimal zi for the calculation was the same as in case R5 with 0.11.

For the simulation with EQ3/6, the following conditions were applied:

1. Starting solution: G4 (the EQ6 pickup file G4.6p of the last reaction for case G4 was used)
2. Solid phase: Bischofite product (chemical composition values in Tab. 2.8)
3. Temperature: 25 °C
4. Pressure: 1 atm
5. Database: data0-V8_extend.bfs
6. Suppressed solid phases are:
   - Trichlorid – $Ca_6Al_2(Cl_2)_3O_6{:}30H_2O$
   - Chrysotil – $Mg_3Si_2O_5(OH)_4$
   - Jennit – $Ca_9Si_6O_{21}{:}11H_2O$
   - Tobermorit – $Ca_5Si_6O_{17}{:}9H_2O$
7. Input files for EQ3/6 of the last reaction (zi = 0.11): G5pickup.3i, G5pickup.6i
8. Output file generated by EQ3/6 at z i= 0.11: G5pickup.6o
9. Pickup file after EQ6 calculation by zi = 0.11: G5pickup.6p
10. Results for all EQ3/6 titration calculations can be found in file G5pickup.xls.

The concentration evolution of Mg^{2+} by adding Bischofite product into G4 is shown in Fig. 5.17. The chemical compositions of G5 at zi = 0.11 are listed in Tab. 5.8 (total elemental concentration) and Tab. 5.13 (species concentration).

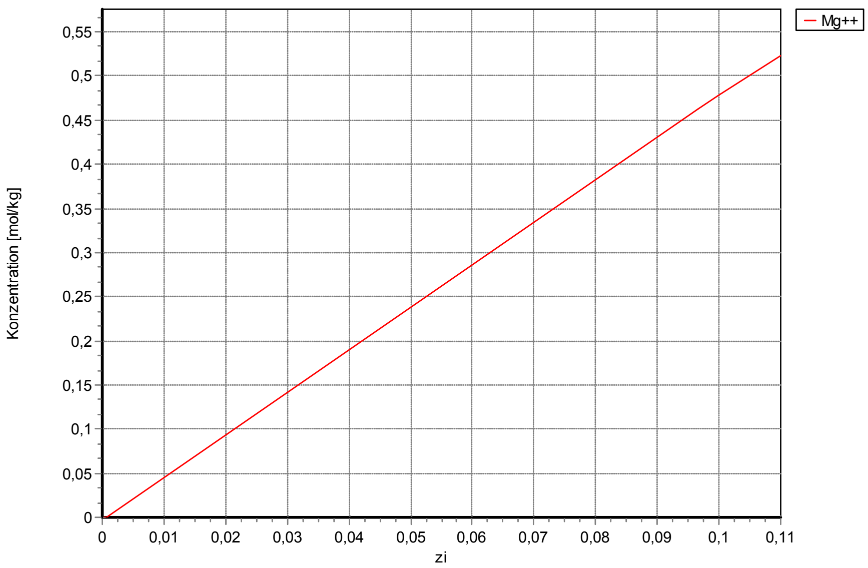

Fig. 5.17 The concentration evolution of Mg^{2+} by adding Bischofite product into corrosion solution G4

Tab. 5.13 Chemical composition of G5 in [mol/kg·H_2O]

Species	Concentration	Species	Concentration
Cl^-	6.38	$SiO_2(aq)$	$6.63 \cdot 10^{-09}$
Na^+	4.32	HCO_3^-	$1.56 \cdot 10^{-07}$
Ca^{++}	$4.55 \cdot 10^{-01}$	$Al(OH)_4^-$	$3.90 \cdot 10^{-10}$
K^+	$1.07 \cdot 10^{-01}$	$MgCO_3(aq)$	$1.69 \cdot 10^{-06}$
OH^-	$1.37 \cdot 10^{-05}$	H^+	$4.81 \cdot 10^{-10}$
SO_4^{--}	$4.60 \cdot 10^{-03}$	$Al(OH)_3$	$1.11 \cdot 10^{-10}$
$CaCO_3(aq)$	$1.43 \cdot 10^{-06}$	HSO_4^-	$1.78 \cdot 10^{-11}$
$MgOH^+$	$1.69 \cdot 10^{-03}$	$CO_2(aq)$	$1.82 \cdot 10^{-10}$
Mg^{++}	$5.23 \cdot 10^{-01}$	$Al(OH)_2^+$	$6.31 \cdot 10^{-13}$
$H_3SiO_4^-$	$8.89 \cdot 10^{-10}$	$Al(OH)^{++}$	$2.85 \cdot 10^{-15}$
$H_2SiO_4^{--}$	$1.56 \cdot 10^{-12}$	Al^{+++}	$7.68 \cdot 10^{-21}$
$CO3^{--}$	$2.44 \cdot 10^{-07}$		

The simulated results showed that the concentration of Mg^{2+} can be increased to the minimum reference value 0.5 M by adding 0.082 kg/kg solution Bischofite product into the layer. As the solution density was 1220 kg/m^3, porosity of the material containing the Bischofite product is 20 %, the minimum amount of Bischofite product needed would be 0.02 kg/L solid. The total amount of Bischofite product needed depends on the G5 solution amount generated and reached the sorel concrete. It is to note that the concentration value of $MgOH^+$ were relatively high in G5 (Tab. 5.13). Therefore, pickup file was used for the followed geochemical simulation.

5.2.6 Case G6

The solution of G5 flows further through the last sealing material sorel concrete and resulted corrosion solution G6.

For the simulation with EQ3/6, the following conditions were applied:

1. Starting solution: G5 (using the EQ6 pickup file G5pickup.6p of last reaction)
2. Solid phase: Sorel concrete (sorel concrete in Tab. 2.8)
3. Temperature: 25 °C
4. Pressure: 1 atm
5. Database: data0-V8_extend.bfs
6. Suppressed solid phases are:
    - Trichlorid – $Ca_6Al_2(Cl_2)_3O_6{:}30H_2O$
    - Chrysotil – $Mg_3Si_2O_5(OH)_4$
    - Jennit – $Ca_9Si_6O_{21}{:}11H_2O$
    - Tobermorit – $Ca_5Si_6O_{17}{:}9H_2O$
7. Input files for EQ3/6 of the last reaction (zi = 4): G6pickup.3i, G6pickup.6i
8. Output file for EQ3/6: G6pickup.6o
9. Pickup file after EQ6 calculation by zi = 4: G6pickup.6p
10. Results for all EQ3/6 titration calculations can be found in file G6pickup.xls.
11. The concentration evolution of main species by adding sorel concrete into G5 is shown in Fig. 5.18, while the mineral evolution in Fig. 5.19. The chemical compositions of G6 at zi = 4 are listed in Tab. 5.8 (total elemental concentration) and Tab. 5.14 (species concentration).

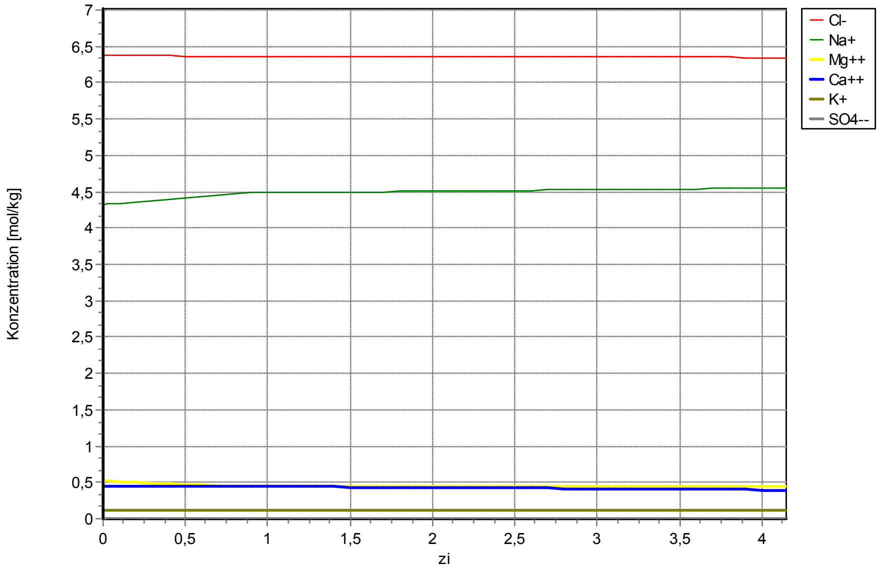

Fig. 5.18 Concentration evolution of main species with the addition of sorel concrete into solution G5

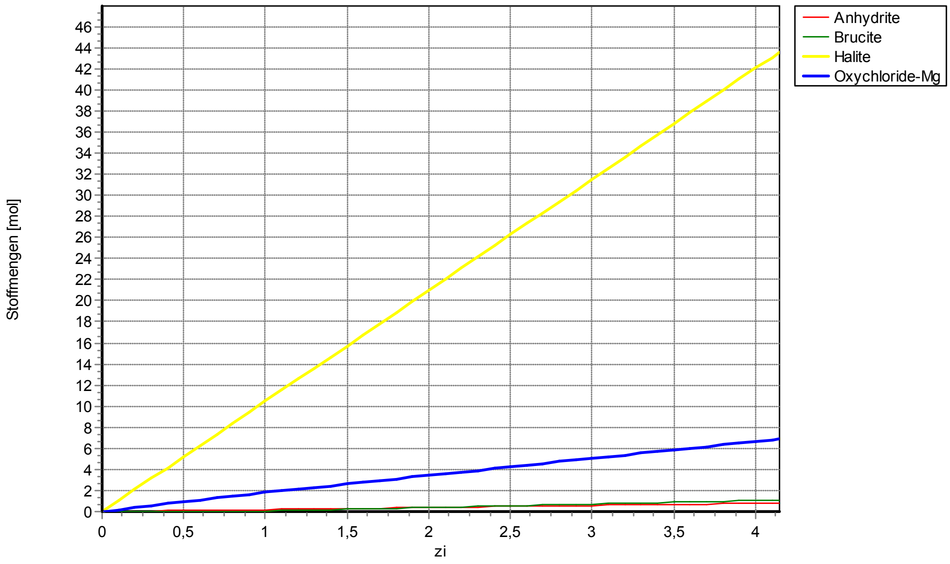

Fig. 5.19 Mineral composition evolution with the addition of sorel concrete into solution G5

Tab. 5.14 Chemical composition of G6 in [mol/kg·H_2O]

Species	Concentration	Species	Concentration
Cl^-	6.35	$SiO_2(aq)$	$6.14 \cdot 10^{-09}$
Na^+	4.55	$H_3SiO_4^-$	$9.65 \cdot 10^{-10}$
Mg^{++}	$4.46 \cdot 10^{-01}$	H^+	$4.29 \cdot 10^{-10}$
Ca^{++}	$3.96 \cdot 10^{-01}$	$Al(OH)_4^-$	$4.08 \cdot 10^{-10}$
K^+	$1.21 \cdot 10^{-01}$	$CO_2(aq)$	$1.67 \cdot 10^{-10}$
SO_4^{--}	$5.26 \cdot 10^{-03}$	$Al(OH)_3$	$9.54 \cdot 10^{-11}$
$MgOH^+$	$1.58 \cdot 10^{-03}$	HSO_4^-	$1.95 \cdot 10^{-11}$
OH^-	$1.39 \cdot 10^{-05}$	$H_2SiO_4^{--}$	$1.77 \cdot 10^{-12}$
$MgCO_3(aq)$	$1.67 \cdot 10^{-06}$	$Al(OH)_2^+$	$4.74 \cdot 10^{-13}$
$CaCO_3(aq)$	$1.45 \cdot 10^{-06}$	$Al(OH)^{++}$	$1.96 \cdot 10^{-15}$
CO_3^{--}	$2.42 \cdot 10^{-07}$	Al^{+++}	$4.94 \cdot 10^{-21}$
HCO_3^-	$1.71 \cdot 10^{-07}$		

The simulated results of the mineral composition evolution showed that the binder Mg-Oxychloride precipitated even from the starting adding sorel concrete into the G5 solution (zi approaching 0) with $1.63 \cdot 10^{-7}$ kg/kg H_2O (Fig. 5.19). The dissolution capacity Ku corresponds to $6.72 \cdot 10^{-8}$ m^3/m^3 (Tab. 5.24). The solution G5 is thus not corrosive to sorel concrete.

5.3 IP9 serial

IP9 serial represents a worst case scenario for the corrosion of salt concrete. This is because IP9 solution is rich in Mg^{2+} with 1.04 mol/kg H_2O, which is relatively corrosive against salt concrete /HAG 2009/. Solution IP9 flows through salt concrete, sorel concrete and the layer between them, and resulting solution H4, H6 and H5 respectively. Simulated total element concentration values are listed in Tab. 5.15. Detailed description can be found in the following sections.

Tab. 5.15 The total elemental concentrations of the corrosion solutions for the IP9

	Ca	Cl	K	Mg	Na	S	Si	Al	pcH	ρ_L*
H4	$1.64 \cdot 10^{-01}$	6.77	1.24	$2.38 \cdot 10^{-06}$	5.24	$1.18 \cdot 10^{-02}$	$2.87 \cdot 10^{-06}$	$1.90 \cdot 10^{-09}$	12.34	1.22
H5	$1.55 \cdot 10^{-01}$	6.87	1.18	$5.10 \cdot 10^{-01}$	4.39	$1.30 \cdot 10^{-02}$	$7.86 \cdot 10^{-09}$	$1.80 \cdot 10^{-09}$	9.36	1.22
H6	$8.88 \cdot 10^{-02}$	6.77	1.07	$4.83 \cdot 10^{-01}$	4.59	$2.23 \cdot 10^{-02}$	$6.84 \cdot 10^{-09}$	$9.95 \cdot 10^{-11}$	9.37	1.22

*- ρ_L – solution density in kg/m^3

Tab. 5.16 Dissolution capacity of solutions against salt concrete (H4) andsorel concrete (H6) for the IP9 serial

	m_c [kg/kg H_2O]	m_L [kg/kg H_2O]	ρ_L [kg/m^3]	ρ_c [kg/m^3]	Ku [m^3/m^3]	Km [kg/kg]	Corrosion evaluation
H4	0.96	1.400	1220	2100	0.397	0.686	high
H6	0.00	1.41	1220	2100	0.00	0.000	non corosive

5.3.1 Case H4

The solution of IP9 flows downwards through the salt concrete and results the corrosion solution H4. For the simulation, the following conditions were applied:

1. Solution: IP9 containing 1 kg H_2O (Tab. 2.11)
2. Solid phase: Salt concrete (chemical composition of salt concrete in Tab. 2.8)
3. Temperature: 25 °C
4. Pressure: 1 atm
5. Database: data0-V8_extend.bfs
6. Suppressed solid phases are:
    - Trichlorid – $Ca_6Al_2(Cl_2)_3O_6:30H_2O$
    - Chrysotil – $Mg_3Si_2O_5(OH)_4$
    - Jennit – $Ca_9Si_6O_{21}:11H_2O$
    - Tobermorit – $Ca_5Si_6O_{17}:9H_2O$
    - Ca5Si5O14(OH)2:4H2O – $Ca_5Si_5O_{14}(OH)_2:4H_2O$
    - Talcit – $Mg_3Si_4O_{11}:H_2O$
    - Hydrotalcit – $Mg_4Al_2(OH)_{14}:3H_2O$
    - Hydrotalcit-Semi-CO3 – $Mg_4Al_2(OH)_{12}CO_3:2H_2O$
7. Input files for EQ3/6 of the last reaction (zi = 4): H4.3i, H4.6i
8. Output file for EQ3/6: H4.6o
9. Pickup file after EQ6 calculation by zi = 4: H4.6p
10. Results for all EQ3/6 titration calculations can be found in file H4.xls.

11. The concentration evolution of main species by adding rock salt into IP9 solution is showed in Fig. 5.20, while the mineral evolution in Fig. 5.21. The chemical compositions of G4 at zi = 4 are listed in Tab. 5.15 (total elemental concentration) and Tab. 5.17 (species concentration).

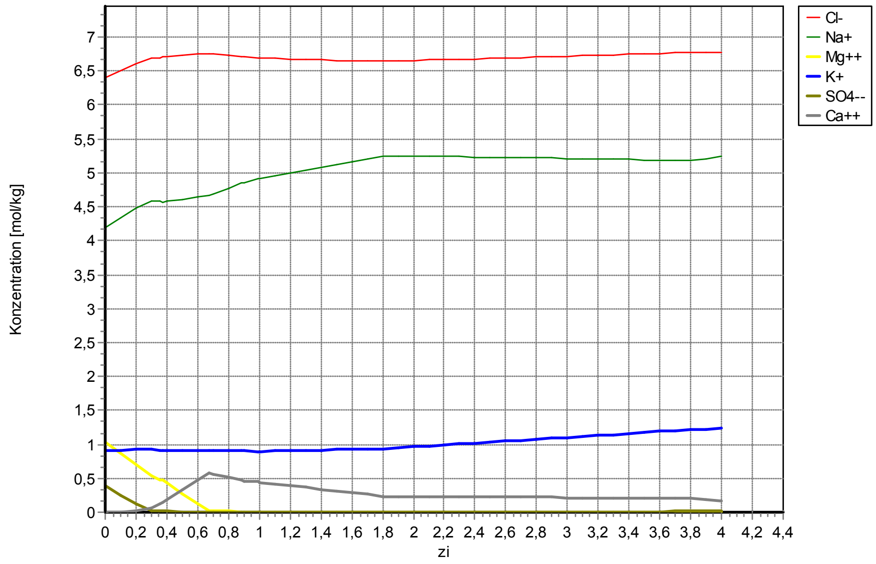

Fig. 5.20 The concentration evolution of main species by adding salt concrete into IP9 solution

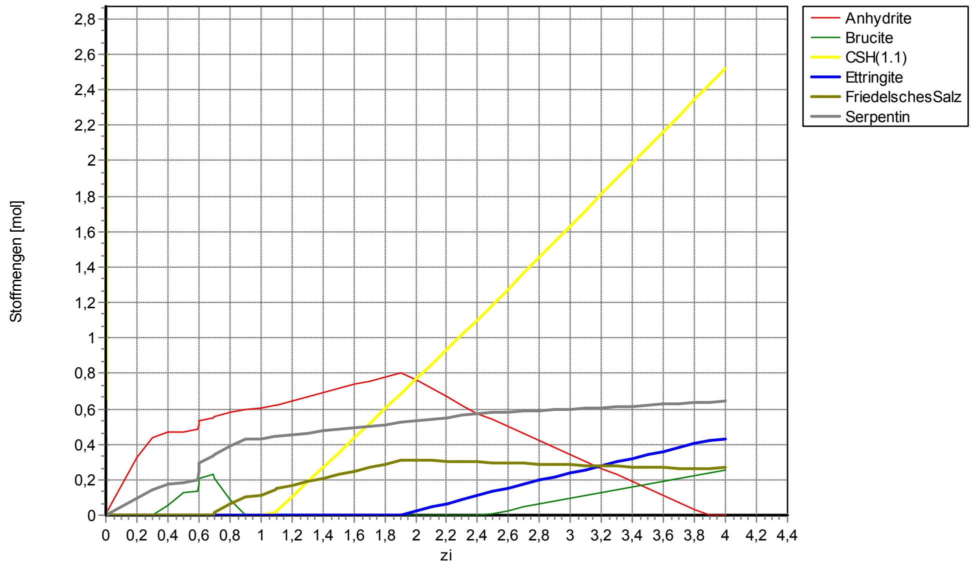

Fig. 5.21 The mineral composition evolution by adding salt concrete into IP9 solution

Tab. 5.17 Chemical composition of H4 in [mol/kg·H_2O]

Species	Concentration	Species	Concentration
Cl^-	6.77	H^+	$4.55 \cdot 10^{-13}$
Na^+	5.24	$SiO_2(aq)$	$7.48 \cdot 10^{-09}$
Mg^{++}	$5.54 \cdot 10^{-07}$	$Al(OH)_3$	$3.03 \cdot 10^{-13}$
K^+	1.24	$Al(OH)_2^+$	$1.70 \cdot 10^{-18}$
SO_4^{--}	$1.18 \cdot 10^{-02}$	$Al(OH)^{++}$	$1.08 \cdot 10^{-23}$
Ca^{++}	$1.64 \cdot 10^{-01}$	$Al(OH)_4^-$	$1.90 \cdot 10^{-09}$
$MgOH^+$	$1.82 \cdot 10^{-06}$	$H_3SiO_4^-$	$1.35 \cdot 10^{-06}$
OH^-	$6.36 \cdot 10^{-03}$	Al^{+++}	$2.28 \cdot 10^{-32}$
HSO_4^-	$7.64 \cdot 10^{-14}$	$H_2SiO_4^{--}$	$1.33 \cdot 10^{-06}$

The simulated results showed that the pH value increased up to 12.3. The C-S-H phase CSH(1.1) is totally dissolved at zi = 0.96. The corresponding mass of solution is 1.40 kg, the density of salt concrete is 2100 kg/m^3, while the density of solution G4 is 1220 kg/m^3. Dissolution capacity Ku can be thus calculated with 0.397 m^3/m^3 (Tab. 5.23). The Mg^{2+} concentration is very low owing to brucite precipitation.

5.3.2 Case H5

The solution of H4 flows further downwards and reacts with bischofite which serves as Mg-donator in the layer between salt concrete and the sorel concrete. Consequently, the resulted solution approaching the sorel concrete has a minimal Mg^{2+} concentration of 0.5 M. The required minimal zi for the calculation is 0.09.

For the simulation with EQ3/6, the following conditions were applied:

1. Starting solution: H4 (the EQ6 pickup file (H4.6p) of the last reaction for H4 was used)
2. Solid phase: Bischofite product (chemical composition values in Tab. 2.8)
3. Temperature: 25 °C
4. Pressure: 1 atm
5. Database: data0-V8_extend.bfs
6. Input files for EQ3/6 of the last reaction (zi = 0.09): H5pickup.3i, H5pickup.6i
7. Output file for EQ3/6: H5pickup.6o

8. Pickup file after EQ6 calculation by zi = 0.09: H5pickup.6p

9. Results for all EQ3/6 titration calculations can be found in file H5pickup.xls.

The concentration evolution of Mg^{2+} by adding Bischofite product into H4 is shown in Fig. 5.22. The chemical compositions of H5 at zi = 0.09 are listed in Tab. 5.15 (total elemental concentration) and Tab. 5.18 (species concentration).

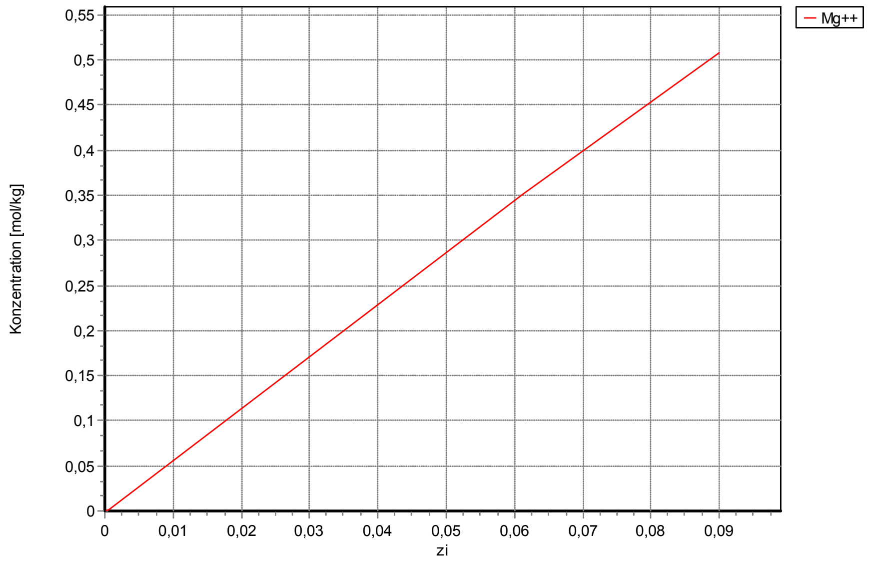

Fig. 5.22 The concentration evolution of Mg^{2+} by adding Bischofite product into corrosion solution H4

Tab. 5.18 Chemical composition of H5 in [mol/kg·H_2O]

Species	Concentration	Species	Concentration
Cl^-	6,87	Mg^{++}	$5{,}08 \cdot 10^{-01}$
Na^+	4,39	$SiO_2(aq)$	$6{,}87 \cdot 10^{-09}$
K^+	1,18	$Al(OH)_4^-$	$1{,}46 \cdot 10^{-09}$
Ca^{++}	$1{,}55 \cdot 10^{-01}$	H^+	$4{,}40 \cdot 10^{-10}$
SO_4^{--}	$1{,}30 \cdot 10^{-02}$	$Al(OH)_3$	$3{,}40 \cdot 10^{-10}$
OH^-	$8{,}54 \cdot 10^{-06}$	HSO_4^-	$6{,}03 \cdot 10^{-11}$
$MgOH^+$	$1{,}82 \cdot 10^{-03}$	$Al(OH)_2^+$	$1{,}95 \cdot 10^{-12}$
$H2SiO_4^{--}$	$1{,}52 \cdot 10^{-12}$	$Al(OH)^{++}$	$1{,}07 \cdot 10^{-14}$
$H3SiO_4^-$	$9{,}85 \cdot 10^{-10}$	Al^{+++}	$1{,}90 \cdot 10^{-20}$

The simulated results showed that the concentration of Mg^{2+} can be increased to the minimum reference value 0.5 M by adding 0.077 kg/kg▪solution Bischofite product into the layer. As the solution density is 1220 kg/m^3, if the porosity of the material containing the Bischofite product is 20 %, the minimum amount of Bischofite product needed would be 0.019 kg/L solid. The total amount of Bischofite product needed depends on the H5 solution amount generated and reached the sorel concrete.

5.3.3 Case H6

The solution of H5 flows further through the last sealing material sorel concrete and results corrosion solution H6.

For the simulation with EQ3/6, the following conditions were applied:

1. Starting solution: H5 (EQ6 pickup file H5pickup.6p of last reaction was not used owing to numerical problems). As the concentration of $MgOH^+$ is fairly high, it was ignored and the concentration of Cl- was also modified for charge balance (compare Tab. 5.18). The chemical compositions of solution H5 were (in mol/kg H_2O):

   ```
   Cl-        6.86
   Na+        4.39
   Mg++       0.508
   K+         1.178
   SO4--      0.013
   Ca++       0.155
   SiO2(aq)   6.87E-09
   Al+++      1.90E-20
   pH         9.36
   ```

2. Solid phase: Sorel concrete (sorel concrete in Tab. 2.8)

3. Temperature: 25 °C

4. Pressure: 1 atm

5. Database: data0-V8_extend.bfs

6. Input files for EQ3/6 of the last reaction (zi = 4): H6.3i, H6.6i

7. Output file for EQ3/6: H6.6o

8. Pickup file after EQ6 calculation by zi = 4: H6.6p

9. Results for all EQ3/6 titration calculations can be found in file H6.xls.

10. The concentration evolution of main species by adding sorel concrete into H5 is showed in Fig. 5.23, while the mineral evolution in Fig. 5.24. The chemical compo-

sitions of G6 at zi = 4 are listed in Tab. 5.15 (total elemental concentration) and Tab. 5.19 (species concentration).

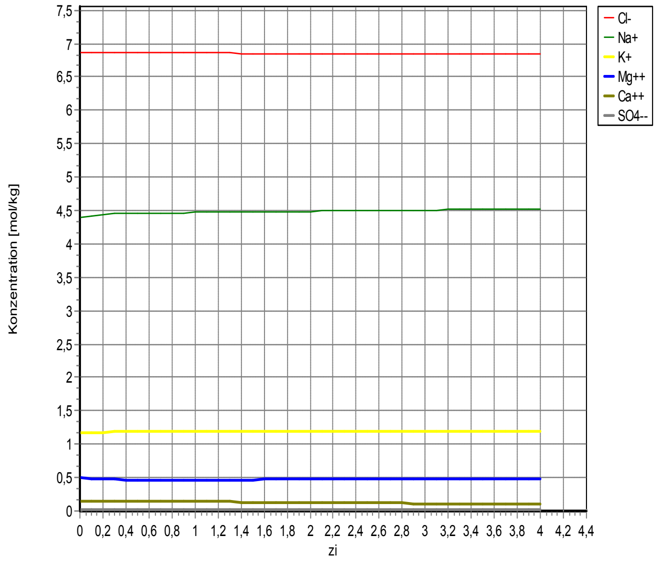

Fig. 5.23 Concentration evolution of main species with the addition of sorel concrete into solution H5

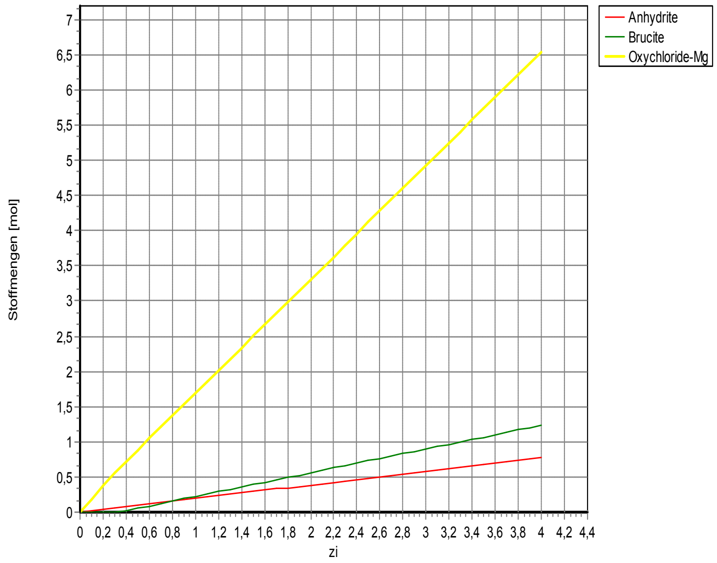

Fig. 5.24 Mineral composition evolution with the addition of sorel concrete into solution H5

Tab. 5.19 Chemical composition of H6 in [mol/kg·H_2O]

Species	Concentration	Species	Concentration
Cl^-	6.77	$H_3SiO_4^-$	$9.05 \cdot 10^{-10}$
Na^+	4.59	H^+	$4.24 \cdot 10^{-10}$
K^+	1.07	HSO_4^-	$1.05 \cdot 10^{-10}$
Mg^{++}	$4.82 \cdot 10^{-01}$	$Al(OH)_4^-$	$8.19 \cdot 10^{-11}$
Ca^{++}	$8.88 \cdot 10^{-02}$	$Al(OH)_3$	$1.75 \cdot 10^{-11}$
SO_4^{--}	$2.23 \cdot 10^{-02}$	$H2SiO_4^{--}$	$1.38 \cdot 10^{-12}$
$MgOH^+$	$1.74 \cdot 10^{-03}$	$Al(OH)_2^+$	$9.43 \cdot 10^{-14}$
OH^-	$8.32 \cdot 10^{-06}$	$Al(OH)^{++}$	$4.97 \cdot 10^{-16}$
$SiO_2(aq)$	$5.94 \cdot 10^{-09}$	Al^{+++}	$9.53 \cdot 10^{-22}$

The simulated results of the mineral composition evolution showed that the binder Mg-Oxychloride precipitated even from the starting adding sorel concrete into the H5 solution (zi approaching 0) with zi = 0.0 (Fig. 5.24). The dissolution capacity Ku corresponds to 0.0 m^3/m^3 (Tab. 5.24). The solution G5 is thus not corrosive to sorel concrete.

5.4 IP21 serial

IP21 serial represents another case scenario. Solution IP21 flows through sorel concrete and resulting solution I6. Simulated total element concentration values are listed in Tab. 5.20.

Tab. 5.20 The total elemental concentrations of the corrosion solutions for IP21 serial

	Ca	Cl	K	Mg	Na	S	Si	pcH	Density [g/cm³]
I6	$2.35 \cdot 10^{-03}$	8.459	0.439	3.920	0.627	0.224	$1.06 \cdot 10^{-10}$	8.75	1.28

Tab. 5.21 Dissolution capacity of solution IP21 against sorel concrete for the IP21 serial

	m_c [kg/kg H_2O]	m_L [kg/kg H_2O]	ρ_L [kg/m³]	ρ_c [kg/m³]	Ku [m³/m³]	Km [kg/kg]	Corrosion evaluation
I6	$9.86 \cdot 10^{-4}$	1.48	1280	2100	$4.06 \cdot 10^{-4}$	$6.66 \cdot 10^{-4}$	Very low

For the simulation with EQ3/6, the following conditions were applied:

1. EQ3/6 version 8.0a failed to calculate, therefore, EQ3/6 version 8.0 was applied.
2. Starting solution: IP21 solution
3. Solid phase: Sorel concrete (sorel concrete in Tab. 2.8)
4. Temperature: 25 °C
5. Pressure: 1 atm
6. Database: data0-V8_extend.bfs
7. Input files for EQ3/6 of the last reaction (zi = 4): I6ver8.3i, I6ver8.6i
8. Output file for EQ3/6: I6ver8.6o
9. Pickup file after EQ6 calculation by zi = 4: I6ver8.6p
10. Results for all EQ3/6 titration calculations can be found in file I6ver8.xls.
11. The concentration evolution of main species by adding sorel concrete into IP21 solution is showed in Fig. 5.25, while the mineral evolution in Fig. 5.26. The chemical compositions of I6 at zi = 4 are listed in Tab. 5.20 (total elemental concentration) and Tab. 5.19 (species concentration).

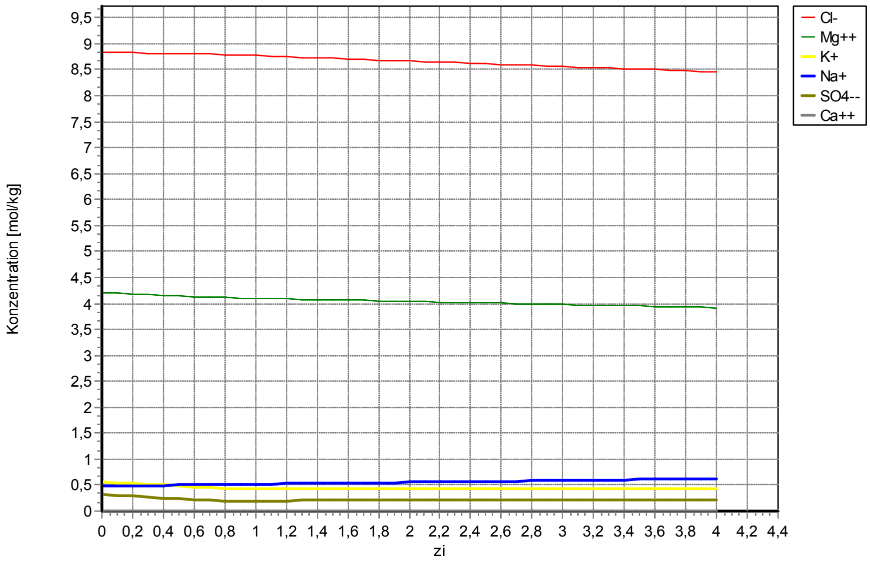

Fig. 5.25 Concentration evolution of main species with the addition of sorel concrete into solution IP21

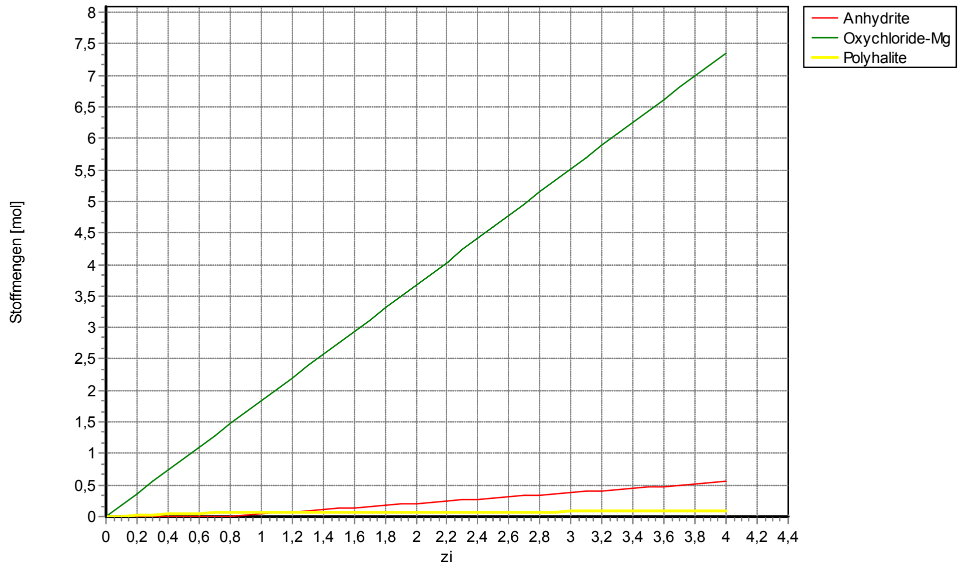

Fig. 5.26 Mineral composition evolution with the addition of sorel concrete into IP21 solution

Tab. 5.22 Chemical composition of I6 in [mol/kg·H_2O]

Species	Concentration	Species	Concentration
Cl^-	8.46	H^+	$1.80 \cdot 10^{-09}$
Mg^{++}	3.92	$SiO_2(aq)$	$1.06 \cdot 10^{-10}$
K^+	$4.39 \cdot 10^{-01}$	$Al(OH)^{++}$	$2.84 \cdot 10^{-13}$
Na^+	$6.27 \cdot 10^{-01}$	$Al(OH)_2^+$	$7.21 \cdot 10^{-12}$
SO_4^{--}	$2.24 \cdot 10^{-01}$	$Al(OH)_3$	$9.57 \cdot 10^{-11}$
Ca^{++}	$2.35 \cdot 10^{-03}$	$Al(OH)_4^-$	$2.84 \cdot 10^{-12}$
$MgOH^+$	$4.56 \cdot 10^{-03}$	$H3SiO_4^-$	$2.76 \cdot 10^{-13}$
OH^+	$3.50 \cdot 10^{-06}$	Al^{+++}	$8.43 \cdot 10^{-19}$
HSO_4^-	$1.45 \cdot 10^{-09}$	$H_2SiO_4^{--}$	$2.91 \cdot 10^{-16}$

The simulated results of the mineral composition evolution showed that the binder Mg-Oxychloride precipitated even from the starting adding sorel concrete into the H5 solution (zi approaching 0) with zi = $9.86 \cdot 10^{-4}$ (Fig. 5.26 and Tab. 5.24). The dissolution capacity Ku corresponds to $4.06 \cdot 10^{-4}$ m^3/m^3 (Tab. 5.24). The solution IP21 is thus not corrosive against sorel concrete.

5.5 Correlation of Mg^{2+} and Dissolution capacity

Based on the simulated results mentioned above, the dissolution capacity values Ku of various solutions against normal and salt concretes linearly depend on the initial Mg^{2+}

concentration in the percolating solutions (Fig. 5.27). The correlation of the dissolution capacity values Ku and the initial Mg^{2+} concentration in the percolating solutions is not very clear for the cases mentioned above because of the high initial Mg^{2+} concentration, which will be discussed in section 7.3.6.

Tab. 5.23 Dissolution capacity of solutions against normal and salt concretes

	m_c [kg/kg H_2O]	m_L [kg/kg H_2O]	Ku [m^3/m^3]	Km [kg/kg]	Mg^{2+} Concentration [M]	Corrosion evaluation
R1	0.0015	1.000	$7.12 \cdot 10^{-3}$	0.0015	$1.00 \cdot 10^{-10}$	very low
R4	0.54	1.370	0.225	0.3942	0.531	medium
G1	0.0713	1.300	0.03	0.0548	$5.64 \cdot 10^{-02}$	low
G4	0.572	1.372	0.24	0.4169	0.563	medium
H4	0.96	1.400	0.397	0.6857	1.04	high

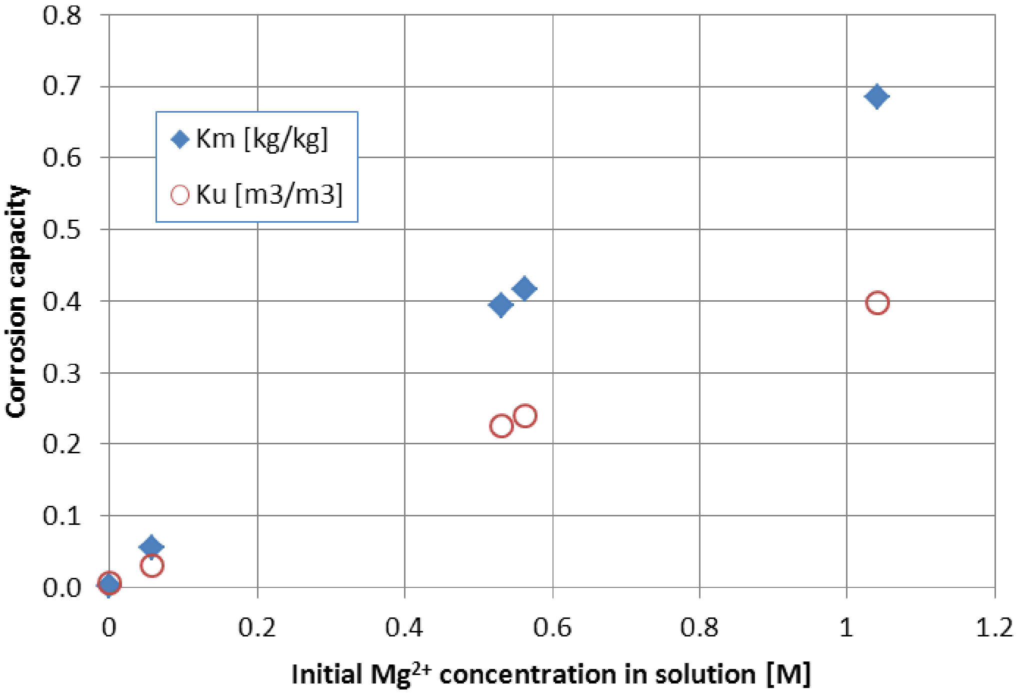

Fig. 5.27 Relation of the corrosion capacities Ku and the Mg^{2+} concentration of solution

Tab. 5.24 Dissolution capacity of solutions against sorel concrete

	m_c [kg/kg H_2O]	m_L [kg/kg H_2O]	Ku [m^3/m^3]	Km [kg/kg]	Mg^{2+} # [M]	Corrosion evaluation
R6	$1.59 \cdot 10^{-7}$	1.37	$6.73 \cdot 10^{-8}$	$1.16 \cdot 10^{-7}$	0.517	very low
G6	$1.63 \cdot 10^{-7}$	1.411	$6.72 \cdot 10^{-8}$	$1.16 \cdot 10^{-7}$	0.525	Very low
H6	0.00	1.41	0.00	0.00	0.51	non-corrosive
I6	$9.86 \cdot 10^{-4}$	1.48	$4.06 \cdot 10^{-4}$	$6.66 \cdot 10^{-4}$	4.21	Very low

- Mg^{2+} concentration

6 Estimation of maximum amount of corroded concrete

The amount of concrete to be corroded depends on both the dissolution capacity (Km) and the amount of the solution encountered. The dissolution capacity of a solution depends largely on its Mg^{2+} concentration. The relatively high fraction of exchangeable Mg^{2+} in the Ca-bentonite (22.4 meq/100 g) can act as Mg^{2+} source for solution through liquid/solid interaction (see section 2.2.1). Therefore, it is important to evaluate the impact of the exchangeable Mg^{2+} in the Ca-bentonite on the corrosion of the salt concrete. The maximal change of Mg^{2+} concentration of a solution penetrating the bentonite layer should be less than the Mg^{2+} concentration calculated under the assumption that all of the exchangeable Mg^{2+} is released. Based on the design of the shafts /LIN 2012/ , the diameter of the shafts is 7.63 m, after cutting depth is 0.50 m. The diameter of Ca-bentonite layer is 8.63 m. The thickness of the layer is 60 m. The total volume of the bentonite is 3510 m^3. The dry density of bentonite is designed to be 1650 kg/m^3. Total amount of exchange Mg^{2+} will be 648581 mol.

The amount of solution penetrating bentonite layer is assumed to be the same of the pore space volume between bentonite layer and the salt concrete layer, which was calculated according to /LIN 2012/ and listed in Tab. 6.1. The total amount is 2327 m^3. Therefore, the maximal variation of averaged Mg^{2+} concentration due to the Mg^{2+} in bentonite should be the total amount of exchangeable Mg^{2+} in mol divided by the amount of water in the solution in kg, which will be calculated for rain water serial and Gipshut-solution serial in the following subsections respectively.

Tab. 6.1 Size and pore space volume of material layers between bentonite and salt concrete layers broken/crushed rock (basalt), Crushed salt

Parameter	Filter	Broken/crushed rock (basalt)	Crushed salt
Thickness [m]	14	190	30
Diameter [m]	7.63	7.63	7.63
Volume of layer [m^3]	640	8687	1372
Porosity [%]	30	23	10
Pore volume [m^3]	192	1998	137

In the previous geochemical simulations, it is clear to see that the rain water and Gipshut-solution serials are most likely cases in the shafts. The dominant factor for concrete corrosion is the Mg^{2+} concentration in the solutions. For standard concrete and salt concrete, the correlation of the mass dissolution capacity (Km) and the Mg^{2+} concentration of solutions can be derived as (Fig. 6.1):

$$Km = 0.1598 \cdot C^2 + 0.8207 \cdot C + 0.0049 \qquad (6.1)$$

In which C is the Mg^{2+} concentration of a solution in mol/kg H_2O.

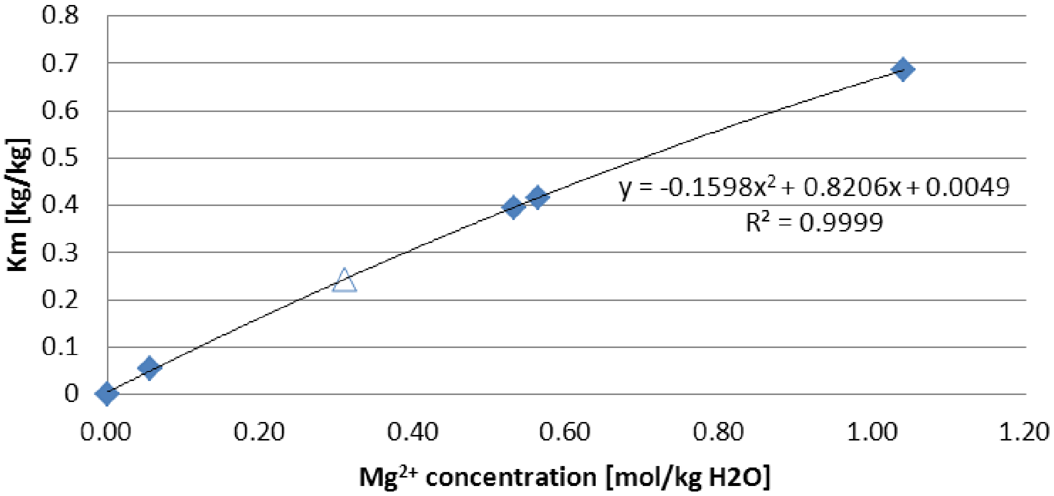

Fig. 6.1 Correlation of the mass dissolution capacity ($\boldsymbol{Km}$) and the Mg^{2+} concentration of solutions for Normal- and salt concrete

6.1 Rain water case

For the rain water case it is assumed that rain water is the dominant solution which can reach the fundament, reacts with salt and then penetrate bentonite layer and by the end contact with salt concrete. During these processes, the Mg^{2+} concentration can increase and might reach the maximum if all the exchangeable Mg^{2+} in bentonite would be fully released into the solution assuming no other Mg^{2+} sources and sinks exist. Take the chemical concentration of rain water serial, case R2 as starting point (Tab. 5.1). The total Mg^{2+} increase should be less than 0.312 mol/kg H_2O. Taking the Mg^{2+} in R2 into consideration, the total Mg^{2+} concentration should less than 0.364 mol/kg H_2O, which corresponds a mass dissolution capacity Km in 0.2825 kg/kg according to the equation mentioned above. The maximal total amount of salt concrete to be corroded by the 2327 m^3 solution (density 1220 kg/m^3) is 802 t.

6.2 Gipshut-solution case

For the Gipshut-solution case it is assumed that Gipshut-solution is the dominant solution which can reach the fundament, reacts with salt and then penetrate bentonite layer and by the end contact with salt concrete. During these processes, the Mg^{2+} concentration can increase and might reach the maximum if all the exchangeable Mg^{2+} in bentonite would be fully released into the solution assuming no other Mg^{2+} sources and sinks exist. Take the chemical concentration of Gipshut-solution serial, case G2 as starting point (Tab. 5.8). The total increase of Mg^{2+} concentration should be less than 0.32 mol/kg H_2O. Taking the Mg^{2+} in solution G2 into consideration, the total Mg^{2+} concentration should less than 0.377 mol/kg H_2O, which corresponds a mass dissolution capacity Km in 0.2914 kg/kg according to the equation mentioned above. The maximal total amount of salt concrete to be corroded by the 2327 m^3 solution (density 1220 kg/m^3) is 827 t.

7 Concrete corrosion by shaft solutions

The total amount of concrete corrosion depends not only on the corrosion capacity but also the amount of a solution. Continuous observations of the saline solutions emerged at different locations during the shaft excavation and later on operation phases showed that such solution was limited. All solution intrusions ceased after a certain time period. /HAM 2011/. Therefore it is reasonable to evaluate the total amount of potential corrosion of each concrete in shaft by the limited amount of solutions gathered in the shafts during the excavation time. These solutions were separately collected and analyzed (Appendix VI).

7.1 Shaft solutions gathered

The solutions from the stratigraphic horizons z3OSM, z3BK/BD, z3OSO and z2/z3Grenze collected in the shafts (Appendix VII) are analytic data provided by Hammer et al (2011) /HAM 2011/ as listed in Tab. 7.1. Their volumes of each solution type vary from 0.045 m^3 to 146.502 m^3. The Mg^{2+} concentration of the solution z3BK/BD is the highest in 4.455 mol/(kg H_2O), which is comparable to IP21 solution (Tab. 2.11). The chemical composition of solutions z3OSO and z2/z3Grenze is similar to that of IP9 solution, while that of the solution z3OSM is close to the composition of Gipshut-solution (Tab. 2.11).

It is important to point out that three of the solutions (z3OSM, z3OSO and z2/z3Grenze) were collected at the depth above the concrete foundation in the shafts in -340.0 m.

Tab. 7.1 The measured chemical composition of the four shaft solutions (in [mol/kg H_2O]) /HAM 2011/

	Na^+	K^+	Mg^{2+}	Ca^{2+}	Cl^-	SO_4^{2-}	Density [g/cm^3]	Volume [m^3]	Depth [m]
z3OSM	5.638	0.088	0.145	0.050	6.000	0.057	1.206	146.502	-286.05 to -236.69
z3BK/BD	0.333	0.217	4.455	0.053	9.384	0.091	1.294	0.0528	-816.6 to -311.04
z3OSO	4.543	0.240	0.503	0.089	5.897	0.035	1.203	84.655	-236.68
z2/z3Grenze	4.927	0.199	0.339	0.084	5.874	0.049	1.202	0.045	-242.78

pH – not available

7.2 Simulation cases

The geochemical simulations were undertaken in two groups (Tab. 7.2). The first group calculations were batch reactions between each solutions in Tab. 7.1 and each concrete layers (i.e. standard concrete, salt concrete and sorel concrete). The solution z3OSM reacts for example with the standard concrete layer and can result in solution M1. The second group calculations consider the Mg^{2+} concentration and ionic exchange in bentonite and its influence on the corrosion properties of the resulting solution of the salt concrete . In such cases each solution is in equilibrium first with bentonite through ionic exchange and the resulting solution reacts with salt concrete .

An overview of all calculation cases is listed in Tab. 7.2. The calculations were conducted under the same assumptions described in Section 2.3. The only difference lies in that no fixed solid/solution ratio (as one pore volume) was applied. Instead the calculations were conducted like the following: Taking a solution including one kg of H_2O, adding gradually concretes until the binder of concretes totally dissolved (see Section 4). The corresponding chemical composition of the resulting solution together with the solution and solid phase amount are used for the dissolution capacity calculation (Km). Based on the Km value and the total amount of each solution the maximal amount of concrete to be corroded Cc can be calculated.

Tab. 7.2 Corrosion solutions produced by the reactions between solutions and solid phases in shaft

Group	Layers	Solutions			
		z3OSM	z3BK/BD	z3OSO	z2/z3 Grenze
Group 1	standard concrete	M1	D1	O1	E1
	salt concrete	M4	D4	O4	E4
	sorel concrete	M6	D6	O6	E6
Group 2	Bentonite	M3	D3	O3	E3
	salt concrete	M4B	D4B	O4B	E4B

7.3 Simulation results

In this section the corrosion properties of each solution collected in shafts are investigated. Such solutions are most likely to occur in the shaft. Bentonite is also considered in the analysis owing to the exchangeable Mg^{2+} embedded in bentonite.

7.3.1 Ionic exchange with bentonite

The geochemical simulations of Group 2 step 1 were undertaken for equilibrium ionic exchange with PhreeqC. The resulted solutions are listed in Tab. 7.3. It is clear to see that bentonite acts as buffer for Mg^{2+} concentration in the solutions. The Mg^{2+} concentration in solution z3BK/BD decreased from 4.455 mol/kg H_2O to 3.459 mol/kg H_2O, while the Mg^{2+} concentration of other three solutions increased. Details of all ionic exchange calculations are described individually in the following subsections.

Tab. 7.3 The calculated chemical composition values of the four shaft solutions after equilibrium with Ca-bentonite in [mol/kg H_2O]

Solution	Na^+	K^+	Mg^{2+}	Ca^{2+}	Cl^-	SO_4^{2-}	Density [g/cm^3]	pH
M3 (z3OSM + bentonite)	2.946	$2.75 \cdot 10^{-05}$	0.5373	1.047	6.000	0.05727	1.211	6.14
D3 (z3BK/BD + bentonite)	0.3107	$2.87 \cdot 10^{-04}$	3.459	1.169	9.384	0.09125	1.301	6.99
O3 (z3OSO + bentonite)	2.362	$6.86 \cdot 10^{-05}$	0.7383	1.064	5.897	0.03515	1.206	6.48
E3 (z2/z3Grenze + bentonite)	2.552	$5.62 \cdot 10^{-05}$	0.6459	1.064	5.874	0.0494	1.207	6.36

7.3.1.1 Case M3 (z3OSM +bentonite)

The solution of z3OSM flows through the compacted bentonite. Through ionic exchange, Mg^{2+} and Ca^{2+} in bentonite are released from the calcigel and Na^+ in the z3OSM solution is partially absorbed. The calculation was conducted with PHREEQC. The important ionic exchange equations and log_k values are the same as described in section 5.1.3. The amount of exchangeable ions in the calcigel was:

```
EXCHANGE 1
        #equilibrate 1
NaX   0.111379104  #mol of exchange species/kg H2O
KX    0.01263916
MgX2  0.693025539
CaX2  1.163292869
```

For the simulation, the following conditions were applied:

1. Solution: z3OSM as the following

   ```
   SOLUTION 0  #z3OSM solution
   units           mol/kgw
   ```

```
temp            25.0
pH              6.9
pe              4.0
Na       5.637564589
K        0.088490365
Ca       0.049953913
Mg       0.144518004
Cl       6.000457506
S(6)     0.057270642
```

2. Solid phase: Calcigel

3. Temperature: 25 °C

4. Pressure: 1 atm

5. Database: phreeqc_NAGRA_PSI.dat

6. Input files for PHREEQC calculation: M3

7. Output or result file of PHREEQC: M3.out

The results of the simulated solution M3 were:

```
------------------------Exchange composition-------------------

X               3.836e+000 mol

                                 Equiv-    Equivalent      Log
Species              Moles       alents      Fraction     Gamma

NaX              2.803e+000  2.803e+000  7.307e-001     0.000
MgX2             3.003e-001  6.005e-001  1.565e-001     0.000
CaX2             1.659e-001  3.318e-001  8.648e-002     0.000
KX               1.008e-001  1.008e-001  2.628e-002     0.000
HX               4.670e-006  4.670e-006  1.217e-006     0.000

------------------------Solution composition-------------------

Elements            Molality       Moles

Ca               1.047e+000  1.047e+000
Cl               6.000e+000  6.000e+000
K                2.752e-005  2.752e-005
Mg               5.373e-001  5.373e-001
Na               2.946e+000  2.946e+000
S                5.727e-002  5.727e-002
 pH  =   6.142
```

The elemental compositions of M3 are listed in Tab. 7.3. The concentration of Ca in the solution increases from 0.050 M to 1.05 M; the concentration of Mg changes from 0.144 M to 0.537 M respectively, while that of Na decreases from 5.64 M to 2.95 M.

7.3.1.2 Case D3 (z3BK/BD +bentonite)

The solution of z3BK/BD flows through the compacted bentonite. Through ionic exchange, Mg^{2+} and Ca^{2+} in bentonite are released from the calcigel and Na^{+} in the z3OSM solution is partially absorbed. The calculation was conducted with PHREEQC. The important ionic exchange equations and log_k values are the same as described in section 5.1.3. The amount of exchangeable ions in the calcigel was:

```
EXCHANGE 1
        #equilibrate 1
NaX   0.11231221  #mol of exchange species/kg H2O
KX    0.012479134
MgX2  0.69883153
CaX2  1.17303864
```

For the simulation, the following conditions were applied:

1. Solution: z3BK/BD as the following

```
SOLUTION 0  #z3OSM solution
units           mol/kgw
temp            25.0
pH              6.9
pe              4.0
Na      5.637564589
K       0.088490365
Ca      0.049953913
Mg      0.144518004
Cl      6.000457506
S(6)    0.057270642
```

2. Solid phase: Calcigel
3. Temperature: 25 °C
4. Pressure: 1 atm
5. Database: phreeqc_NAGRA_PSI.dat
6. Input files for PHREEQC calculation: D3
7. Output or result file of PHREEQC: D3.out

The results of the simulated solution D3 were:

```
-----------------Exchange composition------------------------
X               3.869e+000 mol

                               Equiv-    Equivalent      Log
Species              Moles      alents      Fraction     Gamma

MgX2              1.695e+000  3.390e+000  8.764e-001    -0.000
KX                2.296e-001  2.296e-001  5.934e-002    -0.000
NaX               1.351e-001  1.351e-001  3.493e-002    -0.000
CaX2              5.672e-002  1.134e-001  2.932e-002    -0.000
HX                1.325e-007  1.325e-007  3.425e-008    -0.000

------------------Solution composition-----------------------

Elements            Molality       Moles

Ca                1.169e+000  1.169e+000
Cl                9.384e+000  9.384e+000
K                 2.869e-004  2.869e-004
Mg                3.459e+000  3.459e+000
Na                3.107e-001  3.107e-001
S                 9.125e-002  9.125e-002
 pH  =   6.985
```

The elemental compositions of D3 are listed in Tab. 7.3. The concentration of Ca in the solution increases from 0.053 M to 1.17 M; the concentration of Mg decreases significantly from 4.456 M to 3.459 M, which buffers its corrosion capacity against Portland cement. However, this concentration remains relatively high, which will still be very corrosive to salt concrete.

7.3.1.3 Case O3 (z3OSO +bentonite)

The solution of z3OSO flows through the compacted bentonite. Through ionic exchange, Mg^{2+} and Ca^{2+} in bentonite are released from the calcigel and Na^{+} in the z3OSO solution is partially absorbed. The calculation was conducted with PHREEQC. The important ionic exchange equations and log_k values are the same as described in section 5.1.3. The amount of exchangeable ions in the calcigel was:

```
EXCHANGE 1
        #equilibrate 1
NaX   0.111379104  #mol of exchange species/kg H2O
KX    0.01263916
MgX2  0.693025539
CaX2  1.163292869
```

For the simulation, the following conditions were applied:

1. Solution: z3OSO as the following

   ```
   SOLUTION 0  #z3OSM solution
   units       mol/kgw
   temp        25.0
   pH          6.9
   pe          4.0
   Na      4.542998816
   K       0.240341918
   Ca      0.088809947
   Mg      0.503256365
   Cl      5.897165483
   S(6)    0.035153937
   ```

2. Solid phase: Calcigel
3. Temperature: 25 °C
4. Pressure: 1 atm
5. Database: phreeqc_NAGRA_PSI.dat
6. Input files for PHREEQC calculation: O3
7. Output or result file of PHREEQC: O3.out

The results of the simulated solution O3 were:

```
---------------------Exchange composition-----------------------

X               3.804e+000 mol

                               Equiv-    Equivalent      Log
Species              Moles     alents      Fraction     Gamma

NaX              2.291e+000  2.291e+000  6.023e-001     0.000
MgX2             4.522e-001  9.044e-001  2.377e-001     0.000
KX               2.525e-001  2.525e-001  6.639e-002     0.000
CaX2             1.780e-001  3.560e-001  9.358e-002     0.000
HX               2.169e-006  2.169e-006  5.703e-007     0.000

------------------Solution composition---------------------

Elements           Molality       Moles

Ca               1.064e+000  1.064e+000
Cl               5.897e+000  5.897e+000
K                6.855e-005  6.855e-005
Mg               7.383e-001  7.383e-001
Na               2.362e+000  2.362e+000
S                3.515e-002  3.515e-002
 pH  =   6.476
```

The elemental compositions of O3 are listed in Tab. 7.3. The concentration of Ca in the solution increases from 0.089 M to 1.06 M; the concentration of Mg changes from 0.503 M to 0.738 M respectively, while that of Na decreases from 4.54 M to 2.36 M.

7.3.1.4 Case E3 (z2/z3Grenze +bentonite)

The solution of z2/z3Grenze flows through the compacted bentonite. Through ionic exchange, Mg^{2+} and Ca^{2+} in bentonite are released from the calcigel and Na^{+} in the z2/z3Grenze solution is partially absorbed. The calculation was conducted with PHREEQC. The important ionic exchange equations and log_k values are the same as described in section 5.1.3. The amount of exchangeable ions in the calcigel was:

```
EXCHANGE 1
        #equilibrate 1
NaX   0.110833453  #mol of exchange species/kg H2O
KX    0.012314828
MgX2  0.689630372
CaX2  1.157593839
```

For the simulation, the following conditions were applied:

1. Solution: z2/z3Grenze as the following

   ```
   SOLUTION 0  #z3OSM solution
   units       mol/kgw
   temp        25.0
   pH          6.9
   pe          4.0
   Na      4.927286856
   K       0.198712256
   Ca      0.084369449
   Mg      0.339142984
   Cl      5.874222913
   S(6)    0.049400533
   ```

2. Solid phase: Calcigel
3. Temperature: 25 °C
4. Pressure: 1 atm
5. Database: phreeqc_NAGRA_PSI.dat
6. Input files for PHREEQC calculation: E3
7. Output or result file of PHREEQC: E3.out

The results of the simulated solution E3 were:

```
-----------------Exchange composition--------------------------

X               3.818e+000 mol

                                Equiv-    Equivalent      Log
Species               Moles     alents      Fraction     Gamma

NaX              2.486e+000  2.486e+000  6.512e-001     0.000
MgX2             3.829e-001  7.657e-001  2.006e-001     0.000
KX               2.110e-001  2.110e-001  5.526e-002     0.000
CaX2             1.775e-001  3.550e-001  9.300e-002     0.000
HX               2.864e-006  2.864e-006  7.501e-007     0.000

------------------Solution composition--------------------------

Elements           Molality       Moles

Ca               1.064e+000  1.064e+000
Cl               5.874e+000  5.874e+000
K                5.624e-005  5.624e-005
Mg               6.459e-001  6.459e-001
Na               2.552e+000  2.552e+000
S                4.940e-002  4.940e-002
 pH  =   6.364
```

The elemental compositions of E3 are listed in Tab. 7.3. The concentration of Ca in the solution increases from 0.084 M to 1.06 M; the concentration of Mg changes from 0.339 M to 0.646 M respectively, while that of Na decreases from 4.92 M to 2.55 M.

7.3.1.5 Discussion

In the calculations mentioned in this section, the solid-liquid ratio is assumed to a ratio for saturated bentonite. This is to say, the equilibrium ionic exchange occurs exactly between the liquid amount VL including one kg H_2O and the amount of bentonite Mb (dry density 1650 kg/m^3) including the pore volume that can hold the VL solution. The amount of exchangeable ions for the calculation refers to the total amount of exchangeable ions within the Mb bentonite. The simulated results showed that Na+ concentration of all solutions decreases and Ca^{2+} concentration increases. Three of the solutions showed an increase of Mg^{2+} concentration, while one solution with significantly high Mg^{2+} concentration decreases. This means that three solutions are more corrosive to salt concrete through the ionic exchange with bentonite.

Considering the limited amount of the four solutions in comparison with the large quantity of bentonite, only a small fraction of bentonite can be included. Consequently, the concrete corrosion capacity of the resulting solution might vary accordingly.

7.3.2 Concrete corrosion by z3OSM serial

The calculations of concrete corrosion by z3OSM serial include three batch reactions M1 (solution z3OSM + standard concrete), M4 (solution z3OSM + salt concrete) and M6 (solution z3OSM + sorel concrete), and M4B (M4B + standard concrete). The geochemical simulations calculate the dissolution capacity Km of a solution to concretes, followed by the potential amount of concrete to be corroded. Simulated results are listed in Tab. 7.4 and Tab. 7.5.

Tab. 7.4 The total elemental concentrations of the corrosion solutions for the z2OSM serial

No	Ca	Cl	K	Mg	Na	S	Si	Density [g/cm^3]	pCH
M1	0.146	5.940	0.091	$1.93 \cdot 10^{-06}$	5.584	0.010	$2.98 \cdot 10^{-06}$	1.195	12.30
M4	0.142	6.171	0.092	$2.46 \cdot 10^{-06}$	5.822	0.013	$3.25 \cdot 10^{-05}$	1.202	11.23
M6	0.037	6.184	0.085	$5.19 \cdot 10^{-01}$	5.091	0.051	-	1.205	9.33
M4B	1.377	6.535	0.014	$2.01 \cdot 10^{-05}$	3.771	0.002	$8.14 \cdot 10^{-06}$	1.223	10.76

Tab. 7.5 Dissolution capacity of solutions to concretes for the z2OSM serial

No	m_c [kg/kg H_2O]	m_L [kg/kg H_2O]	Km [kg/kg]	ρ_L [kg/m^3]	V [m^3]	Solution [kg]	Cc [kg]
M1	0.1798	1.3631	0.1319	1207	146.502	1.77e5	2.33e4
M4	0.1684	1.3535	0.1244	1207	146.502	1.77e5	2.20e4
M6	0.5000	1.4393	0.3474	1207	146.502	1.77e5	6.14e4
M4B	0.5500	1.3947	0.3943	1207	146.502	1.77e5	6.97e4

m_c – mass of concrete, m_L – mass of solution, Km – dissolution capacity, ρ_L – density of solution, V – total amount of solution, Solution – total amount of solution in kg, Cc – corroded amount of concrete by encountered volume of solution

The simulated results showed that the z2OSM solution is relatively corrosive to sorel concrete owing to its low Mg^{2+} concentration in 0.145 mol/kg H_2O. The total amount of 146.5 m^3 z2OSM solution has the potential to corrode 64.4 tons sorel concrete. This solution is less corrosive to standard concrete and salt concrete with the potential of 23 tons and 22 tons respectively. However, if the solution is in equilibrium with Ca-bentonite it turns to be more corrosive to salt concrete. The 146.5 m^3 z2OSM solution has the potential to corrode nearly 70 tons salt concrete.

7.3.3 Concrete corrosion by z3BK/BD serial

The calculations of concrete corrosion by z3BK/BD serial include three batch reactions D1 (solution z3BK/BD + standard concrete), D4 (solution z3BK/BD + salt concrete) and D6 (solution z3BK/BD + sorel concrete), and D4B (D4B + standard concrete). The geochemical simulations calculate the dissolution capacity Km of a solution to concretes, followed by the potential amount of concrete to be corroded. Simulated results are listed in Tab. 7.6 and Tab. 7.7.

Tab. 7.6 The total elemental concentrations of the corrosion solutions for the z3BK/BD serial

No	Ca	Cl	K	Mg	Na	S	Si	Density [g/cm^3]	pCH
D1	2.6012	5.6404	0.2075	$1.80\cdot10^{-05}$	0.2703	$1.80\cdot10^{-03}$	$4.48\cdot10^{-07}$	1.2138	11.63
D4	2.9552	7.8019	0.3014	$3.46\cdot10^{-05}$	1.5929	$7.64\cdot10^{-04}$	$3.43\cdot10^{-06}$	1.2728	10.71
D6	0.0062	9.3945	0.2174	4.46	0.3436	$4.50\cdot10^{-02}$	0.00	1.2872	8.69
D4B	3.3670	8.0535	0.0856	$3.72\cdot10^{-05}$	1.2383	$5.93\cdot10^{-04}$	$2.72\cdot10^{-06}$	1.2826	10.71

Tab. 7.7 Dissolution capacity of solutions to concretes for the z3BK/BD serial

No	m_c [kg/kg H_2O]	m_L [kg/kg H_2O]	Km [kg/kg]	ρ_L [kg/m^3]	V [m^3]	Solution [kg]	Cc [kg]
D1	4.94	1.9655	2.515	1306	0.0528	68.96	173.43
D4	4.60	1.6203	2.839	1306	0.0528	68.96	195.77
D6	$9.57\cdot10^{-4}$	1.4626	$6.54\cdot10^{-}4$	1306	0.0528	68.96	0.045
D4B	3.55	1.5907	2.2358	1306	0.0528	68.96	154.17

m_c – mass of concrete, m_L – mass of solution, Km – dissolution capacity, ρ_L – density of solution, V – total amount of solution, Solution – total amount of solution in kg, Cc – corroded amount of concrete by encountered volume of solution

The simulated results showed that the z3BK/BD solution is very corrosive to normal and salt concretes (Normal- and salt concrete) owing to its high Mg^{2+} concentration in 4.455 mol/kg H_2O. The dissolution capacities Km to standard concrete or salt concrete are 2.5 or 2.8 kg/kg. Fortunately such solution occurs only in very small amount

(52.8 liter). The total amount of 0.0528 m^3 z3BK/BD solution has the potential to corrode less than 200 kg Normal- or salt concrete. This solution is non-corrosive to sorel concrete. If the solution is in equilibrium with Ca-bentonite, the Mg^{2+} concentration decreases. Consequently it turns to be less corrosive to salt concrete. The 0.0528 m^3 z3BK/BD solution has the potential to corrode 154 kg salt concrete.

7.3.4 Concrete corrosion by z3OSO serial

The calculations of concrete corrosion by z3OSO serial include three batch reactions O1 (solution z3OSO + standard concrete), O4 (solution z3OSO + salt concrete) and O6 (solution z3OSO + sorel concrete), and O4B (O4B + standard concrete). The geochemical simulations calculate the dissolution capacity Km of a solution to concretes, followed by the potential amount of concrete to be corroded. Simulated results are listed in Tab. 7.8 and Tab. 7.9.

Tab. 7.8 The total elemental concentrations of the corrosion solutions for the z3OSO serial

No	Ca	Cl	K	Mg	Na	S	Si	Density [g/cm^3]	pCH
O1	0.4926	5.5483	0.2390	$4.37\cdot10^{-06}$	4.3390	$3.88\cdot10^{-03}$	$1.46\cdot10^{-06}$	1.1884	11.98
O4	0.4275	6.3351	0.2510	$6.79\cdot10^{-06}$	5.2400	$5.14\cdot10^{-03}$	$1.78\cdot10^{-05}$	1.2091	11.00
O6	0.0782	6.2268	0.2398	$5.20\cdot10^{-01}$	4.8424	$2.52\cdot10^{-02}$		1.2045	9.33
O4B	1.5564	6.6194	0.0196	$2.23\cdot10^{-05}$	3.4909	$1.82\cdot10^{-03}$	$7.35\cdot10^{-06}$	1.2276	10.74

Tab. 7.9 Dissolution capacity of solutions to concretes for the z3OSO serial

No	m_c [kg/kg H_2O]	m_L [kg/kg H_2O]	Km [kg/kg]	ρ_L [kg/m^3]	V [m^3]	Solution [kg]	Cc [kg]
O1	0.5591	1.3908	0.4020	1203	84.655	1.02e5	4.09e4
O4	0.5390	1.3913	0.3874	1203	84.655	1.02e5	3.95e4
O6	0.0295	1.3632	0.0217	1203	84.655	1.02e5	2.21e3
O4B	0.7579	1.4063	0.5389	1203	84.655	1.02e5	5.49e4

m_c – mass of concrete, m_L – mass of solution, Km – dissolution capacity, ρ_L – density of solution, V – total amount of solution, Solution – total amount of solution in kg, Cc – corroded amount of concrete by encountered volume of solution

The simulated results showed that the z2OSO solution is minor corrosive to sorel concrete owing to its Mg^{2+} concentration in 0.5 mol/kg H_2O. The total amount of 84.7 m^3

z2OSM solution has the potential to corrode 2.2 tons sorel concrete. However this solution is more corrosive to standard concrete and salt concrete with the potential of about 40 tons. If the solution is in equilibrium with Ca-bentonite it turns to be slightly more corrosive to salt concrete. The 84.7 m^3 z2OSO solution has the potential to corrode nearly 55 tons salt concrete.

7.3.5 Concrete corrosion by z2/z3Grenze serial

The calculations of concrete corrosion by z2/z3Grenze serial include three batch reactions E1 (solution z2/z3Grenze + standard concrete), E4 (solution z2/z3Grenze + salt concrete) and E6 (solution z2/z3Grenze + sorel concrete), and E4B (E4B + standard concrete). The geochemical simulations calculate the dissolution capacity Km of a solution to concretes, followed by the potential amount of concrete to be corroded. Simulated results are listed in Tab. 7.10 and Tab. 7.11.

Tab. 7.10 The total elemental concentrations of the corrosion solutions for the z2/z3Grenze serial

No	Ca	Cl	K	Mg	Na	S	Si	Density [g/cm^3]	pCH
E1	0.3474	5.6676	0.1997	$3.39\cdot10^{-06}$	4.7891	0.0047587	$1.77\cdot10^{-06}$	1.1901	12.07
E4	0.3252	6.2822	0.2042	$4.69\cdot10^{-03}$	5.4312	0.00648257	$3.47\cdot10^{-08}$	1.2065	10.26
E6	0.0615	6.2672	0.1943	$5.07\cdot10^{-01}$	4.9987	0.0309029	-	1.2057	9.34
E4B	1.4775	6.5815	0.0172	$2.13\cdot10^{-05}$	3.6130	0.00190926	$7.69\cdot10^{-06}$	1.2257	10.75

Tab. 7.11 Dissolution capacity of solutions to concretes for the z2/z3Grenze serial

No	m_c [kg/kg H_2O]	m_L [kg/kg H_2O]	Km [kg/kg]	ρ_L [kg/m^3]	V [m^3]	Solution [kg]	Cc [kg]
E1	0.3779	1.3732	0.2752	1202	0.045	54.09	14.89
E4	0.2871	1.3808	0.2079	1202	0.045	54.09	11.25
E6	0.2300	1.3986	0.1645	1202	0.045	54.09	8.90
E4B	0.6648	1.4010	0.4745	1202	0.045	54.09	25.67

m_c – mass of concrete, m_L – mass of solution, Km – dissolution capacity, ρ_L – density of solution, V – total amount of solution, Solution – total amount of solution in kg, Cc – corroded amount of concrete by encountered volume of solution

The simulated results showed that the z2/z3Grenze solution is corrosive to sorel concrete with Km in 0.16 kg/kg owing to its low Mg^{2+} concentration in 0.339 mol/kg H_2O.

The tiny amount of 0.045 m^3 z2/z3Grenze solution has the potential to corrode 8.9 kg sorel concrete. This solution is slightly more corrosive to standard concrete and salt concrete with Km in 0.28 and 0.20 kg/kg respectively. The tiny amount of 0.045 m^3 z2/z3Grenze solution has the corrosion potential of 15 kg standard concrete or 11 kg salt concrete respectively. However, if the solution is in equilibrium with Ca-bentonite it turns to be more corrosive to salt concrete. The potential amount of salt concrete to be corroded can be doubled.

7.3.6 Discussion

The geochemical simulations have revealed that concrete corrosion depends largely on the concrete type and the Mg^{2+} concentration of the solution. Generally the concrete types investigated in this work can be divided into two groups – Portland cement based concretes (i.e. standard concrete and salt concrete) and magnesium binder based concrete. The first group showed a positive correlation of Km and the Mg^{2+} concentration (Fig. 7.1). The sorel concrete revealed a negative correlation of Km and the Mg^{2+} concentration if [Mg^{2+}] < 0.51 mol/kg H_2O. When the Mg^{2+} concentration of a solution is higher than 0.51 mol/kg H_2O, it is non-corrosive to sorel concrete anymore (Fig. 7.2).

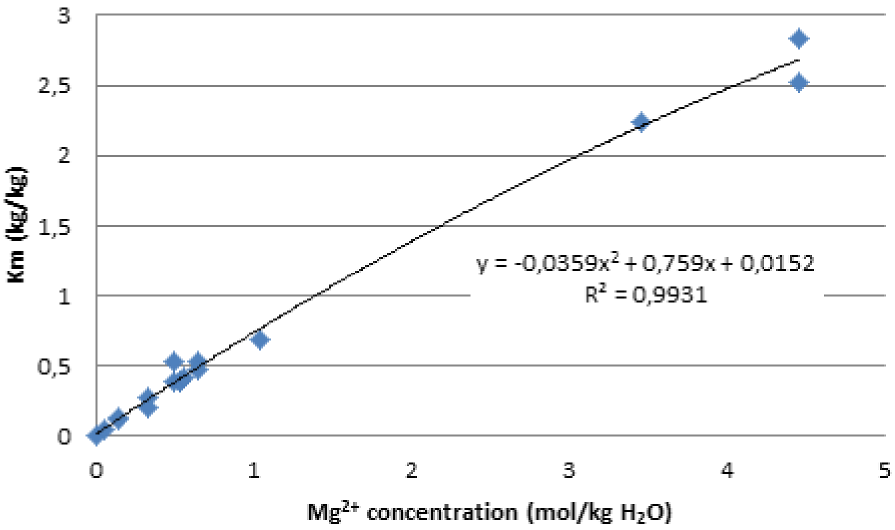

Fig. 7.1 The Mg^{2+} concentration of a solution and its dissolution capacity Km to normal and salt concrete

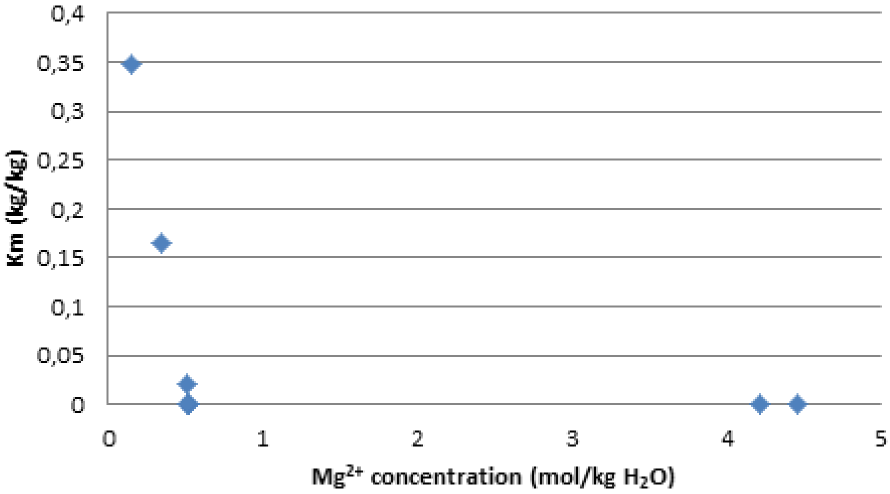

Fig. 7.2 The Mg^{2+} concentration of solutions and their dissolution capacity values Km to sorel concrete

All the calculations are based on specific assumptions e. g. equilibrium geochemical reactions, model phases in cements, ionic exchange only in bentonite and on conservative scenarios. More realistic evaluations can only be made by using the reactive transport approach with well-defined initial and boundary conditions together with realistic scenarios.

8 Geochemical simulation for sorel concrete protection by adding bischofite product

To protect the sorel concrete from salt solution with low Mg concentration, 19000 tons of technical Bischofite product (Appendix I) as magnesium donator is to be implemented in the pore space (41800 m^3) of the filling material at the infrastructure exploration level (Wiederlager plus Erkundungssohle in Fig. 2.1), so that the Mg^{2+} concentration of the solution reached there (through either the salt concrete above it or the contact zone of shaft and host rock) can be increased to a level higher than the minimal value in 0.5 M – noncorrosive against the sorel concrete by penetrating the filling material. Further more, the pore space in the infrastructure area of the storage sole (Einlagerungssohle in Fig. 2.1) might be filled with solution in the long term. The total pore volume of the filling material at both levels amounts 87,400 m^3. Concerning the concentration of magnesium in the solution, there is a dilution effect. To ensure the functionality of the sorel concrete adjacent to the infrastructure area, the maximal amount of solution is 87,400 m^3.

8.1 Materials and solutions

The materials used for the geochemical simulations are Bischofite product (section 2.2.1, Tab. 2.8), saturated NaCl-solution, R4-solution (Fig. 2.1 and Tab. 5.5 in section 5.1). R4-solution is generated through the corrosion of concrete by the rain water, which is the worst case concerning the magnesium concentration. The chemical composition of the saturated NaCl-solution was calculated with EQ3/6 and the same database mentioned in section 3. The concentrations of Na^+ and Cl^- are 6.105 mol/kg H_2O, pH 6.96 (Tab. 8.1).

Tab. 8.1 Chemical compositions of liquids used in the geochemical modeling

Composition	**Concentration [mol/kg H_2O]**		
	NaCl-solution	**R4**	**B4 (R4/NaCl-mixture)**
Na^+	6.105	5.29	5.70
K^+	n.e.	$1.07 \cdot 10^{-01}$	$5.34 \cdot 10^{-02}$
Ca^{++}	n.e.	$4.38 \cdot 10^{-01}$	$2.18 \cdot 10^{-01}$
Mg^{++}	n.e.	$1.58 \cdot 10^{-06}$	$1.07 \cdot 10^{-06}$
Cl^-	6.105	6.26	6.18
SO_4^{--}	n.e.	$5.04 \cdot 10^{-03}$	$2.51 \cdot 10^{-03}$
SiO_2(aq)	n.e.	$6.83 \cdot 10^{-09}$	$6.61 \cdot 10^{-09}$
Al^{+++}	n.e.	$8.02 \cdot 10^{-32}$	$2.56 \cdot 10^{-31}$
HCO_3^-	n.e.	$6.14 \cdot 10^{-10}$	$1.16 \cdot 10^{-09}$
pH	6.96	12.09	11.89
Amount [m^3]	**45600**	**41800**	**87400**

n.e. – not existing

8.2 Geochemical simulations

The geochemical calculations are undertaken with EQ3/6.

The simulations are undertaken as the following:

1. Take 41800 m^3 R4-solution and mixing with (87400 - 41800) = 45600 m^3 NaCl-solution, which is named here B4 solution (Tab. 8.1);
2. Calculate the geochemical reaction of all B4 with 19000 ton bischofite, the resulted solution is named B5;
3. The chemical composition of B5 is given in Tab. 8.2.

It is generally recognized that saline solution rich in Mg^{2+} is not corrosive to sorel concrete. The minimum concentration of Mg^{2+} for a solution to be non-corrosive to sorel concrete is about 0.5 mol/kg H_2O at 25°C and 1 atm. It is clear to see that the concentration of Mg^{2+} in B5 is 0.98 mol/kg H_2O, which is much higher than the minimum Mg^{2+} concentration 0.5 mol/kg H_2O. Therefore the 19000 ton bischofite is enough for the protection of sorel concrete from geochemical corrosion.

Tab. 8.2 The chemical composition of B5

Species	**Concentration [mol/kg H_2O]**	**Species**	**Concentration [mol/kg H_2O]**
Cl^-	6.36	SiO_2(aq)	$9.29\cdot10^{-09}$
Na^+	4.02	HCO_3^-	$1.04\cdot10^{-07}$
Ca^{++}	$1.68\cdot10^{-01}$	$Al(OH)_4^-$	$1.45\cdot10^{-10}$
K^+	$5.14\cdot10^{-02}$	$MgCO_3$(aq)	$1.02\cdot10^{-06}$
OH-	$8.27\cdot10^{-06}$	H^+	$7.42\cdot10^{-10}$
SO_4*	$6.65\cdot10^{-03}$	$Al(OH)_3$	$8.29\cdot10^{-11}$
$CaCO_3$(aq)	$1.60\cdot10^{-07}$	HSO_4^-	$3.69\cdot10^{-11}$
Mg^{++}	$9.80\cdot10^{-01}$	CO_2(aq)	$1.41\cdot10^{-10}$
$MgOH^+$	$1.95\cdot10^{-03}$	$Al(OH)_2^+$	$7.36\cdot10^{-13}$
$H3SiO_4^-$	$6.50\cdot10^{-10}$	$Al(OH)^{++}$	$4.91\cdot10^{-15}$
CO_3^{--}	$9.54\cdot10^{-08}$	Al^{+++}	$2.08\cdot10^{-20}$
$H_2SiO_4^{--}$	$7.84\cdot10^{-13}$		

9 Discussion

The current report deals with geochemical calculations for the evaluation of the long-term stability of the solid materials considered in the shaft sealing system under the framework of VSG. Solid/solution interactions were analyzed by geochemical calculations. The solids considered in this study and the solutions interacting with these solids are illustrated in Fig. 2.1 and Fig. 2.2.

With respect to solutions rain water (RW) and Gipshut-solution (GH) were considered. RW and GH are of special interest because they are present in high amounts in the immediate neighborhood of the shaft. Any ratio of mixture of both solutions should have the corrosion potential within the range of both solutions alone. Accordingly, no mixtures of these two solutions were considered. One of the critical situations is the rain water infiltration into the shaft, because rain water has a very low ion strength and possesses a large dissolution potential in contact with rock salt. The simulated results showed that RW was not corrosive to the standard concrete, but it can dissolve rather high amounts of rock salt and lead to a rapid increase of ionic strength. As large amounts of rock salt are available above the bentonite sealing element RW becomes NaCl-saturated. Consequently, increasing porosity and permeability of salt aggregates in sealing materials was not considered in the current simulations. GH is NaCl-saturated, naturally.

The other solutions used in the calculations have a higher corrosion potential to individual sealing materials but they occur in very small amounts. Therefore these solutions have a very low impact on the chemical stability of the considered materials.

The analyzed cases are systematic and cover a wide range of potential scenarios. We think that the calculated cases cover the reasonable scenarios and thus the possible evolution of the shaft sealing system. However, no guarantee for absolute completeness can be given as there are many factors that might influence the mineralogical and geochemical stability of materials in the sealing system.

In the calculations the temperature was assumed to be 25 °C. According to the current estimation, the temperature at different positions in the lower part of the shaft is higher than 25 °C. After the closure of the shaft, the temperature at the compacted bentonite level will increase from 300 to 308 K (or 26.8 to 34.8 °C); While that at the salt concrete from 307 to 319 K (or 33.8 to 45.8 °C); And that at the sorel concrete level from 311 to

324 K (or 37.8 to 50.8 °C). This indicates that the temperature are well below 60 °C, which should have limited influence on the results of the calculated geochemical reactions /HER 2002/, /KAU 2009/, /KAU 2010/ and /KAU 2011/.

Bentonite is a natural clay rock containing clay minerals which arequite stable under normal thermodynamic and geochemical conditions. However, its long-term stability under special conditions (e. g. contact with highly saline solutions and/or elevated temperatures) is still under investigation. Experimental studies of MX-80 bentonite in saturated pure NaCl-solution and IP21 solution at 25 °C, 50 °C and 150 °C by Herbert et al. /HER 2002/ observed montmorillonite alteration after about 50 days at higher temperatures. Kaufhold and Dohrmann studied the alteration processes for different kinds of bentonite in pure NaCl-solution /KAU 2009/, in pure KCl-solution /KAU 2010/, and in $Ca(OH)_2$ solution /KAU 2011/. No alteration of bentonite was observed in NaCl-solution at 60 °C and moderate pH. But limited smectite dissolution and illite precipitation was determined for bentonite in KCl-solution. However, bentonite is surprisingly resistant against $Ca(OH)_2$ solutions at pH around 12 and up to 90 °C. Above this temperature and at larger pH values dissolution is expected to be much faster /KAU 2011/. Based on the present state of knowledge we assume that our calculations at 25 °C regarding ion exchange in the bentonite are relevant and representative for the temperatures occurring in the shaft, because of the low amount of Mg^{2+} in the crystal structure of the minerals.

The interaction of cement based concrete pore fluids with bentonite was also widely studied /SAV 2007/, /SAV 2011/. Savage et al. in the thorough review papers pointed out that calcium (aluminum) silicate hydrates (C(A)SH), zeolites, feldspars, hydroxides,carbonates, polymorphs of silica, and some sheet silicates (all of varying degrees of crystallinity) are potential products of cement–bentonite interaction on time scales of interest to safety assessment of the geological disposal of radioactive wastes. “The relatively more siliceous zeolites (clinoptilolite, phillipsite) are likely to form at lower pH (distal regions of migrating cement pore fluids), whereas C(A)SH, illite, feldspars, and the more aluminous zeolites (analcime, heulandite) are more likely to format higher pH and hence, the more proximal regions of migrating cement pore fluids” /SAV 2007/. Natural analogue studies revealed that zeolite and K-feldspar can be formed of natural clay minerals under alkaline conditions /SAV 2011/. In the same work the author emphasized the lack of accurate thermodynamic data and related numerical prediction should be undertaken with caution.

The geochemical calculations provide no information of the reaction progress in time and space (exact location of the solution and corrosion front at different times). Such information would be extremely valuable but they cannot be achieved at the time being with the available modeling tools. This is one of the identified important gaps regarding the understanding of the long term corrosion behaviors of cemented materials.

10 Conclusions

The long term stability assessment of the sealing materials bentonite, salt concrete and sorel concrete is important for the engineering design of the shaft sealing system and for the long term safety assessment of the potential Gorleben repository. The assessment of the long term stability has been done by employing geochemical calculations with satisfactory results. However there are some shortcomings of this study which should be mentioned. At the time being it is not possible to provide a really accurate assessment owing to several factors such as: variations in scenario definition and in the chemical composition of materials to be used, partial lack of thermodynamic data for geochemical simulation valid for highly saline solutions and at elevated temperature, reliable tools for the complex natural reactive transport process simulation etc. Therefore, several simplified but representative cases of geochemical simulations were defined, which are considered to be covering for the understanding of the geochemical reaction principles under different geochemical conditions.

Calcigel as natural Ca-bentonite showed favorite properties as potential HLW sealing material. It is supposed to be applied as the first sealing layer in the shaft. If solution in the upper shaft seeps downwards through the calcigel, this solution may reach the second shaft sealing element – the salt concrete. Salt concrete is sensitive to the Mg^{2+} concentration of the solution. As there is a large fraction of Mg^{2+} on the surface, calcigel can act as Mg^{2+} donator for the penetrating solution. Mg^{2+} can be released mainly through ionic exchange into the solution. Therefore, only the ionic exchange process was simulated using PHREEQC together with NAGRA-PSI database in the calculations. Simulation results showed an increase of Mg^{2+} in the solutions after penetrating the calcigel and revealed a potential risk for salt concrete.

Salt concrete showed fairly stable properties under normal geochemical conditions. The critical geochemical condition is the concentration and amount of Mg^{2+}, which coincides with the previous findings /HAG 2009/. The higher the Mg^{2+} concentration in an attacking fluid, the higher is the corrosive potential of the solution against salt concrete. The total amount of Mg^{2+} in the solution in contact with salt concrete has been evaluated. This amount is very low. Accordingly the corrosion of salt concrete is considered to be very low too.

Contrary to salt concrete, the minimal concentration (0.5 M) of Mg^{2+} in a solution is essential for the geochemical stability of sorel concrete. By “adding” enough bischofite in the layer between salt concrete and sorel concrete, the solutions were turned to be all non-corrosive against sorel concrete. However, this is a controversial measure, because diffusion process can also transport Mg^{2+} upwards. In a worst case the salt concrete may thus be corroded from the bottom if the layer between the salt concrete and the sorel concrete is getting fully saturated. In a separate study it should be evaluated whether such a scenario may become relevant.

Considering the actually encountered solutions during shaft sinking and their specific chemical composition, the total amount of corroded material was very small and can be neglected.

Assuming a uniform diffusion driven corrosion the relatively small amounts of corroded concrete materials are not significant and can be optimized in the planning of the sealing system.

Acknowledgements

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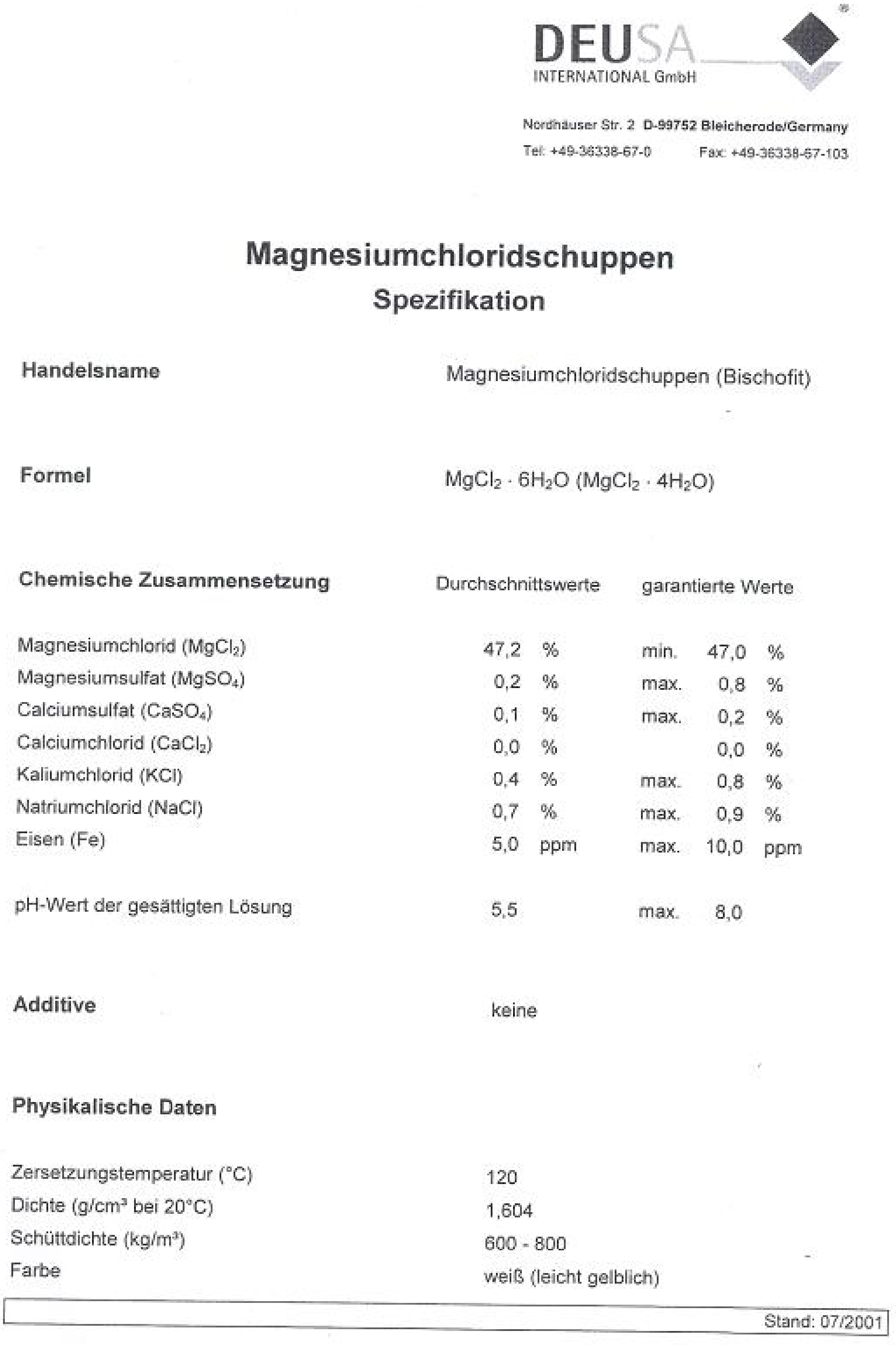
A Appendix

A.1 Appendix 1: Chemical composition of Bischofite



DEUSA
INTERNATIONAL GmbH

Nordhäuser Str. 2 D-99752 Bleicherode/Germany
Tel: +49-36338-67-0 Fax: +49-36338-67-103

Magnesiumchloridschuppen
Spezifikation

Handelsname	Magnesiumchloridschuppen (Bischofit)
Formel	$MgCl_2 \cdot 6H_2O$ ($MgCl_2 \cdot 4H_2O$)

Chemische Zusammensetzung	Durchschnittswerte	garantierte Werte
Magnesiumchlorid ($MgCl_2$)	47,2 %	min. 47,0 %
Magnesiumsulfat ($MgSO_4$)	0,2 %	max. 0,8 %
Calciumsulfat ($CaSO_4$)	0,1 %	max. 0,2 %
Calciumchlorid ($CaCl_2$)	0,0 %	0,0 %
Kaliumchlorid (KCl)	0,4 %	max. 0,8 %
Natriumchlorid (NaCl)	0,7 %	max. 0,9 %
Eisen (Fe)	5,0 ppm	max. 10,0 ppm
pH-Wert der gesättigten Lösung	5,5	max. 8,0

Additive	keine

Physikalische Daten

Zersetzungstemperatur (°C)	120
Dichte (g/cm³ bei 20°C)	1,604
Schüttdichte (kg/m³)	600 - 800
Farbe	weiß (leicht gelblich)

Stand: 07/2001

A.2 Appendix 2: Database for EQ3/6 calculation

```
File Name: data0-V8_extend.bfs

Diese Datenbasis wurde am 22.02.2008 für die Berechnung des
salt concretes M2 für das BfS erstellt .

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,Si, Al, Zementphasen
Daten von EQ3/6 Vers. 7.2c data0.bfs
Reihenfolge der Pitzerkoeffizienten:
HMW
SiO2(aq)
H3SiO4
H2SiO4

+---------------------------------------------------------------
-----
Miscellaneous parameters
+---------------------------------------------------------------
-----
Temperature limits (degC)
        25.0000   25.0000
temperatures
         0.0100   25.0000   60.0000  100.0000
       150.0000  200.0000  250.0000  300.0000
pressures
         1.0132    1.0132    1.0132    1.0132
         4.7572   15.5365   39.7365   85.8378
debye huckel aphi
         0.3791    0.3920    0.4195    0.4602
         0.5261    0.6135    0.7363    0.9345
log k for eh reaction
       -91.0448  -83.1049  -74.0534  -65.8641
       -57.8929  -51.6848  -46.7256  -42.6828
+---------------------------------------------------------------
-----
single-salt parameters
+-------------------------------------------------------------
MgOH+                     SiO2(aq)
  1            0
*
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                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
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*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
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    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
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+------------------------------------------------------------
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                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = Azaroual et al. (1997)
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
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+------------------------------------------------------------
Ca++                       SiO2(aq)
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*
      cphi =  0.00000
    source = Azaroual et al. (1997)
*
*
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    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
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K+                         SiO2(aq)
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```

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      cphi =  0.00000
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*
*
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    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
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*
*
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    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
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+-------------------------------------------------------------
Cl-                       SiO2(aq)
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      cphi =  0.00000
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*
*
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    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
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+-------------------------------------------------------------
SO4--                     SiO2(aq)
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      cphi =  0.00000
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*
*
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    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
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```

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    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
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+--------------------------------------------------------------
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*
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    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
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    source =
+--------------------------------------------------------------
Ca++                      CO2(aq)
  2            0
*
     beta0 =   0.18300   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
```

```
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Ca++                      CO3--
  2            -2
*
     beta0 =   0.00000   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   1.4       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Ca++                      Cl-
  2            -1
*
     beta0 =   0.31590   beta1 =   1.61400   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi = -0.00034
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Ca++                      HCO3-
  2            -1
*
     beta0 =   0.40000   beta1 =   2.97700   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
```

```
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-----------------------------------------------------------------
Ca++                      HSO4-
  2            -1
*
     beta0 =   0.21450   beta1 =   2.53000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-----------------------------------------------------------------
Ca++                      OH-
  2            -1
*
     beta0 =  -0.17470   beta1 =  -0.23030   beta2 =  -5.72000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-----------------------------------------------------------------
Ca++                      SO4--
  2            -2
*
     beta0 =   0.20000   beta1 =   3.19730   beta2 = -54.24000
                         alpha1 =   1.4       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-----------------------------------------------------------------
Ca++                      H3SiO4-
  2            -1
*
     beta0 =   0.21450   beta1 =   2.530000   beta2 = 0
                         alpha1 =   2.0       alpha2 =  12.0
```

```
*
      cphi =  0.00000
    source =  Readon90
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Ca++                      H2SiO4--
  2            -2
*
     beta0 =   0.20000   beta1 =   3.197300   beta2 = -54.24
                         alpha1 =   1.4       alpha2 =  12.0
*
      cphi =  0.00000
    source = Reardon90
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Ca++                      Al(OH)4-
  2            -1
*
     beta0 =   0.21450   beta1 =   2.530000   beta2 = 0
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source =  Readon90
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Cl-                       CO2(aq)
 -1             0
*
     beta0 =  -0.00500   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
```

```
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
H+                       CO2(aq)
  1            0
*
     beta0 =   0.00000   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
H+                       CO3--
  1           -2
*
     beta0 =   0.00000   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
H+                       CaCO3(aq)
  1            0
*
     beta0 =   0.00000   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
H+                       Cl-
  1           -1
*
     beta0 =   0.17750   beta1 =   0.29450   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
```

```
*
      cphi =  0.00080
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
H+                       HCO3-
  1            -1
*
     beta0 =   0.00000   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
H+                       HSO4-
  1            -1
*
     beta0 =   0.20650   beta1 =   0.55560   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
H+                       MgCO3(aq)
  1             0
*
     beta0 =   0.00000   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   0.0       alpha2 =   0.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
```

```
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
H+                        OH-
  1            -1
*
     beta0 =   0.00000   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
H+                        SO4--
  1            -2
*
     beta0 =   0.02980   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.04380
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
H+                        H3SiO4-
  1            -1
*
     beta0 =   0.21060   beta1 =   0.532000   beta2 = 0
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source =  Readon90
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
H+                        H2SiO4--
  1            -2
*
     beta0 =   0.02170   beta1 =   0.000000   beta2 = 0.0000
                         alpha1 =   2.0       alpha2 =  12.0
```

```
*
      cphi =  0.041100
    source = Reardon90
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
H+                        Al(OH)4-
  1            -1
*
     beta0 =   0.21060   beta1 =   0.532000   beta2 = 0
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source =  Readon90
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
HSO4-                     CO2(aq)
 -1             0
*
     beta0 =  -0.00300   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   0.0       alpha2 =   0.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
K+                        CO2(aq)
  1             0
*
     beta0 =   0.05100   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
```

```
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
K+                        CO3--
  1            -2
*
     beta0 =   0.14880   beta1 =   1.43000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi = -0.00150
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
K+                        Cl-
  1            -1
*
     beta0 =   0.04835   beta1 =   0.21220   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi = -0.00084
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
K+                        HCO3-
  1            -1
*
     beta0 =   0.02960   beta1 =  -0.01300   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi = -0.00800
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
K+                        HSO4-
  1            -1
*
     beta0 =  -0.00030   beta1 =   0.17350   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
```

```
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
K+                       OH-
  1            -1
*
     beta0 =   0.12980   beta1 =   0.32000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00410
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
K+                       SO4--
  1            -2
*
     beta0 =   0.04995   beta1 =   0.77930   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
K+                       H3SiO4-
  1            -1
*
     beta0 =   -0.0003   beta1 =   0.173500   beta2 = 0
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source =  Readon90
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
```

```
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
K+                        H2SiO4--
  1            -2
*
     beta0 =   0.04990   beta1 =   0.779300   beta2 = 0.0000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.000000
    source = Reardon90
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
K+                        Al(OH)4-
  1            -1
*
     beta0 =   -0.0003   beta1 =   0.173500   beta2 = 0
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source =  Readon90
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Mg++                      CO2(aq)
  2             0
*
     beta0 =   0.18300   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Mg++                      CO3--
  2            -2
*
     beta0 =   0.00000   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   1.4       alpha2 =  12.0
```

```
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Mg++                      Cl-
  2            -1
*
     beta0 =   0.35235   beta1 =   1.68150   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00519
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Mg++                      HCO3-
  2            -1
*
     beta0 =   0.32900   beta1 =   0.60720   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Mg++                      HSO4-
  2            -1
*
     beta0 =   0.47460   beta1 =   1.72900   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
```

```
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Mg++                      OH-
  2            -1
*
     beta0 =   0.00000   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Mg++                      SO4--
  2            -2
*
     beta0 =   0.22100   beta1 =   3.34300   beta2 = -37.23000
                         alpha1 =   1.4       alpha2 =  12.0
*
      cphi =  0.02500
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Mg++                      H3SiO4-
  2            -1
*
     beta0 =   0.47460   beta1 =   1.729000   beta2 = 0
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source =  Readon90
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Mg++                      H2SiO4--
  2            -2
*
     beta0 =   0.22100   beta1 =   3.343000   beta2 = -37.23
                         alpha1 =   1.4       alpha2 =  12.0
```

```
*
      cphi =  0.02500
    source = Reardon90
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Mg++                         Al(OH)4-
  2            -1
*
     beta0 =   0.47460   beta1 =   1.729000   beta2 = 0
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source =  Readon90
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
MgOH+                        CO2(aq)
  1             0
*
     beta0 =   0.00000   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
MgOH+                        CO3--
  1            -2
*
     beta0 =   0.00000   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
```

```
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
MgOH+                     Cl-
  1           -1
*
     beta0 =  -0.10000   beta1 =   1.65800   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
MgOH+                     HCO3-
  1           -1
*
     beta0 =   0.00000   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
MgOH+                     HSO4-
  1           -1
*
     beta0 =   0.00000   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
MgOH+                     OH-
  1           -1
*
     beta0 =   0.00000   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
```

```
*
      cphi =  0.00000
    source = Reardon90
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
MgOH+                        SO4--
  1            -2
*
     beta0 =   0.00000   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = Reardon90
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
MgOH+                        H3SiO4-
  1            -1
*
     beta0 =   0.00000   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = Reardon90
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
MgOH+                        H2SiO4--
  1            -2
*
     beta0 =   0.00000   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   1.4      alpha2 =  12.0
*
      cphi =  0.00000
    source = Reardon90
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
```

```
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
MgOH+                    Al(OH)4-
  1           -1
*
     beta0 =   0.00000   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = Reardon90
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                      CO2(aq)
  1            0
*
     beta0 =   0.10000   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                      CO3--
  1           -2
*
     beta0 =   0.03990   beta1 =   1.38900   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00440
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                      Cl-
  1           -1
*
     beta0 =   0.07650   beta1 =   0.26440   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
```

```
*
      cphi =  0.00127
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                        HCO3-
  1            -1
*
     beta0 =   0.02770   beta1 =   0.04110   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                        HSO4-
  1            -1
*
     beta0 =   0.04540   beta1 =   0.39800   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                        OH-
  1            -1
*
     beta0 =   0.08640   beta1 =   0.25300   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00440
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
```

```
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                       SO4--
  1            -2
*
     beta0 =   0.01958   beta1 =   1.11300   beta2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00497
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                       H3SiO4-
  1            -1
*
     beta0 =   0.04540   beta1 =   0.398000   beta2 = 0
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.00000
    source =  Readon90
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                       H2SiO4--
  1            -2
*
     beta0 =   0.01960   beta1 =   1.113000   beta2 = 0.0000
                         alpha1 =   2.0       alpha2 =  12.0
*
      cphi =  0.005000
    source = Reardon90
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                       Al(OH)4-
  1            -1
*
     beta0 =   0.04540   beta1 =   0.398000   beta2 = 0
                         alpha1 =   2.0       alpha2 =  12.0
```

```
*
      cphi =  0.00000
    source =  Readon90
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                     CO2(aq)
 -2            0
*
     beta0 =   0.09700   beta1 =   0.00000   beta2 =   0.00000
                         alpha1 =   0.0       alpha2 =   0.0
*
      cphi =  0.00000
    source = 84har/mol
*
*
    db0/dt =  0.000E+00  d2b0/dt2 =  0.000E+00
    db1/dt =  0.000E+00  d2b1/dt2 =  0.000E+00
    db2/dt =  0.000E+00  d2b2/dt2 =  0.000E+00
     dc/dt =  0.000E+00   d2c/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
mixture term parameters
E-theta flag = on
+--------------------------------------------------------------
Ca++                      H+                        CO3--
*
     theta =  0.09200       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Ca++                      H+                        Cl-
*
     theta =  0.09200       psi = -0.01500
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Ca++                      H+                        HCO3-
*
     theta =  0.09200       psi =  0.00000
    source = 84har/mol
*
*
```

```
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Ca++                      H+                        HSO4-
*
     theta =  0.09200       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Ca++                      H+                        OH-
*
     theta =  0.09200       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Ca++                      H+                        SO4--
*
     theta =  0.09200       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Ca++                      Mg++                      CO3--
*
     theta =  0.00700       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Ca++                      Mg++                      Cl-
*
     theta =  0.00700       psi = -0.01200
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Ca++                      Mg++                      HCO3-
*
```

```
     theta =  0.00700       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Ca++                     Mg++                     HSO4-
*
     theta =  0.00700       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Ca++                     Mg++                     OH-
*
     theta =  0.00700       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Ca++                     Mg++                     SO4--
*
     theta =  0.00700       psi =  0.02400
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Ca++                     MgOH+                    CO3--
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Ca++                     MgOH+                    Cl-
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
```

```
    source =
+-------------------------------------------------------------
Ca++                     MgOH+                    HCO3-
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Ca++                     MgOH+                    HSO4-
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Ca++                     MgOH+                    OH-
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Ca++                     MgOH+                    SO4--
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Cl-                      CO3--                    Ca++
*
     theta = -0.02000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Cl-                      CO3--                    H+
*
     theta = -0.02000       psi =  0.00000
    source = 84har/mol
```

```
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Cl-                        CO3--                     K+
*
     theta = -0.02000       psi =  0.00400
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Cl-                        CO3--                     Mg++
*
     theta = -0.02000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Cl-                        CO3--                     MgOH+
*
     theta = -0.02000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Cl-                        CO3--                     Na+
*
     theta = -0.02000       psi =  0.00850
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Cl-                        HCO3-                     Ca++
*
     theta =  0.03000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
```

```
Cl-                        HCO3-                      H+
*
     theta =  0.03000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Cl-                        HCO3-                      K+
*
     theta =  0.03000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Cl-                        HCO3-                      Mg++
*
     theta =  0.03000       psi = -0.09600
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Cl-                        HCO3-                      MgOH+
*
     theta =  0.03000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Cl-                        HCO3-                      Na+
*
     theta =  0.03000       psi = -0.01500
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Cl-                        HSO4-                      Ca++
*
     theta = -0.00600       psi =  0.00000
    source = 84har/mol
*
*
```

```
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Cl-                       HSO4-                    H+
*
     theta = -0.00600       psi =  0.01300
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Cl-                       HSO4-                    K+
*
     theta = -0.00600       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Cl-                       HSO4-                    Mg++
*
     theta = -0.00600       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Cl-                       HSO4-                    MgOH+
*
     theta = -0.00600       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Cl-                       HSO4-                    Na+
*
     theta = -0.00600       psi = -0.00600
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Cl-                       OH-                      Ca++
*
```

```
     theta = -0.05000       psi = -0.02500
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Cl-                       OH-                       H+
*
     theta = -0.05000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Cl-                       OH-                       K+
*
     theta = -0.05000       psi = -0.00600
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Cl-                       OH-                       Mg++
*
     theta = -0.05000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Cl-                       OH-                       MgOH+
*
     theta = -0.05000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Cl-                       OH-                       Na+
*
     theta = -0.05000       psi = -0.00600
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
```

```
    source =
+------------------------------------------------------------
Cl-                     SO4--                     Ca++
*
     theta =  0.02000       psi = -0.01800
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+------------------------------------------------------------
Cl-                     SO4--                     H+
*
     theta =  0.02000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+------------------------------------------------------------
Cl-                     SO4--                     K+
*
     theta =  0.02000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+------------------------------------------------------------
Cl-                     SO4--                     Mg++
*
     theta =  0.02000       psi = -0.00400
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+------------------------------------------------------------
Cl-                     SO4--                     MgOH+
*
     theta =  0.02000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+------------------------------------------------------------
Cl-                     SO4--                     Na+
*
     theta =  0.02000       psi =  0.00140
    source = 84har/mol
```

```
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Cl-                       H3SiO4-                   Ca++
*
     theta = -0.00600       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Cl-                       H3SiO4-                   H+
*
     theta = -0.00600       psi =  0.01300
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Cl-                       H3SiO4-                   K+
*
     theta =  -0.00600      psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Cl-                       H3SiO4-                   Mg++
*
     theta =  -0.00600      psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Cl-                       H3SiO4-                   MgOH+
*
     theta =  -0.00600      psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
```

```
Cl-                       H3SiO4-                   Na+
*
     theta =  -0.00600      psi = -0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Cl-                       H2SiO4--                  Ca++
*
     theta =  0.00000       psi = -0.01800
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Cl-                       H2SiO4--                  H+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Cl-                       H2SiO4--                  K+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Cl-                       H2SiO4--                  Mg++
*
     theta =  0.00000       psi = -0.00400
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Cl-                       H2SiO4--                  MgOH+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
```

```
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Cl-                      H2SiO4--                  Na+
*
     theta =  0.00000       psi =  0.00140
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Cl-                      Al(OH)4-                  Ca++
*
     theta = -0.00600       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Cl-                      Al(OH)4-                  H+
*
     theta = -0.00600       psi =  0.01300
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Cl-                      Al(OH)4-                  K+
*
     theta = -0.00600       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Cl-                      Al(OH)4-                  Mg++
*
     theta = -0.00600       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Cl-                      Al(OH)4-                  MgOH+
*
```

```
     theta = -0.00600       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Cl-                       Al(OH)4-                  Na+
*
     theta = -0.00600       psi = -0.00600
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
HCO3-                     CO3--                     Ca++
*
     theta = -0.04000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
HCO3-                     CO3--                     H+
*
     theta = -0.04000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
HCO3-                     CO3--                     K+
*
     theta = -0.04000       psi =  0.01200
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
HCO3-                     CO3--                     Mg++
*
     theta = -0.04000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
```

```
    source =
+--------------------------------------------------------------
HCO3-                    CO3--                    MgOH+
*
     theta = -0.04000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HCO3-                    CO3--                    Na+
*
     theta = -0.04000       psi =  0.00200
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HCO3-                    H3SiO4-                  Ca++
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HCO3-                    H3SiO4-                  H+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HCO3-                    H3SiO4-                  K+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HCO3-                    H3SiO4-                  Mg++
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
```

```
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
HCO3-                     H3SiO4-                    MgOH+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
HCO3-                     H3SiO4-                    Na+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
HCO3-                     H2SiO4--                   Ca++
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
HCO3-                     H2SiO4--                   H+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
HCO3-                     H2SiO4--                   K+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
```

```
HCO3-                     H2SiO4--                  Mg++
*
     theta =  0.00000       psi = -0.16100
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HCO3-                     H2SiO4--                  MgOH+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HCO3-                     H2SiO4--                  Na+
*
     theta =  0.00000       psi = -0.00500
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HCO3-                     Al(OH)4-                  Ca++
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HCO3-                     Al(OH)4-                  H+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HCO3-                     Al(OH)4-                  K+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
```

```
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HCO3-                     Al(OH)4-                  Mg++
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HCO3-                     Al(OH)4-                  MgOH+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HCO3-                     Al(OH)4-                  Na+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HSO4-                     CO3--                     Ca++
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HSO4-                     CO3--                     H+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HSO4-                     CO3--                     K+
*
```

```
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HSO4-                    CO3--                    Mg++
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HSO4-                    CO3--                    MgOH+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HSO4-                    CO3--                    Na+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HSO4-                    HCO3-                    Ca++
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HSO4-                    HCO3-                    H+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
```

```
    source =
+--------------------------------------------------------------
HSO4-                      HCO3-                     K+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HSO4-                      HCO3-                     Mg++
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HSO4-                      HCO3-                     MgOH+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HSO4-                      HCO3-                     Na+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HSO4-                      OH-                       Ca++
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HSO4-                      OH-                       H+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
```

```
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HSO4-                    OH-                      K+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HSO4-                    OH-                      Mg++
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HSO4-                    OH-                      MgOH+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
HSO4-                    OH-                      Na+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                       Ca++                     CO3--
*
     theta =  0.03200       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
```

```
K+                        Ca++                      Cl-
*
     theta =  0.03200       psi = -0.02500
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        Ca++                      HCO3-
*
     theta =  0.03200       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        Ca++                      HSO4-
*
     theta =  0.03200       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        Ca++                      OH-
*
     theta =  0.03200       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        Ca++                      SO4--
*
     theta =  0.03200       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        H+                        CO3--
*
     theta =  0.00500       psi =  0.00000
    source = 84har/mol
*
*
```

```
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        H+                        Cl-
*
     theta =  0.00500       psi = -0.01100
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        H+                        HCO3-
*
     theta =  0.00500       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        H+                        HSO4-
*
     theta =  0.00500       psi = -0.02650
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        H+                        OH-
*
     theta =  0.00500       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        H+                        SO4--
*
     theta =  0.00500       psi =  0.19700
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        Mg++                      CO3--
*
```

```
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        Mg++                      Cl-
*
     theta =  0.00000       psi = -0.02200
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        Mg++                      HCO3-
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        Mg++                      HSO4-
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        Mg++                      OH-
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        Mg++                      SO4--
*
     theta =  0.00000       psi = -0.04800
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
```

```
    source =
+--------------------------------------------------------------
K+                        MgOH+                         CO3--
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        MgOH+                         Cl-
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        MgOH+                         HCO3-
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        MgOH+                         HSO4-
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        MgOH+                         OH-
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        MgOH+                         SO4--
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
```

```
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Mg++                     H+                        CO3--
*
     theta =  0.10000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Mg++                     H+                        Cl-
*
     theta =  0.10000       psi = -0.01100
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Mg++                     H+                        HCO3-
*
     theta =  0.10000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Mg++                     H+                        HSO4-
*
     theta =  0.10000       psi = -0.01780
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Mg++                     H+                        OH-
*
     theta =  0.10000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
```

```
Mg++                      H+                         SO4--
*
     theta =  0.10000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Mg++                      MgOH+                      CO3--
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Mg++                      MgOH+                      Cl-
*
     theta =  0.00000       psi =  0.02800
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Mg++                      MgOH+                      HCO3-
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Mg++                      MgOH+                      HSO4-
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Mg++                      MgOH+                      OH-
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
```

```
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Mg++                     MgOH+                     SO4--
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
MgOH+                    H+                        CO3--
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
MgOH+                    H+                        Cl-
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
MgOH+                    H+                        HCO3-
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
MgOH+                    H+                        HSO4-
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
MgOH+                    H+                        OH-
*
```

```
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
MgOH+                    H+                          SO4--
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                      Ca++                        CO3--
*
     theta =  0.07000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                      Ca++                        Cl-
*
     theta =  0.07000       psi = -0.00700
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                      Ca++                        HCO3-
*
     theta =  0.07000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                      Ca++                        HSO4-
*
     theta =  0.07000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
```

```
    source =
+-------------------------------------------------------------
Na+                       Ca++                      OH-
*
     theta =  0.07000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                       Ca++                      SO4--
*
     theta =  0.07000       psi = -0.05500
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                       H+                        CO3--
*
     theta =  0.03600       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                       H+                        Cl-
*
     theta =  0.03600       psi = -0.00400
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                       H+                        HCO3-
*
     theta =  0.03600       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                       H+                        HSO4-
*
     theta =  0.03600       psi = -0.01290
    source = 84har/mol
```

```
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                     H+                        OH-
*
     theta =  0.03600       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                     H+                        SO4--
*
     theta =  0.03600       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                     K+                        CO3--
*
     theta = -0.01200       psi =  0.00300
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                     K+                        Cl-
*
     theta = -0.01200       psi = -0.00180
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                     K+                        HCO3-
*
     theta = -0.01200       psi = -0.00300
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
```

```
Na+                       K+                         HSO4-
*
     theta = -0.01200       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                       K+                         OH-
*
     theta = -0.01200       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                       K+                         SO4--
*
     theta = -0.01200       psi = -0.01000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                       Mg++                       CO3--
*
     theta =  0.07000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                       Mg++                       Cl-
*
     theta =  0.07000       psi = -0.01200
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                       Mg++                       HCO3-
*
     theta =  0.07000       psi =  0.00000
    source = 84har/mol
*
*
```

```
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                       Mg++                      HSO4-
*
     theta =  0.07000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                       Mg++                      OH-
*
     theta =  0.07000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                       Mg++                      SO4--
*
     theta =  0.07000       psi = -0.01500
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                       MgOH+                     CO3--
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                       MgOH+                     Cl-
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                       MgOH+                     HCO3-
*
```

```
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                        MgOH+                        HSO4-
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                        MgOH+                        OH-
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Na+                        MgOH+                        SO4--
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
OH-                        CO3--                        Ca++
*
     theta =  0.10000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
OH-                        CO3--                        H+
*
     theta =  0.10000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
```

```
    source =
+--------------------------------------------------------------
OH-                        CO3--                     K+
*
     theta =  0.10000       psi = -0.01000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
OH-                        CO3--                     Mg++
*
     theta =  0.10000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
OH-                        CO3--                     MgOH+
*
     theta =  0.10000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
OH-                        CO3--                     Na+
*
     theta =  0.10000       psi = -0.01700
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
OH-                        HCO3-                     Ca++
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
OH-                        HCO3-                     H+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
```

```
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
OH-                     HCO3-                    K+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
OH-                     HCO3-                    Mg++
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
OH-                     HCO3-                    MgOH+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
OH-                     HCO3-                    Na+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
OH-                     H3SiO4-                  Ca++
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
```

```
OH-                        H3SiO4-                   H+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
OH-                        H3SiO4-                   K+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
OH-                        H3SiO4-                   Mg++
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
OH-                        H3SiO4-                   MgOH+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
OH-                        H3SiO4-                   Na+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
OH-                        H2SiO4--                  Ca++
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
```

```
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
OH-                        H2SiO4--                  H+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
OH-                        H2SiO4--                  K+
*
     theta =  0.00000       psi = -0.05000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
OH-                        H2SiO4--                  Mg++
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
OH-                        H2SiO4--                  MgOH+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
OH-                        H2SiO4--                  Na+
*
     theta =  0.00000       psi = -0.009000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
OH-                        Al(OH)4-                  Ca++
*
```

```
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
OH-                     Al(OH)4-                 H+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
OH-                     Al(OH)4-                 K+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
OH-                     Al(OH)4-                 Mg++
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
OH-                     Al(OH)4-                 MgOH+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
OH-                     Al(OH)4-                 Na+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
```

```
    source =
+--------------------------------------------------------------
SO4--                    CO3--                    Ca++
*
     theta =  0.02000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                    CO3--                    H+
*
     theta =  0.02000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                    CO3--                    K+
*
     theta =  0.02000       psi = -0.00900
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                    CO3--                    Mg++
*
     theta =  0.02000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                    CO3--                    MgOH+
*
     theta =  0.02000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                    CO3--                    Na+
*
     theta =  0.02000       psi = -0.00500
    source = 84har/mol
```

```
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
SO4--                    HCO3-                    Ca++
*
     theta =  0.01000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
SO4--                    HCO3-                    H+
*
     theta =  0.01000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
SO4--                    HCO3-                    K+
*
     theta =  0.01000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
SO4--                    HCO3-                    Mg++
*
     theta =  0.01000       psi = -0.16100
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
SO4--                    HCO3-                    MgOH+
*
     theta =  0.01000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
```

```
SO4--                     HCO3-                     Na+
*
     theta =  0.01000       psi = -0.00500
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                     HSO4-                     Ca++
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                     HSO4-                     H+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                     HSO4-                     K+
*
     theta =  0.00000       psi = -0.06770
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                     HSO4-                     Mg++
*
     theta =  0.00000       psi = -0.04250
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                     HSO4-                     MgOH+
*
     theta =  0.00000       psi =  0.00000
    source = 84har/mol
*
*
```

```
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
SO4--                     HSO4-                     Na+
*
     theta =  0.00000       psi = -0.00940
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
SO4--                     OH-                       Ca++
*
     theta = -0.01300       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
SO4--                     OH-                       H+
*
     theta = -0.01300       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
SO4--                     OH-                       K+
*
     theta = -0.01300       psi = -0.05000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
SO4--                     OH-                       Mg++
*
     theta = -0.01300       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
SO4--                     OH-                       MgOH+
*
```

```
     theta = -0.01300       psi =  0.00000
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                    OH-                      Na+
*
     theta = -0.01300       psi = -0.00900
    source = 84har/mol
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                    H3SiO4-                  Ca++
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                    H3SiO4-                  H+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                    H3SiO4-                  K+
*
     theta =  0.00000       psi = -0.06770
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                    H3SiO4-                  Mg++
*
     theta =  0.00000       psi = -0.04250
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
```

```
    source =
+--------------------------------------------------------------
SO4--                     H3SiO4-                   MgOH+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                     H3SiO4-                   Na+
*
     theta =  0.00000       psi = -0.00940
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                     H2SiO4--                  Ca++
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                     H2SiO4--                  H+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                     H2SiO4--                  K+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                     H2SiO4--                  Mg++
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
```

```
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
SO4--                     H2SiO4--                  MgOH+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
SO4--                     H2SiO4--                  Na+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
SO4--                     Al(OH)4-                  Ca++
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
SO4--                     Al(OH)4-                  H+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
SO4--                     Al(OH)4-                  K+
*
     theta =  0.00000       psi = -0.06770
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
```

```
SO4--                    Al(OH)4-                 Mg++
*
     theta =  0.00000       psi = -0.04250
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                    Al(OH)4-                 MgOH+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
SO4--                    Al(OH)4-                 Na+
*
     theta =  0.00000       psi = -0.00940
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
CO3--                    H3SiO4-                  Ca++
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
CO3--                    H3SiO4-                  H+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
CO3--                    H3SiO4-                  K+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
```

```
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
CO3--                     H3SiO4-                   Mg++
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
CO3--                     H3SiO4-                   MgOH+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
CO3--                     H3SiO4-                   Na+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
CO3--                     H2SiO4--                  Ca++
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
CO3--                     H2SiO4--                  H+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
CO3--                     H2SiO4--                  K+
*
```

```
     theta =  0.00000       psi = -0.00900
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
CO3--                    H2SiO4--                 Mg++
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
CO3--                    H2SiO4--                 MgOH+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
CO3--                    H2SiO4--                 Na+
*
     theta =  0.00000       psi = -0.00500
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
CO3--                    Al(OH)4-                 Ca++
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
CO3--                    Al(OH)4-                 H+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
```

```
    source =
+--------------------------------------------------------------
CO3--                     Al(OH)4-                  K+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
CO3--                     Al(OH)4-                  Mg++
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
CO3--                     Al(OH)4-                  MgOH+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
CO3--                     Al(OH)4-                  Na+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
H3SiO4-                   H2SiO4--                  Ca++
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
H3SiO4-                   H2SiO4--                  H+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
```

```
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
H3SiO4-                  H2SiO4--                 K+
*
     theta =  0.00000       psi = -0.06770
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
H3SiO4-                  H2SiO4--                 Mg++
*
     theta =  0.00000       psi = -0.04250
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
H3SiO4-                  H2SiO4--                 MgOH+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
H3SiO4-                  H2SiO4--                 Na+
*
     theta =  0.00000       psi = -0.00940
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
H3SiO4-                  Al(OH)4-                 Ca++
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
```

```
H3SiO4-                    Al(OH)4-                   H+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
H3SiO4-                    Al(OH)4-                   K+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
H3SiO4-                    Al(OH)4-                   Mg++
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
H3SiO4-                    Al(OH)4-                   MgOH+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
H3SiO4-                    Al(OH)4-                   Na+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
H2SiO4--                   Al(OH)4-                   Ca++
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
```

```
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
H2SiO4--                 Al(OH)4-                 H+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
H2SiO4--                 Al(OH)4-                 K+
*
     theta =  0.00000       psi = -0.06770
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
H2SiO4--                 Al(OH)4-                 Mg++
*
     theta =  0.00000       psi = -0.04250
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
H2SiO4--                 Al(OH)4-                 MgOH+
*
     theta =  0.00000       psi =  0.00000
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
H2SiO4--                 Al(OH)4-                 Na+
*
     theta =  0.00000       psi = -0.00940
    source = Reardon90
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                      K+                       H3SiO4-
*
```

```
     theta = -0.01200       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                      K+                       H2SiO4--
*
     theta = -0.01200       psi = -0.01000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                      K+                       Al(OH)4-
*
     theta = -0.01200       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                      Ca++                     H3SiO4-
*
     theta =  0.07000       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                      Ca++                     H2SiO4--
*
     theta =  0.07000       psi = -0.05500
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                      Ca++                     Al(OH)4-
*
     theta =  0.07000       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
```

```
    source =
+--------------------------------------------------------------
Na+                        Mg++                        H3SiO4-
*
     theta =  0.07000       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                        Mg++                        H2SiO4--
*
     theta =  0.07000       psi = -0.01500
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                        Mg++                        Al(OH)4-
*
     theta =  0.07000       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                        H+                          H3SiO4-
*
     theta =  0.03600       psi = -0.01290
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                        H+                          H2SiO4--
*
     theta =  0.03600       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                        H+                          Al(OH)4-
*
     theta =  0.03600       psi = -0.01290
    source = Reardon
```

```
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                       MgOH+                    H3SiO4-
*
     theta =  0.00000       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                       MgOH+                    H2SiO4--
*
     theta =  0.00000       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Na+                       MgOH+                    Al(OH)4-
*
     theta =  0.00000       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        Ca++                     H3SiO4-
*
     theta =  0.03200       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        Ca++                     H2SiO4--
*
     theta =  0.03200       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
```

```
K+                        Ca++                         Al(OH)4-
*
     theta =  0.03200       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        Mg++                         H3SiO4-
*
     theta =  0.00000       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        Mg++                         H2SiO4--
*
     theta =  0.00000       psi = -0.08400
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        Mg++                         Al(OH)4-
*
     theta =  0.00000       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        H+                           H3SiO4-
*
     theta =  0.00500       psi = -0.02650
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
K+                        H+                           H2SiO4--
*
     theta =  0.00500       psi =  0.19700
    source = Reardon
*
*
```

```
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
K+                         H+                         Al(OH)4-
*
     theta =  0.00500       psi = -0.02650
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
K+                         MgOH+                      H3SiO4-
*
     theta =  0.00000       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
K+                         MgOH+                      H2SiO4--
*
     theta =  0.00000       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
K+                         MgOH+                      Al(OH)4-
*
     theta =  0.00000       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Ca++                       Mg++                       H3SiO4-
*
     theta =  0.00700       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Ca++                       Mg++                       H2SiO4--
*
```

```
     theta =  0.00700       psi =  0.02400
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Ca++                      Mg++                      Al(OH)4-
*
     theta =  0.00700       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Ca++                      H+                        H3SiO4-
*
     theta =  0.09200       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Ca++                      H+                        H2SiO4--
*
     theta =  0.09200       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Ca++                      H+                        Al(OH)4-
*
     theta =  0.09200       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+-------------------------------------------------------------
Ca++                      MgOH+                     H3SiO4-
*
     theta =  0.00000       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
```

```
    source =
+--------------------------------------------------------------
Ca++                     MgOH+                    H2SiO4--
*
     theta =  0.00000       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Ca++                     MgOH+                    Al(OH)4-
*
     theta =  0.00000       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Mg++                     H+                       H3SiO4-
*
     theta =  0.10000       psi = -0.01780
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Mg++                     H+                       H2SiO4--
*
     theta =  0.10000       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Mg++                     H+                       Al(OH)4-
*
     theta =  0.10000       psi = -0.01780
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Mg++                     MgOH+                    H3SiO4-
*
     theta =  0.00000       psi =  0.00000
    source = Reardon
```

```
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Mg++                     MgOH+                    H2SiO4--
*
     theta =  0.00000       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
Mg++                     MgOH+                    Al(OH)4-
*
     theta =  0.00000       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
H+                       MgOH+                    H3SiO4-
*
     theta =  0.00000       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
H+                       MgOH+                    H2SiO4--
*
     theta =  0.00000       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
+--------------------------------------------------------------
H+                       MgOH+                    Al(OH)4-
*
     theta =  0.00000       psi =  0.00000
    source = Reardon
*
*
    dth/dt =   0.0000    d2th/dt2 =  0.000E+00
   dpsi/dt =   0.0000    d2ps/dt2 =  0.000E+00
    source =
```

```
+---------------------------------------------------------------
-----
elements
+---------------------------------------------------------------
-----
O         15.99940
Al        26.98154
C         12.01100
Ca        40.07800
Cl        35.45270
H          1.00794
K         39.09830
Mg        24.30500
Na        22.98977
S         32.06600
Si        28.08550
+---------------------------------------------------------------
-----
basis species
+---------------------------------------------------------------
-----
H2O
     charge  =   0.0
****
     2 element(s):
      2.0000 H              1.0000 O
****
+---------------------------------------------------------------
-----
Al+++
     charge  =   3.0
****
     1 element(s):
      1.0000 Al
****
+---------------------------------------------------------------
-----
HCO3-
     charge  =  -1.0
****
     3 element(s):
      1.0000 C              1.0000 H              3.0000 O
****
+---------------------------------------------------------------
-----
Ca++
     charge  =   2.0
****
     1 element(s):
      1.0000 Ca
****
+---------------------------------------------------------------
-----
Cl-
     charge  =  -1.0
****
```

```
     1 element(s):
      1.0000 Cl
****
+---------------------------------------------------------------
-----
H+
     charge  =   1.0
****
     1 element(s):
      1.0000 H
****
+---------------------------------------------------------------
-----
K+
     charge  =   1.0
****
     1 element(s):
      1.0000 K
****
+---------------------------------------------------------------
-----
Mg++
     charge  =   2.0
****
     1 element(s):
      1.0000 Mg
****
+---------------------------------------------------------------
-----
Na+
     charge  =   1.0
****
     1 element(s):
      1.0000 Na
****
+---------------------------------------------------------------
-----
SO4--
     charge  =  -2.0
****
     2 element(s):
      4.0000 O              1.0000 S
****
+---------------------------------------------------------------
-----
SiO2(aq)
     charge  =   0.0
****
     2 element(s):
      2.0000 O              1.0000 Si
****
+---------------------------------------------------------------
-----
O2(g)
     charge  =   0.0
****
```

```
     1 element(s):
      2.0000 O
****
+----------------------------------------------------------------
-----
auxiliary basis species
+----------------------------------------------------------------
-----
HS-
     charge  =  -1.0
     2 element(s):
      1.0000 H              1.0000 S
****
     4 species in aqueous dissociation reaction:
    -1.0000  HS-                        -2.0000  O2(g)
     1.0000  H+                          1.0000  SO4--
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       146.7859  132.5203  116.0105  100.8144
        85.7147   73.6540   63.7280   55.2988
*
*    gflag = 1 [reported delG0f used]
*    extrapolation algorithm: supcrt92 [92joh/oel]
*    ref-state data  [source: 88sho/hel ]
*         delG0f =      2.860 kcal/mol     [reported]
*         delH0f =     -3.850 kcal/mol     [reported]
*         S0PrTr =     16.300 cal/(mol*K)  [reported]
+----------------------------------------------------------------
-----
aqueous species
+----------------------------------------------------------------
-----
Al(OH)++
     revised =  01-jul-1993
     sp.type =  aqueous
     charge  =    2.0
*    DHazero =    4.0
*    mol.wt. =   78.003559 g/mol
     3 element(s):
      1.0000 H              1.0000 O              1.0000 Al
     4 species in aqueous dissociation reaction:
    -1.0000  Al(OH)++                   -1.0000  H+
     1.0000  Al+++                       1.0000  H2O
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    4.9700  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* gflag = 1  (reported delG0f used)
*    ref-state data   Baes und Mesmer (1976)
*         delG0f =    -180.673 kcal/mol
*         delH0f =     500.000 kcal/mol
*         S0PrTr =     500.000 cal/(mol*K)
+----------------------------------------------------------------
-----
Al(OH)2+
```

```
     revised =  01-jul-1993
     sp.type =  aqueous
     charge  =    1.0
*    DHazero =    4.0
*    mol.wt. =   78.003559 g/mol
     3 element(s):
      2.0000 H              2.0000 O              1.0000 Al
     4 species in aqueous dissociation reaction:
    -1.0000  Al(OH)2+                    -2.0000  H+
     1.0000  Al+++                        2.0000  H2O
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    9.3000  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*    gflag = 1  (reported delG0f used)
*    ref-state data   Baes und Mesmer (1976)
*         delG0f =     -180.673 kcal/mol
*         delH0f =      500.000 kcal/mol
*         S0PrTr =      500.000 cal/(mol*K)
+---------------------------------------------------------------
-----
Al(OH)3
     revised =  01-jul-1993
     sp.type =  aqueous
     charge  =    0.0
*    DHazero =    4.0
*    mol.wt. =   60.996219 g/mol
     3 element(s):
      3.0000 H              3.0000 O              1.0000 Al
     4 species in aqueous dissociation reaction:
    -1.0000  Al(OH)3                     -3.0000  H+
     1.0000  Al+++                        3.0000  H2O
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   15.0000  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*    gflag = 1  (reported delG0f used)
*    ref-state data   Baes und Mesmer (1976)
*         delG0f =     -180.673 kcal/mol
*         delH0f =      500.000 kcal/mol
*         S0PrTr =      500.000 cal/(mol*K)
+---------------------------------------------------------------
-----
Al(OH)4-
     revised =  01-jul-1993
     sp.type =  aqueous
     charge  =   -1.0
*    DHazero =    4.0
*    mol.wt. =   95.07154 g/mol
     3 element(s):
      4.0000 H              4.0000 O              1.0000 Al
     4 species in aqueous dissociation reaction:
    -1.0000  Al(OH)4-                    -4.0000  H+
     1.0000  Al+++                        4.0000  H2O
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
```

```
       500.0000   23.0000  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*    gflag = 1  (reported delG0f used)
*    ref-state data   Baes und Mesmer (1976)1
*         delG0f =     -180.673 kcal/mol
*         delH0f =      500.000 kcal/mol
*         S0PrTr =      500.000 cal/(mol*K)
+---------------------------------------------------------------
-----
CO2(aq)
     sp.type =  aqueous
*    EQ3/6   =  hmw
     revised =  01-jul-1993
*    mol.wt. =  44.010 g/mol
*    DHazero =   3.0
     charge  =   0.0
****
     2 element(s):
      1.0000 C              2.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  CO2(aq)                     -1.0000  H2O
     1.0000  H+                           1.0000  HCO3-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -6.3374  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =    -92.238 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+---------------------------------------------------------------
-----
CO3--
     sp.type =  aqueous
*    EQ3/6   =  hmw
     revised =  01-jul-1993
*    mol.wt. =  60.009 g/mol
*    DHazero =   4.5
     charge  =  -2.0
****
     2 element(s):
      1.0000 C              3.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  CO3--                       -1.0000  H+
     1.0000  HCO3-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   10.3392  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
```

```
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -126.166 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
CaCO3(aq)
     sp.type =  aqueous
*    EQ3/6   =  hmw
     revised =  19-feb-1991
*    mol.wt. = 100.087 g/mol
*    DHazero =   3.0
     charge  =   0.0
****
     3 element(s):
      1.0000 C              1.0000 Ca             3.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  CaCO3(aq)                  -1.0000  H+
     1.0000  Ca++                        1.0000  HCO3-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    7.1880  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -262.767 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
H2(aq)
     sp.type =  aux
*    EQ3/6   =  com, alt, sup
     revised =  13-jun-1988
*    mol.wt. =   2.016 g/mol
*    DHazero =   3.0
     charge  =   0.0
****
     1 element(s):
      2.0000 H
****
     3 species in aqueous dissociation reaction:
    -1.0000  H2(aq)                     -0.5000  O2(g)
     1.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
        49.1500   44.6575   39.4400   34.6224
        29.8242   25.9892   22.8409   20.1881
*
*    gflag = 1 [reported delG0f used]
*    extrapolation algorithm: supcrt92 [92joh/oel]
```

```
*    ref-state data  [source: 89sho/hel ]
*         delG0f =      4.236 kcal/mol     [reported]
*         delH0f =     -1.000 kcal/mol     [reported]
*         S0PrTr =     13.800 cal/(mol*K)  [reported]
+----------------------------------------------------------------
-----
H2S(aq)
     revised =  01-jul-1993
     sp.type =  aqueous
     charge  =   0.0
*    DHazero =   3.0
*    mol.wt. =  34.082 g/mol
     2 element(s):
      2.0000 H              1.0000 S
     3 species in aqueous dissociation reaction:
    -1.0000  H2S(aq)                       1.0000  H+
     1.0000  HS-
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
        -7.4159   -6.9877   -6.6467   -6.4827
        -6.4960   -6.6831   -7.0225   -7.5536
*    gflag = 1 [reported delG0f used]
*    extrapolation algorithm: supcrt92 [92joh/oel]
*    ref-state data  [source: 89sho/hel ]
*         delG0f =     -6.673 kcal/mol     [reported]
*         delH0f =     -9.001 kcal/mol     [reported]
*         S0PrTr =     30.000 cal/(mol*K)  [reported]
+----------------------------------------------------------------
-----
HSO4-
     sp.type =  aqueous
*    EQ3/6   =  hmw
     revised =  01-jul-1993
*    mol.wt. =  97.072 g/mol
*    DHazero =   4.0
     charge  =  -1.0
****
     3 element(s):
      1.0000 H              4.0000 O              1.0000 S
****
     3 species in aqueous dissociation reaction:
    -1.0000  HSO4-                         1.0000  H+
     1.0000  SO4--
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -1.9786  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -180.673 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
```

```
H3SiO4-
     revised =  01-jul-1993
     sp.type =  aqueous
     charge  =   -1.0
*    DHazero =    4.0
*    mol.wt. =   94.10190 g/mol
     3 element(s):
      3.0000 H              4.0000 O              1.0000 Si
     4 species in aqueous dissociation reaction:
    -1.0000  H3SiO4-                   -1.0000  H+
     1.0000  SiO2(aq)                   2.0000  H2O
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    9.8100  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*    gflag = 1  (reported delG0f used)
*    ref-state data   NEA Grenthe et al. (1992)
*         delG0f =      500.000 kcal/mol
*         delH0f =      500.000 kcal/mol
*         S0PrTr =      500.000 cal/(mol*K)
+------------------------------------------------------------------
-----
H2SiO4--
     revised =  01-jul-1993
     sp.type =  aqueous
     charge  =   -2.0
*    DHazero =    4.0
*    mol.wt. =   93.07240 g/mol
     3 element(s):
      2.0000 H              4.0000 O              1.0000 Si
     4 species in aqueous dissociation reaction:
    -1.0000  H2SiO4--                  -2.0000  H+
     1.0000  SiO2(aq)                   2.0000  H2O
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   23.1400  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*    gflag = 1  (reported delG0f used)
*    ref-state data   NEA Grenthe et al. (1992)
*         delG0f =      500.000 kcal/mol
*         delH0f =      500.000 kcal/mol
*         S0PrTr =      500.000 cal/(mol*K)
+------------------------------------------------------------------
-----
MgCO3(aq)
     sp.type =  aqueous
*    EQ3/6   =  hmw
     revised =  19-feb-1991
*    mol.wt. =  84.314 g/mol
*    DHazero =   3.0
     charge  =   0.0
****
     3 element(s):
      1.0000 C              1.0000 Mg             3.0000 O
****
     4 species in aqueous dissociation reaction:
```

```
    -1.0000  MgCO3(aq)                   -1.0000  H+
     1.0000  HCO3-                        1.0000  Mg++
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    7.4108  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -238.863 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
MgOH+
     sp.type =  aqueous
*    EQ3/6   =  hmw
     revised =  19-feb-1991
*    mol.wt. =  41.312 g/mol
*    DHazero =   4.0
     charge  =   1.0
****
     3 element(s):
      1.0000 H              1.0000 Mg             1.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  MgOH+                       -1.0000  H+
     1.0000  H2O                          1.0000  Mg++
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   11.8091  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -149.270 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
OH-
     sp.type =  aqueous
*    EQ3/6   =  hmw
     revised =  30-jun-1993
*    mol.wt. =  17.007 g/mol
*    DHazero =   3.5
     charge  =  -1.0
****
     2 element(s):
      1.0000 H              1.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  OH-                         -1.0000  H+
     1.0000  H2O
```

```
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   13.9967  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =    -37.584 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
solids
+----------------------------------------------------------------
-----
Anhydrite               CaSO4
     sp.type =  solid
*    EQ3/6   =  hmw
     revised =  01-feb-1994
*    mol.wt. =   136.142 g/mol
     V0PrTr  =    45.940 cm**3/mol [source: supcrt92 ]
****
     3 element(s):
      1.0000 Ca             4.0000 O              1.0000 S
****
     3 species in aqueous dissociation reaction:
    -1.0000  Anhydrite                   1.0000  Ca++
     1.0000  SO4--
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -4.3621  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -316.226 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Antarcticite            CaCl2:6H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
     revised =  21-may-1990
*    mol.wt. =   219.075 g/mol
     V0PrTr  =   128.120 cm**3/mol [source: 89wea/lid]
****
     4 element(s):
      1.0000 Ca             2.0000 Cl            12.0000 H
      6.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  Antarcticite                1.0000  Ca++
     2.0000  Cl-                         6.0000  H2O
```

```
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    4.1436  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -529.473 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Aphthitalite            NaK3(SO4)2
     sp.type =  solid   idealized
*    EQ3/6   =  com, alt, pit, hmw
     revised =  11-sep-1990
*    mol.wt. =   332.412 g/mol
     V0PrTr  =   246.230 cm**3/mol [source: 86jen    ]
****
     4 element(s):
      3.0000 K              1.0000 Na              8.0000 O
      2.0000 S
****
     4 species in aqueous dissociation reaction:
    -1.0000  Aphthitalite                 1.0000  Na+
     2.0000  SO4--                        3.0000  K+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -3.8027  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    alternate name = Glaserite
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -626.285 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Aragonite               CaCO3
     sp.type =  solid   polymorph
*    EQ3/6   =  hmw
     revised =  02-aug-1989
*    mol.wt. =   100.087 g/mol
     V0PrTr  =    34.150 cm**3/mol [source: supcrt92 ]
****
     3 element(s):
      1.0000 C              1.0000 Ca              3.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  Aragonite                   -1.0000  H+
     1.0000  Ca++                         1.0000  HCO3-
*
```

```
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    2.1198  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -269.681 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Arcanite                K2SO4
     sp.type =  solid
*    EQ3/6   =  hmw
     revised =  02-may-1990
*    mol.wt. =   174.260 g/mol
     V0PrTr  =    65.500 cm**3/mol [source: 79rob/hem]
****
     3 element(s):
      2.0000 K              4.0000 O              1.0000 S
****
     3 species in aqueous dissociation reaction:
    -1.0000  Arcanite                    1.0000  SO4--
     2.0000  K+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -1.7763  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -315.432 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Bischofite              MgCl2:6H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
     revised =  13-jul-1990
*    mol.wt. =   203.302 g/mol
     V0PrTr  =   129.570 cm**3/mol [source: 89wea/lid]
****
     4 element(s):
      2.0000 Cl            12.0000 H              1.0000 Mg
      6.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  Bischofite                  1.0000  Mg++
     2.0000  Cl-                         6.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    4.4554  500.0000  500.0000
```

```
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -505.448 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Bloedite                Na2Mg(SO4)2:4H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
     revised =  01-feb-1983
*    mol.wt. =   334.473 g/mol
     V0PrTr  =   149.980 cm**3/mol [source: 89wea/lid]
****
     5 element(s):
      8.0000 H              1.0000 Mg             2.0000 Na
     12.0000 O              2.0000 S
****
     5 species in aqueous dissociation reaction:
    -1.0000  Bloedite                     1.0000  Mg++
     2.0000  Na+                          2.0000  SO4--
     4.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -2.3469  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    alternate name = Astrakanite
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -819.760 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Brucite                 Mg(OH)2
     sp.type =  solid
*    EQ3/6   =  hmw
     revised =  17-dec-1986
*    mol.wt. =    58.320 g/mol
     V0PrTr  =    24.630 cm**3/mol [source: supcrt92 ]
****
     3 element(s):
      2.0000 H              1.0000 Mg             2.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  Brucite                     -2.0000  H+
     1.0000  Mg++                         2.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   17.1090  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
```

```
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol];Altmaier et a. 2003
*         delG0f =   -198.719 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+-----------------------------------------------------------------
-----
Burkeite                 Na6CO3(SO4)2
     sp.type =  solid
*    EQ3/6   =  com, alt, hmw
     revised =  03-sep-1985
*    mol.wt. =   390.075 g/mol
     V0PrTr  =   151.190 cm**3/mol [source: 73don    ]
****
     4 element(s):
      1.0000 C              6.0000 Na            11.0000 O
      2.0000 S
****
     5 species in aqueous dissociation reaction:
    -1.0000  Burkeite                    -1.0000  H+
     1.0000  HCO3-                        2.0000  SO4--
     6.0000  Na+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    9.5671  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -858.746 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+-----------------------------------------------------------------
-----
Ca2Cl2(OH)2:H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
     revised =  03-sep-1985
*    mol.wt. =   203.091 g/mol
     V0PrTr  =     0.000 cm**3/mol [source:          ]
****
     4 element(s):
      2.0000 Ca             2.0000 Cl             4.0000 H
      3.0000 O
****
     5 species in aqueous dissociation reaction:
    -1.0000  Ca2Cl2(OH)2:H2O             -2.0000  H+
     2.0000  Ca++                         2.0000  Cl-
     3.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   26.5313  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
```

```
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -461.195 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Ca4Cl2(OH)6:13H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
     revised =  03-sep-1985
*    mol.wt. =   567.460 g/mol
     V0PrTr  =     0.000 cm**3/mol [source:          ]
****
     4 element(s):
      4.0000 Ca             2.0000 Cl            32.0000 H
     19.0000 O
****
     5 species in aqueous dissociation reaction:
    -1.0000  Ca4Cl2(OH)6:13H2O          -6.0000  H+
     2.0000  Cl-                         4.0000  Ca++
    19.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   68.7343  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =  -1575.088 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
CaCl2:4H2O
     sp.type =  solid
*    EQ3/6   =  hmw
     revised =  21-may-1990
*    mol.wt. =   183.045 g/mol
     V0PrTr  =     0.000 cm**3/mol [source:          ]
****
     4 element(s):
      1.0000 Ca             2.0000 Cl             8.0000 H
      4.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  CaCl2:4H2O                  1.0000  Ca++
     2.0000  Cl-                         4.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    5.7171  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
```

```
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -413.968 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Calcite                 CaCO3
     sp.type =  solid   polymorph
*    EQ3/6   =  hmw
     revised =  02-aug-1989
*    mol.wt. =   100.087 g/mol
     V0PrTr  =    36.934 cm**3/mol [source: supcrt92 ]
****
     3 element(s):
      1.0000 C              1.0000 Ca             3.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  Calcite                    -1.0000  H+
     1.0000  Ca++                        1.0000  HCO3-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    1.9330  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -269.936 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Carnallite              KMgCl3:6H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
     revised =  21-may-1990
*    mol.wt. =   277.853 g/mol
     V0PrTr  =   172.580 cm**3/mol [source: 89wea/lid]
****
     5 element(s):
      3.0000 Cl            12.0000 H              1.0000 K
      1.0000 Mg             6.0000 O
****
     5 species in aqueous dissociation reaction:
    -1.0000  Carnallite                  1.0000  K+
     1.0000  Mg++                        3.0000  Cl-
     6.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    4.3304  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
```

```
*         delG0f =   -604.511 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+---------------------------------------------------------------
-----
Dolomite                CaMg(CO3)2
     sp.type =  solid
*    EQ3/6   =  hmw
     revised =  01-feb-1983
*    mol.wt. =   184.401 g/mol
     V0PrTr  =    64.365 cm**3/mol [source: supcrt92 ]
****
     4 element(s):
      2.0000 C              1.0000 Ca             1.0000 Mg
      6.0000 O
****
     5 species in aqueous dissociation reaction:
    -1.0000  Dolomite                   -2.0000  H+
     1.0000  Ca++                        1.0000  Mg++
     2.0000  HCO3-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    3.5960  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -516.640 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+---------------------------------------------------------------
-----
Epsomite                MgSO4:7H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
     revised =  21-may-1990
*    mol.wt. =   246.476 g/mol
     V0PrTr  =   146.800 cm**3/mol [source: 79rob/hem]
****
     4 element(s):
     14.0000 H              1.0000 Mg            11.0000 O
      1.0000 S
****
     4 species in aqueous dissociation reaction:
    -1.0000  Epsomite                    1.0000  Mg++
     1.0000  SO4--                       7.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -1.8811  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -685.995 kcal/mol     [reported]
```

```
*         delH0f =      N/A
*         S0PrTr =      N/A
+---------------------------------------------------------------
-----
Gaylussite              CaNa2(CO3)2:5H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, hmw
     revised =  03-sep-1985
*    mol.wt. =   296.152 g/mol
     V0PrTr  =   148.150 cm**3/mol [source: 73don    ]
****
     5 element(s):
      2.0000 C              1.0000 Ca            10.0000 H
      2.0000 Na            11.0000 O
****
     6 species in aqueous dissociation reaction:
    -1.0000  Gaylussite                 -2.0000  H+
     1.0000  Ca++                        2.0000  HCO3-
     2.0000  Na+                         5.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   11.2576  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -806.074 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+---------------------------------------------------------------
-----
Gibbsite                Al(OH)3
     revised =  23-jul-2003
     sp.type =  solid            polymorph
     V0PrTr  =    31.956 cm**3/mol  (source = supcrt92    )
*    mol.wt. =    78.00356 g/mol
     3 element(s):
      1.0000 Al             3.0000 H              3.0000 O
     4 species in aqueous dissociation reaction:
    -1.0000  Gibbsite                   -3.0000  H+
     1.0000  Al+++                       3.0000  H2O
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    8.0250  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*    gflag = 4    (reported urt data used)
*    ref-state data   Sadiq und Lindsay (1981)
*         delG0f =      500.000 kcal/mol
*         delH0f =      500.000 kcal/mol
*         S0PrTr =      500.000 cal/(mol*K)
+---------------------------------------------------------------
-----
Glauberite              Na2Ca(SO4)2
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
```

```
     revised =  21-may-1990
*    mol.wt. =   278.185 g/mol
     V0PrTr  =   101.120 cm**3/mol [source: 73don    ]
****
     4 element(s):
      1.0000 Ca            2.0000 Na            8.0000 O
      2.0000 S
****
     4 species in aqueous dissociation reaction:
    -1.0000  Glauberite                   1.0000  Ca++
     2.0000  Na+                          2.0000  SO4--
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -5.2445  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -620.597 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Gypsum                  CaSO4:2H2O
     sp.type =  solid
*    EQ3/6   =  hmw
     revised =  18-may-1990
*    mol.wt. =   172.172 g/mol
     V0PrTr  =    74.690 cm**3/mol [source: 79rob/hem]
****
     4 element(s):
      1.0000 Ca            4.0000 H             6.0000 O
      1.0000 S
****
     4 species in aqueous dissociation reaction:
    -1.0000  Gypsum                       1.0000  Ca++
     1.0000  SO4--                        2.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -4.5805  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -429.882 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Halite                  NaCl
     sp.type =  solid
*    EQ3/6   =  hmw
     revised =  02-mar-1990
*    mol.wt. =    58.442 g/mol
```

```
     V0PrTr  =    27.015 cm**3/mol [source: supcrt92 ]
****
     2 element(s):
      1.0000 Cl            1.0000 Na
****
     3 species in aqueous dissociation reaction:
    -1.0000  Halite                      1.0000  Cl-
     1.0000  Na+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    1.5704  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =    -91.829 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Hexahydrite             MgSO4:6H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
     revised =  21-may-1990
*    mol.wt. =   228.460 g/mol
     V0PrTr  =   132.580 cm**3/mol [source: 67rob/bet]
****
     4 element(s):
     12.0000 H             1.0000 Mg            10.0000 O
      1.0000 S
****
     4 species in aqueous dissociation reaction:
    -1.0000  Hexahydrite                 1.0000  Mg++
     1.0000  SO4--                       6.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -1.6351  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -628.981 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Hemihydrate             CaSO4:0.5H2O
     sp.type =  solid
 * Also known as Bassanite (which is probably more proper)
     revised =  21-may-1990
     V0PrTr  =    00.000 cm**3/mol [source:          ]
****
     4 element(s):
      1.0000 Ca            1.0000 H              4.5000 O
```

```
      1.0000 S
****
     4 species in solid dissolution reaction:
    -1.0000  Hemihydrate                  1.0000  Ca++
     1.0000  SO4--                        0.5000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
        -3.4301   -3.7773   -4.2698   -4.9372
        -5.8587   -6.7479   -7.6614   No_Data
* Source: 89Gre/Mol [Minerals_gmo.xls]
*
* Alternate data:
*       -3.4306   -3.6440   -4.0989   -4.7171
*       -5.5895   -6.5815   -7.7514   -9.2445
* Source: 95Bar/Pla [Solids_j_Ca_TJW_1.xls]
*
* Alternate data:
*       No_Data   -4.5805   No_Data   No_Data
*       No_Data   No_Data   No_Data   No_Data
* Source: 84Har/Mol [Minerals_hmw.xls] from data0.ypf
+----------------------------------------------------------------
-----
K2CO3:1.5H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, hmw
     revised =  03-sep-1985
*    mol.wt. =   165.229 g/mol
     V0PrTr  =    80.880 cm**3/mol [source: 89wea/lid]
****
     4 element(s):
      1.0000 C              3.0000 H              2.0000 K
      4.5000 O
****
     5 species in aqueous dissociation reaction:
    -1.0000  K2CO3:1.5H2O                -1.0000  H+
     1.0000  HCO3-                        1.5000  H2O
     2.0000  K+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   13.3720  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -342.082 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
K3H(SO4)2
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
     revised =  17-dec-1986
*    mol.wt. =   310.430 g/mol
```

```
     V0PrTr  =     0.000 cm**3/mol [source:          ]
****
     4 element(s):
      1.0000 H              3.0000 K              8.0000 O
      2.0000 S
****
     4 species in aqueous dissociation reaction:
    -1.0000  K3H(SO4)2                   1.0000  H+
     2.0000  SO4--                       3.0000  K+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -3.5425  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -563.333 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
K8H4(CO3)6:3H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, hmw
     revised =  03-sep-1985
*    mol.wt. =   730.919 g/mol
     V0PrTr  =     0.000 cm**3/mol [source:          ]
****
     4 element(s):
      6.0000 C             10.0000 H              8.0000 K
     21.0000 O
****
     5 species in aqueous dissociation reaction:
    -1.0000  K8H4(CO3)6:3H2O            -2.0000  H+
     3.0000  H2O                         6.0000  HCO3-
     8.0000  K+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   27.6874  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =  -1514.033 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
KNaCO3:6H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, hmw
     revised =  03-sep-1985
*    mol.wt. =   230.189 g/mol
     V0PrTr  =     0.000 cm**3/mol [source:          ]
```

```
****
     5 element(s):
      1.0000 C            12.0000 H              1.0000 K
      1.0000 Na            9.0000 O
****
     6 species in aqueous dissociation reaction:
    -1.0000  KNaCO3:6H2O                -1.0000  H+
     1.0000  HCO3-                       1.0000  K+
     1.0000  Na+                         6.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   10.2233  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -596.513 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Kainite                  KMgClSO4:3H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
     revised =  21-may-1990
*    mol.wt. =   248.965 g/mol
     V0PrTr  =   115.300 cm**3/mol [source: 73don    ]
****
     6 element(s):
      1.0000 Cl            6.0000 H              1.0000 K
      1.0000 Mg            7.0000 O              1.0000 S
****
     6 species in aqueous dissociation reaction:
    -1.0000  Kainite                     1.0000  Cl-
     1.0000  K+                          1.0000  Mg++
     1.0000  SO4--                       3.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -0.1926  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -555.868 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Kalicinite               KHCO3
     sp.type =  solid
*    EQ3/6   =  com, alt, hmw
     revised =  03-sep-1985
*    mol.wt. =   100.115 g/mol
     V0PrTr  =    46.140 cm**3/mol [source: 89wea/lid]
```

```
****
     4 element(s):
      1.0000 C              1.0000 H              1.0000 K
      3.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  Kalicinite                   1.0000  HCO3-
     1.0000  K+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    0.2814  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -207.405 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Kieserite               MgSO4:H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
     revised =  21-may-1990
*    mol.wt. =   138.384 g/mol
     V0PrTr  =    56.600 cm**3/mol [source: 89wea/lid]
****
     4 element(s):
      2.0000 H              1.0000 Mg             5.0000 O
      1.0000 S
****
     4 species in aqueous dissociation reaction:
    -1.0000  Kieserite                    1.0000  H2O
     1.0000  Mg++                         1.0000  SO4--
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -0.1227  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -343.522 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Leonite                 K2Mg(SO4)2:4H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
     revised =  21-may-1990
*    mol.wt. =   366.690 g/mol
     V0PrTr  =   166.300 cm**3/mol [source: 73don    ]
****
     5 element(s):
```

```
      8.0000 H              2.0000 K              1.0000 Mg
     12.0000 O              2.0000 S
****
     5 species in aqueous dissociation reaction:
    -1.0000  Leonite                       1.0000  Mg++
     2.0000  K+                            2.0000  SO4--
     4.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -3.9790  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -831.829 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+-----------------------------------------------------------------
-----
Magnesite               MgCO3
     sp.type =  solid
*    EQ3/6   =  hmw
     revised =  01-feb-1983
*    mol.wt. =    84.314 g/mol
     V0PrTr  =    28.018 cm**3/mol [source: supcrt92 ]
****
     3 element(s):
      1.0000 C              1.0000 Mg             3.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  Magnesite                    -1.0000  H+
     1.0000  HCO3-                         1.0000  Mg++
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    2.5054  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -245.555 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+-----------------------------------------------------------------
-----
Mercallite              KHSO4
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
     revised =  03-sep-1985
*    mol.wt. =   136.170 g/mol
     V0PrTr  =    58.590 cm**3/mol [source: 73don    ]
****
     4 element(s):
      1.0000 H              1.0000 K              4.0000 O
      1.0000 S
```

```
****
     4 species in aqueous dissociation reaction:
    -1.0000  Mercallite                   1.0000  H+
     1.0000  K+                           1.0000  SO4--
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -1.4015  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -247.403 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
MgSO4(wasserfrei)       MgSO4
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
     revised =  19-3-2004
*    mol.wt. =   120.36860 g/mol
     V0PrTr  =    45.250 cm**3/mol [source: 73don    ]
****
     3 element(s):
      1.0000 Mg            4.0000 O             1.0000 S
****
     3 species in aqueous dissociation reaction:
    -1.0000  MgSO4(wasserfrei)            1.0000  Mg++
     1.0000  SO4--
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
         6.2392    4.8781    3.1018    1.2809
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 73bar/kna]
*         delG0f =      N/A
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Mirabilite              Na2SO4:10H2O
     sp.type =  solid
*    EQ3/6   =  hmw
     revised =  15-may-1990
*    mol.wt. =   322.196 g/mol
     V0PrTr  =   219.800 cm**3/mol [source: 79rob/hem]
****
     4 element(s):
     20.0000 H             2.0000 Na           14.0000 O
      1.0000 S
****
     4 species in aqueous dissociation reaction:
    -1.0000  Mirabilite                   1.0000  SO4--
```

```
     2.0000  Na+                          10.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -1.2278  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -871.632 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+-----------------------------------------------------------------
-----
Misenite               K8H6(SO4)7
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
     revised =  03-sep-1985
*    mol.wt. =   991.279 g/mol
     V0PrTr  =     0.000 cm**3/mol [source:          ]
****
     4 element(s):
      6.0000 H              8.0000 K             28.0000 O
      7.0000 S
****
     4 species in aqueous dissociation reaction:
    -1.0000  Misenite                      6.0000  H+
     7.0000  SO4--                         8.0000  K+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000  -10.8061  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =  -1800.700 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+-----------------------------------------------------------------
-----
Na2CO3:7H2O
     sp.type =  solid
*    EQ3/6   =  hmw
     revised =  01-feb-1983
*    mol.wt. =   232.096 g/mol
     V0PrTr  =   153.710 cm**3/mol [source: 89wea/lid]
****
     4 element(s):
      1.0000 C             14.0000 H              2.0000 Na
     10.0000 O
****
     5 species in aqueous dissociation reaction:
    -1.0000  Na2CO3:7H2O                  -1.0000  H+
     1.0000  HCO3-                         2.0000  Na+
     7.0000  H2O
```

```
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    9.8791  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -648.740 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Na3H(SO4)2
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
     revised =  03-apr-1990
*    mol.wt. =   262.104 g/mol
     V0PrTr  =     0.000 cm**3/mol [source:          ]
****
     4 element(s):
      1.0000 H              3.0000 Na             8.0000 O
      2.0000 S
****
     4 species in aqueous dissociation reaction:
    -1.0000  Na3H(SO4)2                  1.0000  H+
     2.0000  SO4--                       3.0000  Na+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -0.8143  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -544.848 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Na4Ca(SO4)3:2H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
     revised =  01-feb-1983
*    mol.wt. =   456.258 g/mol
     V0PrTr  =     0.000 cm**3/mol [source:          ]
****
     5 element(s):
      1.0000 Ca             4.0000 H              4.0000 Na
     14.0000 O              3.0000 S
****
     5 species in aqueous dissociation reaction:
    -1.0000  Na4Ca(SO4)3:2H2O            1.0000  Ca++
     2.0000  H2O                         3.0000  SO4--
     4.0000  Na+
*
```

```
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -5.6723  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =  -1037.706 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+---------------------------------------------------------------
-----
Nahcolite               NaHCO3
     sp.type =  solid
*    EQ3/6   =  hmw
     revised =  17-may-1990
*    mol.wt. =    84.007 g/mol
     V0PrTr  =    38.620 cm**3/mol [source: 73don    ]
****
     4 element(s):
      1.0000 C              1.0000 H              1.0000 Na
      3.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  Nahcolite                    1.0000  HCO3-
     1.0000  Na+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -0.4030  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -203.417 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+---------------------------------------------------------------
-----
Natron                  Na2CO3:10H2O
     sp.type =  solid
*    EQ3/6   =  hmw
     revised =  17-may-1990
*    mol.wt. =   286.142 g/mol
     V0PrTr  =   195.990 cm**3/mol [source: 73don    ]
****
     4 element(s):
      1.0000 C             20.0000 H              2.0000 Na
     13.0000 O
****
     5 species in aqueous dissociation reaction:
    -1.0000  Natron                      -1.0000  H+
     1.0000  HCO3-                        2.0000  Na+
    10.0000  H2O
*
```

```
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    9.5145  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -819.275 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+-----------------------------------------------------------------
-----
Nesquehonite            MgCO3:3H2O
     sp.type =  solid
*    EQ3/6   =  hmw
     revised =  01-feb-1983
*    mol.wt. =   138.360 g/mol
     V0PrTr  =    74.790 cm**3/mol [source: supcrt92 ]
****
     4 element(s):
      1.0000 C              6.0000 H              1.0000 Mg
      6.0000 O
****
     5 species in aqueous dissociation reaction:
    -1.0000  Nesquehonite               -1.0000  H+
     1.0000  HCO3-                       1.0000  Mg++
     3.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    5.1722  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -411.954 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+-----------------------------------------------------------------
-----
Mg-Oxychloride          Mg2Cl(OH)3:4H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
     revised =  03-sep-1985
*    mol.wt. =   207.146 g/mol
     V0PrTr  =     0.000 cm**3/mol [source:          ]
****
     4 element(s):
      1.0000 Cl            11.0000 H              2.0000 Mg
      7.0000 O
****
     5 species in aqueous dissociation reaction:
    -1.0000  Mg-Oxychloride             -3.0000  H+
     1.0000  Cl-                         2.0000  Mg++
     7.0000  H2O
*
```

```
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   26.0297  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol];Altmaier et al. 2003
*         delG0f =   -610.021 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Pentahydrite            MgSO4:5H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, pit
     revised =  01-feb-1983
*    mol.wt. =   210.445 g/mol
     V0PrTr  =   110.760 cm**3/mol [source: 86jen    ]
****
     4 element(s):
     10.0000 H              1.0000 Mg             9.0000 O
      1.0000 S
****
     4 species in aqueous dissociation reaction:
    -1.0000  Pentahydrite                1.0000  Mg++
     1.0000  SO4--                       5.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -1.4274  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    alternate name = Allenite
*    ref-state data  87Pab/Pit [Solids_j_Pabalan_TJW_1.xls]
*         delG0f =   -571.766 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Picromerite             K2Mg(SO4)2:6H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
     revised =  21-may-1990
*    mol.wt. =   402.720 g/mol
     V0PrTr  =   197.500 cm**3/mol [source: 73don    ]
****
     5 element(s):
     12.0000 H              2.0000 K              1.0000 Mg
     14.0000 O              2.0000 S
****
     5 species in aqueous dissociation reaction:
    -1.0000  Picromerite                 1.0000  Mg++
     2.0000  K+                          2.0000  SO4--
     6.0000  H2O
*
```

```
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -4.3277  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    alternate name = Schoenite
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -945.663 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+---------------------------------------------------------------
-----
Pirssonite              Na2Ca(CO3)2:2H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, hmw
     revised =  03-sep-1985
*    mol.wt. =   242.106 g/mol
     V0PrTr  =   102.300 cm**3/mol [source: 73don    ]
****
     5 element(s):
      2.0000 C              1.0000 Ca             4.0000 H
      2.0000 Na             8.0000 O
****
     6 species in aqueous dissociation reaction:
    -1.0000  Pirssonite                 -2.0000  H+
     1.0000  Ca++                        2.0000  H2O
     2.0000  HCO3-                       2.0000  Na+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   11.4354  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -635.794 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+---------------------------------------------------------------
-----
Polyhalite              K2MgCa2(SO4)4:2H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
     revised =  01-feb-1983
*    mol.wt. =   602.943 g/mol
     V0PrTr  =   218.100 cm**3/mol [source: 78don    ]
****
     6 element(s):
      2.0000 Ca             4.0000 H              2.0000 K
      1.0000 Mg            18.0000 O              4.0000 S
****
     6 species in aqueous dissociation reaction:
    -1.0000  Polyhalite                  1.0000  Mg++
     2.0000  Ca++                        2.0000  H2O
     2.0000  K+                          4.0000  SO4--
```

```
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000  -13.7441  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =  -1352.344 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Portlandite             Ca(OH)2
     sp.type =  solid
*    EQ3/6   =  hmw
     revised =  17-may-1990
*    mol.wt. =    74.093 g/mol
     V0PrTr  =    33.056 cm**3/mol [source: 79rob/hem]
****
     3 element(s):
      1.0000 Ca            2.0000 H             2.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  Portlandite                -2.0000  H+
     1.0000  Ca++                        2.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   22.8035  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -214.550 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Starkeyite              MgSO4:4H2O
     sp.type =  solid
*    EQ3/6   =  ult
     revised =  01-feb-1983
*    mol.wt. =    192.42972 g/mol
     V0PrTr  =    95.740 cm**3/mol  (source = 86jen       )
****
     4 element(s):
      8.0000 H             1.0000 Mg            8.0000 O
      1.0000 S
****
     4 species in aqueous dissociation reaction:
    -1.0000  Starkeyite                  1.0000  Mg++
     1.0000  SO4--                       4.0000  H2O
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -1.0359  500.0000  500.0000
```

```
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*            ref-state   data   *   Source:   87Pab/Pit   [Sol-
ids_j_Pabalan_TJW_1.xls]
*         delG0f =      N/A
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Sylvite                 KCl
     sp.type =  solid
*    EQ3/6   =  hmw
     revised =  05-jul-1989
*    mol.wt. =    74.551 g/mol
     V0PrTr  =    37.524 cm**3/mol [source: supcrt92 ]
****
     2 element(s):
      1.0000 Cl             1.0000 K
****
     3 species in aqueous dissociation reaction:
    -1.0000  Sylvite                     1.0000  Cl-
     1.0000  K+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    0.8999  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =    -97.665 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Syngenite               K2Ca(SO4)2:H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
     revised =  21-may-1990
*    mol.wt. =   328.417 g/mol
     V0PrTr  =   124.200 cm**3/mol [source: 73don    ]
****
     5 element(s):
      1.0000 Ca             2.0000 H              2.0000 K
      9.0000 O              2.0000 S
****
     5 species in aqueous dissociation reaction:
    -1.0000  Syngenite                   1.0000  Ca++
     1.0000  H2O                         2.0000  K+
     2.0000  SO4--
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -7.4484  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
```

```
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -690.125 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Tachyhydrite            Mg2CaCl6:12H2O
     sp.type =  solid
*    EQ3/6   =  com, alt, pit, hmw
     revised =  21-may-1990
*    mol.wt. =   517.588 g/mol
     V0PrTr  =   203.780 cm**3/mol [source: 86jen    ]
****
     5 element(s):
      1.0000 Ca             6.0000 Cl            24.0000 H
      2.0000 Mg            12.0000 O
****
     5 species in aqueous dissociation reaction:
    -1.0000  Tachyhydrite                1.0000  Ca++
     2.0000  Mg++                        6.0000  Cl-
    12.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   17.3839  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =  -1194.388 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
Thenardite              Na2SO4
     sp.type =  solid
*    EQ3/6   =  hmw
     revised =  13-jul-1990
*    mol.wt. =   142.043 g/mol
     V0PrTr  =    53.330 cm**3/mol [source: 79rob/hem]
****
     3 element(s):
      2.0000 Na             4.0000 O              1.0000 S
****
     3 species in aqueous dissociation reaction:
    -1.0000  Thenardite                  1.0000  SO4--
     2.0000  Na+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -0.2875  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
```

```
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -303.559 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+-----------------------------------------------------------------
-----
Thermonatrite           Na2CO3:H2O
     sp.type =  solid
*    EQ3/6   =  hmw
     revised =  18-may-1990
*    mol.wt. =   124.004 g/mol
     V0PrTr  =    54.920 cm**3/mol [source: 73don    ]
****
     4 element(s):
      1.0000 C              2.0000 H              2.0000 Na
      4.0000 O
****
     5 species in aqueous dissociation reaction:
    -1.0000  Thermonatrite              -1.0000  H+
     1.0000  H2O                         1.0000  HCO3-
     2.0000  Na+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   10.8211  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -307.381 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+-----------------------------------------------------------------
-----
Trona                   Na3H(CO3)2:2H2O
     sp.type =  solid
*    EQ3/6   =  hmw
     revised =  01-feb-1983
*    mol.wt. =   226.026 g/mol
     V0PrTr  =     0.000 cm**3/mol [source:          ]
****
     4 element(s):
      2.0000 C              5.0000 H              3.0000 Na
      8.0000 O
****
     5 species in aqueous dissociation reaction:
    -1.0000  Trona                      -1.0000  H+
     2.0000  H2O                         2.0000  HCO3-
     3.0000  Na+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    9.2948  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
```

```
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -569.009 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+---------------------------------------------------------------
-----
Trona-K                 K2NaH(CO3)2:2H2O
     sp.type =  solid   idealized
*    EQ3/6   =  com, alt, hmw
     revised =  06-jul-1987
*    mol.wt. =   258.243 g/mol
     V0PrTr  =     0.000 cm**3/mol [source:          ]
****
     5 element(s):
      2.0000 C              5.0000 H              2.0000 K
      1.0000 Na             8.0000 O
****
     6 species in aqueous dissociation reaction:
    -1.0000  Trona-K                   -1.0000  H+
     1.0000  Na+                        2.0000  H2O
     2.0000  HCO3-                      2.0000  K+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   11.5757  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =   -575.740 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+---------------------------------------------------------------
-----
Muscovite               KAl3Si3O10(OH)2
     revised =  08-aug-1984
     sp.type =  solid            idealized
     V0PrTr  =   140.710 cm**3/mol  (source = supcrt92        )
*    mol.wt. =   398.30810 g/mol
     5 element(s):
      3.0000 Al             2.0000 H              1.0000 K
     12.0000 O              3.0000 Si
     6 species in aqueous dissociation reaction:
    -1.0000  Muscovite                -10.0000  H+
     1.0000  K+                         3.0000  Al+++
     3.0000  SiO2(aq)                   6.0000  H2O
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
        14.0189   11.0217    6.9022    2.8284
        -1.4013   -4.9716   -8.1786  -11.2615
* Extrapolation algorithm: supcrt92
*    gflag = 1    (supcrt92 equations and data used)
*    ref-state data   supcrt92
*         delG0f =    -1336.301 kcal/mol
*         delH0f =    -1427.408 kcal/mol
*         S0PrTr =       68.800 cal/(mol*K)
```

```
* cp coefficients   (source = supcrt92                )
* T**0    =  0.97560000E+02
* T**1    =  0.26380000E-01
* T**-2   = -0.25440000E+07
* Tlimit  =  726.85 C
+---------------------------------------------------------------
-----
Trichlorid              Ca6Al2(Cl2)3O6:30H2O
     revised =  25-mar-1998
     sp.type =  solid
     V0PrTr  =    450.000 cm**3/mol   (source = Schätzung! D=2.5
*    mol.wt. =   1143.6135 g/mol
     5 element(s):
      2.0000 Al             6.0000 Ca            36.0000 O
     60.0000 H              6.0000 Cl
     6 species in aqueous dissociation reaction:
    -1.0000  Trichlorid                -12.0000  H+
     2.0000  Al+++                       6.0000  Ca++
    36.0000  H2O                         6.0000  Cl-
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   56.8400  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: constant enthalpy approximation
*    gflag = 1    (reported delG0f used)
*    ref-state data Revertegat et al. (1997)
*         delG0f =      500.000 kcal/mol
*         delH0f =      500.000 kcal/mol
*         S0PrTr =      500.000 cal/(mol*K)
+---------------------------------------------------------------
-----
Hydrogarnet             Ca3Al2O6:6H2O
     revised =  25-mar-1998
     sp.type =  solid
     V0PrTr  =    00.000 cm**3/mol   (source = 90crc         )
*    mol.wt. =   590.45948 g/mol
     4 element(s):
      2.0000 Al             3.0000 Ca            12.0000 O
     12.0000 H
     5 species in aqueous dissociation reaction:
    -1.0000  Hydrogarnet               -12.0000  H+
     2.0000  Al+++                       3.0000  Ca++
    12.0000  H2O
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   80.5500  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: constant enthalpy approximation
*    gflag = 1    (reported delG0f used)
*    ref-state data Revertegat et al. (1997)
*         delG0f =      500.000 kcal/mol
*         delH0f =      500.000 kcal/mol
*         S0PrTr =      500.000 cal/(mol*K)
+---------------------------------------------------------------
-----
Tetracalciumaluminat    Ca4Al2O7:13H3O
```

```
     revised =  25-mar-1998
     sp.type =  solid
     V0PrTr  =    00.000 cm**3/mol  (source = 90crc      )
*    mol.wt. =   590.45948 g/mol
     4 element(s):
      2.0000 Al            4.0000 Ca            20.0000 O
     26.0000 H
     5 species in aqueous dissociation reaction:
    -1.0000  Tetracalciumaluminat      -14.0000  H+
     2.0000  Al+++                       4.0000  Ca++
    20.0000  H2O
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000  104.0000  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: constant enthalpy approximation
*    gflag = 1    (reported delG0f used)
*    ref-state data Revertegat et al. (1997)
*         delG0f =      500.000 kcal/mol
*         delH0f =      500.000 kcal/mol
*         S0PrTr =      500.000 cal/(mol*K)
+---------------------------------------------------------------
-----
Si-Hydrogarnet          Ca3Al2SiO8:4H2O
     revised =  25-mar-1998
     sp.type =  solid
     V0PrTr  =    00.000 cm**3/mol  (source = 90crc         )
*    mol.wt. =   402.34458 g/mol
     5 element(s):
      2.0000 Al            3.0000 Ca            12.0000 O
      8.0000 H             1.0000 Si
     6 species in aqueous dissociation reaction:
    -1.0000  Si-Hydrogarnet            -12.0000  H+
     2.0000  Al+++                       3.0000  Ca++
    10.0000  H2O                         1.0000  SiO2(aq)
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   69.3500  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: constant enthalpy approximation
*    gflag = 1    (reported delG0f used)
*    ref-state data Revertegat et al. (1997)
*         delG0f =      500.000 kcal/mol
*         delH0f =      500.000 kcal/mol
*         S0PrTr =      500.000 cal/(mol*K)
+---------------------------------------------------------------
-----
Jennit                  Ca9Si6O21:11H2O
     revised =  25-mar-1998
     sp.type =  solid
     V0PrTr  =    00.000 cm**3/mol  (source = 90crc          )
*    mol.wt. =  1063.38760 g/mol
     4 element(s):
      6.0000 Si            9.0000 Ca            32.0000 O
     22.0000 H
     5 species in aqueous dissociation reaction:
```

```
    -1.0000  Jennit                     -18.0000  H+
     6.0000  SiO2(aq)                     9.0000  Ca++
    20.0000  H2O
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000  150.8100  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: constant enthalpy approximation
*    gflag = 1    (reported delG0f used)
*    ref-state data  Kulik und Kersten (2002)
*         delG0f =      500.000 kcal/mol
*         delH0f =      500.000 kcal/mol
*         S0PrTr =      500.000 cal/(mol*K)
+---------------------------------------------------------------
-----
Ettringite              Ca6Al2(SO4)3(OH)12:26H2O
     revised =  27-may-1988
     sp.type =  solid
     V0PrTr  =     0.000 cm**3/mol  (source =              )
*    mol.wt. =  1255.10724 g/mol
     5 element(s):
      2.0000 Al             6.0000 Ca            64.0000 H
     50.0000 O              3.0000 S
     6 species in aqueous dissociation reaction:
    -1.0000  Ettringite                 -12.0000  H+
     2.0000  Al+++                        3.0000  SO4--
     6.0000  Ca++                        38.0000  H2O
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
        66.8870   55.3527   54.7045   50.2795
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: constant enthalpy approximation
*    gflag = 2    (calculated delG0f(delH0f,S0PrTr) used)
*    ref-state data   Revertegat et al. (1997)
*         delG0f =    -3628.433 kcal/mol
*         delH0f =    -4193.000 kcal/mol
*         S0PrTr =      427.800 cal/(mol*K)
+---------------------------------------------------------------
-----
Kaolinit                Al2Si2O5(OH)4
     revised =  15-nov-2003
     sp.type =  solid
     V0PrTr  =    00.000 cm**3/mol  (source = 90crc         )
*    mol.wt. =   240.14508 g/mol
     4 element(s):
      2.0000 Si             2.0000 Al             9.0000 O
      4.0000 H
     5 species in aqueous dissociation reaction:
    -1.0000  Kaolinit                    -6.0000  H+
     2.0000  SiO2(aq)                     2.0000  Al+++
     5.0000  H2O
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    7.4350  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: constant enthalpy approximation
```

```
*    gflag = 1    (reported delG0f used)
*    ref-state data   Nordstrom et al (1990): May et al. (1986)
*         delG0f =      500.000 kcal/mol
*         delH0f =      500.000 kcal/mol
*         S0PrTr =      500.000 cal/(mol*K)
+----------------------------------------------------------------
-----
Tobermorit              Ca5Si6O17:9H2O
     revised =  14-nov-2003
     sp.type =  solid
     V0PrTr  =    00.000 cm**3/mol  (source = 90crc         )
*    mol.wt. =   803.03960 g/mol
     4 element(s):
      6.0000 Si             5.0000 Ca            26.0000 O
     18.0000 H
     5 species in aqueous dissociation reaction:
    -1.0000  Tobermorit                -10.0000  H+
     6.0000  SiO2(aq)                    5.0000  Ca++
    14.0000  H2O
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   64.3500  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: constant enthalpy approximation
*    gflag = 1    (reported delG0f used)
*    ref-state data Kulik und Kersten (2002)
*         delG0f =      500.000 kcal/mol
*         delH0f =      500.000 kcal/mol
*         S0PrTr =      500.000 cal/(mol*K)
+----------------------------------------------------------------
-----
Ca5Si5O14(OH)2:4H2O     Ca5Si5O14(OH)2:4H2O
     revised =  14-nov-2003
     sp.type =  solid
     V0PrTr  =    00.000 cm**3/mol  (source = 90crc         )
*    mol.wt. =   803.03960 g/mol
     4 element(s):
      5.0000 Si             5.0000 Ca            20.0000 O
     10.0000 H
     5 species in aqueous dissociation reaction:
    -1.0000  Ca5Si5O14(OH)2:4H2O       -10.0000  H+
     5.0000  SiO2(aq)                    5.0000  Ca++
    10.0000  H2O
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   73.2000  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: constant enthalpy approximation
*    gflag = 1    (reported delG0f used)
*    ref-state data: Tommaseo und Kersten (2002)
*         delG0f =      500.000 kcal/mol
*         delH0f =      500.000 kcal/mol
*         S0PrTr =      500.000 cal/(mol*K)
+----------------------------------------------------------------
-----
Gehlenithydrat          Ca2Al2SiO7:8H2O
```

```
     revised =  25-mar-1998
     sp.type =  solid
     V0PrTr  =    00.000 cm**3/mol  (source = 90crc         )
*    mol.wt. =   418.32598 g/mol
     5 element(s):
      2.0000 Al            2.0000 Ca            15.0000 O
     16.0000 H             1.0000 Si
     6 species in aqueous dissociation reaction:
    -1.0000  Gehlenithydrat            -10.0000  H+
     2.0000  Al+++                       2.0000  Ca++
    13.0000  H2O                         1.0000  SiO2(aq)
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   49.3800  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: constant enthalpy approximation
*    gflag = 1    (reported delG0f used)
*    ref-state data
*         delG0f =      500.000 kcal/mol
*         delH0f =      500.000 kcal/mol
*         S0PrTr =      500.000 cal/(mol*K)
+----------------------------------------------------------------
-----
Dicalciumaluminathydrat Ca2Al2O5:8H2O
     revised =  25-mar-1998
     sp.type =  solid
     V0PrTr  =    00.000 cm**3/mol  (source = 90crc         )
*    mol.wt. =   358.24168 g/mol
     4 element(s):
      2.0000 Al            2.0000 Ca            13.0000 O
     16.0000 H
     5 species in aqueous dissociation reaction:
    -1.0000  Dicalciumaluminathydrat    -10.0000  H+
     2.0000  Al+++                       2.0000  Ca++
    13.0000  H2O
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   59.6700  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: constant enthalpy approximation
*    gflag = 1    (reported delG0f used)
*    ref-state data Revertegat et al. (1997)
*         delG0f =      500.000 kcal/mol
*         delH0f =      500.000 kcal/mol
*         S0PrTr =      500.000 cal/(mol*K)
+----------------------------------------------------------------
-----
Tricalciumaluhemisilik  Ca3Al2Si0.5O7
     revised =  25-mar-1998
     sp.type =  solid
     V0PrTr  =    00.000 cm**3/mol  (source = 90crc         )
*    mol.wt. =   300.24163 g/mol
     4 element(s):
      2.0000 Al            3.0000 Ca             7.0000 O
      0.5000 Si
     6 species in aqueous dissociation reaction:
```

```
    -1.0000  Tricalciumaluhemisilik     -12.0000  H+
     2.0000  Al+++                        3.0000  Ca++
     6.0000  H2O                          0.5000  SiO2(aq)
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   74.1200  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: constant enthalpy approximation
*    gflag = 1    (reported delG0f used)
*    ref-state data Revertegat et al. (1997)
*         delG0f =      500.000 kcal/mol
*         delH0f =      500.000 kcal/mol
*         S0PrTr =      500.000 cal/(mol*K)
+---------------------------------------------------------------
-----
Afwill                  CaSi2O5:3H2O
     revised =  26-mar-1998
     sp.type =  solid
     V0PrTr  =    00.000 cm**3/mol  (source = supcrt92      )
*    mol.wt. =   230.16028 g/mol
     4 element(s):
      1.0000 Ca             6.0000 H              8.0000 O
      2.0000 Si
     5 species in aqueous dissociation reaction:
    -1.0000  Afwill                      -2.0000  H+
     1.0000  Ca++                         4.0000  H2O
     2.0000  SiO2(aq)
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   46.9000  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: supcrt92
*    gflag = 1    (supcrt92 equations and data used)
*    ref-state data   supcrt92
*         delG0f =     500.0000 kcal/mol
*         delH0f =     500.0000 kcal/mol
*         S0PrTr =     500.0000 l/(mol*K)
+---------------------------------------------------------------
-----
Halloy                  Al2Si2O7:2H2O
     revised =  26-mar-1998
     sp.type =  solid
     V0PrTr  =    00.000 cm**3/mol  (source = supcrt92      )
*    mol.wt. =   258.16028 g/mol
     4 element(s):
      2.0000 Al             4.0000 H              9.0000 O
      2.0000 Si
     5 species in aqueous dissociation reaction:
    -1.0000  Halloy                      -6.0000  H+
     2.0000  Al+++                        5.0000  H2O
     2.0000  SiO2(aq)
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   15.1000  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: supcrt92
```

```
*    gflag = 1    (supcrt92 equations and data used)
*    ref-state data supcrt92
*         delG0f =     500.0000 kcal/mol
*         delH0f =     500.0000 kcal/mol
*         S0PrTr =     500.0000 l/(mol*K)
+---------------------------------------------------------------
-----
Chabazit                CaAl2Si4O12:6H2O
     revised =  08-aug-1984
     sp.type =  solid
     V0PrTr  =    00.000 cm**3/mol  (source = supcrt92      )
*    mol.wt. =   506.46908 g/mol
     5 element(s):
      2.0000 Al           12.0000 H             18.0000 O
      1.0000 Ca            4.0000 Si
     6 species in aqueous dissociation reaction:
    -1.0000  Chabazit                   -8.0000  H+
     2.0000  Al+++                      10.0000  H2O
     1.0000  Ca++                        4.0000  SiO2(aq)
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   13.0000  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: supcrt92
*    gflag = 1    (supcrt92 equations and data used)
*    ref-state data supcrt92
*         delG0f =     500.000 kcal/mol
*         delH0f =     500.000 kcal/mol
*         S0PrTr =     500.000 cal/(mol*K)
+---------------------------------------------------------------
-----
Chrysotil               Mg3Si2O5(OH)4
     revised =  15-nov-2003
     sp.type =  solid
     V0PrTr      =         000.000   cm**3/mol      (source   =
www.musee.ensmp.fr/gm/ )
*    mol.wt. =   379.26560 g/mol
     4 element(s):
      3.0000 Mg            4.0000 H              9.0000 O
      2.0000 Si
     5 species in aqueous dissociation reaction:
    -1.0000  Chrysotil                  -6.0000  H+
     3.0000  Mg++                        5.0000  H2O
     2.0000  SiO2(aq)
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   32.2000  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: supcrt92
*    gflag = 1
*    ref-state data Nordstrom et al. (1990)/ Stoessel (1988)
*         delG0f =     500.000 kcal/mol
*         delH0f =     500.000 kcal/mol
*         S0PrTr =     500.000 cal/(mol*K)
+---------------------------------------------------------------
-----
```

```
Sepiolit                Mg2Si3O7.5(OH):3H2O
     revised =  15-nov-2003
     sp.type =  solid
     V0PrTr      =         000.000   cm**3/mol      (source   =
www.musee.ensmp.fr/gm/ )
*    mol.wt. =   379.26560 g/mol
     4 element(s):
      2.0000 Mg            7.0000 H             11.5000 O
      3.0000 Si
     5 species in aqueous dissociation reaction:
    -1.0000  Sepiolit                   -4.0000  H+
     2.0000  Mg++                        5.5000  H2O
     3.0000  SiO2(aq)
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   15.7600  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: supcrt92
*    gflag = 1
*    ref-state data Nordstrom et al. (1990)
*         delG0f =     500.000 kcal/mol
*         delH0f =     500.000 kcal/mol
*         S0PrTr =     500.000 cal/(mol*K)
+---------------------------------------------------------------
-----
Talcit                  Mg3Si4O11:H2O
     revised =  08-aug-1984
     sp.type =  solid
     V0PrTr      =         140.209   cm**3/mol      (source   =
www.musee.ensmp.fr/gm/ )
*    mol.wt. =   379.26560 g/mol
     4 element(s):
      3.0000 Mg            2.0000 H             12.0000 O
      4.0000 Si
     5 species in aqueous dissociation reaction:
    -1.0000  Talcit                     -6.0000  H+
     3.0000  Mg++                        4.0000  H2O
     4.0000  SiO2(aq)
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   22.4100  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: supcrt92
*    gflag = 1
*    ref-state data Nordstrom et al. (1990)/ Stoessel (1988)
*         delG0f =     500.000 kcal/mol
*         delH0f =     500.000 kcal/mol
*         S0PrTr =     500.000 cal/(mol*K)
+---------------------------------------------------------------
-----
Kerolite                Mg3Si4O11:H2O
     revised =  26-jan-2009
     sp.type =  solid
     V0PrTr      =         140.209   cm**3/mol      (source   =
www.musee.ensmp.fr/gm/ )
*    mol.wt. =   379.26560 g/mol
```

```
     4 element(s):
      4.0000 H              3.0000 Mg            13.0000 O
      4.0000 Si
     5 species in aqueous dissociation reaction:
    -1.0000  Kerolite                      -6.0000  H+
     3.0000  Mg++                           4.0000  SiO2(aq)
     5.0000  H2O
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   25.7900  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: supcrt92
*    gflag = 1
*    ref-state data Nordstrom et al. (1990)/ Stoessel (1988)
*         delG0f =     500.000 kcal/mol
*         delH0f =     500.000 kcal/mol
*         S0PrTr =     500.000 cal/(mol*K)
+----------------------------------------------------------------
-----
Hydrotalcit             Mg4Al2(OH)14:3H2O
     revised =  08-aug-1984
     sp.type =  solid
     V0PrTr  =    00.000 cm**3/mol  (source = supcrt92      )
*    mol.wt. =   443.33088 g/mol
     4 element(s):
      4.0000 Mg            20.0000 H             17.0000 O
      2.0000 Al
     5 species in aqueous dissociation reaction:
    -1.0000  Hydrotalcit                  -14.0000  H+
     4.0000  Mg++                          17.0000  H2O
     2.0000  Al+++
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   83.2200  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: SUPCRT92 Johnson et al. (1992)
*    gflag = 1    (supcrt92 equations and data used)
*    ref-state data supcrt92
*         delG0f =     500.000 kcal/mol
*         delH0f =     500.000 kcal/mol
+----------------------------------------------------------------
-----
Hydrotalcit-Semi-CO3    Mg4Al2(OH)12CO3:2H2O
     revised =  08-aug-1984
     sp.type =  solid
     V0PrTr  =    00.000 cm**3/mol  (source = supcrt92      )
*    mol.wt. =   443.33088 g/mol
     5 element(s):
      4.0000 Mg            16.0000 H             17.0000 O
      2.0000 Al             1.0000 C
     6 species in aqueous dissociation reaction:
    -1.0000  Hydrotalcit-Semi-CO3         -13.0000  H+
     4.0000  Mg++                          14.0000  H2O
     2.0000  Al+++                          1.0000  HCO3-
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
```

```
       500.0000   61.2000  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm:
*    gflag = 1
*    ref-state data   Johnson und Glasser (2003)
*         delG0f =     500.000 kcal/mol
*         delH0f =     500.000 kcal/mol
+---------------------------------------------------------------
-----
SiO2(am)                SiO2(am)
     revised =  01-jul-1993
     sp.type =  solid            polymorph
     V0PrTr  =    22.688 cm**3/mol  (source = supcrt92
*    mol.wt. =    60.08430 g/mol
     2 element(s):
      2.0000 O              1.0000 Si
     2 species in aqueous dissociation reaction:
    -1.0000  SiO2(am)                     1.0000  SiO2(aq)
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -2.6600  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm:
*    gflag = 1    ()
*    ref-state data PSI/NAGRA DB: GUNNARSSON & ARNORSSON (2000)
*         delG0f =     XXX kcal/mol
*         delH0f =     XXX kcal/mol
*         S0PrTr =     XXX cal/(mol*K)
* cp coefficients   (source = supcrt92                )
* T**0    =  0.11220000E+02
* T**1    =  0.82000000E-02
* T**-2   = -0.27000000E+06
* Tlimit  =  574.85 C
* delH0tr   =     0.290 kcal/mol
* delV0tr   =     0.372 cm**3/mol
* (dP/dT)tr =    38.500 bars/K
+---------------------------------------------------------------
-----
Quartz                  SiO2(cr)
     revised =  01-jul-1993
     sp.type =  solid            polymorph
     V0PrTr  =    22.688 cm**3/mol  (source = supcrt92      )
*    mol.wt. =    60.08430 g/mol
     2 element(s):
      2.0000 O              1.0000 Si
     2 species in aqueous dissociation reaction:
    -1.0000  Quartz                       1.0000  SiO2(aq)
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -4.0000  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm:
*    gflag = 1    (reported delG0f used)
*    ref-state data PSI/NAGRA: GUNNARSSON & ARNORSSON (2000)
*         delG0f =      500.000 kcal/mol
*         delH0f =      500.000 kcal/mol
```

```
*         S0PrTr =      500.000 cal/(mol*K)
+---------------------------------------------------------------
-----
FriedelschesSalz        Ca4Al2Cl2O6:10H2O
     revised =  25-mar-1998
     sp.type =  solid
     V0PrTr  =    00.000 cm**3/mol  (source = 90crc         )
*    mol.wt. =   561.33748 g/mol
     5 element(s):
      2.0000 Al             4.0000 Ca            16.0000 O
     20.0000 H              2.0000 Cl
     6 species in aqueous dissociation reaction:
    -1.0000  FriedelschesSalz          -12.0000  H+
     2.0000  Al+++                       4.0000  Ca++
    16.0000  H2O                         2.0000  Cl-
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   72.5200  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: constant enthalpy approximation
*    gflag = 1    (reported delG0f used)
*    ref-state data
*         delG0f =      500.000 kcal/mol
*         delH0f =      500.000 kcal/mol
*         S0PrTr =      500.000 cal/(mol*K)
+---------------------------------------------------------------
-----
CSH(0.8)                Ca0.8SiO2.8:H2O
     revised =  25-mar-1998
     sp.type =  solid
     V0PrTr  =    00.000 cm**3/mol  (source = 90crc         )
*    mol.wt. =   122.8 g/mol
     4 element(s):
      0.8000 Ca             1.0000 Si             3.8000 O
      2.0000 H
     5 species in aqueous dissociation reaction:
    -1.0000  CSH(0.8)                   -1.6000  H+
     0.8000  Ca++                        1.0000  SiO2(aq)
     1.8000  H2O
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   11.0700  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: constant enthalpy approximation
*    gflag = 1    (reported delG0f used)
*    ref-state data Revertegat et al. (1997)
*         delG0f =      500.000 kcal/mol
*         delH0f =      500.000 kcal/mol
*         S0PrTr =      500.000 cal/(mol*K)
+---------------------------------------------------------------
-----
CSH(1.1)                Ca1.1SiO3.1:3H2O
     revised =  25-mar-1998
     sp.type =  solid
     V0PrTr  =    00.000 cm**3/mol  (source = 90crc         )
*    mol.wt. =   175.6 g/mol
```

```
     4 element(s):
      1.1000 Ca              1.0000 Si              6.1000 O
      6.0000 H
     5 species in aqueous dissociation reaction:
    -1.0000  CSH(1.1)                    -2.2000  H+
     1.1000  Ca++                         1.0000  SiO2(aq)
     4.1000  H2O
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   16.7100  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: constant enthalpy approximation
*    gflag = 1    (reported delG0f used)
*    ref-state data Revertegat et al. (1997)
*         delG0f =      500.000 kcal/mol
*         delH0f =      500.000 kcal/mol
*         S0PrTr =      500.000 cal/(mol*K)
+----------------------------------------------------------------
-----
CSH(1.8)                Ca1.8SiO3.8:5H2O
     revised =  25-mar-1998
     sp.type =  solid
     V0PrTr  =    00.000 cm**3/mol  (source = 90crc         )
*    mol.wt. =   250.8 g/mol
     4 element(s):
      1.8000 Ca              1.0000 Si              8.8000 O
     10.0000 H
     5 species in aqueous dissociation reaction:
    -1.0000  CSH(1.8)                    -3.6000  H+
     1.8000  Ca++                         1.0000  SiO2(aq)
     6.8000  H2O
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   32.5400  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
* Extrapolation algorithm: constant enthalpy approximation
*    gflag = 1    (reported delG0f used)
*    ref-state data Revertegat et al. (1997)
*         delG0f =      500.000 kcal/mol
*         delH0f =      500.000 kcal/mol
*         S0PrTr =      500.000 cal/(mol*K)
+----------------------------------------------------------------
-----
Serpentin               Mg3Si2O5(OH)4
     revised =  08-aug-1984
     sp.type =  solid
     V0PrTr  =   108.500 cm**3/mol  (source = 90crc         )
*    mol.wt. =  277.11236 g/mol
     4 element(s):
      4.0000 H               3.0000 Mg              9.0000 O
      2.0000 Si
     5 species in aqueous dissociation reaction:
    -1.0000  Serpentin                   -6.0000  H+
     2.0000  SiO2(aq)                     3.0000  Mg++
     5.0000  H2O
```

```
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
        34.4271   36.2000   26.9983   23.1597
        19.4090   16.4625   14.0146   11.8204
* Extrapolation algorithm: constant enthalpy approximation
*    gflag = 1    (reported delG0f used)
*    ref-state data Revertegat et al. (1997)
*         delG0f =     -964.871 kcal/mol
*         delH0f =    -1043.123 kcal/mol
*         S0PrTr =       52.900 cal/(mol*K)
+----------------------------------------------------------------
-----
liquids
+----------------------------------------------------------------
-----
gases
+----------------------------------------------------------------
-----
CO2(g)
     sp.type =  gas
*    EQ3/6   =  hmw
     revised =  01-jul-1993
*    mol.wt. =    44.010 g/mol
     V0PrTr  =     0.000 cm**3/mol [source:          ]
****
     2 element(s):
      1.0000 C              2.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  CO2(g)                      -1.0000  H2O
     1.0000  H+                           1.0000  HCO3-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   -7.8193  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 84har/mol ]
*         delG0f =    -94.259 kcal/mol     [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
+----------------------------------------------------------------
-----
H2(g)
     sp.type =  gas     refstate
*    EQ3/6   =  com, alt, sup, pit
     revised =  22-nov-1996
*    mol.wt. =     2.016 g/mol
     V0PrTr   =        0.000  cm**3/mol  [source:  supcrt92  [see
92joh/oel]]
****
     1 element(s):
      2.0000 H
****
     3 species in aqueous dissociation reaction:
```

```
    -1.0000  H2(g)                       -0.5000  O2(g)
     1.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000   41.5461  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 82wag/eva, 60kel      ]
*         delG0f =      0.000 kcal/mol     [reported]
*         delH0f =      0.000 kcal/mol     [reported]
*         S0PrTr =     31.234 cal/(mol*K)  [reported]
*    Cp coefficients [source: 82wag/eva               ]
*         T**0   =  0.65200000E+01
*         T**1   =  0.78000000E-03
*         T**-2  =  0.12000000E+05
*         Tlimit = 2726.85C
+----------------------------------------------------------------
-----
H2S(g)
     sp.type =  gas
*    EQ3/6   =  com, alt, sup
     revised =  01-jul-1993
*    mol.wt. =    34.082 g/mol
     V0PrTr   =         0.000  cm**3/mol  [source:  supcrt92  [see
92joh/oel]]
****
     2 element(s):
      2.0000 H              1.0000 S
****
     3 species in aqueous dissociation reaction:
    -1.0000  H2S(g)                       1.0000  H+
     1.0000  HS-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
        -8.0781   -7.9759   -7.9295   -7.9572
        -8.0759   -8.2750   -8.5671   -9.0074
*
*    gflag = 1 [reported delG0f used]
*    extrapolation algorithm: supcrt92 [92joh/oel]
*    ref-state data  [source: 82wag/eva, 60kel      ]
*         delG0f =     -8.021 kcal/mol     [reported]
*         delH0f =     -4.931 kcal/mol     [reported]
*         S0PrTr =     49.185 cal/(mol*K)  [reported]
*    Cp coefficients [source: 82wag/eva               ]
*         T**0   =  0.78100000E+01
*         T**1   =  0.29600000E-02
*         T**-2  = -0.46000000E+05
*         Tlimit = 2026.85C
+----------------------------------------------------------------
-----
O2(g)                   O2
     sp.type =  gas     refstate
*    EQ3/6   =  com, alt, sup, pit
```

```
     revised =  18-may-1990
*    mol.wt. =    31.999 g/mol
     V0PrTr   =        0.000  cm**3/mol  [source:  supcrt92  [see
92joh/oel]]
****
     1 element(s):
      2.0000 O
****
     2 species in aqueous dissociation reaction:
    -1.0000  O2(g)                        1.0000  O2(g)
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-
H2O]:
       500.0000    0.0000  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    alternate name = O2(g)
*     ref-state data   [source: supcrt92 [see 92joh/oel], 60kel
]
*         delG0f =      0.000 kcal/mol     [reported]
*         delH0f =      0.000 kcal/mol     [reported]
*         S0PrTr =     49.029 cal/(mol*K)  [reported]
*    Cp coefficients [source: supcrt92 [see 92joh/oel]]
*         T**0   =  0.71600000E+01
*         T**1   =  0.10000000E-02
*         T**-2  = -0.40000000E+05
*         Tlimit = 2726.85C
+----------------------------------------------------------------
-----
solid solutions
+----------------------------------------------------------------
-----
references
+-----------------------------------------------------
ternäre ss ausgelagert!
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ties of
minerals, gases, aqueous species, and reactions from 1 to 5000
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1000degC:  Computers Geosci., 18, 899-947.

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```

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stop.

A.3 Appendix 3: NAGRA-PSI Database for PHREEQC

```
# Nagra/PSI Chemical Thermodynamic Data Base Version 01/01 (Nagra/PSI TDB 01/01)
# NAPSI_290502.DAT                                                                  LAST MOD. 26-AUG-
2002
#
###############################################################################################
#
# This file contains the Nagra/PSI TDB 01/01 formatted for PHREEQC. It was developed by
#
#      W. Hummel, U. Berner, E. Curti, and T. Thoenen from the
#                                                     Waste Management Laboratory
#                                                     Paul Scherrer Institut
#                                                     CH-5232 Villigen PSI
#                                                     Switzerland
#
#                                 and by F.J. Pearson from
#                                                     Ground-Water Geochemistry
#                                                     411 East Front St.
#                                                     New Bern, NC, 28560
#                                                     U.S.A.
#
# The Nagra/PSI Chemical Thermodynamic Data Base has been updated from version 05/92 to 01/01in order
# to support the ongoing safety assessment of a planned Swiss repository for high-level radioactive
# waste. This update is thoroughly documented in  Hummel et al. (2002).
# Data base version 05/92 distinguished between "core data" (Pearson & Berner 1991) and "supplemental
# data" (Pearson, Berner & Hummel 1992). Core data are for elements commonly found as major solutes
in
# natural waters. These data are well established and have not been changed to any significant de-
gree.
# Supplemental data comprise actinides and fission products, as well as Mn, Fe, Si and Al. The update
# from version 05/92 to 01/01 involved major revisions for most of the supplemental data. Altogether,
# more than 70% of the data base contents have been updated.
# Thermodynamic data for Th, Sn, Eu, Pd, Al, and solubility and metal complexation of sulfides and
# silicates were extensively reviewed.
# Data for Zr, Ni and Se were examined less rigorously, since these elements are currently being
# reviewed in phase II of the NEA TDB (Nuclear Energy Agency Thermochemical Data Base) project.
# Data for U, Np, Pu, Am and Tc recommended by the NEA TDB  project were included in the update.
# In several cases NEA recommendations were not accepted, detailed discussions can be found in Hummel
# et al. (2002).
#
#                               WARNING: TEMPERATURE EXTRAPOLATIONS
#
# The Nagra/PSI Chemical Thermodynamic Data Base 01/01 provides thermodynamic data for use at 25 C.
# PHREEQC allows the calculation of equilibria at temperatures other than 25 C. The temperature de-
# pendence of an equilibrium constant is taken care of by either an analytical expression of the form
#                                logK(T) = A + B T + C/T + D logT + E/T^2
# or by the integrated van't Hoff equation
#                        logK(T) = logK(T0) - (1/T - 1/T0) (deltaH[reaction]/(R ln10))
# if only the reaction enthalpy is known.
# Both types of data are available for some but not all of the species and phases contained in the
# data base.
# If a temperature differing from 25 C is used in a PHREEQC calculation, but reaction enthalpies or
# analytical expressions are known only for some of the species, PHREEQC will use the data valid at
```

```
# 25 C for all the other species. This may lead to inconsistencies, and it is therefore essential
that
# users examine outputs carefully to determine whether species with insufficient data for temperature
# extrapolations have had a significant effect on the calculation results.
# Users are advised to restrict their calculations at temperatures other than 25 C to subsets of the
# data base that contain all necessary data.
# In the light of these caveats, all lines containing data for temperature extrapolations (delta_h
for
# the integrated van't Hoff equation and -a_ for the analytical expression) have been commented out.
# In order to use these data, the #-signs at the beginning of the corresponding lines have to be
# deleted.
#
#                           WARNING: LIMITATIONS OF THIS DATA BASE
#
# Some of the stability constants in the Nagra/PSI TDB 01/01 are given as limiting values only or as
# approximate values:
#        Ni+2 + 2 CO3-2 = Ni(CO3)2-2                          logK < 6
#        Ni+2 + HCO3- = NiHCO3+                               logK approximately 1
#        Pd+2 + 2 Cl- + 2 H2O - 2 H+ = PdCl2(OH)2-2           logK < -7.0
#        TcO(OH)2 + 2 H+ - 2 H2O = TcO+2                      logK < 4
#        NpO2+2 + 3 H2O - 3 H+ = NpO2(OH)3-                   logK <= -19
#        NpO2+2 + 4 H2O - 4 H+ = NpO2(OH)4-2                  logK <= -33
#        PuO2+ + H2O - H+ = PuO2OH                            logK <= -9.73
# Since PHREEQC (and other speciation codes) cannot handle inequalities, the logK values of these
# equilibria are given as exact. This has to be kept in mind for the interpretation of calculation
# results.
# In the course of the review process for the Nagra/PSI TDB 01/01 we identified important cases of
# insufficient chemical knowledge leading to gaps in the data base. These are discussed in Hummel et
# al. (2002). In the case of ternary hydroxide-carbonate complexes of tetravalent actinides, reliable
# experimental data are only available for ThCO3(OH)3-, while data for the corresponding complexes of
# U+4, Np+4, and Pu+4 are missing. Hummel and Berner (2001) and Hummel and Berner (submitted) have
# estimated the missing complexation constants. However, these estimates are not part of the
# official Nagra/PSI TDB 01/01 and are therefore not part of this PHREEQC data file. Hummel and
Berner
# (2001) and Hummel and Berner (submitted) also estimated several missing complexation constants for
# hydroxide, carbonate, sulfate, fluoride, chloride, and silicate complexes of Np+3 and Pu+3. These
# constants are also not part of this PHREEQC data file.
#
#                                           NOTE: TIN
#
# Sn+2 and Sn+4 are not redox coupled in the Nagra/PSI TDB 01/01, i.e., there is no redox reaction
# relating Sn+2 with Sn+4. Therefore, two elements for tin appear in this data base, Sn for divalent
# tin (as, e. g., in SnOH+) and Tn for tetravalent tin (as, e. g., in Tn(OH)5-).
#
#
#                          NOTE: ACTIVITY COEFFICIENTS OF UNCHARGED SPECIES
#
# With the Nagra/PSI TDB 01/01 activity coefficients of uncharged species are calculated by PHREEQC
# according to the Setchenow equation:
#                                       ln(gamma) = b*I,
# where I is the ionic strength, and b = 0.1 (default value, because the Nagra/PSI TDB 01/01 does not
# provide any values of b for uncharged species). In order to use an activity coefficient of one for
# uncharged species,the #-signs at the beginning of the lines with "-gamma      0.00    0.00" have to
# be deleted.
#
#                                          REFERENCES:
```

```
#
# Hummel W., Berner U. (2001): Application of the Nagra/PSI Thermochemical Data Base 01/01: Solubili-
ty
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# Hummel W., Berner U. (submitted): Solubility of actinides in a planned underground repository:
#      Application of chemical thermodynamics for estimation of limiting values. Submitted to Applied
#      Geochemistry.
# Hummel W., Berner U., Curti E., Pearson F.J. & Thoenen T. (2002): Nagra/PSI Chemical Thermodynamic
#      Data Base 01/01. Universal Publishers/uPUBLISH.com USA, available from:
#      http://www.upublish.com/books/hummel.htm. Also issued as Nagra Technical Report NTB 02-16,
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# Pearson F.J. & Berner U. (1991): Nagra Thermochemical Data Base I. Core Data. Nagra Technical Re-
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#      NTB 91-17, Nagra, Wettingen, Switzerland.
# Pearson F.J., Berner U. & Hummel W. (1992): Nagra Thermochemical Data Base II. Supplemental Data
#      05/92. Nagra Technical Report NTB 91-18, Nagra, Wettingen, Switzerland.


SOLUTION_MASTER_SPECIES


#        ATOMIC WEIGHTS
#        Naturally occuring elements: IUPAC 1993 Table 1 rounded to 0.001
#        Radioelements: Mass number of longest-lived isotope
#
#
#
#  elemen     species        alk   gfw_formula element_gfw atomic
#                                                          number
#
H                H+          -1.0        H         1.008   #   1
H(0)             H2           0.0        H                 #
H(1)             H+          -1.0        H                 #
E                e-           0.0        0.0        0.0    #
O                H2O          0.0        O        15.999   #   8
O(0)             O2           0.0        O                 #
O(-2)            H2O          0.0        O                 #
Al              Al+3          0.0        Al       26.982   #  13
Am              Am+3          0.0        Am         243    #  95
As             HAsO4-2        0.0        As       74.922   #  33
As(3)          As(OH)3        0.0        As                #
As(5)          HAsO4-2        1.0        As                #
B              B(OH)3         0.0        B        10.812   #   5
Ba              Ba+2          0.0        Ba      137.328   #  56
Br               Br-          0.0        Br       79.904   #  35
C               HCO3-         1.0        C        12.011   #   6
C(+4)           HCO3-         1.0      HCO3-               #
C(-4)            CH4          0.0       CH4                #
Alkalinity      HCO3-         1.0      HCO3-      61.016   #
Ca              Ca+2          0.0        Ca       40.078   #  20
Cl               Cl-          0.0        Cl       35.453   #  17
Cs               Cs+          0.0        Cs      132.905   #  55
Eu              Eu+3          0.0        Eu      151.966   #  63
Eu(2)           Eu+2          0.0        Eu                #
Eu(3)           Eu+3          0.0        Eu                #
```

```
F              F-          0.0      F        18.998   #   9
Fe             Fe+2        0.0      Fe       55.845   #  26
Fe(2)          Fe+2        0.0      Fe                #
Fe(3)          Fe+3        0.0      Fe                #
I              I-          0.0      I        126.904  #  53
I(-1)          I-          0.0      I                 #
I(0)           I2          0.0      I                 #
K              K+          0.0      K        39.098   #  19
Li             Li+         0.0      Li        6.941   #   6
Mg             Mg+2        0.0      Mg       24.305   #  12
Mn             Mn+2        0.0      Mn       54.938   #  25
Mo             MoO4-2      0.0      Mo       95.941   #  42
N              NO3-        0.0      N        14.007   #   7
N(0)           N2          0.0      N2                #
N(-3)          NH4+        0.0      NH4               #
N(5)           NO3-        0.0      NO3               #
Na             Na+         0.0      Na        22.99   #  11
Nb             NbO3-       0.0      Nb       92.906   #  41
Ni             Ni+2        0.0      Ni       58.693   #  28
Np             NpO2+2      0.0      Np         237    #  93
Np(3)          Np+3        0.0      Np                #
Np(4)          Np+4        0.0      Np                #
Np(5)          NpO2+       0.0      Np                #
Np(6)          NpO2+2      0.0      Np                #
P              HPO4-2      1.0      P        30.974   #  15
Pd             Pd+2        0.0      Pd       106.421  #  46
Pu             PuO2+2      0.0      Pu         242    #  94
Pu(3)          Pu+3        0.0      Pu                #
Pu(4)          Pu+4        0.0      Pu                #
Pu(5)          PuO2+       0.0      Pu                #
Pu(6)          PuO2+2      0.0      Pu                #
Ra             Ra+2        0.0      Ra         226    #  88
S              SO4-2       0.0      S        32.067   #  16
S(-2)          HS-         1.0      HS                #
S(2)           S2O3-2      0.0      S2O3              #
S(4)           SO3-2       0.0      SO3               #
S(6)           SO4-2       0.0      SO4               #
Se             SeO3-2      0.0      Se       78.963   #  34
Se(4)          SeO3-2      0.0      Se                #
Se(-2)         H2Se        0.0      Se                #
Se(6)          HSeO4-      0.0      Se                #
Si             Si(OH)4     0.0      Si       28.086   #  14
Sn             Sn+2        0.0      Sn       118.711  #  50
Tn             Tn(OH)4     0.0     Tn(OH)4   186.739  #
Sr             Sr+2        0.0      Sr       87.621   #  38
Tc             TcO4-       0.0      Tc        98      #  43
Tc(7)          TcO4-       0.0      TcO4              #
Tc(4)          TcO(OH)2   -1.0     TcO(OH)2           #
Th             Th+4        0.0      Th       232.038  #  90
U              UO2+2       0.0      U        238.029  #  92
U(4)           U+4         0.0      U                 #
U(5)           UO2+        0.0      U                 #
U(6)           UO2+2       0.0      UO2               #
Zr             Zr+4        0.0      Zr       91.224   #  40

SOLUTION_SPECIES
```

```
# PMATCH MASTER SPECIES

H+                    = H+
    log_k      0.0
    -gamma     9.00    0.00

e-                    = e-
    log_k      0.0

H2O                   = H2O
    log_k      0.0

Al+3                  = Al+3
    log_k      0.0
    -gamma     6.65    0.19

Am+3                  = Am+3
    log_k      0.0
    -gamma     9.00    0.00

HAsO4-2               = HAsO4-2
    log_k      0.0
    -gamma     4.00    0.00

B(OH)3                = B(OH)3
    log_k      0.0
#    -gamma     0.00    0.00

Ba+2                  = Ba+2
    log_k      0.0
    -gamma     4.55    0.09

Br-                   = Br-
    log_k      0.0
    -gamma     3.00    0.00

HCO3-                 = HCO3-
    log_k      0.0
    -gamma     5.40    0.00

Ca+2                  = Ca+2
    log_k      0.0
    -gamma     4.86    0.15

Cl-                   = Cl-
    log_k      0.0
    -gamma     3.71    0.01

Cs+                   = Cs+
    log_k      0.0
    -gamma     2.50    0.00

Eu+3                  = Eu+3
    log_k      0.0
    -gamma     9.00    0.00
```

```
F-                    = F-
    log_k      0.0
    -gamma     3.46    0.08

Fe+2                  = Fe+2
    log_k      0.0
    -gamma     5.08    0.16

I-                    = I-
    log_k      0.0
    -gamma     3.00    0.00

K+                    = K+
    log_k      0.0
    -gamma     3.71    0.01

Li+                   = Li+
    log_k      0.0
    -gamma     4.76    0.20

Mg+2                  = Mg+2
    log_k      0.0
    -gamma     5.46    0.22

Mn+2                  = Mn+2
    log_k      0.0
    -gamma     7.04    0.22

MoO4-2                = MoO4-2
    log_k      0.0
    -gamma     5.00    0.00

NO3-                  = NO3-
    log_k      0.0
    -gamma     3.00    0.00

Na+                   = Na+
    log_k      0.0
    -gamma     4.32    0.06

NbO3-                 = NbO3-
    log_k      0.0
    -gamma     3.00    0.00

Ni+2                  = Ni+2
    log_k      0.0
    -gamma     5.51    0.22

NpO2+2                = NpO2+2
    log_k      0.0
    -gamma     4.00    0.00

HPO4-2                = HPO4-2
    log_k      0.0
    -gamma     4.00    0.00
```

```
Pd+2                = Pd+2
    log_k      0.0
    -gamma     5.50    0.00

PuO2+2              = PuO2+2
    log_k      0.0
    -gamma     4.00    0.00

Ra+2                = Ra+2
    log_k      0.0
    -gamma     5.00    0.00

SO4-2               = SO4-2
    log_k      0.0
    -gamma     5.31   -0.07

SeO3-2              = SeO3-2
    log_k      0.0
    -gamma     4.50    0.00

Si(OH)4             = Si(OH)4
    log_k      0.0
#    -gamma     0.00    0.00

Sn+2                = Sn+2
    log_k      0.0
    -gamma     6.00    0.00

Sr+2                = Sr+2
    log_k      0.0
    -gamma     5.48    0.11

TcO4-               = TcO4-
    log_k      0.0
    -gamma     3.50    0.00

Th+4                = Th+4
    log_k      0.0
    -gamma    11.00    0.00

UO2+2               = UO2+2
    log_k      0.0
    -gamma     4.00    0.00

Zr+4                = Zr+4
    log_k      0.0
    -gamma    11.00    0.00

Tn(OH)4             = Tn(OH)4
    log_k      0.0
#    -gamma     0.00    0.00


# PMATCH SECONDARY MASTER SPECIES
```

```
 +2.000H+                  +2.000e-                  = H2
    log_k      -3.1055
#    delta_h    -4.0390
#     -a_e   -7.645285E+01 -6.533210E-03  3.037267E+03  2.631234E+01 -0.000000E+00
#    -gamma       0.00    0.00

 +2.000H2O                 -4.000H+                  -4.000e-                  = O2
    log_k     -85.9862
#    delta_h   559.6010
#     -a_e   -2.163762E+01  4.101330E-03 -2.747501E+04  1.074196E+01 -0.000000E+00
#    -gamma       0.00    0.00

 +1.000HAsO4-2                +4.000H+                     +2.000e-                      -1.000H2O
= As(OH)3
    log_k      28.4412
#    delta_h  -121.6899
#     -a_e   -4.012500E+00  0.000000E+00  6.852070E+03  3.827857E+00  0.000000E+00
#    -gamma       0.00    0.00

 +1.000HCO3-                  +9.000H+                     +8.000e-                      -3.000H2O
= CH4
    log_k      27.8493
#    delta_h  -255.8820
#     -a_e    1.366894E+02  4.100659E-02  2.778061E+03 -5.730937E+01  1.015550E+06
#    -gamma       0.00    0.00

 +2.000NO3-                  +12.000H+                    +10.000e-                      -6.000H2O
= N2
    log_k     207.2676
#    delta_h -1311.7170
#     -a_e   -2.637226E+02  0.000000E+00  7.925347E+04  8.291702E+01 -0.000000E+00
#    -gamma       0.00    0.00

 +1.000NO3-                  +10.000H+                     +8.000e-                      -3.000H2O
= NH4+
    log_k     119.1372
#    delta_h  -783.9000
#     -a_e   -1.151682E+02  0.000000E+00  4.526337E+04  3.333745E+01 -0.000000E+00
    -gamma       2.50    0.00

 +1.000NpO2+2                 +4.000H+                     +3.000e-                      -2.000H2O
= Np+3
    log_k      33.5000
#    delta_h  -238.1600
#     -a_e   -8.213169E+00  0.000000E+00  1.244018E+04  0.000000E+00 -0.000000E+00
    -gamma       9.00    0.00

 +1.000NpO2+2                 +4.000H+                     +2.000e-                      -2.000H2O
= Np+4
    log_k      29.8000
#    delta_h  -266.9600
#     -a_e   -1.695543E+01  0.000000E+00  1.394454E+04  0.000000E+00 -0.000000E+00
    -gamma      11.00    0.00

 +1.000NpO2+2              +1.000e-                  = NpO2+
    log_k      19.5900
```

```
#    delta_h  -117.5000
#    -a_e   -9.810953E-01  0.000000E+00  6.137562E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000PuO2+2                 +4.000H+                      +3.000e-                      -2.000H2O
= Pu+3
    log_k      50.9700
#    delta_h  -341.4600
#    -a_e   -8.861393E+00  0.000000E+00  1.783602E+04  0.000000E+00 -0.000000E+00
    -gamma      9.00    0.00

 +1.000PuO2+2                 +4.000H+                      +2.000e-                      -2.000H2O
= Pu+4
    log_k      33.2800
#    delta_h  -289.5600
#    -a_e   -1.746350E+01  0.000000E+00  1.512504E+04  0.000000E+00 -0.000000E+00
    -gamma     11.00    0.00

 +1.000PuO2+2              +1.000e-                  = PuO2+
    log_k      15.8200
#    delta_h   -88.1000
#    -a_e    3.679107E-01  0.000000E+00  4.601865E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +2.000SO4-2                 +10.000H+                      +8.000e-                      -5.000H2O
= S2O3-2
    log_k      38.0145
#    delta_h  -258.9700
#    -a_e   -3.450029E+02  0.000000E+00  2.855787E+04  1.160806E+02 -0.000000E+00
    -gamma      4.00    0.00

 +1.000SO4-2                  +9.000H+                      +8.000e-                      -4.000H2O
= HS-
    log_k      33.6900
#    delta_h  -250.2800
#    -a_e   -1.956803E+02  0.000000E+00  2.133208E+04  6.378207E+01 -0.000000E+00
    -gamma      3.50    0.00

 +1.000TcO4-                  +4.000H+                      +3.000e-                      -1.000H2O
= TcO(OH)2
    log_k      29.4000
#    -a_e    2.940000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000UO2+2                  +4.000H+                      +2.000e-                      -2.000H2O
= U+4
    log_k       9.0380
#    delta_h  -143.8600
#    -a_e   -1.616564E+01  0.000000E+00  7.514465E+03  0.000000E+00 -0.000000E+00
    -gamma     11.00    0.00

 +1.000UO2+2               +1.000e-                  = UO2+
    log_k       1.4840
#    delta_h    -6.1270
#    -a_e    4.105766E-01  0.000000E+00  3.200412E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00
```

```
 +1.000H2O                 -1.000H+                  = OH-
    log_k     -13.9995
#    delta_h    55.9043
#    -a_e   -2.839710E+02 -5.069842E-02  1.332300E+04  1.022445E+02 -1.119669E+06
    -gamma     10.65    0.00

 +1.000H+                  -1.000H2O                 +1.000HCO3-               = CO2
    log_k       6.3519
#    delta_h    -9.1092
#    -a_e    3.563094E+02  6.091964E-02 -2.183437E+04 -1.268339E+02  1.684915E+06
#    -gamma      0.00    0.00

 -1.000H+                  +1.000HCO3-               = CO3-2
    log_k     -10.3289
#    delta_h    14.9007
#    -a_e   -1.078871E+02 -3.252849E-02  5.151790E+03  3.892561E+01 -5.637139E+05
    -gamma      5.40    0.00

 +1.000HPO4-2              +2.000H+                  = H3PO4
    log_k       9.3520
#    delta_h     4.8800
#    -a_e    1.020695E+01  0.000000E+00 -2.549047E+02  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +1.000HPO4-2              +1.000H+                  = H2PO4-
    log_k       7.2120
#    delta_h    -3.6000
#    -a_e    6.581296E+00  0.000000E+00  1.880444E+02  0.000000E+00 -0.000000E+00
    -gamma      4.50    0.00

 +1.000HPO4-2              -1.000H+                  = PO4-3
    log_k     -12.3500
#    delta_h    14.6000
#    -a_e   -9.792144E+00  0.000000E+00 -7.626247E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000NH4+                -1.000H+                  = NH3
    log_k      -9.2370
#    delta_h    52.0900
#    -a_e   -1.110615E-01  0.000000E+00 -2.720899E+03  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +1.000Fe+2                -1.000e-                  = Fe+3
    log_k     -13.0200
#    delta_h    40.5000
#    -a_e   -5.924578E+00  0.000000E+00 -2.115500E+03  0.000000E+00 -0.000000E+00
    -gamma      9.00    0.00

 +1.000Eu+3                +1.000e-                  = Eu+2
    log_k      -5.9200
#    delta_h    78.1000
#    -a_e    7.761165E+00  0.000000E+00 -4.079520E+03  0.000000E+00 -0.000000E+00
    -gamma      6.00    0.00

 +1.000Si(OH)4             -1.000H+                  = SiO(OH)3-
```

```
    log_k      -9.8100
#    delta_h    25.6000
#    -a_e   -5.324993E+00  0.000000E+00 -1.337205E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Si(OH)4              -2.000H+                  = SiO2(OH)2-2
    log_k     -23.1400
#    delta_h    75.0000
#    -a_e   -1.000033E+01  0.000000E+00 -3.917592E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Al+3                 +4.000H2O                 -4.000H+                  = Al(OH)4-
    log_k     -22.8797
#    delta_h   180.8990
#    -a_e    2.886657E+01  0.000000E+00 -1.034188E+04 -6.894257E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000SO4-2                   +2.000H+                      +2.000e-                      -1.000H2O
= SO3-2
    log_k      -3.3974
#    delta_h   -11.9900
#    -a_e   -1.576202E+02  0.000000E+00  7.398158E+03  5.229849E+01 -0.000000E+00
    -gamma      4.50    0.00

 +2.000I-                   -2.000e-                  = I2
    log_k      20.9500
#    -a_e    2.095000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      0.00    0.00

 +1.000SeO3-2                  +1.000H2O                     -1.000H+                      -2.000e-
= HSeO4-
    log_k     -25.5800
#    -a_e   -2.558000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000SeO3-2                  +8.000H+                      +6.000e-                      -3.000H2O
= H2Se
    log_k      57.3900
#    -a_e    5.739000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00


# PMATCH PRODUCT SPECIES

 +1.000Al+3                 +1.000F-                  = AlF+2
    log_k       7.0800
#    delta_h     4.8000
#    -a_e    7.920939E+00  0.000000E+00 -2.507259E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Al+3                 +2.000F-                  = AlF2+
    log_k      12.7300
#    delta_h     8.1000
#    -a_e    1.414908E+01  0.000000E+00 -4.231000E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00
```

```
 +1.000Al+3                 +3.000F-                   = AlF3
    log_k      16.7800
#    delta_h      8.9000
#    -a_e    1.833924E+01  0.000000E+00 -4.648876E+02  0.000000E+00 -0.000000E+00
#    -gamma       0.00    0.00

 +1.000Al+3                 +4.000F-                   = AlF4-
    log_k      19.2900
#    delta_h     10.1000
#    -a_e    2.105948E+01  0.000000E+00 -5.275691E+02  0.000000E+00 -0.000000E+00
    -gamma       4.00    0.00

 +1.000Al+3                 +5.000F-                   = AlF5-2
    log_k      20.3000
#    delta_h      7.0000
#    -a_e    2.152637E+01  0.000000E+00 -3.656420E+02  0.000000E+00 -0.000000E+00
    -gamma       4.00    0.00

 +1.000Al+3                 +6.000F-                   = AlF6-3
    log_k      20.3000
#    delta_h      0.5000
#    -a_e    2.038760E+01  0.000000E+00 -2.611728E+01  0.000000E+00 -0.000000E+00
    -gamma       4.00    0.00

 +1.000Al+3                 +2.000H2O                  -2.000H+                   = Al(OH)2+
    log_k     -10.5943
#    delta_h     98.2820
#    -a_e   -4.036210E+01  0.000000E+00 -3.042071E+03  1.615359E+01  0.000000E+00
    -gamma       4.00    0.00

 +1.000Al+3                 +3.000H2O                  -3.000H+                   = Al(OH)3
    log_k     -16.4328
#    delta_h    144.7040
#    -a_e   -4.553311E+01  0.000000E+00 -5.134577E+03  1.872013E+01  0.000000E+00
#    -gamma       0.00    0.00

 +1.000Al+3                 +1.000SO4-2                = AlSO4+
    log_k       3.9000
#    -a_e    3.900000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma       4.00    0.00

 +1.000As(OH)3              +1.000H2O                  -1.000H+                   = As(OH)4-
    log_k      -9.2314
#    delta_h     27.3399
#    -a_e   -4.441558E+00  0.000000E+00 -1.428089E+03  0.000000E+00 -0.000000E+00
    -gamma       4.50    0.00

 +1.000HAsO4-2              -1.000H+                   = AsO4-3
    log_k     -11.6036
#    delta_h     18.2000
#    -a_e   -8.414995E+00  0.000000E+00 -9.506691E+02  0.000000E+00 -0.000000E+00
    -gamma       4.00    0.00

 +1.000B(OH)3               +1.000H2O                  -1.000H+                   = B(OH)4-
    log_k      -9.2352
#    delta_h     14.0528
```

```
#    -a_e    3.496000E+00 -1.722150E-02 -2.264920E+03  0.000000E+00  0.000000E+00
    -gamma      4.50    0.00

 +1.000Ba+2                 -1.000H+                   +1.000HCO3-                = BaCO3
    log_k      -7.6157
#    delta_h    29.7422
#    -a_e   -1.077741E+02 -2.380749E-02  5.151790E+03  3.892561E+01 -5.637139E+05
#    -gamma      0.00    0.00

 +1.000Ba+2                 +1.000HCO3-                = BaHCO3+
    log_k       0.9816
#    delta_h    23.2621
#    -a_e   -3.093800E+00  1.366900E-02  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Ba+2                 +1.000H2O                  -1.000H+                   = BaOH+
    log_k     -13.4700
#    -a_e   -1.347000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Ba+2                 +1.000SO4-2                = BaSO4
    log_k       2.7000
#    -a_e    2.700000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Ca+2                 -1.000H+                   +1.000HCO3-                = CaCO3
    log_k      -7.1048
#    delta_h    29.7327
#    -a_e   -1.336619E+03 -3.319725E-01  4.066454E+04  5.247436E+02 -5.637139E+05
#    -gamma      0.00    0.00

 +1.000Ca+2                 +1.000F-                   = CaF+
    log_k       0.9400
#    delta_h    17.2381
#    -a_e    3.960036E+00  0.000000E+00 -9.004236E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Ca+2                 +1.000HCO3-                = CaHCO3+
    log_k       1.1057
#    delta_h    11.2630
#    -a_e    1.209120E+03  3.129400E-01 -3.476505E+04 -4.787820E+02  0.000000E+00
    -gamma      4.00    0.00

 +1.000Ca+2                 +1.000H2O                  -1.000H+                   = CaOH+
    log_k     -12.7800
#    -a_e   -1.278000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Ca+2                 +1.000SO4-2                = CaSO4
    log_k       2.3000
#    delta_h     6.9036
#    -a_e    3.509480E+00  0.000000E+00 -3.606066E+02  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +2.000H2O                  -2.000H+                   +1.000Fe+3                 = Fe(OH)2+
    log_k      -5.6700
```

```
#    delta_h    71.5475
#    -a_e    6.864807E+00  0.000000E+00 -3.737253E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +3.000H2O                  -3.000H+                   +1.000Fe+3                 = Fe(OH)3
    log_k     -12.5600
#    delta_h   103.7643
#    -a_e    5.619048E+00  0.000000E+00 -5.420083E+03  0.000000E+00 -0.000000E+00
#    -gamma       0.00    0.00

 +4.000H2O                  -4.000H+                   +1.000Fe+3                 = Fe(OH)4-
    log_k     -21.6000
#    delta_h   133.4707
#    -a_e    1.783479E+00  0.000000E+00 -6.971784E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +2.000SO4-2                +1.000Fe+3                 = Fe(SO4)2-
    log_k       5.3800
#    delta_h    19.2475
#    -a_e    8.752077E+00  0.000000E+00 -1.005385E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +2.000H2O                  -2.000H+                   +2.000Fe+3                 = Fe2(OH)2+4
    log_k      -2.9500
#    delta_h    56.4862
#    -a_e    6.946133E+00  0.000000E+00 -2.950532E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +4.000H2O                  -4.000H+                   +3.000Fe+3                 = Fe3(OH)4+5
    log_k      -6.3000
#    delta_h    59.8345
#    -a_e    4.182741E+00  0.000000E+00 -3.125429E+03  0.000000E+00 -0.000000E+00
    -gamma      9.00    0.00

 +1.000Fe+2                 +1.000Cl-                  = FeCl+
    log_k       0.1400
#    -a_e    1.400000E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Cl-                  +1.000Fe+3                 = FeCl+2
    log_k       1.4800
#    delta_h    23.4315
#    -a_e    5.585096E+00  0.000000E+00 -1.223934E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +2.000Cl-                  +1.000Fe+3                 = FeCl2+
    log_k       2.1300
#    -a_e    2.130000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +3.000Cl-                  +1.000Fe+3                 = FeCl3
    log_k       1.1300
#    -a_e    1.130000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma       0.00    0.00

 +1.000Fe+2                 +1.000CO3-2                = FeCO3
```

```
    log_k      5.5
#    -a_e   -5.949000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Fe+2                 +2.000CO3-2                 = Fe(CO3)2-2
    log_k      7.1
#    -a_e    0.000000E+00   0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Fe+2                 +1.000F-                    = FeF+
    log_k       1.0000
#    -a_e    1.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000F-                   +1.000Fe+3                  = FeF+2
    log_k       6.2000
#    delta_h    11.2970
#    -a_e    8.179185E+00  0.000000E+00 -5.900939E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +2.000F-                   +1.000Fe+3                  = FeF2+
    log_k      10.8000
#    delta_h    20.0840
#    -a_e    1.431863E+01  0.000000E+00 -1.049079E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +3.000F-                   +1.000Fe+3                  = FeF3
    log_k      14.0000
#    delta_h    22.5950
#    -a_e    1.795854E+01  0.000000E+00 -1.180240E+03  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

# +1.000Fe+2                 +1.000HCO3-                 = FeHCO3+
#    log_k       2.0000
##    -a_e    2.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      4.00    0.00

 +1.000Fe+2                 +1.000H+                    +1.000SO4-2                 = FeHSO4+
    log_k       3.0680
#    -a_e    3.068000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000H+                   +1.000SO4-2                 +1.000Fe+3                  = FeHSO4+2
    log_k       4.4680
#    -a_e    4.468000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Fe+2                 +1.000H2O                   -1.000H+                    = FeOH+
    log_k      -9.5000
#    delta_h    55.2288
#    -a_e    1.758424E-01  0.000000E+00 -2.884852E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000H2O                  -1.000H+                    +1.000Fe+3                  = FeOH+2
    log_k      -2.1900
#    delta_h    43.5147
```

```
#    -a_e    5.433584E+00  0.000000E+00 -2.272971E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000SO4-2                +1.000Fe+3                 = FeSO4+
    log_k       4.0400
#    delta_h    16.3605
#    -a_e    6.906288E+00  0.000000E+00 -8.545836E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Fe+2                 +1.000SO4-2                = FeSO4
    log_k       2.2500
#    delta_h    13.5143
#    -a_e    4.617649E+00  0.000000E+00 -7.059146E+02  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +1.000HAsO4-2              +1.000H+                   = H2AsO4-
    log_k       6.7645
#    delta_h    -3.2200
#    -a_e    6.200347E+00  0.000000E+00  1.681953E+02  0.000000E+00 -0.000000E+00
    -gamma      4.50    0.00

 +1.000SeO3-2               +2.000H+                   = H2SeO3
    log_k      11.2000
#    delta_h    12.0900
#    -a_e    1.331811E+01  0.000000E+00 -6.315159E+02  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +1.000HAsO4-2              +2.000H+                   = H3AsO4
    log_k       9.0273
#    delta_h     3.8400
#    -a_e    9.700054E+00  0.000000E+00 -2.005807E+02  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +1.000H+                   +1.000F-                   = HF
    log_k       3.1760
#    delta_h    13.3063
#    -a_e   -2.033000E+00  1.264500E-02  4.290100E+02  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000H+                   +2.000F-                   = HF2-
    log_k       3.6201
#    delta_h    15.2000
#    -a_e   -8.943484E+01  0.000000E+00  3.467009E+03  3.290711E+01 -0.000000E+00
    -gamma      4.00    0.00

 +1.000H2Se                 -1.000H+                   = HSe-
    log_k      -3.8000
#    -a_e   -3.800000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      3.50    0.00

 +1.000SeO3-2               +1.000H+                   = HSeO3-
    log_k       8.4000
#    delta_h     5.0200
#    -a_e    9.279482E+00  0.000000E+00 -2.622175E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00
```

```
 +1.000H+                   +1.000SO3-2                = HSO3-
    log_k       7.2202
#    delta_h   120.9500
#    -a_e    2.841007E+01  0.000000E+00 -6.317771E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000H+                   +1.000SO4-2                = HSO4-
    log_k       1.9878
#    delta_h    16.1276
#    -a_e   -5.688900E+01  6.473000E-03  2.307900E+03  1.988580E+01  0.000000E+00
    -gamma      4.00    0.00

 +1.000K+                   +1.000H2O                  -1.000H+                   = KOH
    log_k     -14.4600
#    -a_e   -1.446000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000K+                   +1.000SO4-2                = KSO4-
    log_k       0.8500
#    delta_h     9.4140
#    -a_e    2.499291E+00  0.000000E+00 -4.917362E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Li+                  +1.000H2O                  -1.000H+                   = LiOH
    log_k     -13.6400
#    -a_e   -1.364000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Li+                  +1.000SO4-2                = LiSO4-
    log_k       0.6400
#    -a_e    6.400000E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Mg+2                 -1.000H+                   +1.000HCO3-                = MgCO3
    log_k      -7.3492
#    delta_h    26.2518
#    -a_e   -1.068961E+02 -2.585849E-02  5.151790E+03  3.892561E+01 -5.637139E+05
#    -gamma      0.00    0.00

 +1.000Mg+2                 +1.000F-                   = MgF+
    log_k       1.8200
#    delta_h    13.3888
#    -a_e    4.165659E+00  0.000000E+00 -6.993582E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Mg+2                 +1.000HCO3-                = MgHCO3+
    log_k       1.0682
#    delta_h     3.2881
#    -a_e   -5.921500E+01  0.000000E+00  2.537455E+03  2.092298E+01  0.000000E+00
    -gamma      4.00    0.00

 +1.000Mg+2                 +1.000H2O                  -1.000H+                   = MgOH+
    log_k     -11.4400
#    -a_e   -1.144000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00
```

```
 +1.000Mg+2                 +1.000SO4-2                = MgSO4
    log_k       2.3700
#    delta_h    19.0372
#    -a_e    5.705234E+00  0.000000E+00 -9.943999E+02  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +1.000Mn+2                 +1.000Cl-                  = MnCl+
    log_k       0.6100
#    -a_e    6.100000E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Mn+2                 +2.000Cl-                  = MnCl2
    log_k       0.2500
#    -a_e    2.500000E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Mn+2                 +3.000Cl-                  = MnCl3-
    log_k      -0.3100
#    -a_e   -3.100000E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Mn+2                 +1.000HCO3-                -1.000H+                   = MnCO3
    log_k      -5.4290
#    -a_e   -5.429000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Mn+2                 +1.000F-                   = MnF+
    log_k       0.8400
#    -a_e    8.400000E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Mn+2                 +1.000HCO3-                = MnHCO3+
    log_k       1.9500
#    -a_e    1.950000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Mn+2                 +1.000H2O                  -1.000H+                   = MnOH+
    log_k     -10.5900
#    delta_h    60.2496
#    -a_e   -3.453554E-02  0.000000E+00 -3.147112E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Mn+2                 +1.000SO4-2                = MnSO4
    log_k       2.2500
#    delta_h    14.1001
#    -a_e    4.720272E+00  0.000000E+00 -7.365116E+02  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +1.000Na+                  -1.000H+                   +1.000HCO3-                = NaCO3-
    log_k      -9.0590
#    delta_h    52.1800
#    -a_e    8.270610E-02  0.000000E+00 -2.725600E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Na+                  +1.000F-                   = NaF
    log_k      -0.2400
```

```
#    -a_e   -2.400000E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Na+                  +1.000HCO3-                = NaHCO3
    log_k      -0.2500
#    -a_e   -2.500000E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Na+                  +1.000H2O                  -1.000H+                   = NaOH
    log_k     -14.1800
#    -a_e   -1.418000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Na+                  +1.000SO4-2                = NaSO4-
    log_k       0.7000
#    delta_h     4.6861
#    -a_e    1.520981E+00  0.000000E+00 -2.447754E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000NbO3-                +2.000H+                   +1.000H2O                  = Nb(OH)4+
    log_k       6.896
# log_k entered manually, -a_e changed accordingly
#    -a_e    6.896000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000NbO3-                +1.000H+                   +2.000H2O                  = Nb(OH)5
    log_k       7.344
# log_k entered manually, -a_e changed accordingly
#    -a_e    7.344000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Pd+2                 +1.000Cl-                  = PdCl+
    log_k       5.1000
#    -a_e    5.100000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Pd+2                 +2.000Cl-                  = PdCl2
    log_k       8.3000
#    -a_e    8.300000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Pd+2                 +3.000Cl-                  = PdCl3-
    log_k      10.9000
#    -a_e    1.090000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Pd+2                 +4.000Cl-                  = PdCl4-2
    log_k      11.7000
#    -a_e    1.170000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Pd+2                 +1.000NH3                  = PdNH3+2
    log_k       9.6000
#    -a_e    9.600000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00
```

```
 +1.000Pd+2                 +2.000NH3                  = Pd(NH3)2+2
    log_k      18.5000
#    -a_e    1.850000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Pd+2                 +3.000NH3                  = Pd(NH3)3+2
    log_k      26.0000
#    -a_e    2.600000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Pd+2                 +4.000NH3                  = Pd(NH3)4+2
    log_k      32.8000
#    -a_e    3.280000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Pd+2                 -2.000H+                   +2.000H2O                  = Pd(OH)2
    log_k      -4.0000
#    -a_e   -4.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Pd+2                 -3.000H+                   +3.000H2O                  = Pd(OH)3-
    log_k     -15.5000
#    -a_e   -1.550000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000HSeO4-               -1.000H+                   = SeO4-2
    log_k      -1.8000
#    delta_h   -23.8000
#    -a_e   -5.969655E+00  0.000000E+00  1.243183E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Sr+2                 -1.000H+                   +1.000HCO3-                = SrCO3
    log_k      -7.5238
#    delta_h     36.7281
#    -a_e   -1.089061E+02 -1.970249E-02  5.151790E+03  3.892561E+01 -5.637139E+05
#    -gamma      0.00    0.00

 +1.000Sr+2                 +1.000HCO3-                = SrHCO3+
    log_k       1.1846
#    delta_h     25.3008
#    -a_e   -3.248000E+00  1.486700E-02  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Sr+2                 +1.000H2O                  -1.000H+                   = SrOH+
    log_k     -13.2900
#    -a_e   -1.329000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Sr+2                 +1.000SO4-2                = SrSO4
    log_k       2.2900
#    delta_h      8.7027
#    -a_e    3.814678E+00  0.000000E+00 -4.545828E+02  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +1.000Am+3                 +1.000H2O                  -1.000H+                   = AmOH+2
    log_k      -7.3000
```

```
#    -a_e   -7.300000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Am+3                 +2.000H2O                  -2.000H+                   = Am(OH)2+
    log_k     -15.2000
#    -a_e   -1.520000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Am+3                 +3.000H2O                  -3.000H+                   = Am(OH)3
    log_k     -25.7000
#    -a_e   -2.570000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Am+3                 +1.000F-                   = AmF+2
    log_k       3.4000
#    -a_e    3.400000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Am+3                 +2.000F-                   = AmF2+
    log_k       5.8000
#    -a_e    5.800000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Am+3                 +1.000Cl-                  = AmCl+2
    log_k       1.0500
#    -a_e    1.050000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Am+3                 +1.000SO4-2                = AmSO4+
    log_k       3.8500
#    -a_e    3.850000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Am+3                 +2.000SO4-2                = Am(SO4)2-
    log_k       5.4000
#    -a_e    5.400000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Am+3                 +1.000NO3-                 = AmNO3+2
    log_k       1.3300
#    -a_e    1.330000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Am+3                 +1.000H2PO4-               = AmH2PO4+2
    log_k       3.0000
#    -a_e    3.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Am+3                 +1.000CO3-2                = AmCO3+
    log_k       7.8000
#    -a_e    7.800000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Am+3                 +2.000CO3-2                = Am(CO3)2-
    log_k      12.3000
#    -a_e    1.230000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
```

```
    -gamma      4.00    0.00

 +1.000Am+3                 +3.000CO3-2                = Am(CO3)3-3
    log_k      15.2000
#    -a_e    1.520000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Eu+3                 +1.000H2O                  -1.000H+                   = EuOH+2
    log_k      -7.6400
#    -a_e   -7.640000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Eu+3                 +2.000H2O                  -2.000H+                   = Eu(OH)2+
    log_k     -15.1000
#    -a_e   -1.510000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Eu+3                 +3.000H2O                  -3.000H+                   = Eu(OH)3
    log_k     -23.7000
#    -a_e   -2.370000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Eu+3                 +4.000H2O                  -4.000H+                   = Eu(OH)4-
    log_k     -36.2000
#    -a_e   -3.620000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Eu+3                 +1.000CO3-2                = EuCO3+
    log_k       8.1000
#    -a_e    8.100000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Eu+3                 +2.000CO3-2                = Eu(CO3)2-
    log_k      12.1000
#    -a_e    1.210000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Eu+3                 +1.000SO4-2                = EuSO4+
    log_k       3.9500
#    -a_e    3.950000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Eu+3                 +2.000SO4-2                = Eu(SO4)2-
    log_k       5.7000
#    -a_e    5.700000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Eu+3                 +1.000F-                   = EuF+2
    log_k       3.8000
#    -a_e    3.800000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Eu+3                 +2.000F-                   = EuF2+
    log_k       6.5000
#    -a_e    6.500000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00
```

```
 +1.000Eu+3                 +1.000Cl-                  = EuCl+2
    log_k       1.1000
#    -a_e    1.100000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Eu+3                 +2.000Cl-                  = EuCl2+
    log_k       1.5000
#    -a_e    1.500000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Ni+2                 +1.000H2O                  -1.000H+                   = NiOH+
    log_k      -9.5000
#    delta_h    50.0000
#    -a_e   -7.402203E-01  0.000000E+00 -2.611728E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Ni+2                 +2.000H2O                  -2.000H+                   = Ni(OH)2
    log_k     -18.0000
#    delta_h    85.7600
#    -a_e   -2.975226E+00  0.000000E+00 -4.479636E+03  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +1.000Ni+2                 +3.000H2O                  -3.000H+                   = Ni(OH)3-
    log_k     -29.7000
#    delta_h   120.5900
#    -a_e   -8.573163E+00  0.000000E+00 -6.298966E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Ni+2                 +4.000H2O                  -4.000H+                   = Ni(OH)4-2
    log_k     -44.9000
#    -a_e   -4.490000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +2.000Ni+2                 +1.000H2O                  -1.000H+                   = Ni2OH+3
    log_k      -9.8000
#    delta_h    35.0000
#    -a_e   -3.668154E+00  0.000000E+00 -1.828210E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +4.000Ni+2                 +4.000H2O                  -4.000H+                   = Ni4(OH)4+4
    log_k     -27.9000
#    delta_h   170.0000
#    -a_e    1.883251E+00  0.000000E+00 -8.879876E+03  0.000000E+00 -0.000000E+00
    -gamma      5.00    0.00

 +1.000Ni+2                 +1.000F-                   = NiF+
    log_k       1.3000
#    -a_e    1.300000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Ni+2                 +1.000Cl-                  = NiCl+
    log_k       0.4000
#    -a_e    4.000000E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00
```

```
 +1.000Ni+2                 +2.000Cl-                  = NiCl2
    log_k       0.9600
#    -a_e    9.600000E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Ni+2                 +1.000HS-                  = NiHS+
    log_k       5.5000
#    -a_e    5.500000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Ni+2                 +1.000SO4-2                = NiSO4
    log_k       2.3100
#    delta_h    13.9750
#    -a_e    4.758358E+00  0.000000E+00 -7.299781E+02  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +1.000Ni+2                 +2.000SO4-2                = Ni(SO4)2-2
    log_k       3.2000
#    -a_e    3.200000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Ni+2                 +1.000NO3-                 = NiNO3+
    log_k       0.4000
#    -a_e    4.000000E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Ni+2                 +2.000NO3-                 = Ni(NO3)2
    log_k      -0.6000
#    -a_e   -6.000000E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Ni+2                 +1.000NH3                  = NiNH3+2
    log_k       2.7000
#    -a_e    2.700000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Ni+2                 +2.000NH3                  = Ni(NH3)2+2
    log_k       4.9000
#    -a_e    4.900000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Ni+2                 +3.000NH3                  = Ni(NH3)3+2
    log_k       6.5000
#    -a_e    6.500000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Ni+2                 +4.000NH3                  = Ni(NH3)4+2
    log_k       7.6000
#    -a_e    7.600000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Ni+2                 +5.000NH3                  = Ni(NH3)5+2
    log_k       8.3000
#    -a_e    8.300000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00
```

```
 +1.000Ni+2                +6.000NH3                 = Ni(NH3)6+2
    log_k       8.2000
#    -a_e    8.200000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Ni+2                +1.000H2PO4-              = NiH2PO4+
    log_k       1.5440
#    -a_e    1.544000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Ni+2                +1.000HPO4-2              = NiHPO4
    log_k       2.9340
#    -a_e    2.934000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Ni+2                +1.000PO4-3               = NiPO4-
    log_k       8.3740
#    -a_e    8.374000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Ni+2                   +2.000HPO4-2                 +1.000H+                       -1.000H2O
= NiHP2O7-
    log_k       9.2580
#    -a_e    9.258000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Ni+2                +2.000HPO4-2              -1.000H2O                 = NiP2O7-2
    log_k       3.0880
#    delta_h     9.9170
#    -a_e    4.825415E+00  0.000000E+00 -5.180102E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Ni+2                +1.000CO3-2               = NiCO3
    log_k       4.0000
#    -a_e    4.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Ni+2                +2.000CO3-2               = Ni(CO3)2-2
    log_k       6.0000
#    -a_e    6.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Ni+2                +1.000HCO3-               = NiHCO3+
    log_k       1.0000
#    -a_e    1.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Np+3                +1.000H2O                 -1.000H+                  = NpOH+2
    log_k      -6.8000
#    -a_e   -6.800000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      5.00    0.00

 +1.000Np+4                +1.000H2O                 -1.000H+                  = NpOH+3
    log_k      -0.2900
#    -a_e   -2.900000E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00
```

```
 +1.000Np+4                 +4.000H2O                  -4.000H+                   = Np(OH)4
    log_k      -9.8000
#    -a_e   -9.800000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Np+4                 +1.000F-                   = NpF+3
    log_k       8.9600
#    delta_h     1.5000
#    -a_e    9.222793E+00  0.000000E+00 -7.835185E+01  0.000000E+00 -0.000000E+00
    -gamma      6.00    0.00

 +1.000Np+4                 +2.000F-                   = NpF2+2
    log_k      15.7000
#    -a_e    1.570000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Np+4                 +1.000Cl-                  = NpCl+3
    log_k       1.5000
#    -a_e    1.500000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      6.00    0.00

 +1.000Np+4                 +1.000SO4-2                = NpSO4+2
    log_k       6.8500
#    delta_h    29.8000
#    -a_e    1.207083E+01  0.000000E+00 -1.556590E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Np+4                 +2.000SO4-2                = Np(SO4)2
    log_k      11.0500
#    delta_h    55.4000
#    -a_e    2.075584E+01  0.000000E+00 -2.893795E+03  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +1.000Np+4                 +1.000NO3-                 = NpNO3+3
    log_k       1.9000
#    -a_e    1.900000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      6.00    0.00

 +1.000Np+4                 +4.000CO3-2                = Np(CO3)4-4
    log_k      36.6900
#    -a_e    3.669000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      6.00    0.00

 +1.000Np+4                 +5.000CO3-2                = Np(CO3)5-6
    log_k      35.6200
#    -a_e    3.562000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      9.00    0.00

 +1.000NpO2+                +1.000H2O                  -1.000H+                   = NpO2(OH)
    log_k     -11.3000
#    -a_e   -1.130000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000NpO2+                +2.000H2O                  -2.000H+                   = NpO2(OH)2-
    log_k     -23.6000
```

```
#    -a_e   -2.360000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000NpO2+               +1.000F-                    = NpO2F
    log_k       1.2000
#    -a_e    1.200000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000NpO2+               +1.000SO4-2                 = NpO2SO4-
    log_k       0.4400
#    delta_h    23.2000
#    -a_e    4.504538E+00  0.000000E+00 -1.211842E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000NpO2+               +1.000HPO4-2                = NpO2HPO4-
    log_k       2.9500
#    -a_e    2.950000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000NpO2+               +1.000CO3-2                 = NpO2CO3-
    log_k       4.9600
#    -a_e    4.960000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000NpO2+               +2.000CO3-2                 = NpO2(CO3)2-3
    log_k       6.5300
#    -a_e    6.530000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000NpO2+               +3.000CO3-2                 = NpO2(CO3)3-5
    log_k       5.5000
#    delta_h   -13.3000
#    -a_e    3.169899E+00  0.000000E+00  6.947197E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000NpO2+                   +2.000CO3-2                   +1.000H2O                     -1.000H+
= NpO2(CO3)2OH-4
    log_k      -5.3000
#    -a_e   -5.300000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000NpO2+2              +1.000H2O                   -1.000H+                    = NpO2OH+
    log_k      -5.1000
#    -a_e   -5.100000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000NpO2+2              +3.000H2O                   -3.000H+                    = NpO2(OH)3-
    log_k     -19.0000
#    -a_e   -1.900000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000NpO2+2              +4.000H2O                   -4.000H+                    = NpO2(OH)4-2
    log_k     -33.0000
#    -a_e   -3.300000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00
```

```
 +2.000NpO2+2               +2.000H2O                  -2.000H+                   = (NpO2)2(OH)2+2
    log_k      -6.2700
#    -a_e  -6.270000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +3.000NpO2+2               +5.000H2O                  -5.000H+                   = (NpO2)3(OH)5+
    log_k     -17.1200
#    -a_e  -1.712000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      3.00    0.00

 +1.000NpO2+2               +1.000F-                   = NpO2F+
    log_k       4.5700
#    -a_e   4.570000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000NpO2+2               +2.000F-                   = NpO2F2
    log_k       7.6000
#    -a_e   7.600000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000NpO2+2               +1.000Cl-                  = NpO2Cl+
    log_k       0.4000
#    -a_e   4.000000E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000NpO2+2               +1.000SO4-2                = NpO2SO4
    log_k       3.2800
#    delta_h    16.7000
#    -a_e   6.205766E+00  0.000000E+00 -8.723173E+02  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +1.000NpO2+2               +2.000SO4-2                = NpO2(SO4)2-2
    log_k       4.7000
#    delta_h    26.0000
#    -a_e   9.255085E+00  0.000000E+00 -1.358099E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000NpO2+2               +1.000CO3-2                = NpO2CO3
    log_k       9.3200
#    -a_e   9.320000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000NpO2+2               +2.000CO3-2                = NpO2(CO3)2-2
    log_k      16.5200
#    -a_e   1.652000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000NpO2+2               +3.000CO3-2                = NpO2(CO3)3-4
    log_k      19.3700
#    delta_h   -41.9000
#    -a_e   1.202930E+01  0.000000E+00  2.188628E+03  0.000000E+00 -0.000000E+00
    -gamma      3.00    0.00

 +3.000NpO2+2               +6.000CO3-2                = (NpO2)3(CO3)6-6
    log_k      49.8400
#    -a_e   4.984000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
```

```
    -gamma      4.00    0.00

 +1.000Pu+3                 +1.000H2O                  -1.000H+                   = PuOH+2
    log_k      -6.9000
#    -a_e   -6.900000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Pu+3                 +1.000Cl-                  = PuCl+2
    log_k       1.2000
#    -a_e    1.200000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Pu+3                 +1.000SO4-2                = PuSO4+
    log_k       3.9000
#    delta_h    17.2000
#    -a_e    6.913364E+00  0.000000E+00 -8.984345E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Pu+3                 +2.000SO4-2                = Pu(SO4)2-
    log_k       5.7000
#    delta_h    12.0000
#    -a_e    7.802347E+00  0.000000E+00 -6.268148E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Pu+4                 +1.000H2O                  -1.000H+                   = PuOH+3
    log_k      -0.7800
#    delta_h    36.0000
#    -a_e    5.527041E+00  0.000000E+00 -1.880444E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Pu+4                 +4.000H2O                  -4.000H+                   = Pu(OH)4
    log_k      -8.4000
#    -a_e   -8.400000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Pu+4                 +1.000F-                   = PuF+3
    log_k       8.8400
#    delta_h     9.1000
#    -a_e    1.043428E+01  0.000000E+00 -4.753346E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Pu+4                 +2.000F-                   = PuF2+2
    log_k      15.7000
#    delta_h    11.0000
#    -a_e    1.762715E+01  0.000000E+00 -5.745802E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Pu+4                 +1.000Cl-                  = PuCl+3
    log_k       1.8000
#    -a_e    1.800000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Pu+4                 +1.000SO4-2                = PuSO4+2
    log_k       6.8900
#    -a_e    6.890000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00
```

```
 +1.000Pu+4                 +2.000SO4-2                = Pu(SO4)2
    log_k      11.1400
#    -a_e    1.114000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Pu+4                 +1.000NO3-                 = PuNO3+3
    log_k       1.9500
#    -a_e    1.950000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Pu+4                 +1.000H3PO4                = PuH3PO4+4
    log_k       2.4000
#    -a_e    2.400000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Pu+4                 +4.000CO3-2                = Pu(CO3)4-4
    log_k      35.9000
#    -a_e    3.590000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Pu+4                 +5.000CO3-2                = Pu(CO3)5-6
    log_k      34.5000
#    -a_e    3.450000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      6.00    0.00

 +1.000PuO2+                +1.000H2O                  -1.000H+                   = PuO2OH
    log_k      -9.7300
#    -a_e   -9.730000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000PuO2+                +1.000CO3-2                = PuO2CO3-
    log_k       5.1200
#    -a_e    5.120000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000PuO2+                +3.000CO3-2                = PuO2(CO3)3-5
    log_k       5.0000
#    delta_h   -19.1100
#    -a_e    1.652012E+00  0.000000E+00  9.982026E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000PuO2+2               +1.000H2O                  -1.000H+                   = PuO2OH+
    log_k      -5.5000
#    delta_h    28.0000
#    -a_e   -5.945234E-01  0.000000E+00 -1.462568E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000PuO2+2               +2.000H2O                  -2.000H+                   = PuO2(OH)2
    log_k     -13.2000
#    -a_e   -1.320000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +2.000PuO2+2               +2.000H2O                  -2.000H+                   = (PuO2)2(OH)2+2
    log_k      -7.5000
#    -a_e   -7.500000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
```

```
    -gamma      4.00    0.00

 +1.000PuO2+2               +1.000F-                   = PuO2F+
    log_k       4.5600
#    -a_e    4.560000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000PuO2+2               +2.000F-                   = PuO2F2
    log_k       7.2500
#    -a_e    7.250000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000PuO2+2               +1.000Cl-                  = PuO2Cl+
    log_k       0.7000
#    -a_e    7.000000E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000PuO2+2               +2.000Cl-                  = PuO2Cl2
    log_k      -0.6000
#    -a_e   -6.000000E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000PuO2+2               +1.000SO4-2                = PuO2SO4
    log_k       3.3800
#    delta_h    16.1000
#    -a_e    6.200649E+00  0.000000E+00 -8.409765E+02  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +1.000PuO2+2               +2.000SO4-2                = PuO2(SO4)2-2
    log_k       4.4000
#    delta_h    43.0000
#    -a_e    1.193341E+01  0.000000E+00 -2.246086E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000PuO2+2               +1.000CO3-2                = PuO2CO3
    log_k       9.3000
#    -a_e    9.300000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000PuO2+2               +2.000CO3-2                = PuO2(CO3)2-2
    log_k      14.6000
#    delta_h   -27.0000
#    -a_e    9.869719E+00  0.000000E+00  1.410333E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000PuO2+2               +3.000CO3-2                = PuO2(CO3)3-4
    log_k      17.7000
#    delta_h   -38.6000
#    -a_e    1.093745E+01  0.000000E+00  2.016254E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Ra+2                 +1.000OH-                  = RaOH+
    log_k       0.5000
#    delta_h     4.6000
#    -a_e    1.305900E+00  0.000000E+00 -2.402790E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00
```

```
 +1.000Ra+2                 +1.000Cl-                  = RaCl+
    log_k      -0.1000
#    delta_h     2.1000
#    -a_e    2.679107E-01  0.000000E+00 -1.096926E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Ra+2                 +1.000CO3-2                = RaCO3
    log_k       2.5000
#    delta_h     4.4800
#    -a_e    3.284876E+00  0.000000E+00 -2.340109E+02  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +1.000Ra+2                 +1.000SO4-2                = RaSO4
    log_k       2.7500
#    delta_h     5.4000
#    -a_e    3.696056E+00  0.000000E+00 -2.820667E+02  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +1.000TcO(OH)2             +2.000H+                   -2.000H2O                  = TcO+2
    log_k       4.0000
#    -a_e    4.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.50    0.00

 +1.000TcO(OH)2             +1.000H+                   -1.000H2O                  = TcO(OH)+
    log_k       2.5000
#    -a_e    2.500000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000TcO(OH)2             +1.000H2O                  -1.000H+                   = TcO(OH)3-
    log_k     -10.9000
#    -a_e   -1.090000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000TcO(OH)2                +1.000CO3-2                   +2.000H+                       -1.000H2O
= TcCO3(OH)2
    log_k      19.3000
#    -a_e    1.930000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000TcO(OH)2             +1.000H+                   +1.000CO3-2                = TcCO3(OH)3-
    log_k      11.0000
#    -a_e    1.100000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000UO2+2                +1.000H2O                  -1.000H+                   = UO2OH+
    log_k      -5.2000
#    -a_e   -5.200000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000UO2+2                +2.000H2O                  -2.000H+                   = UO2(OH)2
    log_k     -12.0000
#    -a_e   -1.200000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000UO2+2                +3.000H2O                  -3.000H+                   = UO2(OH)3-
```

```
    log_k     -19.2000
#    -a_e   -1.920000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000UO2+2                +4.000H2O                 -4.000H+                   = UO2(OH)4-2
    log_k     -33.0000
#    -a_e   -3.300000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +2.000UO2+2                +1.000H2O                 -1.000H+                   = (UO2)2OH+3
    log_k      -2.7000
#    -a_e   -2.700000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +2.000UO2+2                +2.000H2O                 -2.000H+                   = (UO2)2(OH)2+2
    log_k      -5.6200
#    -a_e   -5.620000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +3.000UO2+2                +4.000H2O                 -4.000H+                   = (UO2)3(OH)4+2
    log_k     -11.9000
#    -a_e   -1.190000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +3.000UO2+2                +5.000H2O                 -5.000H+                   = (UO2)3(OH)5+
    log_k     -15.5500
#    -a_e   -1.555000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +3.000UO2+2                +7.000H2O                 -7.000H+                   = (UO2)3(OH)7-
    log_k     -31.0000
#    -a_e   -3.100000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +4.000UO2+2                +7.000H2O                 -7.000H+                   = (UO2)4(OH)7+
    log_k     -21.9000
#    -a_e   -2.190000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000U+4                  +1.000H2O                 -1.000H+                   = UOH+3
    log_k      -0.5400
#    delta_h    46.9100
#    -a_e    7.678481E+00  0.000000E+00 -2.450324E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000U+4                  +4.000H2O                 -4.000H+                   = U(OH)4
    log_k      -9.0000
#    -a_e   -9.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000UO2+2                +1.000F-                   = UO2F+
    log_k       5.0900
#    delta_h     1.7000
#    -a_e    5.387833E+00  0.000000E+00 -8.879876E+01  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00
```

```
 +1.000UO2+2               +2.000F-                  = UO2F2
    log_k       8.6200
#    delta_h     2.1000
#    -a_e    8.987911E+00  0.000000E+00 -1.096926E+02  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +1.000UO2+2               +3.000F-                  = UO2F3-
    log_k      10.9000
#    delta_h     2.3500
#    -a_e    1.131171E+01  0.000000E+00 -1.227512E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000UO2+2               +4.000F-                  = UO2F4-2
    log_k      11.7000
#    delta_h     0.2900
#    -a_e    1.175081E+01  0.000000E+00 -1.514802E+01  0.000000E+00 -0.000000E+00
    -gamma      6.00    0.00

 +1.000U+4                 +1.000F-                  = UF+3
    log_k       9.2800
#    delta_h    -5.6000
#    -a_e    8.298905E+00  0.000000E+00  2.925136E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000U+4                 +2.000F-                  = UF2+2
    log_k      16.2300
#    delta_h    -3.5000
#    -a_e    1.561682E+01  0.000000E+00  1.828210E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000U+4                 +3.000F-                  = UF3+
    log_k      21.6000
#    delta_h     0.5000
#    -a_e    2.168760E+01  0.000000E+00 -2.611728E+01  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000U+4                 +4.000F-                  = UF4
    log_k      25.6000
#    delta_h    -4.2060
#    -a_e    2.486365E+01  0.000000E+00  2.196986E+02  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +1.000U+4                 +5.000F-                  = UF5-
    log_k      27.0100
#    -a_e    2.701000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000U+4                 +6.000F-                  = UF6-2
    log_k      29.0800
#    -a_e    2.908000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000UO2+2               +1.000Cl-                 = UO2Cl+
    log_k       0.1700
#    delta_h     8.0000
#    -a_e    1.571565E+00  0.000000E+00 -4.178765E+02  0.000000E+00 -0.000000E+00
```

```
    -gamma      4.00    0.00

 +1.000UO2+2                +2.000Cl-                  = UO2Cl2
    log_k      -1.1000
#    delta_h    15.0000
#    -a_e    1.527934E+00  0.000000E+00 -7.835185E+02  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +1.000U+4                  +1.000Cl-                  = UCl+3
    log_k       1.7200
#    delta_h   -19.0000
#    -a_e   -1.608716E+00  0.000000E+00  9.924568E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000UO2+2                +1.000SO4-2                = UO2SO4
    log_k       3.1500
#    delta_h    19.5000
#    -a_e    6.566314E+00  0.000000E+00 -1.018574E+03  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +1.000UO2+2                +2.000SO4-2                = UO2(SO4)2-2
    log_k       4.1400
#    delta_h    35.1000
#    -a_e    1.028937E+01  0.000000E+00 -1.833433E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000U+4                  +1.000SO4-2                = USO4+2
    log_k       6.5800
#    delta_h     8.0000
#    -a_e    7.981565E+00  0.000000E+00 -4.178765E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000U+4                  +2.000SO4-2                = U(SO4)2
    log_k      10.5100
#    delta_h    32.7000
#    -a_e    1.623890E+01  0.000000E+00 -1.708070E+03  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +1.000UO2+2                +1.000NO3-                 = UO2NO3+
    log_k       0.3000
#    -a_e    3.000000E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000U+4                  +1.000NO3-                 = UNO3+3
    log_k       1.4700
#    -a_e    1.470000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000U+4                  +2.000NO3-                 = U(NO3)2+2
    log_k       2.3000
#    -a_e    2.300000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000UO2+2                +1.000PO4-3                = UO2PO4-
    log_k      13.2300
#    -a_e    1.323000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
```

```
    -gamma      4.00    0.00

 +1.000UO2+2                +1.000HPO4-2               = UO2HPO4
    log_k       7.2400
#    -a_e    7.240000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000UO2+2                +1.000H3PO4                -1.000H+                   = UO2H2PO4+
    log_k       1.1200
#    -a_e    1.120000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000UO2+2                +1.000H3PO4                = UO2H3PO4+2
    log_k       0.7600
#    -a_e    7.600000E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000UO2+2                +2.000H3PO4                -2.000H+                   = UO2(H2PO4)2
    log_k       0.6400
#    -a_e    6.400000E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000UO2+2                +1.000CO3-2                = UO2CO3
    log_k       9.6700
#    delta_h     5.0000
#    -a_e    1.054598E+01  0.000000E+00 -2.611728E+02  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +1.000UO2+2                +2.000CO3-2                = UO2(CO3)2-2
    log_k      16.9400
#    delta_h    18.5000
#    -a_e    2.018112E+01  0.000000E+00 -9.663395E+02  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000UO2+2                +3.000CO3-2                = UO2(CO3)3-4
    log_k      21.6000
#    delta_h   -39.2000
#    -a_e    1.473233E+01  0.000000E+00  2.047595E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +3.000UO2+2                +6.000CO3-2                = (UO2)3(CO3)6-6
    log_k      54.0000
#    delta_h   -62.7000
#    -a_e    4.301524E+01  0.000000E+00  3.275107E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +2.000UO2+2                  +3.000H2O                    -3.000H+                      +1.000CO3-2
= (UO2)2CO3(OH)3-
    log_k      -0.8600
#    -a_e   -8.600000E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000U+4                  +4.000CO3-2                = U(CO3)4-4
    log_k      35.2200
#    -a_e    3.522000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00
```

```
 +1.000U+4                  +5.000CO3-2                = U(CO3)5-6
    log_k      34.1000
#    delta_h   -20.0000
#    -a_e    3.059609E+01  0.000000E+00  1.044691E+03  0.000000E+00 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Th+4                 +1.000H2O                  -1.000H+                   = ThOH+3
    log_k      -2.4000
#    -a_e   -2.400000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Th+4                 +4.000H2O                  -4.000H+                   = Th(OH)4
    log_k     -18.4000
#    -a_e   -1.840000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Th+4                 +1.000F-                   = ThF+3
    log_k       8.0000
#    -a_e    8.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Th+4                 +2.000F-                   = ThF2+2
    log_k      14.2000
#    -a_e    1.420000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Th+4                 +3.000F-                   = ThF3+
    log_k      18.9000
#    -a_e    1.890000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Th+4                 +4.000F-                   = ThF4
    log_k      22.3000
#    -a_e    2.230000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Th+4                 +5.000CO3-2                = Th(CO3)5-6
    log_k      29.8000
#    -a_e    2.980000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Th+4                    +1.000CO3-2                    -3.000H+                       +3.000H2O
= ThCO3(OH)3-
    log_k      -3.1000
#    -a_e   -3.100000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Th+4                 +1.000HPO4-2               = ThHPO4+2
    log_k      13.0000
#    -a_e    1.300000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Th+4                 +1.000SO4-2                = ThSO4+2
    log_k       7.6000
#    -a_e    7.600000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
```

```
    -gamma      4.00    0.00

 +1.000Th+4                 +2.000SO4-2                = Th(SO4)2
    log_k      11.6000
#    -a_e    1.160000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma       0.00    0.00

 +1.000Th+4                 +3.000SO4-2                = Th(SO4)3-2
    log_k      12.4000
#    -a_e    1.240000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +2.000UO2+2                +1.000PuO2+2               +6.000CO3-2                = (UO2)2PuO2(CO3)6-
6
    log_k      52.7000
#    -a_e    5.270000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      6.00    0.00

 +2.000NpO2+2                  +1.000CO3-2                    +3.000H2O                      -3.000H+
= (NpO2)2CO3(OH)3-
    log_k      -2.8700
#    -a_e   -2.870000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +2.000UO2+2                +1.000NpO2+2               +6.000CO3-2                = (UO2)2NpO2(CO3)6-
6
    log_k      53.5900
#    -a_e    5.359000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      6.00    0.00

 +1.000UO2+2                +2.000H3PO4                -1.000H+                   = UO2H2PO4H3PO4+
    log_k       1.6500
#    -a_e    1.650000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000UO2+                 +3.000CO3-2                = UO2(CO3)3-5
    log_k       7.4100
#    -a_e    7.410000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Zr+4                 +1.000H2O                  -1.000H+                   = ZrOH+3
    log_k       0.3000
#    -a_e    3.000000E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Zr+4                 +4.000H2O                  -4.000H+                   = Zr(OH)4
    log_k      -9.7000
#    -a_e   -9.700000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma       0.00    0.00

 +1.000Zr+4                 +5.000H2O                  -5.000H+                   = Zr(OH)5-
    log_k     -16.0000
#    -a_e   -1.600000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Zr+4                 +2.000F-                   = ZrF2+2
```

```
    log_k      18.5000
#    -a_e    0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Zr+4                 +3.000F-                   = ZrF3+
    log_k      24.7000
#    -a_e    0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Zr+4                 +4.000F-                   = ZrF4
    log_k      30.1000
#    -a_e    0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Zr+4                 +1.000SO4-2                = ZrSO4+2
    log_k       7.0000
#    -a_e    7.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Zr+4                 +6.000F-                   = ZrF6-2
    log_k      38.4000
#    -a_e    3.840000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Zr+4                 +1.000F-                   = ZrF+3
    log_k      10.2000
#    -a_e    0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Zr+4                 +5.000F-                   = ZrF5-
    log_k      34.7000
#    -a_e    3.470000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Zr+4                 +1.000Cl-                  = ZrCl+3
    log_k       1.5000
#    -a_e    1.500000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Sn+2                 +1.000H2O                  -1.000H+                   = SnOH+
    log_k      -3.8000
#    -a_e   -3.800000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Sn+2                 +3.000H2O                  -3.000H+                   = Sn(OH)3-
    log_k     -17.5000
#    -a_e   -1.750000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +3.000Sn+2                 +4.000H2O                  -4.000H+                   = Sn3(OH)4+2
    log_k      -5.6000
#    -a_e   -5.600000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Sn+2                 +1.000Cl-                  = SnCl+
    log_k       1.7000
```

```
#    -a_e    1.700000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Sn+2              +3.000Cl-                 = SnCl3-
    log_k       2.1000
#    -a_e    2.100000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Sn+2              +1.000F-                  = SnF+
    log_k       5.0000
#    -a_e    5.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000HS-               -1.000H+                  = S-2
    log_k     -19.0000
#    -a_e   -1.900000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      5.00    0.00

 +1.000Sn+2              +2.000H2O                 -2.000H+                  = Sn(OH)2
    log_k      -7.7000
#    -a_e   -7.700000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Ni+2              +2.000HS-                 = Ni(HS)2
    log_k      11.1000
#    -a_e    1.110000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000HS-               +1.000H+                  = H2S
    log_k       6.9900
#    delta_h   -22.3000
#    -a_e    3.083138E+00  0.000000E+00  1.164831E+03  0.000000E+00 -0.000000E+00
#    -gamma      0.00    0.00

 +1.000Sn+2              +1.000SO4-2               = SnSO4
    log_k       2.6000
#    -a_e    2.600000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Sn+2                 +1.000H2O                     +1.000Cl-                     -1.000H+
= SnOHCl
    log_k      -3.1000
#    -a_e   -3.100000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Sn+2              +2.000Cl-                 = SnCl2
    log_k       2.3600
#    -a_e    2.360000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Tn(OH)4           +1.000H2O                 -1.000H+                  = Tn(OH)5-
    log_k      -8.0000
#    -a_e   -8.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Tn(OH)4           +2.000H2O                 -2.000H+                  = Tn(OH)6-2
```

```
    log_k     -18.4000
#    -a_e   -1.840000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Pd+2                   +3.000Cl-                     +1.000H2O                          -1.000H+
= PdCl3OH-2
    log_k       2.5000
#    -a_e    2.500000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Pd+2                   +2.000Cl-                     +2.000H2O                          -2.000H+
= PdCl2(OH)2-2
    log_k      -7.0000
#    -a_e   -7.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Al+3                +2.000SO4-2                = Al(SO4)2-
    log_k       5.9000
#    -a_e    5.900000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +3.000UO2+2                  +1.000CO3-2                   +3.000H2O                          -3.000H+
= (UO2)3O(OH)2HCO3+
    log_k       0.6600
#    -a_e    6.600000E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000NpO2+2              +1.000HPO4-2               = NpO2HPO4
    log_k       6.2000
#    -a_e    6.200000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000NpO2+2              +1.000H2PO4-               = NpO2H2PO4+
    log_k       3.3200
#    -a_e    3.320000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000NpO2+2              +2.000HPO4-2               = NpO2(HPO4)2-2
    log_k       9.5000
#    -a_e    9.500000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Ca+2                +1.000SiO(OH)3-            = CaSiO(OH)3+
    log_k       1.2000
#    -a_e    1.200000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Ca+2                +1.000SiO2(OH)2-2          = CaSiO2(OH)2
    log_k       4.6000
#    -a_e    4.600000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Mg+2                +1.000SiO(OH)3-            = MgSiO(OH)3+
    log_k       1.5000
#    -a_e    1.500000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00
```

```
 +1.000Mg+2                 +1.000SiO2(OH)2-2          = MgSiO2(OH)2
    log_k       5.7000
#    -a_e    5.700000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
#    -gamma      0.00    0.00

 +1.000Al+3                 +1.000SiO(OH)3-            = AlSiO(OH)3+2
    log_k       7.4000
#    -a_e    7.400000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Fe+3                 +1.000SiO(OH)3-            = FeSiO(OH)3+2
    log_k       9.7000
#    -a_e    9.700000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Eu+3                 +1.000SiO(OH)3-            = EuSiO(OH)3+2
    log_k       7.9000
#    -a_e    7.900000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Eu+3                 +2.000SiO(OH)3-            = Eu(SiO(OH)3)2+
    log_k      12.8000
#    -a_e    1.280000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Am+3                 +1.000SiO(OH)3-            = AmSiO(OH)3+2
    log_k       8.1000
#    -a_e    8.100000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000Al+3                 +1.000H2O                  -1.000H+                   = AlOH+2
    log_k      -4.9573
#    delta_h    49.7980
#    -a_e   -4.073126E+01  0.000000E+00 -6.202912E+02  1.529820E+01 -0.000000E+00
    -gamma      4.00    0.00

 +1.000Al(OH)4-             +1.000Si(OH)4              -1.000H2O                  = Al(OH)6SiO-
    log_k       3.6000
#    -a_e    3.600000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

 +1.000I-                   +1.000I2                   = I3-
    log_k       2.8700
#    -a_e    2.870000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
    -gamma      4.00    0.00

PHASES

# PMATCH MINERALS

Anhydrite
CaSO4                  =  +1.000Ca+2                 +1.000SO4-2
    log_k      -4.3575
#    delta_h    -7.1558
#    -a_e    1.975200E+02 -0.000000E+00 -8.668800E+03 -6.983500E+01 -0.000000E+00
```

```
Aragonite
CaCO3                  =  +1.000Ca+2                 -1.000H+                   +1.000HCO3-
    log_k       1.9928
#    delta_h   -25.7343
#    -a_e   -6.409020E+01 -4.546451E-02 -2.248497E+03  3.266939E+01  5.637139E+05

As(cr)
As                          =   +1.000HAsO4-2                 +7.000H+                         +5.000e-
-4.000H2O
    log_k     -40.9902
#    delta_h   236.9800
#    -a_e    5.276891E-01 -0.000000E+00 -1.237855E+04 -0.000000E+00  0.000000E+00

Barite
BaSO4                  =  +1.000Ba+2                 +1.000SO4-2
    log_k      -9.9704
#    delta_h    26.5742
#    -a_e    1.360350E+02 -0.000000E+00 -7.680410E+03 -4.859500E+01 -0.000000E+00

Brucite
Mg(OH)2                =  +1.000Mg+2                 +2.000H2O                  -2.000H+
    log_k      16.8400
#    delta_h  -113.3864
#    -a_e   -3.024798E+00 -0.000000E+00  5.922689E+03 -0.000000E+00  0.000000E+00

Calcite
CaCO3                  =  +1.000Ca+2                 -1.000H+                   +1.000HCO3-
    log_k       1.8490
#    delta_h   -24.5095
#    -a_e   -6.401940E+01 -4.546451E-02 -2.312471E+03  3.266939E+01  5.637139E+05

Celestite
SrSO4                  =  +1.000Sr+2                 +1.000SO4-2
    log_k      -6.6319
#    delta_h    -4.3389
#    -a_e   -1.480596E+04 -2.466092E+00  7.569685E+05  5.436359E+03 -4.055360E+07

Dolomite(dis)
CaMg(CO3)2                 =   +1.000Ca+2                     +1.000Mg+2                       -2.000H+
+2.000HCO3-
    log_k       4.1180
#    delta_h   -76.2020
#    -a_e   -9.232255E+00 -0.000000E+00  3.980378E+03 -0.000000E+00  0.000000E+00

Dolomite(ord)
CaMg(CO3)2                 =   +1.000Ca+2                     +1.000Mg+2                       -2.000H+
+2.000HCO3-
    log_k       3.5680
#    delta_h   -69.2820
#    -a_e   -8.569901E+00 -0.000000E+00  3.618915E+03 -0.000000E+00  0.000000E+00

Fe(cr)
Fe                     =  +1.000Fe+2                 +2.000e-
    log_k      13.8229
#    delta_h   -89.1000
```

```
#    -a_e   -1.786995E+00 -0.000000E+00  4.654100E+03 -0.000000E+00  0.000000E+00

Fluorite
CaF2                   =  +1.000Ca+2                 +2.000F-
    log_k     -10.5997
#    delta_h    19.6419
#    -a_e    6.634800E+01 -0.000000E+00 -4.298200E+03 -2.527100E+01 -0.000000E+00

Goethite
FeOOH                  =  +2.000H2O                  -3.000H+                   +1.000Fe+3
    log_k      -1.0000
#    -a_e   -1.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Graphite
C                           =   +1.000HCO3-                   +5.000H+                        +4.000e-
-3.000H2O
    log_k     -21.8197
#    delta_h   167.2750
#    -a_e   -2.081775E+02 -4.106888E-02  4.606129E+03  7.863525E+01 -1.015550E+06

Gypsum
CaSO4:2H2O             =  +1.000Ca+2                 +1.000SO4-2                +2.000H2O
    log_k      -4.5809
#    delta_h    -0.4543
#    -a_e    6.824010E+01 -0.000000E+00 -3.221510E+03 -2.506270E+01 -0.000000E+00

Hausmannite
Mn3O4                       =   +3.000Mn+2                    +4.000H2O                       -8.000H+
-2.000e-
    log_k      61.0300
#    delta_h  -421.0778
#    -a_e   -1.274097E+01 -0.000000E+00  2.199481E+04 -0.000000E+00  0.000000E+00

Manganite
MnOOH                       =   +1.000Mn+2                    +2.000H2O                       -3.000H+
-1.000e-
    log_k      25.3400
#    -a_e    2.534000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Melanterite
FeSO4:7H2O             =  +1.000Fe+2                 +1.000SO4-2                +7.000H2O
    log_k      -2.2093
#    delta_h    20.5364
#    -a_e    1.447000E+00 -4.153000E-03 -0.000000E+00 -0.000000E+00 -2.149490E+05

Mo(cr)
Mo                          =   +1.000MoO4-2                  +8.000H+                        +6.000e-
-4.000H2O
    log_k     -19.6675
#    delta_h   145.4200
#    -a_e    5.809486E+00 -0.000000E+00 -7.595951E+03 -0.000000E+00  0.000000E+00

Tugarinovite
MoO2                        =   +1.000MoO4-2                  +4.000H+                        +2.000e-
-2.000H2O
    log_k     -29.9567
```

```
#    delta_h   162.7000
#    -a_e   -1.452371E+00 -0.000000E+00 -8.498564E+03 -0.000000E+00  0.000000E+00

Molybdite
MoO3                   =  +1.000MoO4-2              +2.000H+                   -1.000H2O
    log_k     -12.0552
#    delta_h    33.0200
#    -a_e   -6.270250E+00 -0.000000E+00 -1.724785E+03 -0.000000E+00  0.000000E+00

Nb2O5(cr)
Nb2O5                  =  +2.000NbO3-               +2.000H+                   -1.000H2O
    log_k     -24.3417
#    -a_e   -2.434168E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

NbO2(cr)
NbO2                        =   +1.000NbO3-                  +2.000H+                        +1.000e-
-1.000H2O
    log_k      -7.9784
#    -a_e   -7.978407E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Portlandite
Ca(OH)2                =  +1.000Ca+2                +2.000H2O                  -2.000H+
    log_k      22.8000
#    delta_h  -129.7040
#    -a_e    7.643067E-02 -0.000000E+00  6.775032E+03 -0.000000E+00  0.000000E+00

Pyrochroite
Mn(OH)2                =  +1.000Mn+2                +2.000H2O                  -2.000H+
    log_k      15.2000
#    -a_e    1.520000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Pyrolusite
MnO2                        =   +1.000Mn+2                   +2.000H2O                       -4.000H+
-2.000e-
    log_k      41.3800
#    delta_h  -272.4202
#    -a_e   -6.346826E+00 -0.000000E+00  1.422975E+04 -0.000000E+00  0.000000E+00

Rhodochrosite
MnCO3                  =  +1.000Mn+2                +1.000HCO3-                -1.000H+
    log_k      -0.8011
#    delta_h   -20.8838
#    -a_e    9.570888E+01  3.252849E-02 -4.839264E+03 -3.892561E+01  5.637139E+05

Rhodochrosite(syn)
MnCO3                  =  +1.000Mn+2                +1.000HCO3-                -1.000H+
    log_k      -0.0611
#    delta_h   -14.9007
#    -a_e    9.749710E+01  3.252849E-02 -5.151790E+03 -3.892561E+01  5.637139E+05

Siderite
FeCO3                  =  +1.000Fe+2                +1.000CO3-2
    log_k    -10.8
#original    log_k      -0.5612
#    delta_h   -25.2770
#    -a_e    9.517921E+01  3.252849E-02 -4.609790E+03 -3.892561E+01  5.637139E+05
```

```
FeCO3(pr)
FeCO3                  =  +1.000Fe+2                +1.000HCO3-               -1.000H+
    log_k      -0.1211
#    delta_h   -14.9007
#    -a_e    9.743710E+01  3.252849E-02 -5.151790E+03 -3.892561E+01  5.637139E+05

Strontianite
SrCO3                  =  +1.000Sr+2                -1.000H+                  +1.000HCO3-
    log_k       1.0583
#    delta_h   -16.5756
#    -a_e    2.629176E+02  3.252849E-02 -1.239138E+04 -9.551199E+01  5.637139E+05

Witherite
BaCO3                  =  +1.000Ba+2                -1.000H+                  +1.000HCO3-
    log_k       1.7672
#    delta_h   -11.9609
#    -a_e    7.155291E+02  1.536265E-01 -2.516304E+04 -2.754204E+02  5.637139E+05

Hematite
Fe2O3                  =  +3.000H2O                 -6.000H+                  +2.000Fe+3
    log_k       1.1200
#    -a_e    1.120000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Pyrite
FeS2                       =   +1.000Fe+2                    +2.000HS-                      -2.000H+
-2.000e-
    log_k     -18.5000
#    -a_e   -1.850000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Troilite
FeS                    =  +1.000Fe+2                +1.000HS-                 -1.000H+
    log_k      -5.3100
#    -a_e   -5.310000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Magnesite
MgCO3                  =  +1.000Mg+2                -1.000H+                  +1.000HCO3-
    log_k       2.0410
#    -a_e    2.041000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Am(OH)3(cr)
Am(OH)3                =  +1.000Am+3                +3.000H2O                 -3.000H+
    log_k      15.2000
#    -a_e    1.520000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Am(OH)3(am)
Am(OH)3                =  +1.000Am+3                +3.000H2O                 -3.000H+
    log_k      17.0000
#    -a_e    1.700000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

AmCO3OH(cr)
AmCO3OH                =  +1.000Am+3                +1.000CO3-2               +1.000OH-
    log_k     -21.2000
#    -a_e   -2.120000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Am(CO3)1.5(cr)
```

```
Am(CO3)1.5             =  +1.000Am+3                 +1.500CO3-2
    log_k     -16.7000
#    -a_e   -1.670000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Eu(OH)3(cr)
Eu(OH)3                =  +1.000Eu+3                 +3.000H2O                  -3.000H+
    log_k      14.9000
#    delta_h  -124.3900
#    -a_e   -6.892580E+00 -0.000000E+00  6.497458E+03 -0.000000E+00  0.000000E+00

Eu(OH)3(am)
Eu(OH)3                =  +1.000Eu+3                 +3.000H2O                  -3.000H+
    log_k      17.6000
#    -a_e    1.760000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Eu2(CO3)3(cr)
Eu2(CO3)3              =  +2.000Eu+3                 +3.000CO3-2
    log_k     -35.0000
#    -a_e   -3.500000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

EuOHCO3(cr)
EuOHCO3                =  +1.000Eu+3                 +1.000OH-                  +1.000CO3-2
    log_k     -21.7000
#    -a_e   -2.170000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

EuF3(cr)
EuF3                   =  +1.000Eu+3                 +3.000F-
    log_k     -17.4000
#    -a_e   -1.740000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Theophrastite
Ni(OH)2                =  +1.000Ni+2                 +2.000H2O                  -2.000H+
    log_k      10.5000
#    -a_e    1.050000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

NiCO3(cr)
NiCO3                  =  +1.000Ni+2                 +1.000CO3-2
    log_k     -11.2000
#    -a_e   -1.120000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

NpO2(am,hyd)
NpO2                   =  +1.000Np+4                 +2.000H2O                  -4.000H+
    log_k       1.5000
#    -a_e    1.500000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

NpO2OH(am,fr)
NpO2OH                 =  +1.000NpO2+                +1.000H2O                  -1.000H+
    log_k       5.3000
#    delta_h   -41.1000
#    -a_e   -1.900539E+00 -0.000000E+00  2.146841E+03 -0.000000E+00  0.000000E+00

NpO2CO3(s)
NpO2CO3                =  +1.000NpO2+2               +1.000CO3-2
    log_k     -14.6000
#    -a_e   -1.460000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00
```

```
Pu(OH)3(cr)
Pu(OH)3                 =  +1.000Pu+3                 +3.000H2O                 -3.000H+
    log_k      15.8000
#    -a_e    1.580000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Pu(HPO4)2(am,hyd)
Pu(HPO4)2               =  +1.000Pu+4                 +2.000HPO4-2
    log_k     -30.4500
#    -a_e   -3.045000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

PuO2OH(am)
PuO2OH                  =  +1.000PuO2+                +1.000H2O                 -1.000H+
    log_k       5.0000
#    -a_e    5.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

RaCO3(cr)
RaCO3                   =  +1.000Ra+2                 +1.000CO3-2
    log_k      -8.3000
#    delta_h    11.7000
#    -a_e   -6.250212E+00 -0.000000E+00 -6.111444E+02 -0.000000E+00  0.000000E+00

RaSO4(cr)
RaSO4                   =  +1.000Ra+2                 +1.000SO4-2
    log_k     -10.2600
#    delta_h    39.3000
#    -a_e   -3.374813E+00 -0.000000E+00 -2.052818E+03 -0.000000E+00  0.000000E+00

TcO2:1.6H2O(s)
TcO2:1.6(H2O)           =  +1.000TcO(OH)2             +0.600H2O
    log_k      -8.4000
#    -a_e   -8.400000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

UO2(s)
UO2                     =  +1.000U+4                  +2.000H2O                 -4.000H+
    log_k      -0.0000
#    -a_e   -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Schoepite
UO3:2H2O                =  +1.000UO2+2                +3.000H2O                 -2.000H+
    log_k       5.9600
#    -a_e    5.960000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

UF4:2.5H2O(cr)
UF4:2.5H2O              =  +1.000U+4                  +4.000F-                  +2.500H2O
    log_k     -29.3800
#    -a_e   -2.938000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

U(OH)2SO4(cr)
U(OH)2SO4                  =   +1.000U+4                      +1.000SO4-2                   +2.000H2O
-2.000H+
    log_k      -3.1700
#    -a_e   -3.170000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Rutherfordine
UO2CO3                  =  +1.000UO2+2                +1.000CO3-2
    log_k     -14.4900
```

```
#    -a_e   -1.449000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

NpO2OH(am,ag)
NpO2OH                 =  +1.000NpO2+                +1.000H2O                  -1.000H+
    log_k       4.7000
#    delta_h   -41.1000
#    -a_e   -2.500539E+00 -0.000000E+00  2.146841E+03 -0.000000E+00  0.000000E+00

PuO2(hyd,ag)
PuO2                   =  +1.000Pu+4                 +2.000H2O                  -4.000H+
    log_k      -2.0000
#    -a_e   -2.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

ThO2(s)
ThO2                   =  +1.000Th+4                 +2.000H2O                  -4.000H+
    log_k       9.9000
#    -a_e    9.900000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

ThF4(cr)
ThF4                   =  +1.000Th+4                 +4.000F-
    log_k     -30.2000
#    -a_e   -3.020000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

PuO2(OH)2:H2O(cr)
PuO2(OH)2:H2O          =  +1.000PuO2+2               +3.000H2O                  -2.000H+
    log_k       5.5000
#    -a_e    5.500000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

PuO2CO3(s)
PuO2CO3                =  +1.000PuO2+2               +1.000CO3-2
    log_k     -14.2000
#    -a_e   -1.420000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

NaNpO2CO3:3.5H2O(s,fr)
NaNpO2CO3:3.5H2O         =   +1.000Na+                      +1.000NpO2+                    +1.000CO3-2
+3.500H2O
    log_k     -11.1600
#    -a_e   -1.116000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

NaNpO2CO3(s,ag)
NaNpO2CO3              =  +1.000Na+                  +1.000NpO2+                +1.000CO3-2
    log_k     -11.6600
#    -a_e   -1.166000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Na3NpO2(CO3)2(s)
Na3NpO2(CO3)2          =  +3.000Na+                  +1.000NpO2+                +2.000CO3-2
    log_k     -14.7000
#    -a_e   -1.470000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

NpO3:H2O(cr)
NpO3H2O                =  +1.000NpO2+2               +2.000H2O                  -2.000H+
    log_k       5.4700
#    -a_e    5.470000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

K4NpO2(CO3)3(s)
K4NpO2(CO3)3           =  +4.000K+                   +1.000NpO2+2               +3.000CO3-2
```

```
    log_k     -26.4000
#    -a_e   -2.640000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

(NH4)4NpO2(CO3)3(s)
(NH4)4NpO2(CO3)3       =  +4.000NH4+                 +1.000NpO2+2               +3.000CO3-2
    log_k     -26.8100
#    -a_e   -2.681000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Chernikovite
UO2HPO4:4H2O              =   +1.000UO2+2                     +1.000H3PO4                    +4.000H2O
-2.000H+
    log_k      -2.5000
#    -a_e   -2.500000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

USiO4(s)
USiO4                  =  +1.000U+4                  +1.000Si(OH)4              -4.000H+
    log_k      -2.988
# log_k entered manually, -a_e changed accordingly
#    -a_e   -2.988000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Sn(cr)
Sn                     =  +1.000Sn+2                 +2.000e-
    log_k       4.6300
#    delta_h    -7.7000
#    -a_e    3.281413E+00 -0.000000E+00  4.022062E+02 -0.000000E+00  0.000000E+00

SnO(s)
SnO                    =  +1.000Sn+2                 +1.000H2O                  -2.000H+
    log_k       2.5000
#    -a_e    2.500000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

SnS(pr)
SnS                    =  +1.000Sn+2                 +1.000HS-                  -1.000H+
    log_k     -14.7000
#    -a_e   -1.470000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

S(rhomb)
S                      =  +1.000HS-                  -1.000H+                   -2.000e-
    log_k      -2.1440
#    delta_h   -16.3000
#    -a_e   -5.000608E+00 -0.000000E+00  8.514234E+02 -0.000000E+00  0.000000E+00

Cassiterite
TnO2                   =  +1.000Tn(OH)4              -2.000H2O
    log_k      -8.0000
#    -a_e   -8.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

SnO2(am)
TnO2                   =  +1.000Tn(OH)4              -2.000H2O
    log_k      -7.3000
#    -a_e   -7.300000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

CaSn(OH)6(s)
CaTn(OH)6                 =   +1.000Tn(OH)4                  +2.000H2O                      +1.000Ca+2
-2.000H+
    log_k       8.7000
```

```
#    -a_e    8.700000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Baddeleyite
ZrO2                  =  +1.000Zr+4                +2.000H2O                  -4.000H+
    log_k      -1.9000
#    -a_e   -1.900000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Fe(OH)3(am)
Fe(OH)3               =  +3.000H2O                 -3.000H+                   +1.000Fe+3
    log_k       5.0000
#    -a_e    5.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Fe(OH)3(mic)
Fe(OH)3               =  +3.000H2O                 -3.000H+                   +1.000Fe+3
    log_k       3.0000
#    -a_e    3.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Pd(cr)
Pd                    =  +1.000Pd+2                +2.000e-
    log_k     -30.8000
#    delta_h   177.2000
#    -a_e    2.452738E-01 -0.000000E+00 -9.255965E+03 -0.000000E+00  0.000000E+00

Pd(OH)2(s)
Pd(OH)2               =  +1.000Pd+2                -2.000H+                   +2.000H2O
    log_k      -3.3000
#    -a_e   -3.300000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Magnetite
Fe3O4                     =  +1.000Fe+2                   +4.000H2O                        -8.000H+
+2.000Fe+3
    log_k      10.0200
#    -a_e    1.002000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

PuPO4(s,hyd)
PuPO4                 =  +1.000Pu+3                +1.000PO4-3
    log_k     -24.6000
#    -a_e   -2.460000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Quartz
SiO2                  =  +1.000Si(OH)4             -2.000H2O
    log_k      -3.7460
#    delta_h    20.6370
#    -a_e   -1.325045E+01 -0.000000E+00 -4.939341E+02  4.510415E+00  0.000000E+00

SiO2(am)
SiO2                  =  +1.000Si(OH)4             -2.000H2O
    log_k      -2.7140
#    delta_h    14.5940
#    -a_e   -1.571955E-01 -0.000000E+00 -7.623113E+02 -0.000000E+00  0.000000E+00

Kaolinite
Al2Si2O5(OH)4            =  +2.000Al+3                   +2.000Si(OH)4                    +1.000H2O
-6.000H+
    log_k       7.4350
#    delta_h  -147.7000
```

```
#    -a_e   -1.844139E+01 -0.000000E+00  7.715045E+03 -0.000000E+00  0.000000E+00

Gibbsite
Al(OH)3                 =  +1.000Al+3                 +3.000H2O                  -3.000H+
    log_k       7.7561
#    delta_h  -102.7840
#    -a_e   -1.069028E+01 -0.000000E+00  5.388423E+03  1.509445E-01  0.000000E+00

(UO2)3(PO4)2:4H2O(cr)
(UO2)3(PO4)2:4H2O        =   +3.000UO2+2                     +2.000H3PO4                      +4.000H2O
-6.000H+
    log_k      -5.9600
#    -a_e   -5.960000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00

Se(cr)
Se                           =   +1.000SeO3-2                  +6.000H+                         +4.000e-
-3.000H2O
    log_k     -61.2900
#    -a_e   -6.129000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00


# PMATCH GASES

CH4(g)
CH4                     =  +1.000CH4
    log_k      -2.8565
#    delta_h   -13.7966
#    -a_e   -7.806599E+01 -6.229365E-05  3.957200E+03  2.503828E+01 -0.000000E+00

CO2(g)
CO2                     =  +1.000H+                   -1.000H2O                  +1.000HCO3-
    log_k      -7.8198
#    delta_h   -10.8748
#    -a_e   -2.479229E+02 -4.106888E-02  1.491484E+04  8.638236E+01 -1.015550E+06

H2(g)
H2                      =  +1.000H2
    log_k      -3.1056
#    delta_h    -4.0394
#    -a_e   -7.645288E+01 -6.533210E-03  3.037284E+03  2.631230E+01 -0.000000E+00

N2(g)
N2                      =  +1.000N2
    log_k      -3.1864
#    delta_h   -10.4374
#    -a_e   -6.990691E+01  3.663863E-03  3.662355E+03  2.155827E+01 -0.000000E+00

O2(g)
O2                      =  +1.000O2
    log_k      -2.8944
#    delta_h   -12.0593
#    -a_e   -6.096651E+01  4.101330E-03  3.376712E+03  1.839764E+01 -0.000000E+00

H2S(g)
H2S                     =  +1.000HS-                  +1.000H+
    log_k      -8.0100
```

```
#    delta_h     4.3000
#    -a_e   -7.256659E+00 -0.000000E+00 -2.246086E+02 -0.000000E+00  0.000000E+00


END

#09.2.0.3_korr
#Parameterfile adapted to data related to Siderit.
#Source:
#Bruno, J.; Wersin, P.; Stumm, W. (1992): On the influence of carbonate in mineral dissolution: II.
The solubility of FeCO3 (s) at 25°C and 1 atm total pressure, Geochim. Cosmochim. Acta (56), 1149-
1155.
#Modifications:
#FeHCO3<+> deleted
#DFG298 for FeCO3_Siderite modified with logK = 10.8
#DFG298 for FeCO3<0> (formerly FeCO3) modified with logK = 5.5
#New: Fe(CO3)2<2-> with logK = 7.1: Fe<2+> + 2CO3<2-> --> Fe(CO3)2<2->
```

A.4 Appendix 4: IP9 calculation

IP9 solution was calculated according to Herbert /HER 2000/. To be consistent, this is calculated using EQ3/6 version 8.0a and the database mentioned in section 3 and Appendix A.3. The starting solution is:

Component	**Concentration [in mol/kg H_2O]**
Na^+	0.5
K^+	$1 \cdot 10^{-10}$
Ca^{++}	$1 \cdot 10^{-10}$
Mg^{++}	2
Cl^-	4.5
$SO4^{--}$	$1 \cdot 10^{-10}$

The solid phases are:

Halite – NaCl

Anhydrite – $CaSO_4$

Glauberite – $Na_2Ca(SO_4)_2$

Syngenite – $K_2Ca(SO_4)_2{:}H_2O$

Polyhalite – $K_2MgCa_2(SO_4)_4{:}2H_2O$

The calculation was undertaken by adding the solid material into the solution with the amount including 1 kg H_2O, until equilibrium was reached.

A.5 Appendix 5: IP21 calculation

IP21 solution was calculated according to Herbert /HER 2000/. To be consistent, this is calculated using EQ3/6 version 8.0a and the database mentioned in section 3 and Appendix A.3.

The starting solution is:

Component	**Concentration [in mol/kg H_2O]**
Na^+	0.5
K^+	$1 \cdot 10^{-10}$
Ca^{++}	$1 \cdot 10^{-10}$
Mg^{++}	2
Cl^-	4.5
$SO4^{--}$	$1 \cdot 10^{-10}$

The solid phases are:

Halite – NaCl
Carnallite – $KMgCl_3:6H_2O$
Kainite – $KMgClSO_4:3H_2O$
Sylvite – KCl
Polyhalite – $K_2MgCa_2(SO_4)_4:2H_2O$

The calculation was undertaken by adding the solid material into the solution with the amount including 1 kg H2O, until equilibrium was reached.

A.6 Appendix 6: Analytical chemical composition of salt solutions z3OSM, z3BK/BD, z3OSO and z2/z3Grenze collected in the shafts (based on /HAM 2011/)

Tab. A.6.1 Analytical chemical composition of salt solutions z3OSM

Type	**KeyNo**	**SampleNo**	**No.**	**Concentration in [mol/kg H2O]**						**Density**	**Volume**	**Depth**
				Na^+	**K^+**	**Mg^{2+}**	**Ca^{2+}**	**Cl^-**	**SO_4^{2-}**	**[g/cm^3]**	**in [m^3]**	**[m]**
z3OSM Sohle	11000004	11000004.1	1	5.717	0.093	0.195	0.037	6.155	0.060	1.206	79.662	-286.05
	11000004	11000004.2	2	5.729	0.098	0.144	0.043	6.073	0.064	1.206		
	11000004	11000004.3	3	5.684	0.093	0.144	0.043	6.026	0.063	1.206		
	11000004	11000004.4	4	5.647	0.092	0.144	0.042	5.987	0.062	1.206		
	11000004	11000004.5	5	5.676	0.089	0.139	0.042	6.007	0.059	1.206		
	11000004	11000004.6	6	5.656	0.085	0.134	0.043	6.049	0.023	1.206		
	11000004	11000004.7	7	5.664	0.084	0.129	0.045	5.981	0.058	1.206		
	11000004	11000004.8	8	5.573	0.085	0.162	0.043	5.958	0.055	1.206		
	11000004	11000004.9	9	5.581	0.094	0.158	0.041	5.946	0.063	1.206		
	11000004	11000004.10	10	5.676	0.097	0.148	0.039	6.025	0.061	1.206		
	11000004	11000004.11	11	5.682	0.080	0.120	0.046	5.967	0.064	1.206		
	11000004	11000004.12	12	5.673	0.068	0.139	0.042	5.972	0.065	1.206		
z3OSM Stoß	11000024	11000024.1	13	5.696	0.089	0.111	0.042	5.973	0.059	1.206	15.17	-286.01
	11000024	11000024.2	14	5.639	0.084	0.129	0.044	5.947	0.061	1.206		
	11000024	11000024.3	15	5.636	0.083	0.120	0.043	5.926	0.059	1.206		
	11000024	11000024.4	16	5.628	0.075	0.110	0.044	5.896	0.058	1.206		
	11000024	11000024.5	17	5.702	0.072	0.102	0.049	5.967	0.054	1.206		
	11000024	11000024.6	18	5.789	0.062	0.092	0.047	6.013	0.058	1.206		
	11000024	11000024.7	19	5.800	0.064	0.088	0.044	6.017	0.056	1.206		

Tab. A.6.1 [Continued] Analytical chemical composition of salt solutions z3OSM

Type	KeyNo	SampleNo	No.	Concentration in [mol/kg H_2O]						Density	Volume	Depth
				Na^+	K^+	Mg^{2+}	Ca^{2+}	Cl^-	SO_4^{2-}	[g/cm³]	in [m³]	[m]
	11000024	11000024.8	20	5.787	0.055	0.102	0.046	6.026	0.056	1.206		
	11000024	11000024.9	21	5.688	0.055	0.097	0.046	5.913	0.057	1.206		
	11000024	11000024.10	22	5.787	0.050	0.092	0.048	6.007	0.056	1.206		
	11000024	11000024.11	23	5.798	0.044	0.097	0.048	6.022	0.056	1.206		
	11000024	11000024.12	24	5.819	0.042	0.079	0.044	5.997	0.055	1.206		
	11000024	11000024.13	25	5.845	0.043	0.074	0.044	6.011	0.057	1.206		
	11000024	11000024.14	26	5.522	0.123	0.231	0.033	6.042	0.067	1.206		
	11000024	11000024.15	27	5.582	0.119	0.241	0.036	6.100	0.077	1.206		
	11000024	11000024.16	28	5.457	0.129	0.223	0.046	5.975	0.074	1.206		
	11000024	11000024.17	29	5.502	0.108	0.190	0.043	5.923	0.076	1.206		
	11000024	11000024.18	30	5.570	0.098	0.177	0.044	5.968	0.070	1.206		
	11000024	11000024.19	31	5.727	0.043	0.062	0.039	5.869	0.052	1.206		
z3OSM	12000045	12000045.1	32	5.134	0.152	0.240	0.164	6.064	0.015	1.208	51.67	-236.69
	12000045	12000045.2	33	4.975	0.271	0.355	0.149	6.213	0.021	1.208		
Total amount of collected solution											146.502	
Averaged concentration of species				5.638	0.088	0.145	0.050	6.000	0.057	1.207		

Tab. A.6.2 Analytical chemical composition of salt solutions z2/z3Grenze collected in the shafts (based on /HAM 2011/

Type	KeyNo	SampleNo	No.	Concentration in [mol/kg H2O]						Density	Volume	Depth
				Na^+	K^+	Mg^{2+}	Ca^{2+}	Cl^-	SO_4^{2-}	[g/cm³]	in [m³]	[m]
z2/z3-Grenze	11000005	11000005.1	1	4.9273	0.1987	0.3391	0.0844	5.8742	0.0494	1.202	0.045	-242.78

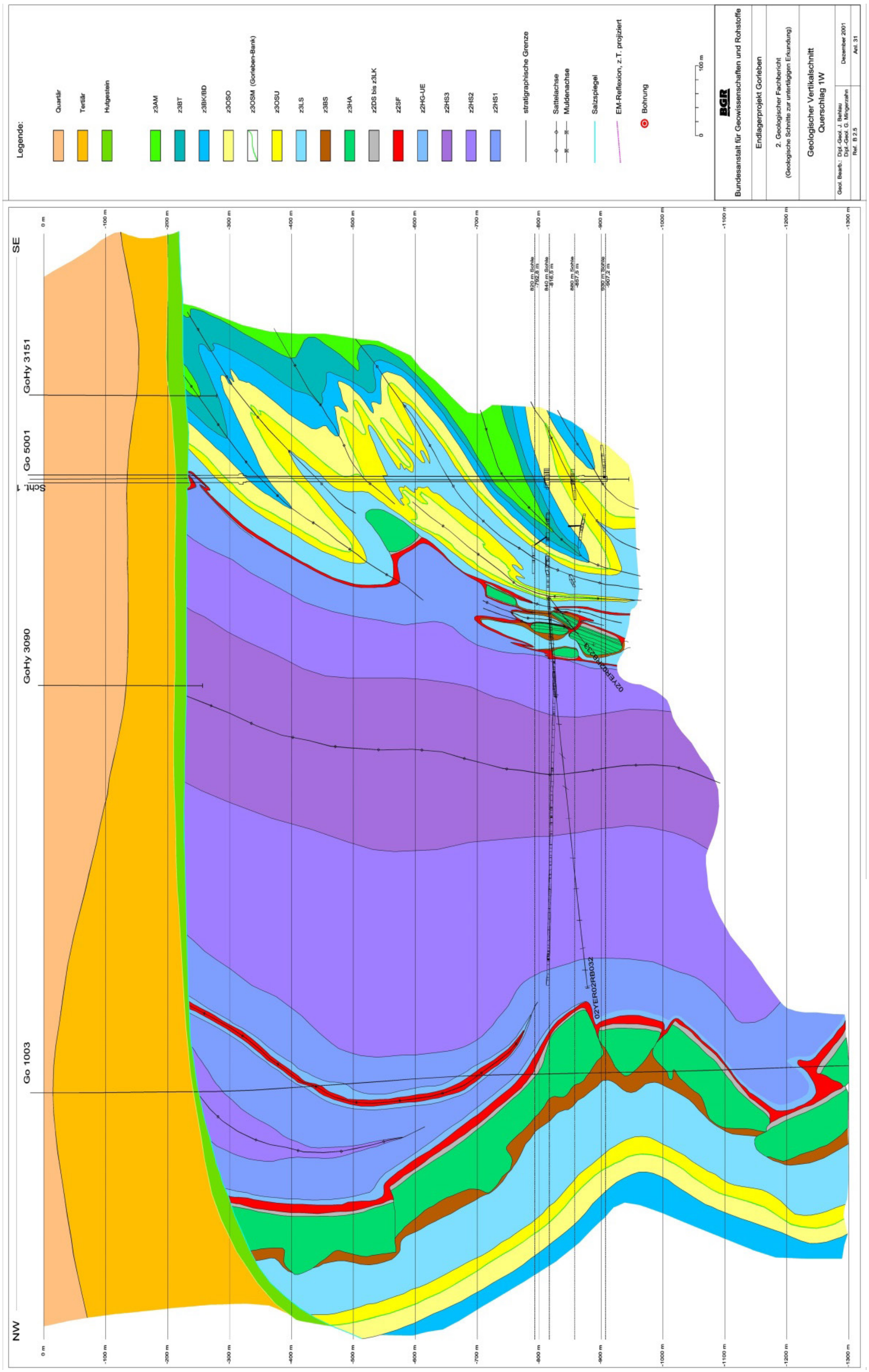
Tab. A.6.3 Analytical chemical composition of salt solutions z3BK/BD

Type	KeyNo	SampleNo	No.	Concentration in [mol/kg H2O]						Density	Volume	Depth
				Na^+	K^+	Mg^{2+}	Ca^{2+}	Cl^-	SO_4^{2-}	[g/cm^3]	in [m^3]	[m]
z3BK/BD	12000044	12000044.1	1	0.3452	0.2437	4.2984	0.0028	9.0281	0.0816	1.287	0.006	-811.8
	12000044	12000044.2	2	0.3774	0.3047	4.2113	0.0006	8.9437	0.0810	1.287		
z3BK/BD	11000002	11000002.1	3	0.2564	0.1610	4.8079	0.2509	10.5273	0.0039	1.31	0.04	-816.6
z3BK/BD	12000036	12000036.1	4	0.3758	0.1865	4.4433	0.0022	9.1080	0.1726	1.29	0.0016	-311.04
z3BK/BD	12000038	12000038.1	5	0.3125	0.1909	4.5165	0.0061	9.3145	0.1171	1.298	0.0052	-453.02
Total amount of collected solution											0.0528	
Averaged concentration of species				0.3335	0.2174	4.4555	0.0525	9.3843	0.0913	1.306		

Tab. A.6.4 Analytical chemical composition of salt solutions z3OSO

Type	KeyNo	SampleNo	No.	Concentration in [mol/kg H2O]						Density	Volume	Depth
				Na^+	K^+	Mg^{2+}	Ca^{2+}	Cl^-	SO_4^{2-}	[g/cm^3]	in [m^3]	[m]
Z3OSO	12000035	12000035.1	1	5.282	0.072	0.100	0.111	5.734	0.021	1.203	84.655	-236.68
	12000035	12000035.2	2	4.299	0.308	0.709	0.074	6.113	0.031	1.203		
	12000035	12000035.3	3	4.048	0.341	0.700	0.081	5.844	0.054	1.203		
Total amount of collected solution											84.655	
Averaged concentration of species				4.543	0.240	0.503	0.089	5.897	0.035	1.203		

A.7 Appendix 7: Geological profile of the Gorleben shafts



The legend z2HS1 and z2HS3 was exchanged by BGR.

Fig. A.7.1 Geological profile of the Gorleben shafts

Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH

Schwertnergasse 1
50667 Köln
Telefon +49 221 2068-0
Telefax +49 221 2068-888

Forschungszentrum
85748 Garching b. München
Telefon +49 89 32004-0
Telefax +49 89 32004-300

Kurfürstendamm 200
10719 Berlin
Telefon +49 30 88589-0
Telefax +49 30 88589-111

Theodor-Heuss-Straße 4
38122 Braunschweig
Telefon +49 531 8012-0
Telefax +49 531 8012-200

www.grs.de

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