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Project SAFE

Modelling of long-term concrete degradation processes in the Swedish SFR repository

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Modelling of long-term concrete degradation processes in the Swedish SFR repository

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Abstract

This study concerns the leaching of concrete barriers, in particular the silo construction, in the Swedish SFR repository for low and intermediate level radioactive waste. A conceptual model for the leaching of concrete in a saline groundwater has been proposed based on the increased understanding achieved from research studies presented in the literature. The conceptual model has been used to set up a numerical model for the complex chemical interactions beween the cement minerals of the concrete with the groundwater. The calculations show that various chemical reactions are expected to occur in the concrete over time. Different cases have been calculated. The results show that the chemical conditions in the concrete barriers will maintain alkaline for long time. In the most exposed parts of the concrete a high degree of leaching can be expected during the considered 10 000 years, whereas only for the most unfavourable assumptions (initially fractured concrete with groundwater flow-through) the inner parts of the concrete will be degraded to any significant degree.

Sammanfattning

Denna studie behandlar lakning av betongbarriärer, främst i siloförvaret, i SFR där låg- och medelaktivt radioaktivt avfall slutförvaras. En konceptuell modell för betonglakning i salthaltigt grundvatten har föreslagits som grundas på litteraturuppgifter från de senaste årens forskning. Den konceptuella modellen har legat till grund för en numerisk modell som tagits fram där komplex kemisk växelverkan mellan betongens cementmineral och grundvattnet beaktas.Beräkningarna visar att olika kemiska reaktioner successivt kan förväntas uppträda i betongen med tiden. Olika beräkningsfall har genomförts. Resultaten visar att de kemiska betingelserna i betongen kommer att förbli alkaliska under lång tid. I de mest utsatta delarna av betongen kan en höggradig urlaking förväntas ske under den beaktade 10 000-årsperioden. Betydande påverkan av betongens inre delar förväntas däremot endast för de mest ofördelaktiga antagandena (dvs en initialt sprucken betong med genomströmmande grundvatten).

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1 Introduction

The aim of this study is to estimate the leaching of concrete in groundwater. This information will be used in the safety assessment of the SFR repository. The work is based on recent years research, which has increased our possibilities to calculate reactions in concrete.

2 Groundwater conditions in the SFR area

The chemical conditions in the groundwater in the SFR area are of importance for the calculations of long-term chemical degradation of the concrete structures in the repository. Data on the present day groundwater chemistry, representative for the salt water period, have been compiled and a set of data for the geochemical model calculations have been proposed, see Table 2.1. Data from the control program of SFR (1989-99), data from before the building of SFR (undisturbed, 1984-86) and data from the counties of Östhammar, Finnsjön and Äspö have been used in this assessment.

Table 2.1 Chemistry data proposed for the salt-water period (i.e. the coming 1000-5000 years) and the associated variation interval. Data from the previous assessment is shown for comparison.

Parameter	**Previous assessment***			**New assessment**		
(mg/l)	assumed	min	max	proposed	Min	Max
HCO_3^- (alk)	100	40	110	100	40	110
SO_4^{2-}	500	20	600	500	20	600
Cl^-	5000	3000	6000	5000	3000	6000
Na^+	2500	1000	2600	2500	1000	2600
K^+	-	-	-	20	6	30
Ca^{2+}	1000	800	1600	430	200	1600
Mg^{2+}	300	100	300	270	100	300
pH	7.5	6.5	7.8	7.3	6.5	7.8
Eh**	-	50	-300	Reducing	-100	-400
Si as SiO_2(aq)	-	-	-	5.66	-	-
Electrical balance %				-0.04 %		

* undisturbed rock, based on measurements in HK1, HK7, HK10 and HK11 (SKB, 1987)
**-100--400 = proposed interval in SKB, 1999 (annual report for SFR).

Results from geochemical speciation modelling of the proposed salt-water suggest that the proposed water composition would be likely to be in thermodynamical equilibrium with common mineral phases in the rock. In particular the above-proposed composition of the SFR groundwater during the salt water period has been adjusted with respect to the contents of calcium and magnesium in order to reach an initial equilibrium with respect to both calcite and dolomite. In addition, silica has been added to the water definition, 5.66 mg/l SiO_2 (equilibrium with quartz), since the absence of silica in the water would give an artificial dissolution of different silicates in the following concrete degradation calculations. As a result of these adjustments of the groundwater composition the pH was slightly reduced in order to maintain electrical balance. The resulting water would have a composition according to Table 2.1. The electrical balance between cations and anions is quite good.

For the period after land rise, rounded values from the County of Östhammar are proposed (Table 2.2). The proposed value for potassium and its variation interval is based on general measurements made by SGU in Sweden ("SGUs grundvattennät" and "PMK-grundvatten") and proposed values for a standard water (SNV/SGU, 1995 and Höglund et al., 1997). The latter are based on observed concentrations in deep groundwaters in igneous rock.

It is important to include potassium in the groundwater since potassium is present in significant amounts in the concrete pore water. The content of potassium in the groundwater will therefore influence the rate of leaching of potassium from the concrete.

Table 2.2 Chemistry data proposed for the fresh water period (i.e. following 1000-5000 years from today) and the associated variation interval.

Parameter (mg/l)	**Proposed value**	**Min**	**max**
HCO_3^- (alk)	300	170	540
SO_4^{2-}	50	3	110
Cl^-	45	5	1000
Na^+	100	20	200
K^+*	4	0.2	10
Ca^{2+}	35	25	140
Mg^{2+}	9	3	10
pH	7.49	6.7	8.7
Eh	Reducing	-100	-400
Si as SiO_2(aq)	5.9		
Electrical balance %	-0.08 %		

*proposed value= rounded "Allard standard water" (SNV, 1997). Min and max are taken from measurements made by SGU in Swedish groundwater ("SGUs grundvattennät" and "PMK-grundvatten"; (SNV/SGU, 1995).

Results from geochemical speciation modelling of the proposed fresh-water suggest that the proposed water composition would be likely to be in thermodynamical equilibrium with common mineral phases in the rock. In particular the above-proposed water is in equilibrium with respect to calcite and slightly sub-saturated with respect to dolomite. In addition, silica has been added to the water definition, 5.9 mg/l SiO_2 (equilibrium with quartz), since the absence of silica in the water would give an artificial dissolution of different silicates in the following concrete degradation calculations. The resulting water would have a composition according to Table 2.2. The electrical balance between cations and anions is quite good.

3 Composition of concrete barrier materials in SFR

3.1 Composition of the cement used in SFR

The cement used for major concrete constructions in SFR, such as the silo bottom, silo walls and silo top, concrete walls in BMA etc, is Degerhamn Anläggningscement. The chemical composition of this cement is presented in Table 3.1.

Table 3.1 Chemical composition of Degerhamn Anläggningscement, including both the oxide composition and the corresponding clinker mineral composition (Alemo, 1992).

Component	***Content % by weight***
Ca	64
SiO_2	21
Al_2O_3	3.5
Fe_2O_3	4.6
MgO	0.7
K_2O	0.62
Na_2O	0.07
SO_3	2.2
Cl	<0.1
Free $CaCO_3$	0.9
Corresponding clinker components	
Tricalcium silicate, C_3S	64.4
Dicalcium silicate, C_2S	10.9
Tricalcium aluminate, C_3A	2.0
Tetracalcium aluminate ferrite, C_4AF	13.9
Calcium sulphate (gypsum), $C\hat{s}H_2$	3.7
Alkali hydroxides, $N + K$	0.7
Abbreviations used for the clinker components:	
C=CaO, S=SiO_2, A=Al_2O_3, F=Fe_2O_3, H=H_2O, $C\hat{s}H_2$=$CaSO_4\cdot 2H_2O$, N=Na_2O, K=K_2O	

Degerhamn Anläggningscement conforms with requirement in the Swedish standard for sulphate resistant cements SS 13 42 01, as well as according to ASTM, DIN and BS standards. This cement also complies with the requirements for low alkali cements that do not give rise to alkali-silica reactions according to Swedish standard SS 13 42 01.

3.2 Mixing proportions for concrete in SFR

The mixing proportions used for concrete components in SFR are presented in Table 3.2.

Table 3.2 Mixing proportions for concrete structures in SFR, amounts given in kg/m^3.

Component	**Construction concrete** *(Jacobsen and Gjörv, 1987)*	**Silo grout** *(Björkenstam, 1997)*	**Conditioning cement**
Degerhamn anläggningscement	350	325	1180
Water	164.5	366	437
Ballast	1829 (total)	1302	-
	0-8 mm 920 kg/m^3 8-16 mm 374 kg/m^3 16-32 mm 535 kg/m^3		
Additives (anti-foaming, cellulose)	0.5% Sika Plastiment BV-40 0.05–0.2% Sika Retarder	6.5	-
Air	-	2.5 % by volume	-
w/c ratio	0.47 (0.46 – 0.49)	1.125	0.37

The ballast material is selected to comply with Swedish standards on resistance to alkali-silica reactions.

4 Composition of bentonite and sand/bentonite barrier materials in SFR

The bentonite used in SFR is a sodium bentonite. Pure bentonite has been used in the slot between the silo walls and the rock. The sand/bentonite bed below the silo bottom is a 90/10 mixture, specially composed to withstand the weight of the silo construction without settling. At the top of the silo a 90/10 sand/bentonite mixture will be applied with moderate compaction supplied by a concrete layer and filling of crushed rock in the top of the silo excavation. The properties of the different bentonite barriers are summarised in Table 4.1.

The bentonite material contains different assessory minerals in addition to the montmorillonite. The mineralogical and chemical composition of the bentonite used in SFR is presented in Table 4.2, whereas the porewater composition is given in Table 4.3.

Table 4.1 Properties of the bentonite barrier materials used in SFR.

Component	**Mixture Sand/bentonite**	**Bulk density, dry (kg/m^3)**	**Porosity (m^3/m^3)**
Sand/ bentonite			
Silo bottom	90/10	2000 a)	0.15
Silo top	90/10	2000 a)	0.25 a)
Pure bentonite			
Silo wall slot	0/100	1050 a) (950 at the top – 1120 at the bottom) b)	0.61 a)

a) Neretnieks et al. (1987); b) Pusch (1985)

Table 5.2 Mineralogical and chemical composition of the bentonite barrier materials used in SFR.

Mineral phase	**Chemical formula**	**Content in 90/10 mixture**	**Content in pure bentonite**	**Comment**
Montmorillonite				72% Na-form 27% Mg-form small amounts of K- and Ca-forms
Calcite	$CaCO_3$	0.14 wt%	1.4 wt% *)	
Pyrite	FeS_2	-	-	Not considered
Brucite	$Mg(OH)_2$	0.087 wt%	0.87 wt% **)	Data missing for GEKO/QI. Assumed value
Gypsum	$CaSO_4 \cdot 2H_2O$	0.034 wt%	0.34 wt% *)	Data missing for GEKO/QI. Data for MX-80 assumed
Cristobalite	SiO_2	-	-	Not considered
$C_{organic}$	$-(CH_2)_n-$		<1%?	Not considered

*) Wanner et al (1994); **) Neretnieks et al. (1987)

Table 5.3 Reported data on pore water composition for bentonite/sand barriers and data assumed in the calculations.

Species	**Reported data (mg/l) [1] [2] for GEKO/QI in Stripa groundwater**	**Assumed values in the calculations (mg/l)**
CO_3^{2-}	1455-2125	2000
SO_4^{2-}	896-1158	1000
Cl^-	234-295	250
Na^+	2246-4126	3000
K^+	-	1
Ca^{2+}	14-30	20
Mg^{2+}	2	2
$H_4SiO_4^0$	-	9
F^-	28-72	Not considered in the calculations

1) Skagius and Karlsson (1987); 2) Neretnieks (1986)

5 Hydration and degradation processes for concrete

5.1 Introduction

Hydration is the process by which the anhydrous cement clinker minerals react with water and form new hydrated solid compounds that give the cement its mechanical strength. The amount of water added to the cement will influence the properties of the hardened cement. The relation between the water and cement added to the mixture is termed the w/c-ratio. Since water is consumed when the hydrated minerals are formed, at low w/c-ratio (less than about 0.3) the cement clinker minerals will not be completely hydrated due to lack of water. At high w/c-ratios, the water remaining after full hydration has occurred will contribute to an increased porosity. In general terms, a low w/c-ratio would give more dense and stronger cement than cement with high w/c-ratio. The choice of mixing proportions is, however, a compromise between factors such as strength, desire to reach full hydration, workability of the fresh paste, special demands on the permeability etc. Commonly, a w/c-ratio between 0.3 and 0.6 is used for normal construction work. In SFR, the construction concrete has a w/c-ratio of 0.47, the conditioning cement a w/c-ratio of 0.37 and the silo grout a w/c-ratio of 1.125.

The porosity of the concrete barriers in SFR has been calculated from the mixing proportions in Table 3.2 and a simple hydration model presented by Höglund (1992) which follow the methodology described by Ahlgren et al (1976). The results are presented in Table 5.1. The stated porosity refers to the total porosity of the concrete, taking into the account the presence of significant amounts of non-porous ballast in some constructions.

Table 5.1 Porosity calculated using the hydration model by Höglund (1992).

Component	**Construction concrete**	**Silo grout**	**Conditioning cement for ion exchange resins**
Degerhamn anläggningscement (kg/m^3)	350	325	1100
Water (kg/m^3)	164.5	366	462
Ballast (kg/m^3)	1829	1302	-
w/c ratio (kg/kg)	0.47	1.125	0.42
Capillary pores	0.03	0.24	0.038
Gel pores	0.047	0.044	0.149
Contraction pores	0.022	0.02	0.069
Total porosity	0.099	0.309	0.256

5.2 Leaching

In their review, Lagerblad and Trägårdh (1994, TR 95-21) have pointed out that the models previously used for studies of the leaching of alkali and calcium hydroxides in the SFR safety assessment were oversimplified. The criticism reflects the simplifications made when calculating the leaching of alkali hydroxides as dissolved substances, and the fact that the counter effect of alkali ions in the groundwater was neglected, leading to a rapid depletion of alkali ions in the concrete material. Furthermore, the leaching of calcium hydroxide and calcium silicate hydrates (*CSH*-gel) were represented as processes independent of the alkali leaching. In the present study, the leaching of alkali hydroxides have been represented by ion exchange processes, also taking into account the counter ion effect of the surrounding groundwater. The results show a significantly different leaching behaviour for the alkali hydroxides compared to the previous estimates.

Further, in the present study the leaching of different calcium compounds, e.g. portlandite and *CSH*-gel, has been coupled to the leaching of alkali hydroxides. This has the effect that during the early period, the leaching of calcium compounds is suppressed by the high pH maintained by the alkali hydroxides in the pore water. The available data for thermodynamic calculations have significantly improved since the previous studies for SFR, especially regarding the preferential leaching of calcium from *CSH*-gels with variable *C/S*-ratio. In the previous study, the limiting *C/S*-ratio for the *CSH*-gel was assumed to be 2.5, whereas this value has been shown by more recent studies to be a too high value (Stronach and Glasser, 1997). It has now been shown that the *CSH*-gels are generally a solid solution series that varies in composition between $C_{1.8}SH$ and $C_{0.8}SH$. In the present study, the *CSH*-gel has been represented by three discrete *CSH* mineral phases: $C_{1.8}SH$, $C_{1.1}SH$ and $C_{0.8}SH$. The $C_{1.8}SH$-phase may coexist with portlandite in the more alkaline regime, whereas $C_{0.8}SH$ may coexist with amorphous SiO_2 in highly leached concrete. In the intermediate regime, between highly alkaline and highly leached conditions, $C_{1.1}SH$ coexist with either $C_{1.8}SH$ or $C_{0.8}SH$ depending on the C/S-ratio. The present model accounts for the gradual transformation of portlandite and *CSH*-gel between these different mineral phases.

Compared to the previous investigations this will have the effects that:

- The amount of free portlandite will be higher, from which follows that the leachable amount of this mineral is increased.

- A high pH will be maintained for an extended period of time when all other assumptions remain the same.

- The amount of leachable *CSH*-gel will decrease accordingly.

5.3 Reactions with calcium aluminates/ferrites

The presence of significant amounts of different calcium aluminate/ferrite phases in the cement must be considered in the leaching model. The calcium aluminates/ferrites are usually alkaline and may influence the long-term leaching process. During an initial stage of the cement hydration, the calcium aluminates play an important role as retardants for the settling process in cement. By adding a small amount of gypsum to the cement, calcium aluminates rapidly forms a thin surface coating of ettringite (a hydrated calcium sulphoaluminate) at the reactive unhydrated cement grains, thereby temporarily retarding the settling. Ettringite may also form due to exposure to high sulphate concentrations at a later stage; a reaction potentially accompanied by large volume expansion that may deteriorate the solid concrete structure. The chemical interactions between calcium aluminates in the cement and different components in the groundwater are complex.

Table 5.1 Composition of hydrated cement used in SFR. Composition calculated from the chemical composition of the SFR cement and the mixing proportions stated in Table 3.2 using the hydration model by Höglund (1992); Höglund and Bengtsson (1991).

Hydrate	Amount kmol/m^3 concrete	Fictive concentration kmol/m^3 pore water
C_3FH_6	0.1008	1.020
C_3AH_6	0.02397	0.2424
Monosulphate	0.09613	0.9722
Ettringite	0	0
CSH-gel	1.225	12.39
Portlandite	1.036	10.48
Brucite	0.06079	0.6149
KOH	0.04607	0.4660
NaOH	0.007903	0.07993
$CaCO_3$	0.06295	0.6367
Porosity	0.099	m^3/m^3 concrete

For the purpose of geochemical modelling the amount of hydration products have been transformed to a fictive pore water concentration in the table. This does not infer that these concentrations would be expected in the pore water, but rather reflects the total amount of these components, in dissolved and solid phases, that are brought in contact with the pore water in the calculations.

The most soluble components, i.e. the alkali hydroxides, are present in significant amounts in the cement phase. However, comparisons with measured pore water data for cement show that only parts of the alkali ions are present in dissolved form. In the present study, the pore water concentrations reported in Table 7:1 in Lagerblad and Trägårdh (1995), have been used to calibrate an ion exchange model that fits both the total concentrations and the soluble phase concentrations that are observed.

6 Conceptual model chemical interaction of concrete with groundwater and bentonite

The objective of this chapter is to present an overview of different processes considered in the modelling work. A conceptual model of different chemical interactions between concrete, groundwater, and bentonite is illustrated in Figure 6.1. Of course, this is not a comprehensive and complete description of the complex geochemical system. However, it does comprise a reasonable representation of components that may influence the properties of barrier materials in the long-term.

When brought in contact with groundwater a number of chemical reactions in the cementitious materials will start. A simple form of reaction is dissolution of soluble components that may be released by diffusion into the groundwater. For low soluble components, a solubility limit is reached, which may reduce the leaching rate. Different components in the groundwater may also react with components in the concrete pore water or with the solid cement minerals and form new minerals. Also different ion exchange processes may need to be considered.

In the present calculations, the interaction between multiple components in groundwater and the concrete are considered simultaneously, using the coupled chemistry-transport model PHREEQC-2 (Parkhurst and Appelo, 1999). The model allows the different processes to occur in parallel and at different locations in the studied model domain. Thereby, the present model gives an assessment on the combined impacts of the different considered processes, which is a further development compared to previous assessments, e.g. Höglund and Bengtsson (1991). Below a description is given for the different chemical sub-systems used in the model.

Alkali metals, Na and K

Generally, the alkali metal hydroxides are soluble, and would therefore, be easily leached from the concrete materials. Studies of the composition of solid phases and pore water of concrete show, however, that the alkali hydroxides are associated with the solid phases, likely the *CSH*-gel phases or the ballast. In the present study, the contents of alkali hydroxides in solid phases and pore water have been coarsely calibrated against measured data for Degerhamn Standard Portland cement (Lagerblad and Trägårdh, 1995) assuming an ion exchange process. A comparison between measured data and model results are presented in Table 6.1. Berner (1990) discussed this phenomenon and used a different approach where 5% of the remaining alkali metals were assumed to dissolve for each pore water exchange cycle.

Table 6.1 Measured data (Lagerblad and Trägårdh, 1995) and results from calibrated ion exchange model calculations of the alkali metal concentrations in fresh cement paste.

Component	Solid phase concentration (% as oxide in cement)	Hypothetical pore water concentration assuming all soluble (mM)	Measured pore water concentration (mM)	Calibrated model results for pore water (mM)
Na	0.07	96	28	26
K	0.62	560	83	90

Portlandite, CSH-gel and SiO_2-gel

In the previous studies of SFR, the upper boundary of the C_xSH-gel composition was assumed to correspond to x=2.5. This assumption was conservative with respect to the amount of portlandite available for leaching. Recent studies have confirmed that the limiting compositions of the solid solutions series, commonly denoted C_xSH-gel, extends from x= 0.8 to about 1.8. At calcium contents below x= 0.8, a separate phase consisting of SiO_2-gel is formed, whereas, for high calcium contents, above x = 1.8 (in the range 1.7 – 2 (Glasser, 2000)), portlandite will precipitate as a separate phase. Initially, concrete made of Ordinary Portland cement will contain an excess of calcium, which means equilibrium between portlandite and $C_{1.8}SH$-gel is maintained. Since portlandite is the more soluble phase, leaching will lead to depletion of portlandite in the first hand. In the next phase, $C_{1.8}SH$-gel will be gradually transformed into $C_{1.1}SH$-gel while expelling calcium into the pore water. This will continue in the next steps by transformation of $C_{1.1}SH$-gel into $C_{0.8}SH$-gel, then of $C_{0.8}SH$-gel into SiO_2-gel. This type of process, where the more soluble component of a solid solution series is gradually leached, is denoted incongruent dissolution. It has been shown that the *CSH*-gels are persistent in nature over periods exceeding 10^4 years, despite the metastability with respect to crystalline mineral phases such as tobermorite[1] and jennite (Stronach and Glasser, 1997). The possible formation of thaumasite by reaction with carbonate has been disregarded and is unlikely to be stable above 20^0C (Glasser, 2000).

In the present study, the incongruent dissolution of the *CSH*-gel has been represented by three distinct mineral phases, $C_{1.8}SH$, $C_{1.1}SH$ and $C_{0.8}SH$ respectively, each with a separate solubility. The used numerical model is capable of handling a more rigorous formulation of the dissolution of solid solution series, whereas, in the present study it has been judged that the selected approach would give sufficient level of detail. It is expected that the conclusions reached would not be significantly changed by a more elaborate approach to model the incongruent dissolution of the *CSH*-gel. Example calculations for incongruent dissolution of *CSH*-gels can be found in Berner (1990) and Savage et al. (2000).

Calcium aluminates and reactions with chloride, sulphate and carbonate

Calcium aluminates are important components of the cement. During early stages of hydration they react rapidly and may be responsible for the mechanical properties during the first hours. The clinker minerals C_3A and C_4AF react with water to form C_3AH_6, C_3FH_6 and/or other related mineral phases by reaction with sulphate, chloride and carbonate in the cement.

In particular the formation of the mineral ettringite, a hydrated calcium aluminate sulphate, is of importance. In the early hydration process, ettringite formation is deliberately enforced by adding gypsum to the cement to slow the settling speed of the cement. The ettringite forms a surface coating on unhydrated calcium silicates, which retard their reaction with water temporarily. Monosulphate is a similar compound, but containing less sulphate.

In later stages, the reaction between concrete and components in the groundwater may lead to further precipitation of calcium aluminate related compounds. This has potentially a large impact on the longevity of concrete materials. The reason is that the calcium aluminates have the ability to bind substantial quantities of crystal water, potentially

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[1] See Table 7.1 for chemical formulas of the various minerals mentioned

leading to expansion in the solid matrix of the cementitious material. In particular, the late formation of ettringite may occur by a solid phase transformation reaction, as opposed to the more common dissolution - precipitation reactions. The late reactions with calcium aluminates may therefore result in the formation of cracks or a disintegration of the material.

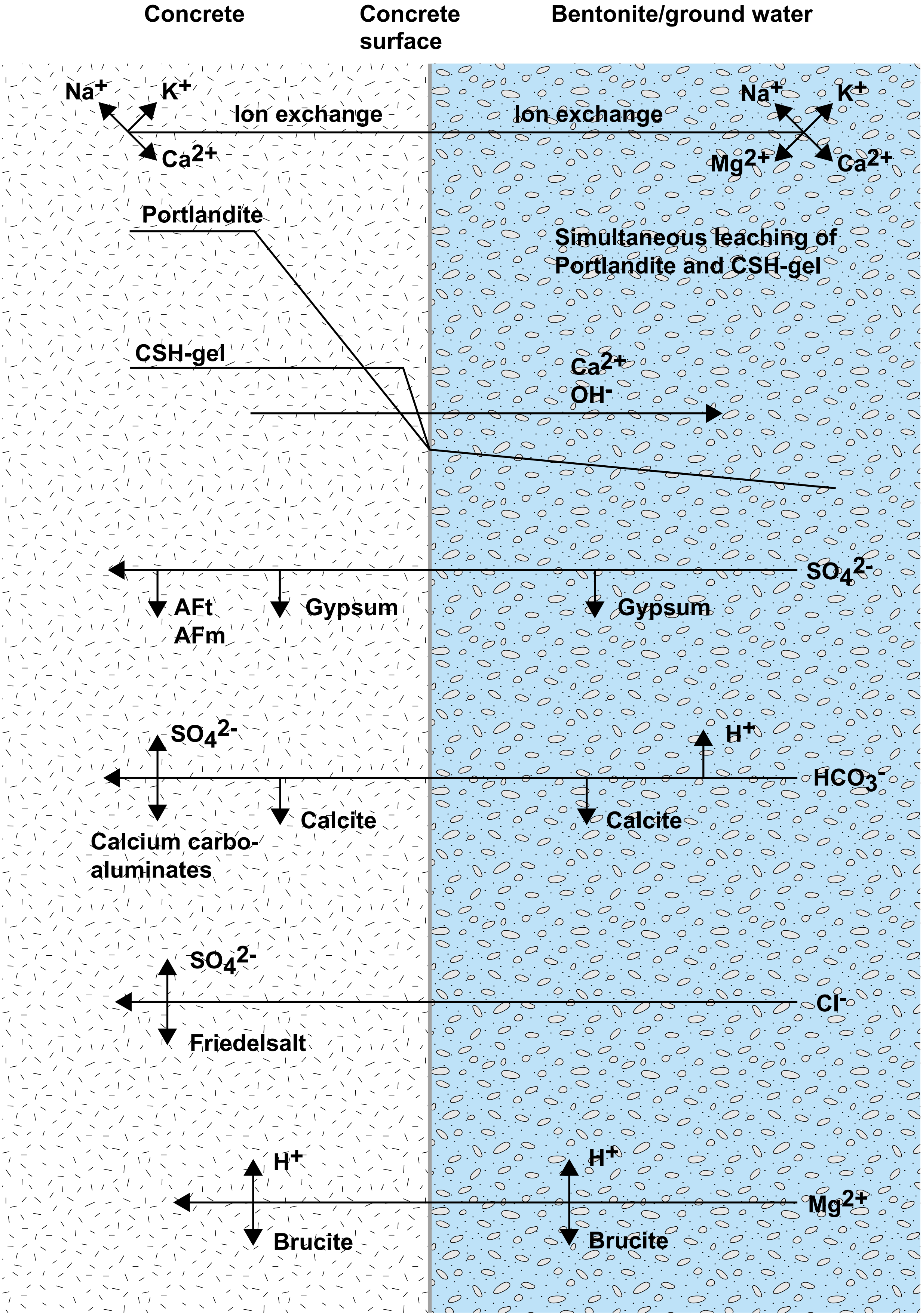

Figure 6.1 Schematic model for the interaction of groundwater with concrete.

7 Compilation of relevant thermodynamic data for concrete, bentonite and rock systems

The thermodynamic data necessary for the calculations have significantly improved as a result of recent research activities. Evaluations of thermodynamic stability constants have been made within the present study based on literature data. A variety of experimental and theoretical investigations on the chemistry of cements have been presented over the last years, e.g. (Damidot and Glasser (1993), Damidot et al (1992,1994a, b; 1995), Birnin-Yauri and Glasser (1998), Atkins and Glasser (1992), Atkins et al (1992), Stronach and Glasser (1997), Perkins and Palmer (1999)). The methodologies applied in different experimental studies differ to some extent, as do the way data are interpreted in terms of stability constants. This makes a direct use of interpreted stability constants assembled from different literature sources uncertain. The approach used in this study is to use the primary data on measured aqueous concentrations and pH-values from different literature sources, and to re-evaluate the thermodynamic data, i.e. log K_s-values for the desired mineral phases, in a consistent way. In the first hand, data for invariant points have been used where the variability of the aqueous concentrations would be expected to be low. Chemical conditions, characterised by equilibrium conditions with one or more pure mineral phases, such that the aqueous composition can not change without disrupting the equilibrium conditions, are denoted invariant points.

The present study presents calculations for about 90 experiments, all calculations made with a common set of basic thermodynamic constants, MINTEQ (Allison, 1991), and a consistent method for ionic strength corrections, Davies (Parkhurst, 1995). Complementary log K_s-values have been calculated for the mineral phases C_xSH-gel (x = 0.8, 1.1, 1.8), gibbsite, brucite, hydrotalcite[2] ($Mg_4Al_2O_7\cdot 10H_2O$), SiO_2-gel, portlandite, ettringite, monosulphate, C_3AH_6, Friedelsalt (7 different phases with compositions ranging from $C_3A\cdot CaCl_2\cdot 10H_2O$ to $C_3A\cdot 0.39CaCl_2\cdot 0.61Ca(OH)_2\cdot 10H_2O$), Kuzel´s salt $C_3A(CaCl_2)_{0.5}(CaSO_4)_{0.5}\cdot 10H_2O$, $CaCl_2\cdot 6H_2O$, $CaO\cdot CaCl_2\cdot 2H_2O$, syngenite, hemicarbo aluminate ($C_2A\cdot 0.5CaCO_3\cdot 0.5Ca(OH)_2\cdot 11.5H_2O$ and monocarbo aluminate ($C_3A\cdot CaCO_3\cdot 11H_2O$). The chemical composition and stoichiometry of the assumed dissociation reactions are presented in Table 7.1. The table also shows the span of calculated log K_s-values, references to the source of data and the selected log K_s-value for the geochemical modelling. Details of the calculations are presented in appendix A. To ensure a consistent approach, the same database and ionic strength corrections have also been used in all calculations in this study.

Apart from pure ion exchange reactions of the bentonite, only the accessory minerals brucite, calcite and gypsum are considered as active geochemical components in the bentonite in the present calculations. Hence, the possible chemical interaction between the montmorillonite mineral and the alkaline concrete leachate water, which would require consideration of kinetic factors, has not been considered in this study. Reactions with christobalite have not been considered in the present calculations. However, this is a topic to be further studied in a recently launched research project within EU, the ECOCLAY-II project.

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[2] This name is also used for a mineral with the composition $Mg_6Al_2(CO3)(OH)_{16}\cdot 4H_2O$

Table 7.1 Calculated thermodynamic stability constants for specific hydrated cement minerals used in the calculations.

Mineral name and chemical composition	**Reaction formula and stability constants (log K_s) calculated in this study using experimental data in the stated references**	**Literature data for log K_s**
$C_{1.8}SH$-gel $(CaO)_{1.8}SiO_2{\cdot}nH_2O$	$Ca_{1.8}SiO_{3.8}:H_2O+3.6\ H^+=H_4SiO_4+1.8\ Ca^{2+}+0.8\ H_2O$ 32.7 (Stronach et al., 1997)	
$C_{1.1}SH$-gel $(CaO)_{1.1}SiO_2.nH_2O$	$Ca_{1.1}SiO_{3.1}:H_2O+2.2H^+=H_4SiO_4+1.1Ca^{2+}+0.1H_2O$ 16.72 (Stronach et al., 1997)	
$C_{0.8}SH$-gel $(CaO)_{0.8}SiO_2{\cdot}nH_2O$	$Ca_{0.8}SiO_{2.8}:H_2O+1.6H^++0.2H_2O=H_4SiO_4+0.8Ca^{2+}$ 11.08 (Stronach et al., 1997)	
Portlandite $Ca(OH)_2$	$Ca(OH)_2+2H^+=Ca^{2+}+2H_2O$ 22.9 (Stronach et al., 1997)	22.9 used value (MINTEQ data base) 22.8* (Reardon, 1992) 22.815 (Glasser et al, 1999)
Gibbsite $Al(OH)_3$	$Al(OH)_3+3H^+=Al^{3+}+3H_2O$	8.77 used value (MINTEQ data base) 8.1* (Reardon, 1992)
Brucite $Mg(OH)_2$	$Mg(OH)_2+2H^+=Mg^{2+}+2H_2O$	16.792 used value (MINTEQ data base) 17.12* (Reardon, 1992)
Hydrotalcite $Mg_4Al_2O_7{\cdot}10H_2O$	$Mg_4Al_2O_7:10H_2O=4Mg^{2+}+2Al(OH)_3+8OH^-+3H_2O$ -65.0 (Glasser et al, 1999)	-68.56* (Glasser et al, 1999)
Ettringite $(CaO)_3Al_2O_3(CaSO_4)_3{\cdot}32H_2O$	$Ca_6Al_2(SO_4)_3(OH)_{12}:26H_2O=6Ca^{2+}+2Al(OH)_4^-+3SO_4^{2-}+4OH^-+26H_2O$ -44.55 (Damidot et al., 1992)	-44.9 used value (Perkins et al., 1999)
Monosulphate $(CaO)_3Al_2O_3CaSO_4{\cdot}12H_2O$	$Ca_4Al_2SO_4(OH)_{12}:6H_2O=4Ca^{2+}+2Al(OH)_4^-+SO_4^{2-}+4OH^-+6H_2O$	-29.43 used value (Lee et al. 1995)- 29.25 (Reardon, 1992) -30.64* (Glasser et al, 1999)
Hemicarbo aluminate $(CaO)_3Al_2O_3{\cdot}(CaCO_3)_{0.5}{\cdot}$ $(Ca(OH)_2)_{0.5}{\cdot}11.5H_2O$	$Ca_3Al_2O_{6.5}C_{0.5}(OH):11.5H_2O=3Ca^{2+}+2Al(OH)_4^-+0.5CO_3^{2-}+3OH^-+6.5H_2O$ -22.44 (Damidot et al, 1994)	
Monocarbo aluminate $(CaO)_3Al_2O_3{\cdot}CaCO_3{\cdot}11H_2O$	$(CaO)_3Al_2O_3CaCO_3:11H_2O=4Ca^{2+}+2Al(OH)_4^-+CO_3^{2-}+4OH^-+5\ H_2O$ -31.5 (Damidot et al, 1994)	

Mineral name and chemical composition	**Reaction formula and stability constants (log K_s) calculated in this study using experimental data in the stated references**	**Literature data for log K_s**
SiO_2 -gel	-2.85 (Stronach et al., 1997)	
C_3AH_6	-22.5 used value (Damidot et al., 1993) -20.04 – -25.32 (Damidot et al., 1992) -22.77 – -22.69 (Damidot et al., 1995) -21.01 (Atkins et al., 1992)	
Friedelsalt	Compositions ranging from $C_3A \cdot CaCl_2 \cdot 10H_2O$ to $C_3A \cdot 0.39CaCl_2 \cdot 0.61Ca(OH)_2 \cdot 10H_2O$ -27.1 to -23.6 (Birnin-Yauri et al., 1998)	
Kuzel´s salt $(CaO)_3Al_2O_3(CaCl_2)_{0.5}(CaSO_4)_{0.5} \cdot 10H_2O$	$Ca_4Al_2(SO_4)_{0.5}Cl(OH)_{12}:6H_2O = 4Ca^{2+} + 2Al(OH)_4^- + 0.5SO_4^{2-} + Cl^- + 4OH^- + 6H_2O$ -27.10 (Glasser et al., 1999)	
Syngenite $CaK_2(SO_4)_2 \cdot H_2O$	$CaK_2(SO_4)_2:H_2O = Ca^{2+} + 2K^+ + 2SO_4^{2-} + H_2O$ -7.48 (Stronach et al., 1997)	-7.45 (Reardon, 1992) -7.45 (Glasser et al, 1999)
$CaCl_2 \cdot 6H_2O$	$CaCl_2:6H_2O = Ca^{2+} + 2Cl^- + 6H_2O$ 2.45 (Stronach et al., 1997)	
$CaO \cdot CaCl_2 \cdot 2H_2O$	$CaOCaCl_2:2H_2O = 2Ca^{2+} + 2Cl^- + 2OH^- + H_2O$ 25.49 (Stronach et al., 1997)	
Tobermorite $(CaO)_5(SiO_2)_6 \cdot 5.5H_2O$	Not considered	
Jennite $Ca_9Si_6O_{18}H_2(OH)_8 \cdot 6H_2O$	Not considered	
Thaumasite $Ca_3Si(CO_3)(SO_4)(OH)_6 \cdot 12H_2O$	Not considered	
Gehlenite hydrate $(CaO)_2Al_2O_3SiO_2 \cdot 8H_2O$	Not considered	
Siliceous hydrogarnet $(CaO)_3Al_2O_3SiO_2 \cdot 4H_2O$	Not considered	
* The stability constant for the reaction is recalculated from data given in the reference to allow comparison		

8 Model calculations

This chapter presents some basic assumptions made in the modelling for different cases. For each of the three considered cases the results are extensively presented in diagrams and commented in the text.

The purpose of the modelling has been to study:

- Effects on concrete integrity (extent and rate of leaching and degradation, tentative interpretation to transport properties, changes of chemical properties)

- Effects on bentonite (extent and rate of degradation as represented by ion exchange effects (Na, K, Ca)-forms of bentonite, changes of porosity)

In the calculations for Case 1 and Case 3, diffusion is assumed to control the mass transfer in concrete and sand/bentonite. The effective diffusivity in concrete has been assigned a constant value of $1 \cdot 10^{-11}$ m^2/s. The effective diffusivity in sand/bentonite has been assigned a constant value of $1 \cdot 10^{-10}$ m^2/s. In the calculations for Case 2, a groundwater flow rate has been assumed that correspond to a total flow of 3.8 m^3/year through the silo construction during steady-state conditions (Holmén and Stigsson, 2001, local model – first silo definition).

8.1 Case 1 - Diffusion with constant groundwater composition as boundary condition

This is a limiting case with constant external conditions. Only diffusion and chemical effects are considered. The composition of the groundwater has been assumed constant, independent of time. This represents a case where the exchange of groundwater is fast compared with the exchange of dissolved components between the groundwater and the concrete. When only diffusion is considered, it therefore represents the most rapid exchange. A complex set of chemical processes is considered in the calculations, i.e. multi-species aqueous complexation, ion exchange, and dissolution and precipitation of selected mineral phases. The concrete slab is represented by five cells (0.05, 0.05, 0.1, 0.2 and 0.6 m respectively), see Figure 8.1.

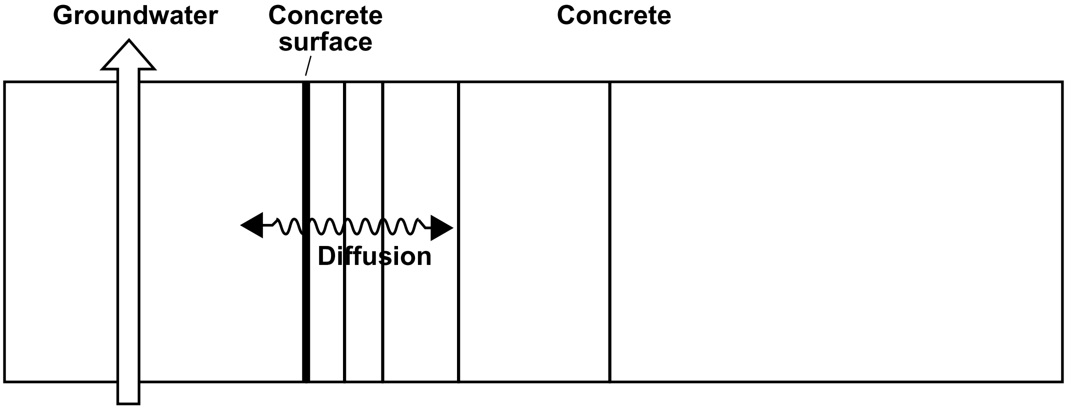

Figure 8.1 Simplified representation of a concrete barrier exposed to leaching by groundwater at one side. Leaching is assumed to be governed by diffusion.

8.1.1 Concentration profiles at different times - Case 1

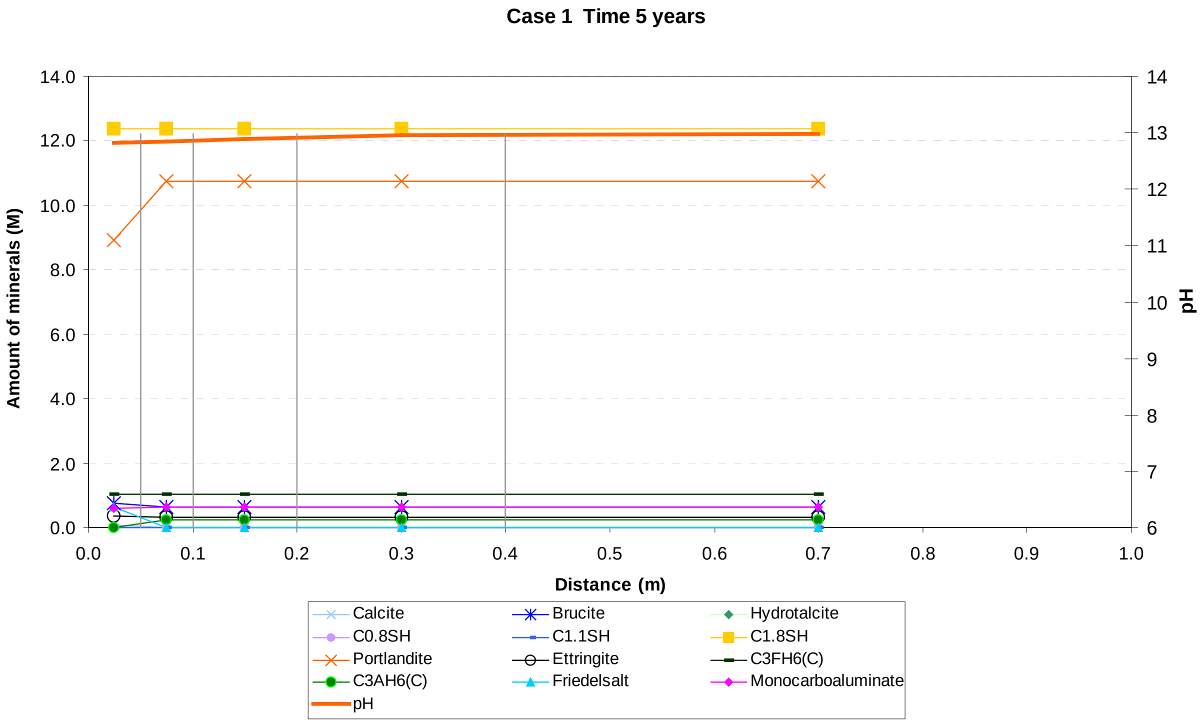

Figure 8.1a Results from leaching calculations for Case 1 after 5 years. Concentration profiles through a 1 m thick concrete slab exposed to groundwater at the left side. The positions of the markers refer to the centre in each cell. The vertical grey lines indicate the borders of the cells.

Figure 8.1a shows a cross-section through a 1 m concrete slab, at one side exposed to groundwater of constant composition. The figure shows the predicted amount of different minerals[3] versus depth after 5 years of leaching.

The calculations show that brucite, $Mg(OH)_2$, is precipitated near the surface exposed to groundwater. Portlandite is leached to about 17% to a depth of 0.05 m.

The interaction with the saline groundwater is indicated by the formation of a form of Friedelsalt, $C_3A{\cdot}0.39CaCl_2{\cdot}0.61Ca(OH)_2{\cdot}10H_2O$, to a depth of about 0-0.05 m. This is caused by an intrusion of chloride ions from the groundwater. Monocarbo calcium aluminate has decreased by 7% at a depth of 0-0.05 m after 5 years as a result of reaction with chloride to form Friedelsalt. C_3AH_6 has been depleted after 30 years forming Friedelsalt. A minor formation of ettringite, $C_3A{\cdot}3CaSO_4{\cdot}32H_2O$, is apparent at a depth of 0-0.05 m. These processes are accompanied by a drop in pH to about 12.8 near the surface. At depth, pH remains about 13.

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[3] In the figures an abbreviated notation common in cement literature is used for many of the calcium minerals, see explanation for abbreviations in Table 3.1 and chemical formula for different minerals in Table 7.1.

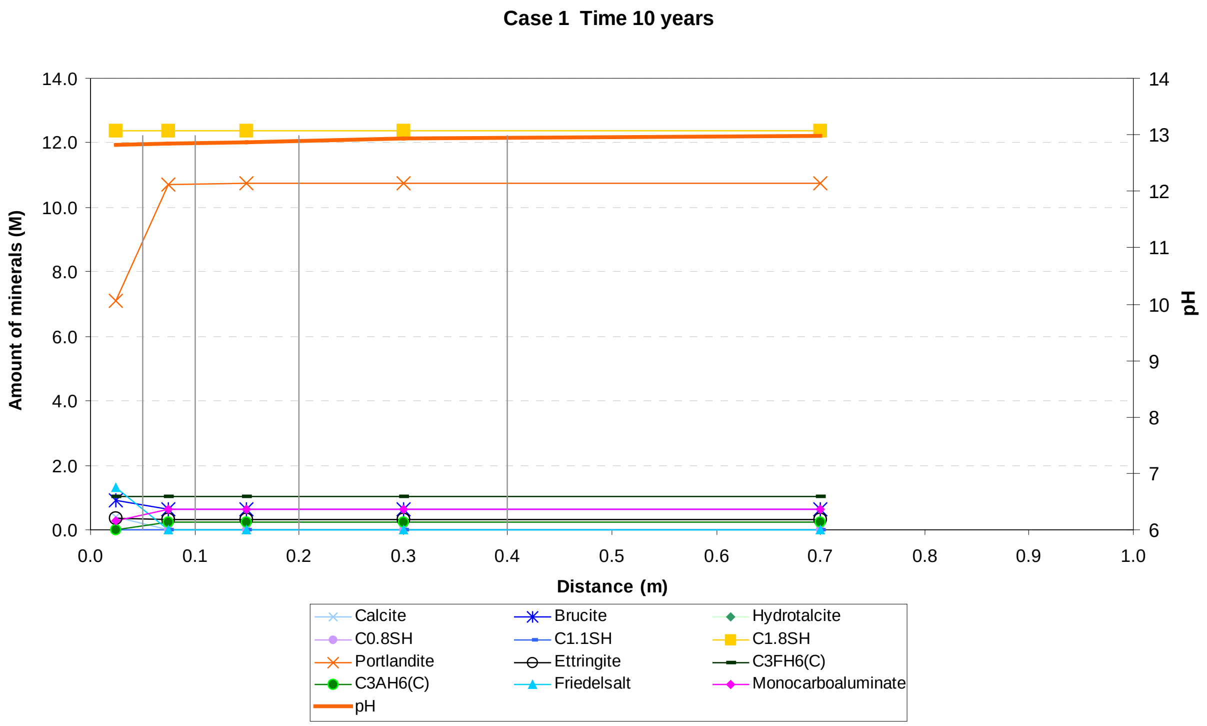


Figure 8.1b Results from leaching calculations for Case 1 after 10 years. Concentration profiles through a 1 m thick concrete slab exposed to groundwater at the left side. The positions of the markers refer to the centre in each cell. The vertical grey lines indicate the borders of the cells.

Chloride intrusion to a depth of 0-0.05 m after 10 years, see Figure 8.1b, is apparent from the formation of Friedelsalt, accompanied by a decrease in free portlandite, which is partly incorporated in the Friedelsalt, partly released into the groundwater, and partly reacts with carbonate to precipitate calcite.

A minor formation of ettringite, $C_3A\cdot 3CaSO_4\cdot 32H_2O$, is apparent near the surface. The monocarbo calcium aluminate is depleted to 54% near the surface.

Near the surface, the pH remains at 12.8, reaching a value of about 13 for depths more than about 0.5 m.

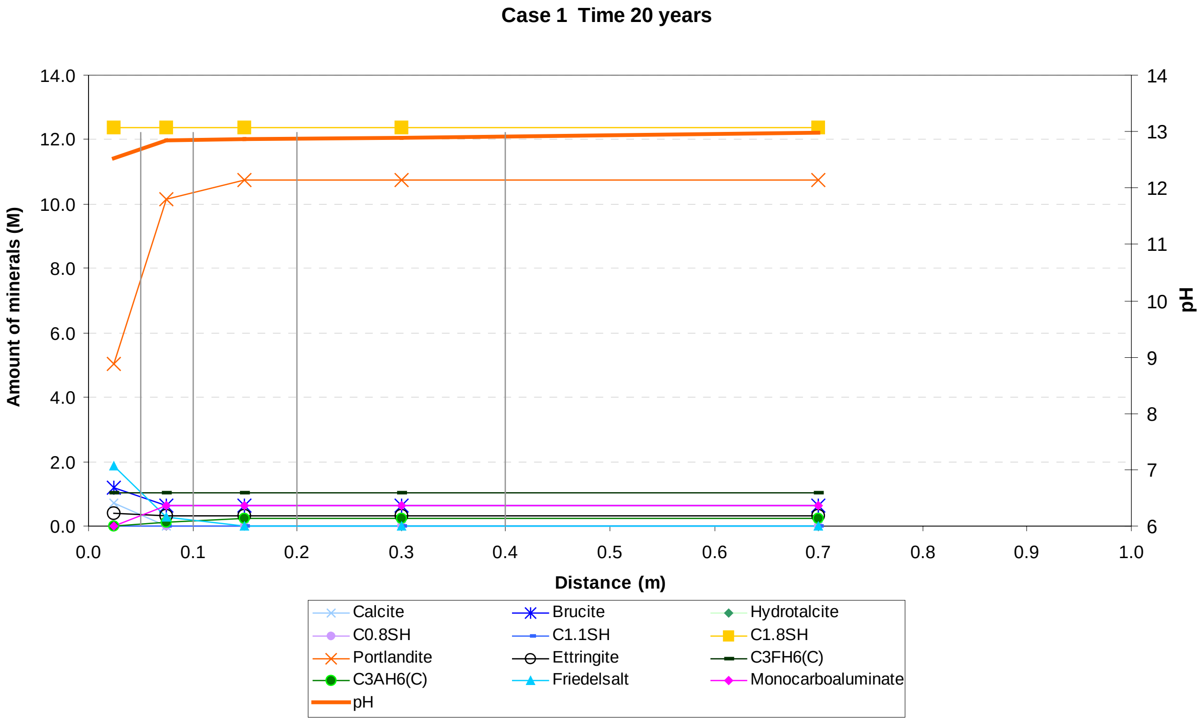


Figure 8.1c Results from leaching calculations for Case 1 after 20 years. Concentration profiles through a 1 m thick concrete slab exposed to groundwater at the left side. The positions of the markers refer to the centre in each cell. The vertical grey lines indicate the borders of the cells.

The gradual depletion of calcium continues at 20 years. Near the exposed surface at 0-0.05 m depth, Portlandite has been depleted to about 53%, see Figure 8.1c. At a depth of about 0.05-0.1 m, the dissolution of Portlandite has started, whereas, at depths of more than 0.15 m Portlandite remains unchanged.

A drop in pH to 12.5 occurs in the first 0-0.05 m. The precipitation of brucite close to the exposed surface continues. Monocarbo calcium aluminate has now been fully converted to Friedelsalt, which is found at a depth of 0.05-0.1 m.

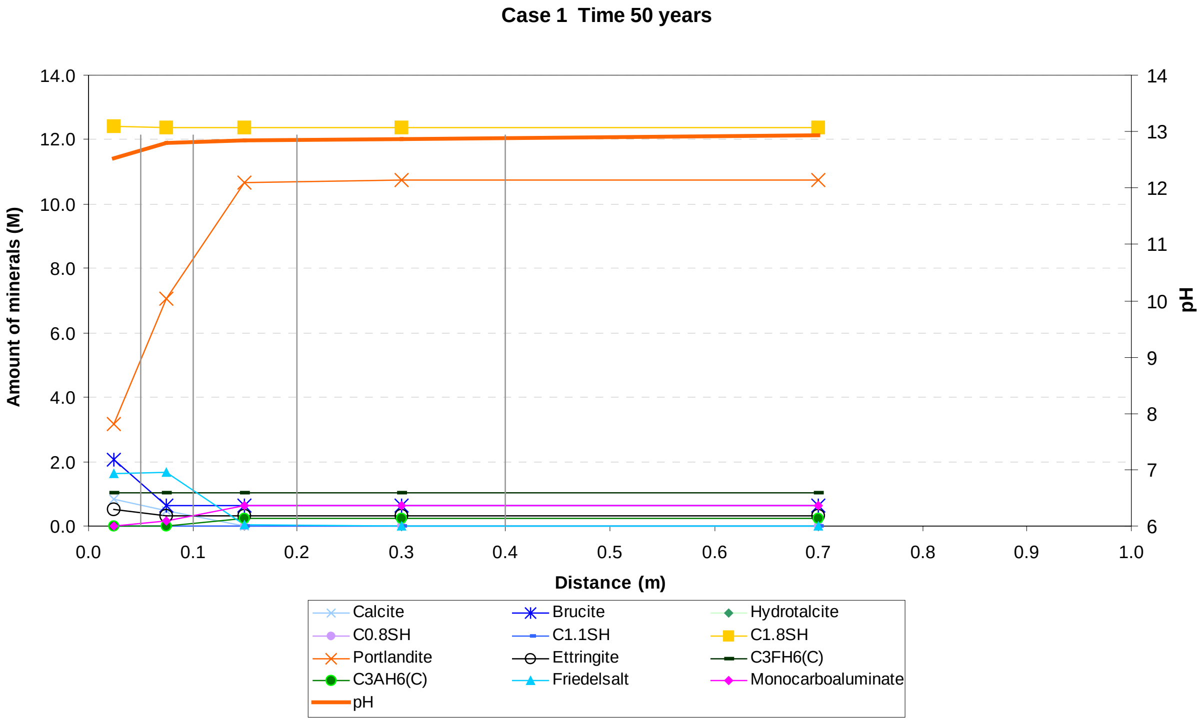


Figure 8.1d Results from leaching calculations for Case 1 after 50 years. Concentration profiles through a 1 m thick concrete slab exposed to groundwater at the left side. The positions of the markers refer to the centre in each cell. The vertical grey lines indicate the borders of the cells.

The dissolution of Portlandite continues, see Figure 8.1d. At a depth of 0-0.05 m about 70% of the Portlandite has disappeared, and about 34% at 0.05-0.1 m depth. It should be noted that there are no signs of dissolution of $C_{1.8}SH$-gel at 50 years.

At the surface the pH remains about 12.5. At depths more than 0.3 m the pH remains constant at 12.8. The precipitation of brucite, calcite and ettringite close to the exposed surface continues. The Friedelsalt has now started to decrease slightly near the surface, whereas ettringite increases.

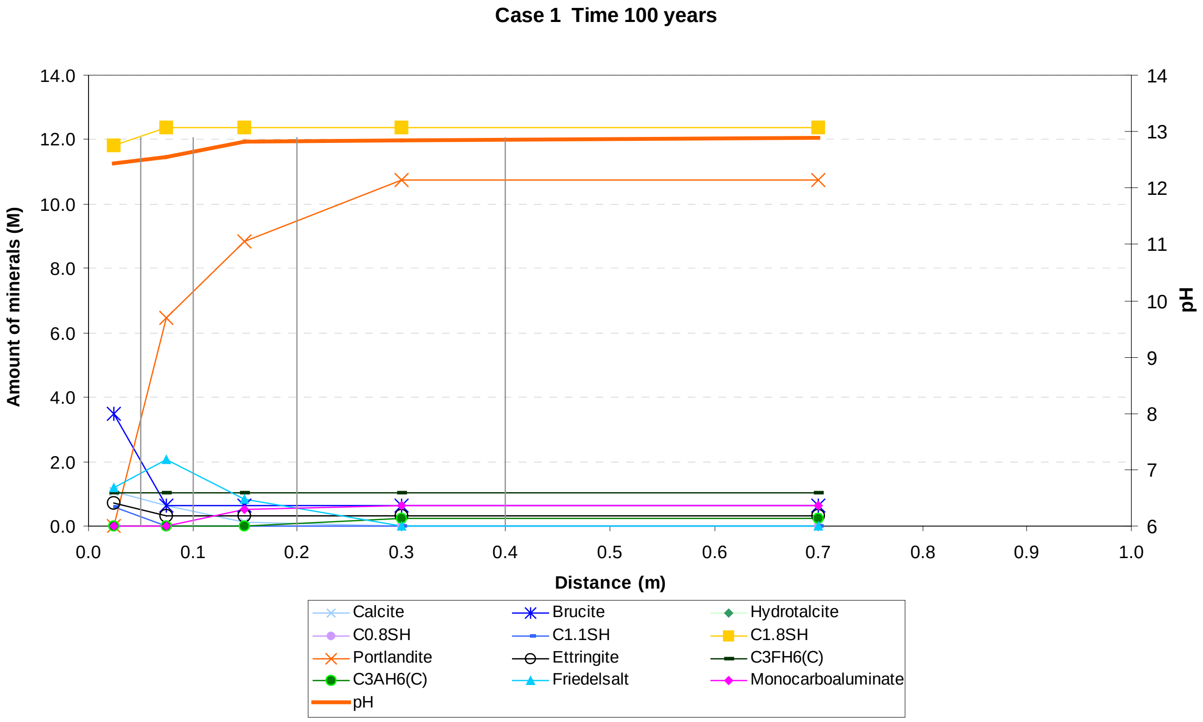


Figure 8.1e Results from leaching calculations for Case 1 after 100 years. Concentration profiles through a 1 m thick concrete slab exposed to groundwater at the left side. The positions of the markers refer to the centre in each cell. The vertical grey lines indicate the borders of the cells.

The transformation of $C_{1.8}SH$ to $C_{1.1}SH$ starts after 100 years, see Figure 8.1e. Portlandite has been depleted to a depth of 0.05 m and is partly depleted also at depths of 0.05-0.2 m.

A drop in pH to about 12.4, occurs in the first 0.1 m. At depths more than 0.15 m the pH remains constant at 12.8. The precipitation of brucite, calcite and ettringite close to the exposed surface continues. Friedelsalt is destabilised by the depletion of Portlandite and now starts to transform to ettringite near the surface.

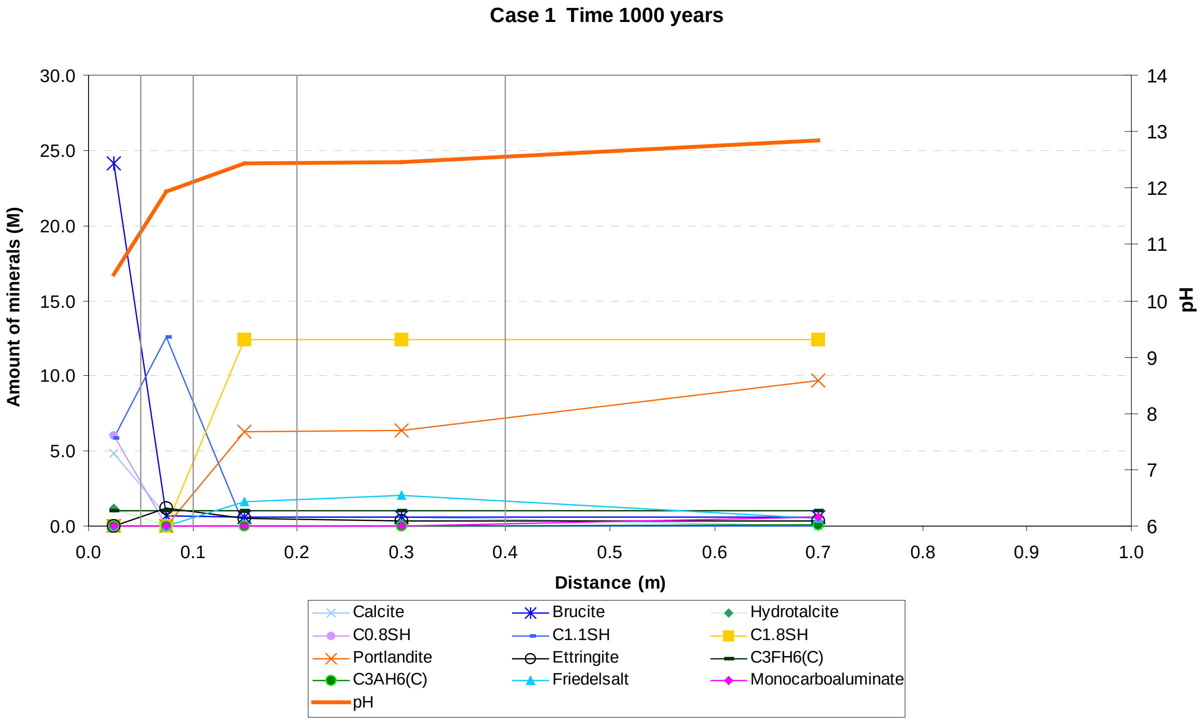


Figure 8.1f Results from leaching calculations for Case 1 after 1000 years. Concentration profiles through a 1 m thick concrete slab exposed to groundwater at the left side. The positions of the markers refer to the centre in each cell. The vertical grey lines indicate the borders of the cells.

The $C_{1.8}SH$ has now been depleted to a depth of 0.1 m. The transformation of $C_{1.1}SH$ continues after 1000 years, see Figure 8.1f. At a depth of 0-0.05 m, $C_{1.1}SH$ is gradually replaced by $C_{0.8}SH$, at 0.05-0.1 m depth $C_{1.1}SH$ is the only calcium silicate phase present. At depths more than 0.1 m, $C_{1.8}SH$ remains intact after 1000 years. Formation of hydrotalcite also occurs near the surface.

A drop in pH to about 10.5 occurs in the first 0.05 m. At depths more than 0.1 m the pH remains constant at 12.4, buffered by Portlandite equilibrium. Ettringite has been depleted close to the exposed surface.

8.1.2 Changes of aqueous composition and ion exchange species versus time in different cells - Case 1

During the initial period, sodium is introduced into the concrete from the groundwater. In the calculations, an ion exchange process for sodium, potassium and calcium has been assumed, presumably with the *CSH*-gel or the ballast providing the necessary ion exchange sites. The model has been calibrated with respect to the analytical (total) content of sodium and potassium, as well as measured pore water data reported by Lagerblad and Trägårdh (1995). Calibration was achieved by adjustment of the assumed amount of ion exchange sites. The relevance and applicability of this approach may certainly need further discussion from a scientific point of view, but never the less provides a feasible model to explain some aspects of the early leaching behaviour of concrete. Hence, it may prove feasible as a performance assessment model for the chemical long-term behaviour of concrete.

The calculated changes of the pore water composition for Case 1 are shown in Figures 8.1g-j. The initially high content of potassium in the concrete is released into the groundwater, whereas the sodium content is recharged by the groundwater. This exchange is rapid and is accompanied by a reduction in pH from about 13.0 to 12.8, where a plateau is reached at 5 years (barely visible in the diagram for the displayed time scale). In Cell 1 (representing the 5 cm surface layer in contact with the groundwater), the ion exchange is 80-90% completed in about 15-30 years, whereas in Cell 5 (0.4-1 m from the concrete surface) the time for exchange of potassium for sodium is estimated to about 3000 years.

As expected, equilibrium is rapidly reached with the concentrations in the groundwater for sodium and potassium. In Cell 1, an equilibrium is also reached for calcium when the potassium has been reduced in the cement as indicated by the next plateau value for pH at 12.5 reached after 20 years, see further details presented in Figure 8.1k.

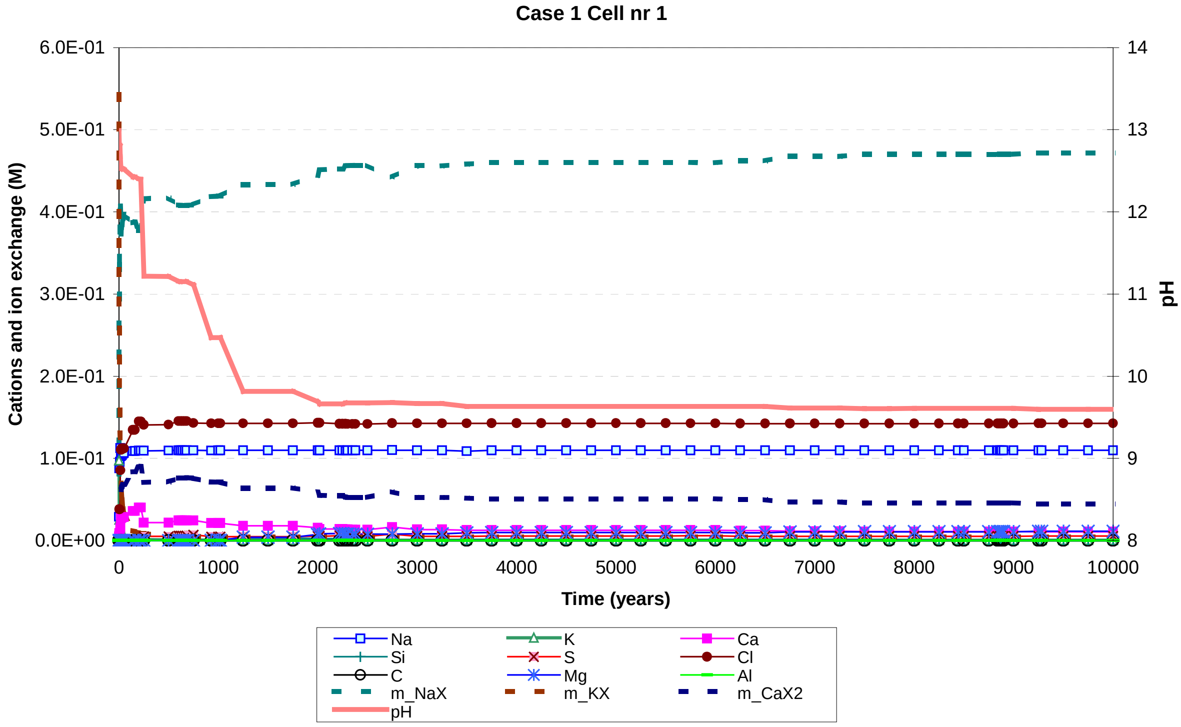


Figure 8.1g Results from leaching calculations for Case 1, Cell 1. The figure shows the development of aqueous concentrations and ion exchange species with time.

Comparing the recharge of sodium and chloride, both initially in higher concentrations in the SFR groundwater than in the concrete pore water, an interesting difference in the intrusion rate is observed. Sodium reaches its maximum concentration about 5 times faster than chloride. A comparison of e.g. Figure 8.1h (showing the aqueous concentrations in Cell 2) and Figure 8.1m (showing the amount of solid mineral phases in Cell 2) offers an explanation to this phenomenon. The chloride intrusion rate is retarded by the formation of a mineral phase, Friedelsalt, containing chloride. This means that chloride is consumed near the concrete surface as long as the chemical conditions are locally favourable for the formation of the Friedelsalt. The sodium is retarded by the assumed ion exchange process, but less effectively than the uptake of chloride in the Friedelsalts. As a consequence, chloride seemingly moves slower than sodium in the concrete. In a study on corrosion of steel in concrete, Tuutti (1982) found experimental evidence for retardation of the chloride diffusion in concrete.

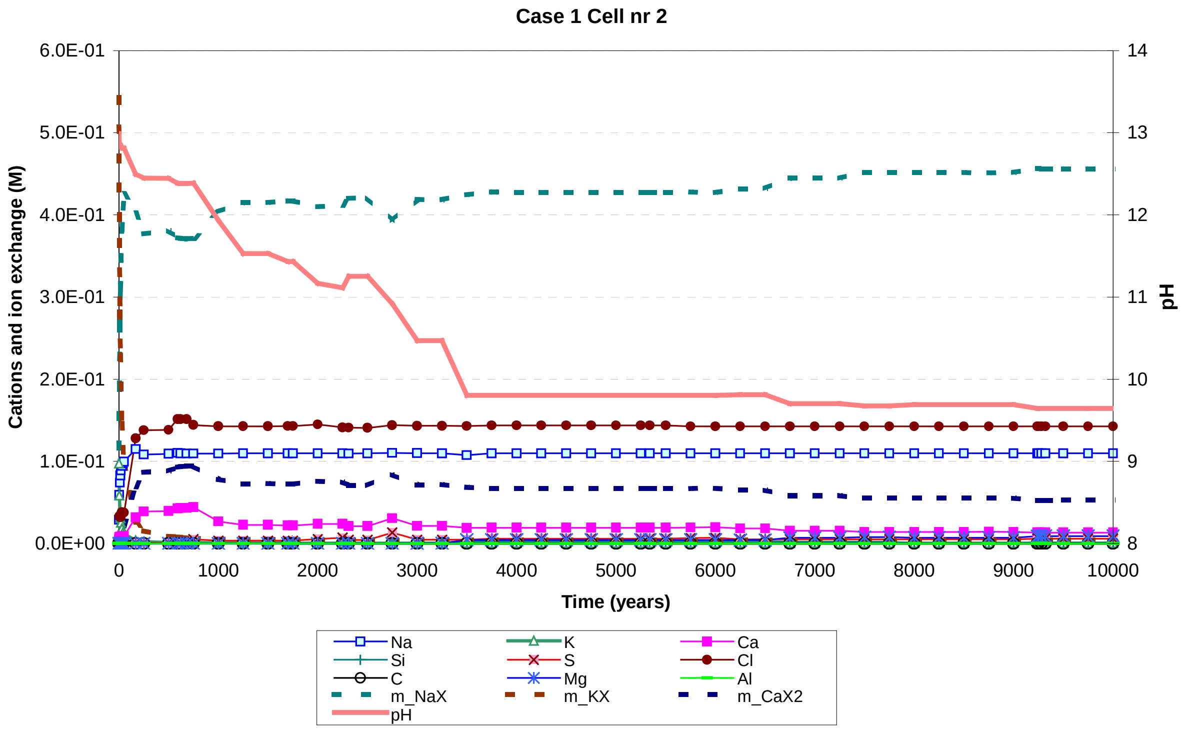


Figure 8.1h Results from leaching calculations for Case 1, Cell 2. The figure shows the development of aqueous concentrations and ion exchange species with time.

The aqueous concentrations of magnesium remain at low levels throughout the calculations, but will increase in the first cell over the period 850-2000 years in response to a gradual drop in pH, see Figures 8.1g-j, whereas the amount of brucite ($Mg(OH)_2$) gradually increases, most pronounced in Cell 1 and Cell 2, at a late stage (after 6500 years) in Cell 3, and to a limited extent also in Cell 4. This shows an ongoing precipitation of brucite formed by reaction between magnesium-rich groundwater and the alkaline concrete pore water. After about 2000 years, brucite starts to dissolve in Cell 1, but still remains to about 50% of the peak amount after 10 000 years.

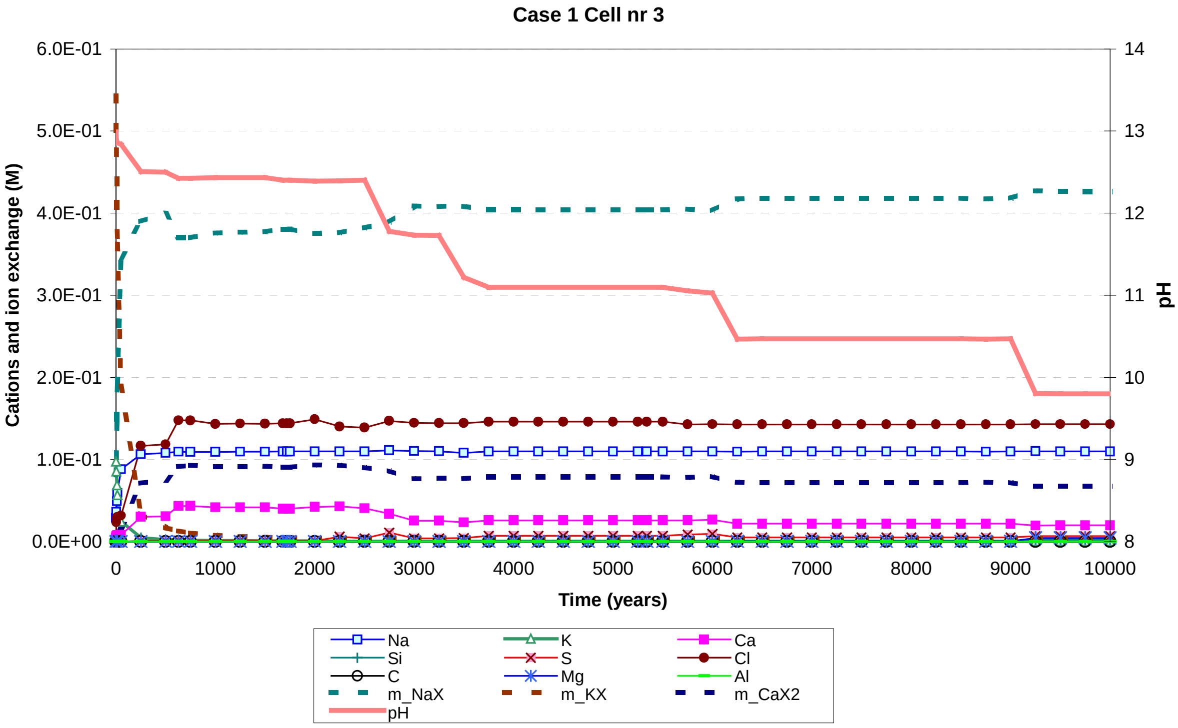


Figure 8.1i Results from leaching calculations for Case 1, Cell 3. The figure shows the development of aqueous concentrations and ion exchange species with time.

Figure 8.1i shows the chemical evolution in the porewater of Cell 3. The chemical changes resemble those shown in Figure 8.1h for Cell 2, but with a significant shift to later times.

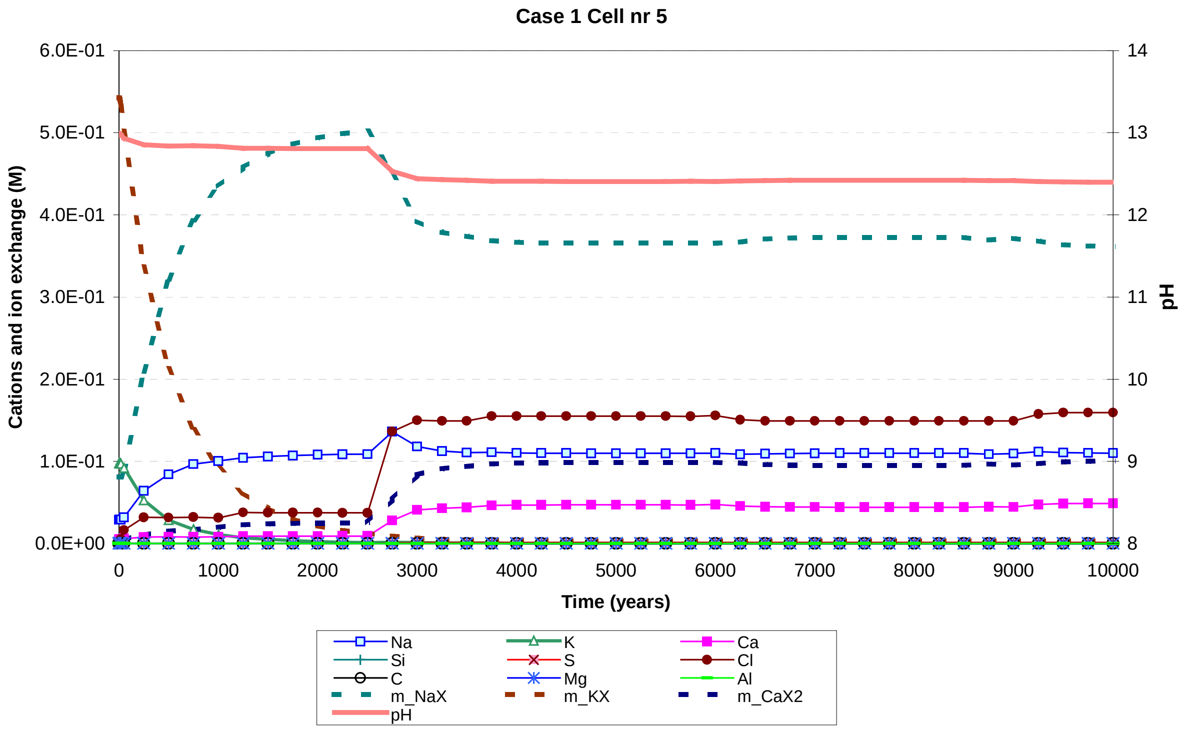


Figure 8.1j Results from leaching calculations for Case 1, Cell 5. The figure shows the development of aqueous concentrations and ion exchange species with time.

The results for Cell 5 are shown in Figure 8.1j. The changes of the chemical conditions in the concrete are slow at this depth. The initial ion exchange between potassium and sodium is still in progress during the first 2600 years. The pH slowly decreases to a value of 12.5 after 2700 years and remains almost invariant at 12.4 until10 000 years.

8.1.3 Changes of mineral composition and ion exchange species versus time in different cells - Case 1

An early formation of Friedelsalt is observed in all cells, cf. Figures 8.1k-o and Figures 8.1q-u, gradually being replaced by ettringite starting from the concrete surface and moving inwards. Ettringite is in turn apparently replaced by hydrotalcite.

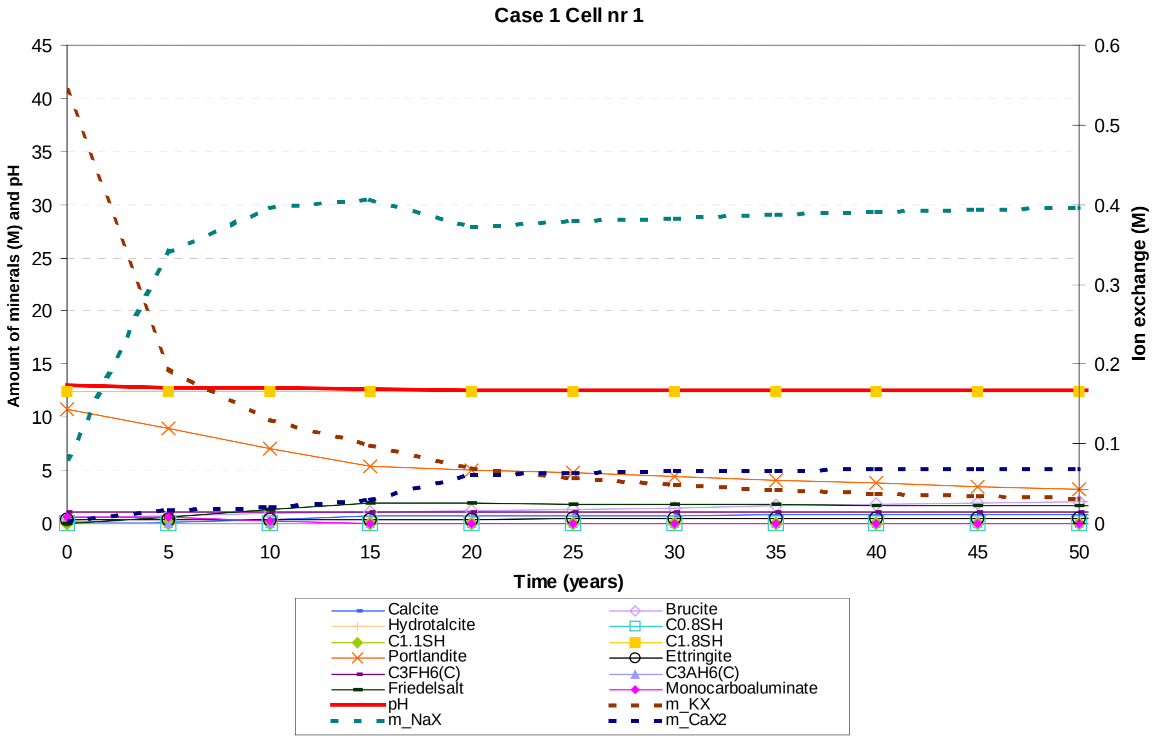


Figure 8.1k Assembly of different mineral phases in Case 1, Cell 1 during the first 50 years. The figure also shows the changes of ion exchange species with time.

At an early stage C_3AH_6 (depleted after 5 years) and monocarbo calcium aluminate (depleted after 15 years) react with chloride and sulphate in the groundwater to form Friedelsalt and ettringite, cf. Figures 8.1k and 8.1q. Portlandite in Cell 1 dissolves during the first 95 years, at which time $C_{1.8}SH$ starts to transform into $C_{1.1}SH$. $C_{1.8}SH$ becomes exhausted after 225 years.

When monocarbo calcium aluminate is exhausted, Friedelsalt destabilises and starts to react with sulphate and transforms gradually to ettringite. Friedelsalt is depleted after 230 years. Following this, ettringite will react with magnesium to form hydrotalcite, which slows down the rate of brucite precipitation slightly. At 840 years, ettringite is depleted and the precipitation of new hydrotalcite stops. The rate of brucite precipitation again increases. At this point in time $C_{1.1}SH$ starts to form $C_{0.8}SH$, a reaction which is completed after 1085 years. Calcite precipitation occurs when C_3AH_6 has been depleted after 5 years and continues throughout the considered 10 000 years.

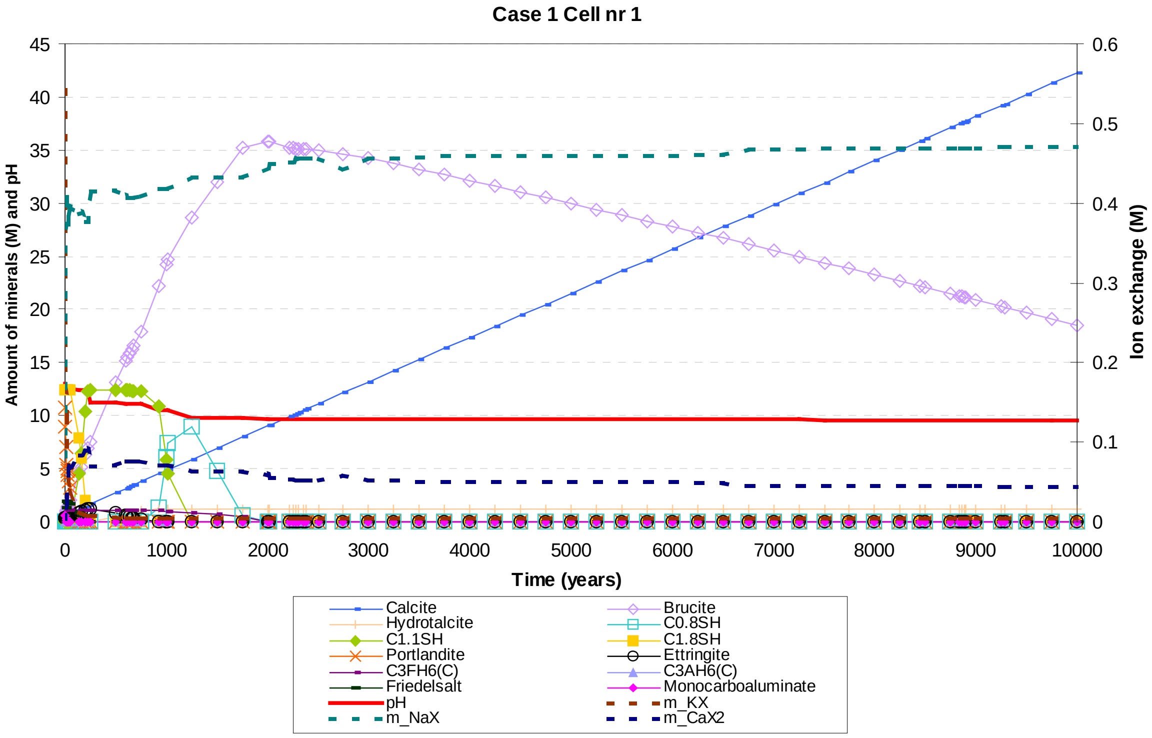


Figure 8.1l Assembly of different mineral phases in Case 1, Cell 1 for the period 0-10 000 years. The figure also shows the changes of ion exchange species with time.

The slight pH drop occurring after 840 years in Cell 1 is a result of the onset of transformation of $C_{1.1}SH$ to $C_{0.8}SH$ and also marks the end of the neoformation of hydrotalcite. The magnesium diffusing into the concrete from the groundwater instead reacts to form brucite at a slightly increased rate. Despite the somewhat increased rate, this slight pH drop results in a less efficient quantitative brucite precipitation in Cell 1. Instead, part of the magnesium is transported deeper into the concrete and starts to precipitate in Cell 2, see Figure 8.1m.

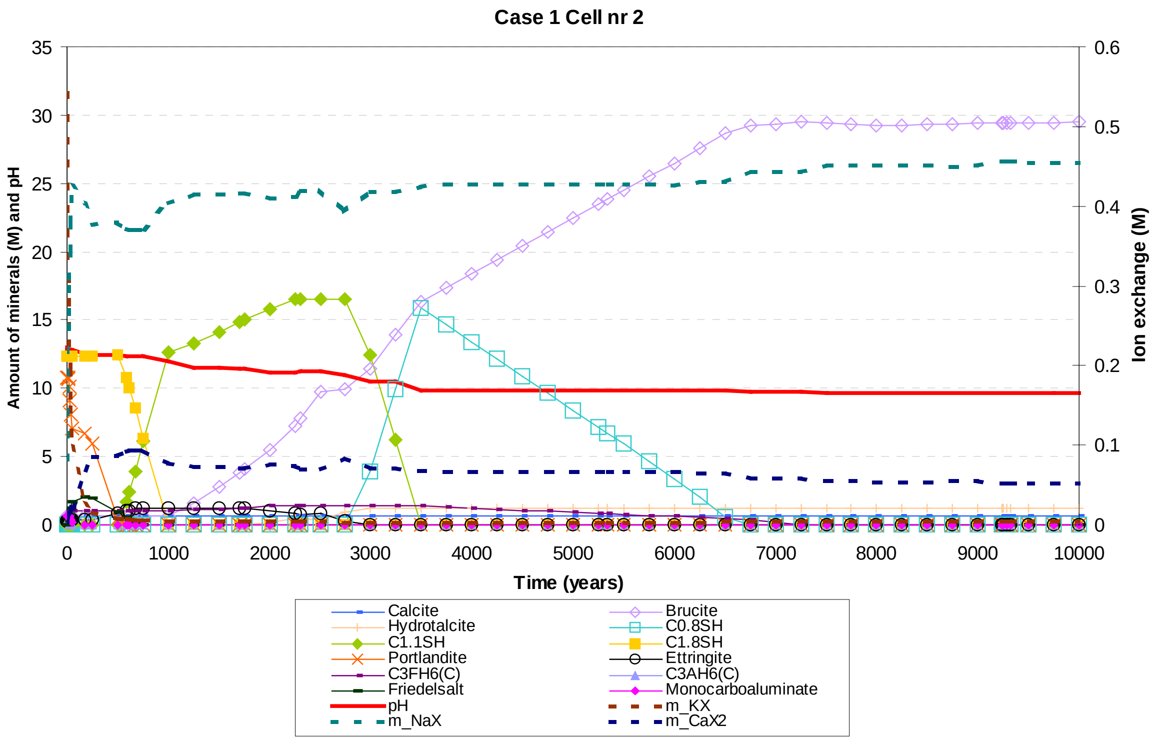


Figure 8.1m Assembly of different mineral phases in Case 1, Cell 2 for the period 0-10 000 years. The figure also shows the changes of ion exchange species with time.

In Case 1, Cell 2, the conditions remain practically unchanged during the first 10 years. At this point, the chloride concentration has increased to enable reaction with C_3AH_6, which is rapidly converted to Friedelsalt, cf. Figures 8.1m and 8.1r. After 30 years C_3AH_6 is exhausted and chloride now reacts with monocarbo calcium aluminate to Friedelsalt. The released carbonate precipitates as calcite.

Monocarbo calcium aluminate is depleted after 60 years. An invariant period follows which ends after about 230 years when Friedelsalt start to be transformed into ettringite. This reaction is completed after 705 years. At 525 years, Portlandite is depleted and the transformation of $C_{1.8}SH$ to $C_{1.1}SH$ starts which is completed at 920 years.

The results for Case 1, Cell 3, are shown in Figure 8.1n. The reaction sequence is equivalent to the description for Case 2, but is stretched out over a much longer period of time. Hence, Portlandite is depleted after 1645 years and the Friedelsalt is converted to ettringite after 2145 years, cf. Figures 8.1n and 8.1s. In Cell 4 (see Figure 8.1t), Portlandite becomes depleted after 5850 years, and in Cell 5 (see figures 8.1o and 8.1u), Portlandite is still present at 10 000 years. The mineral assembly indicates is a transformation of C_3AH_6 to Friedelsalt by reaction with chloride after 1100 years and a depletion of monocarbo calcium aluminate after 2660 years to yield Friedelsalt.

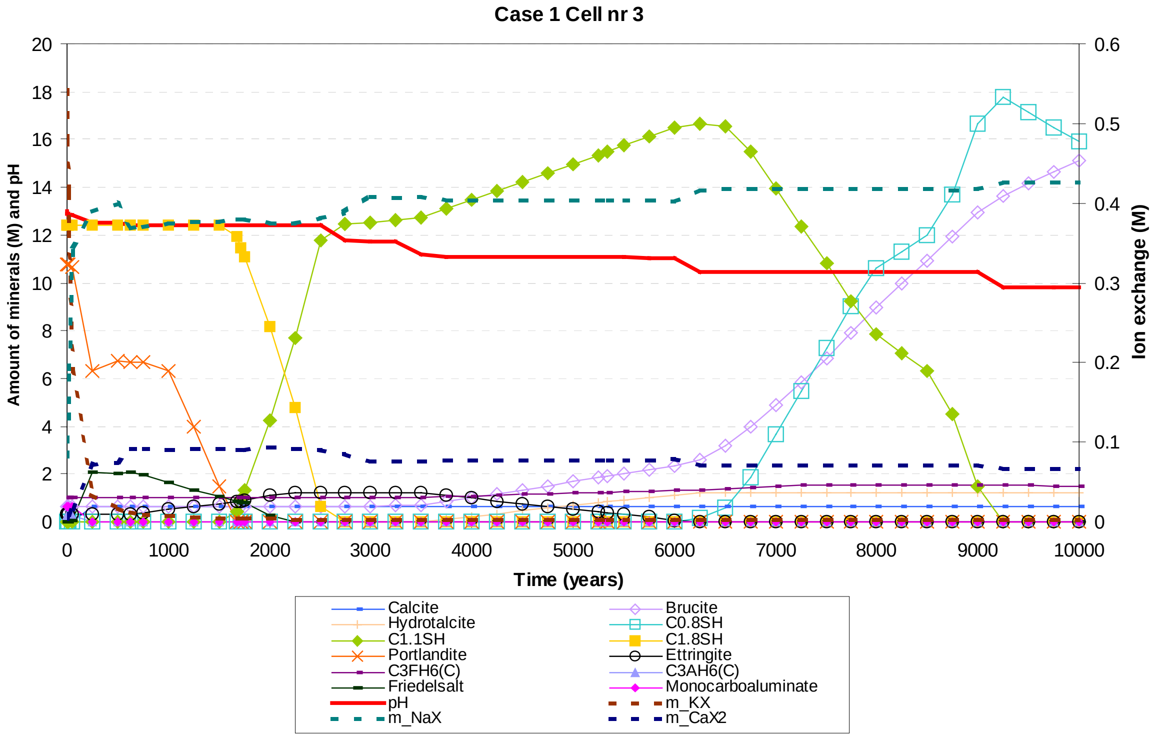


Figure 8.1n Assembly of different mineral phases in Case 1, Cell 3 for the period 0-10 000 years. The figure also shows the changes of ion exchange species with time.

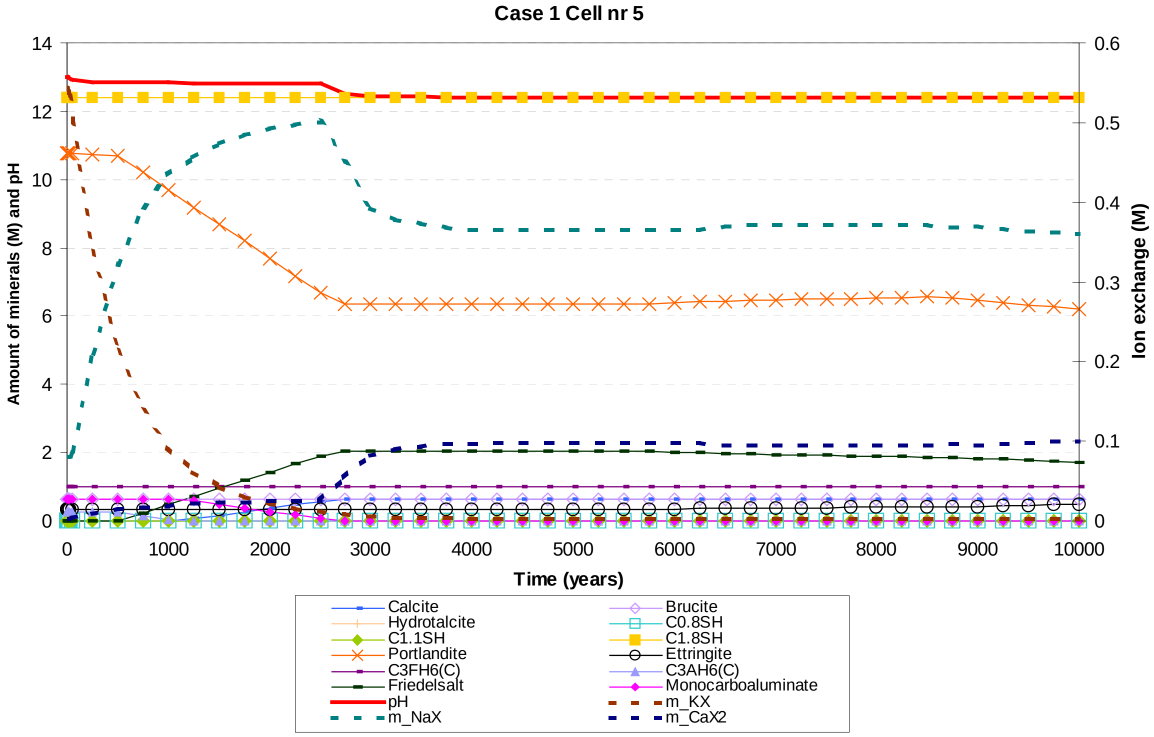
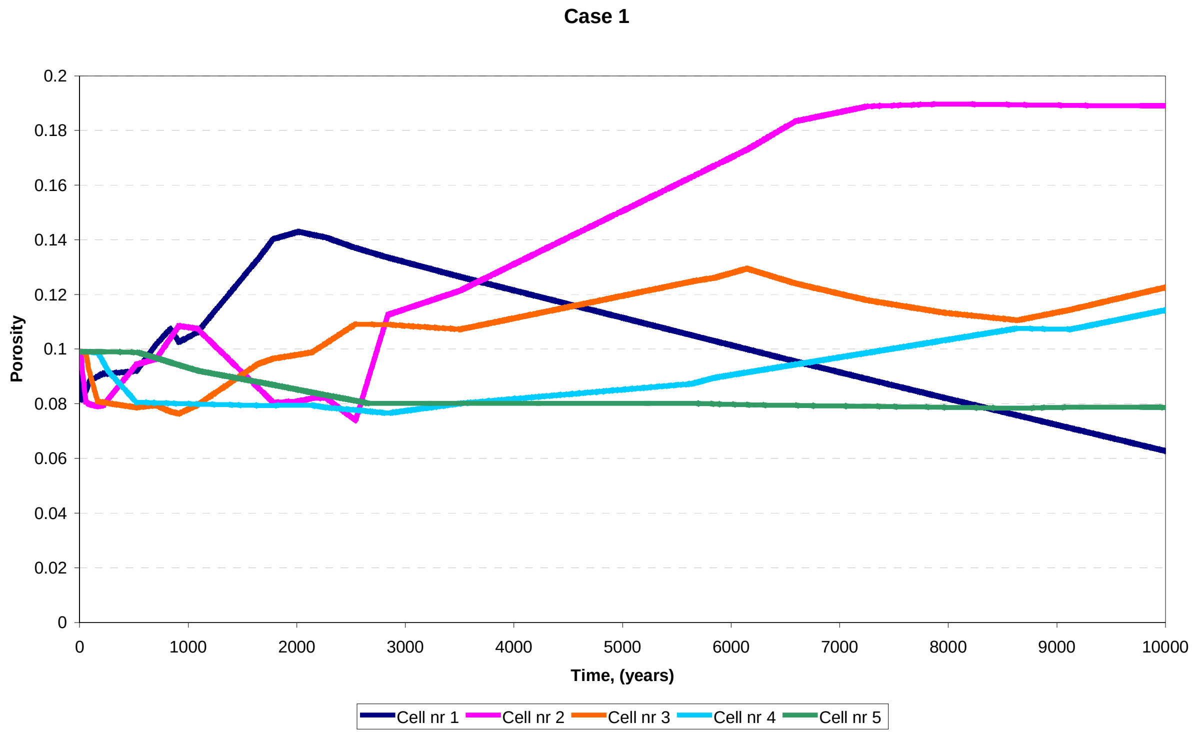


Figure 8.1o Assembly of different mineral phases in Case 1, Cell 5 for the period 0-10 000 years. The figure also shows the changes of ion exchange species with time.

8.1.4 Changes of porosity versus time in different cells - Case 1

The change of porosity has been calculated for the different cells in the model. The calculations are based on the changes of the amounts of individual minerals calculated by the geochemical model. Using data for mineral densities and molar weights of the individual minerals, the molar volumes of the considered minerals have been estimated. These data have been used to estimate the changes in total mineral volumes in the different cells in Case 1. The net changes in mineral volumes have then been related to the initial pore volume to calculate the porosity changes. Figure 8.1p shows the compiled results for porosity changes in different cells in Case 1 as function of time. In Figures 8.1q the contribution of the individual mineral volumes to the total volume of reactive minerals are summarised for Case 1.

The results in Figure 8.1p show that following a rapid drop in porosity during the initial stage the porosity gradually increases. A similar pattern is followed for the porosity changes in the different cells but occur at different times. In Cell 1 the porosity has reached its minimum value of about 8.2 % at an early time (20 years) and will increase to a value equivalent to the initial porosity of about 10 % after 655 years. The porosity steadily increases to about 10.8 % after 835 years, drops slightly to 10.3 % at 930 years, then again increasing to a maximum of 14.3 % after 2015 years, thereafter slowly decreasing to a final value of 6.3 % at 10 000 years. In Cell 2, the porosity varies more than in Cell 1, climbing to a fairly steady value of 18.9 % after 7200 years. In Cell 3, the porosity will steadily decrease reaching a minimum value of 7.6 % after 915 years, thereafter increasing to 13 % after 6100 years. In Cell 4, the porosity levels off at 8 %, starting to increase slowly after 3000 years, reaching a final value of 11.5 % at 10 000 years. In Cell 5 the porosity slowly decreases to 8 % during the first 2700 years, and remains almost constant up to 10 000 years.



Figurer 8.1p Compiled results for calculated changes of porosities in different cells in Case 1. The changes in porosity are shown as a function of time.

The magnitude of porosity variations in Case 1 is summarised in Table 8.1.

Table 8.1 Initial, maximum and minimum porosities in different cells in Case 1.

Cell	**Initial porosity**	**Maximum porosity**	**Minimum porosity**
1	0.099	0.143	0.062
2	0.099	0.189	0.074
3	0.099	0.130	0.076
4	0.099	0.115	0.076
5	0.099	0.099	0.079

Comments and interpretations to the results presented in Figures 8.1q-8.1u can be found in section 8.1.3.

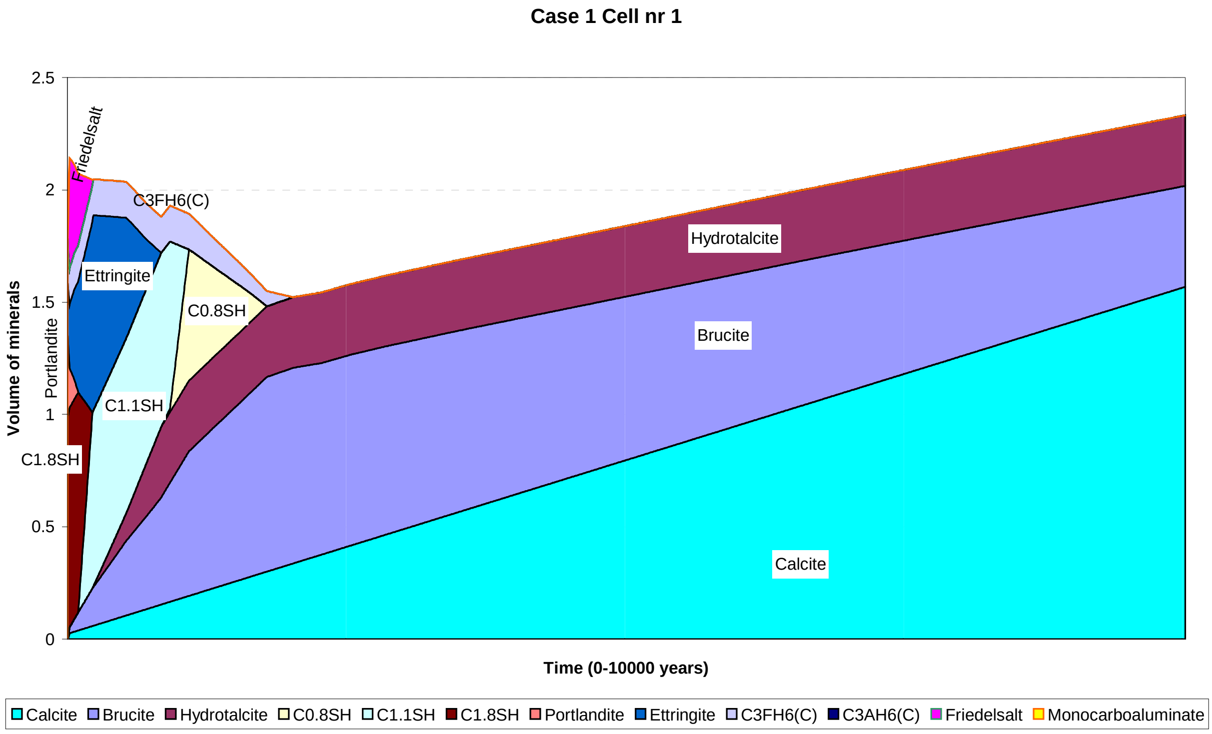


Figure 8.1q *Contribution to the total volume of reactive minerals considered in the calculations for Case 1, Cell 1 for the period 0-10 000 years. The changes of the amounts of individual minerals have been used in the estimates of porosity changes. The total volume is expressed as (m*^{3} *of reactive minerals per m*^{3} *of initial pore volume of the material).*

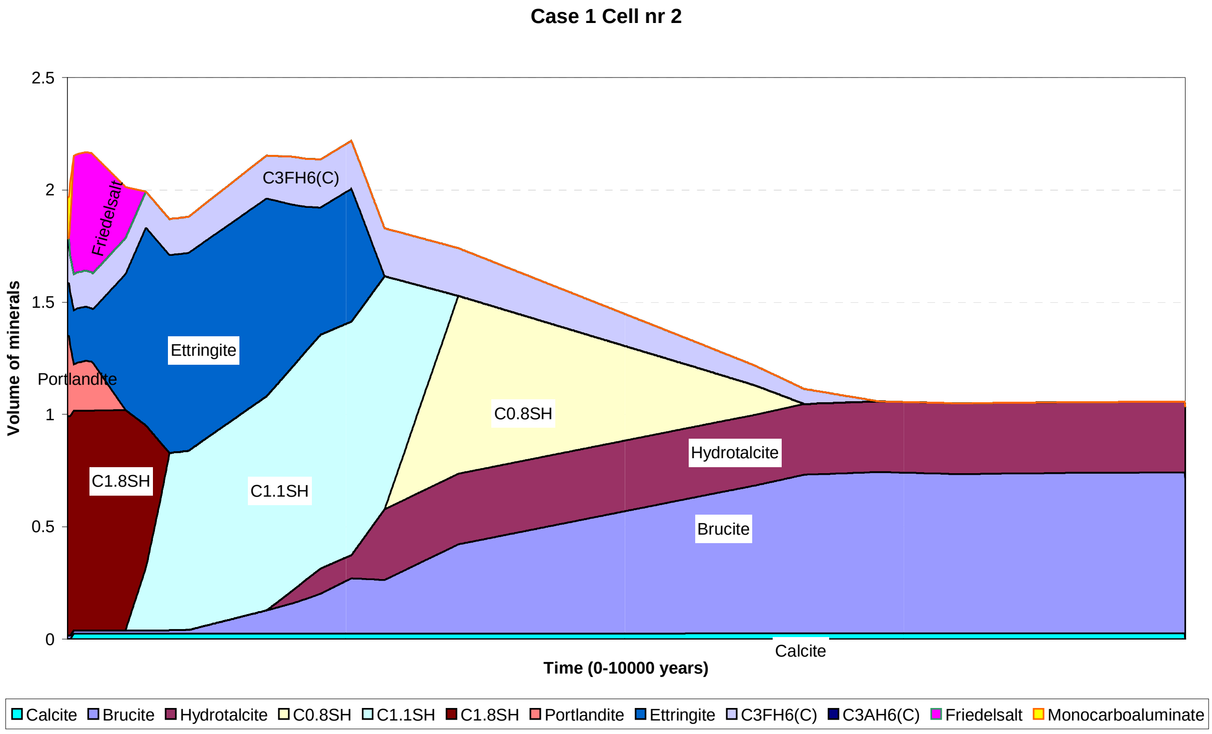


Figure 8.1r *Contribution to the total volume of reactive minerals considered in the calculations for Case 1, Cell 2 for the period 0-10 000 years. The changes of the amounts of individual minerals have been used in the estimates of porosity changes. The total volume is expressed as (m^3 of reactive minerals per m^3 of initial pore volume of the material).*

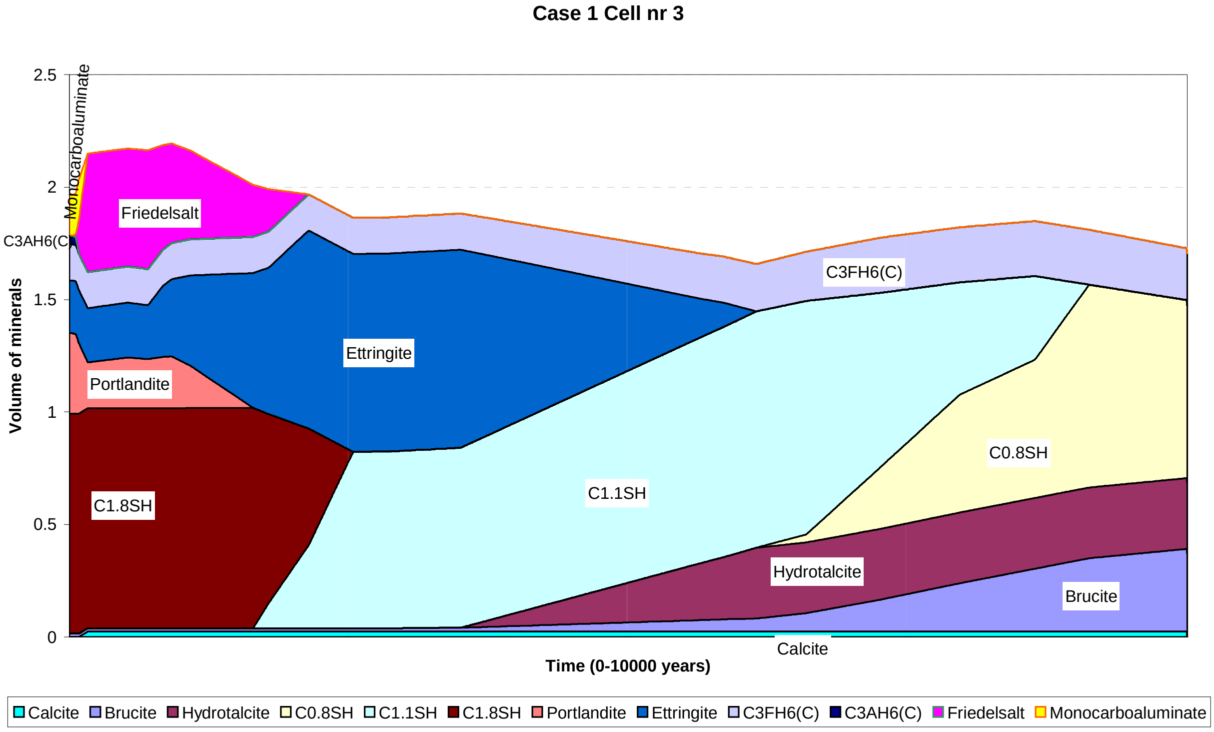


Figure 8.1s *Contribution to the total volume of reactive minerals considered in the calculations for Case 1, Cell 3 for the period 0-10 000 years. The changes of the amounts of individual minerals have been used in the estimates of porosity changes. The total volume is expressed as (m^3 of reactive minerals per m^3 of initial pore volume of the material).*

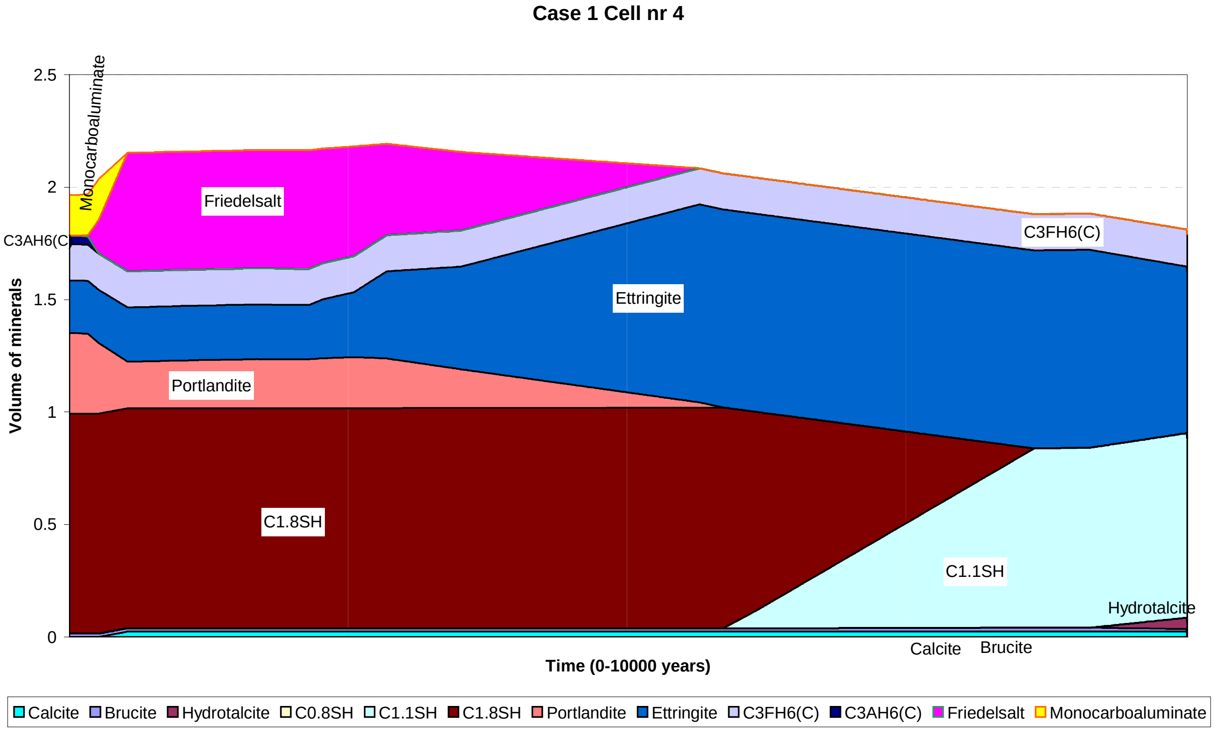


Figure 8.1t *Contribution to the total volume of reactive minerals considered in the calculations for Case 1, Cell 4 for the period 0-10 000 years. Changes of the amounts of individual minerals have been used in the estimates of porosity. The total volume is expressed as (m*^{3} *of reactive minerals per m*^{3} *of initial pore volume of the material).*

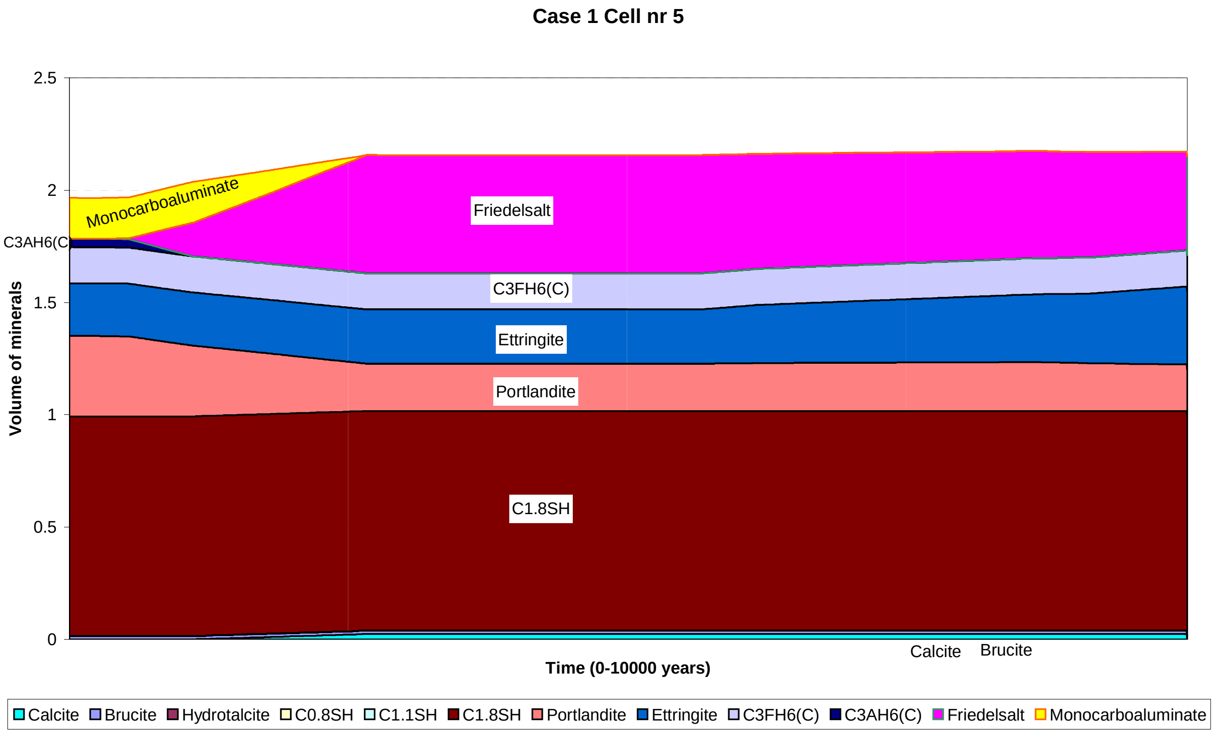


Figure 8.1u *Contribution to the total volume of reactive minerals considered in the calculations for Case 1, Cell 5 for the period 0-10 000 years. Changes of the amounts of individual minerals have been used in the estimates of porosity. The total volume is expressed as (m^3 of reactive minerals per m^3 of initial pore volume of the material).*

8.2 Case 2 – Advective flow of groundwater through a fractured concrete barrier

This is a limiting case where only advection and chemical effects are considered. The results give estimates on the maximum calcium depletion in concrete and interaction between dissolved components in groundwater and concrete porewater. Adding bentonite and near-field rock on upstream and downstream sides would be possible for further studies of interactions, e.g. between a pH-plume and the near-field rock, but has not been included in the present calculations. The calculations shown in the following may be representative for a case with fractured concrete silo allowing a flow of water vertically through the silo bottom (but may be used also as a basis for estimates of horizontal flow through through the silo walls disregarding any bentonite in the slots, or through fractured concrete structures in the BMA and the BTF rock caverns).

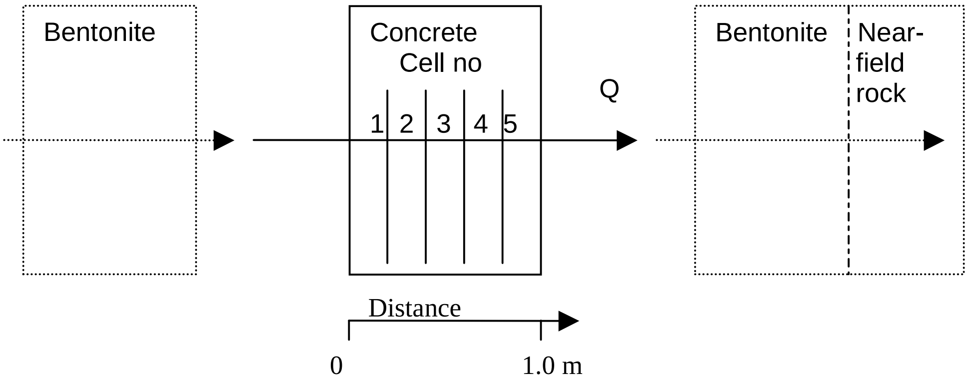


Figure 8.2 Simplified representation of a concrete barrier exposed to leaching by percolating groundwater. Leaching is assumed to be governed by advection.

8.2.1 Concentration profiles at different times - Case 2

Figures 8.2a-e show concentration profiles at different times in a 1 m thick concrete slab developed when groundwater flows through the concrete. The figures show the amount of minerals in the concrete versus distance from the concrete surface exposed to the in-flowing groundwater.

A small amount of brucite has formed close to the exposed surface after 100 years, gradually increasing with time, cf. Figures 8.2a-e. After 10000 years, brucite has precipitated to a depth of about 0.5-0.6 m.

As a result of chloride intrusion with the groundwater, a form of Friedelsalt, $C_3A \cdot 0.39\mathrm{CaCl_2} \cdot 0.61\mathrm{Ca(OH)_2} \cdot 10\mathrm{H_2O}$ has formed to a depth of about 0.3-0.4 m at 100 years. After 500 years, Friedelsalt is found through the entire slab, with a tendency to decrease near the exposed surface. This is more pronounced after 1000 years where Friedelsalt is depleted to a depth of 0.2-0.3 m. After about 5000 years the Friedelsalt is depleted throughout the whole profile, cf. Figure 8.2m. The early-formed Friedelsalt is gradually replaced by ettringite, which results from intrusion of sulphate from the groundwater. After 1000 years the amount of ettringite is increased to a depth of 0.3-0.4 m, whereas after 2500 years ettringite formation is observed to a depth of 0.5-0.6 m and at 5000 years to 0.9-1.0 m, cf. Figures 8.2k-8.2m. Simultaneously, the ettringite is gradually replaced by hydrotalcite, starting from the outer surface. After 1000 years the first hydrotalcite appears, cf. Figures 8.2c and 8.2j, and after 5000 years hydrotalcite is formed at a depth of about 0.3-0.4 m. It is interesting to note that the formation of Friedelsalt is accompanied by an uptake of free portlandite, which is depicted in the figures by a decrease for portlandite (*CH*) when Friedelsalt is increased.

Portlandite (*CH*) is gradually depleted; at 100 years to a depth of 0.05-0.1 m, at 500 years to a depth of 0.1-0.2 m, at 5000 years completely depleted. The interaction with Friedelsalt discussed above will also give rise to a regain of portlandite when Friedelsalt is gradually depleted, an effect clearly shown in Figure 8.2m for Cell 5 after about 4000 years.

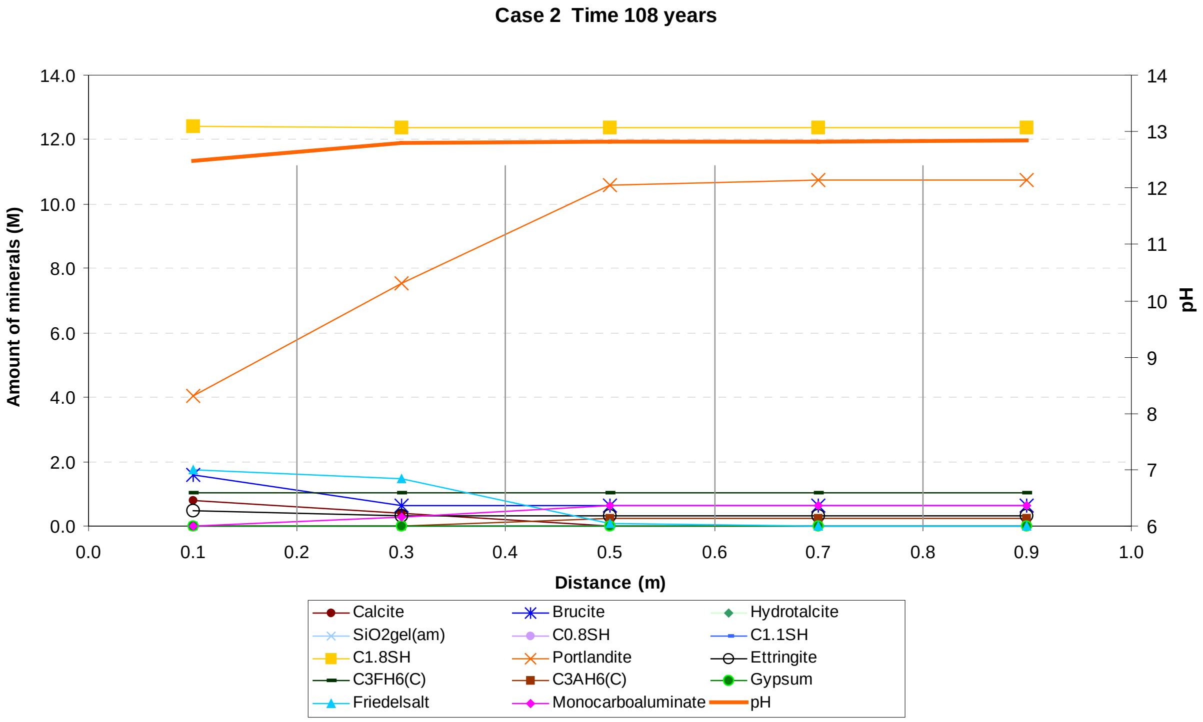


Figure 8.2a Results from leaching calculations for Case 2 after approximately 100 years. Concentration profiles through a 1 m thick concrete slab percolated by groundwater flowing from the left to the right side. The positions of the markers refer to the centre in each cell. The vertical grey lines indicate the borders of the cells.

Figure 8.2a shows a cross-section through a 1 m concrete slab, percolated by groundwater of constant composition. The figure shows the predicted amount of different minerals[4] versus depth after 100 years of leaching.

The calculations show that brucite, $Mg(OH)_2$, is precipitated near the surface exposed to groundwater. Portlandite is partly leached to a depth of 0.3-0.4 m. These processes are accompanied by a hardly noticeable drop in pH to about 12.4 near the surface.

The interaction with the saline groundwater is indicated by the formation of a form of Friedelsalt, $C_3A \cdot 0.39CaCl_2 \cdot 0.61Ca(OH)_2 \cdot 10H_2O$, to a depth of about 0.3-0.4 m. This is caused by an intrusion of chloride ions from the groundwater. A minor formation of calcite has occurred to a depth of about 0.3 m.

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[4] In the figures an abbreviated notation common in cement literature is used for many of the calcium minerals, see explanation for abbreviations in Table 3.1 and chemical formula for different minerals in Table 7.1.

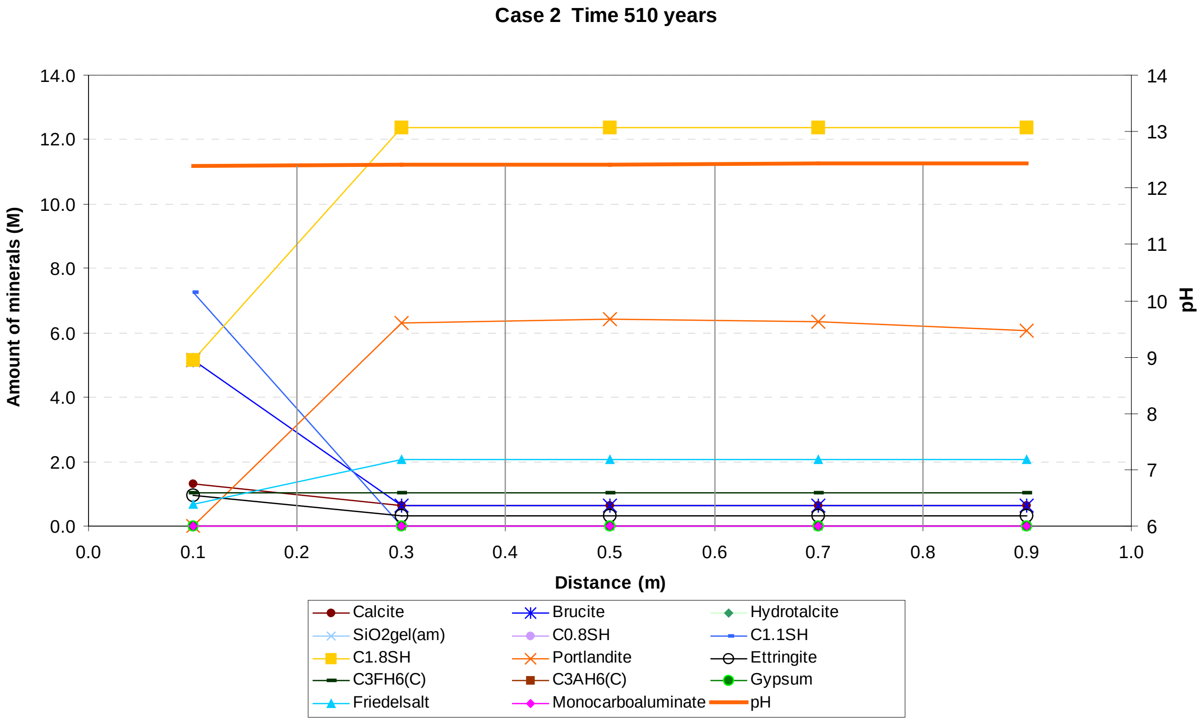

Figure 8.2b Results from leaching calculations for Case 2 after approximately 500 years. Concentration profiles through a 1 m thick concrete slab percolated by groundwater flowing from the left to the right side. The positions of the markers refer to the centre in each cell. The vertical grey lines indicate the borders of the cells.

After 500 years, chloride intrusion throughout the entire depth of 1.0 m is apparent from the formation of Friedelsalt, see Figure 8.2b. This is accompanied by a decrease in free portlandite, which is incorporated in the Friedelsalt, compare Figures 8.2a and 8.2b. It can also be noticed that a decline for Friedelsalt is indicated near the upstream side of the concrete slab. This is interpreted as an effect depletion of free portlandite which destabilises the Friedelsalt in the first cell. A transformation of about half of the initial amount of $C_{1.8}SH$ to $C_{1.1}SH$ has occurred in the first 0.2 m.

A minor additional formation of ettringite, $C_3A \cdot 3CaSO_4 \cdot 32H_2O$, is apparent at a depth of 0.1-0.2 m. A slight precipitation of calcite has occurred near the exposed surface.

The pH is constant in the slab at a value of about 12.4.

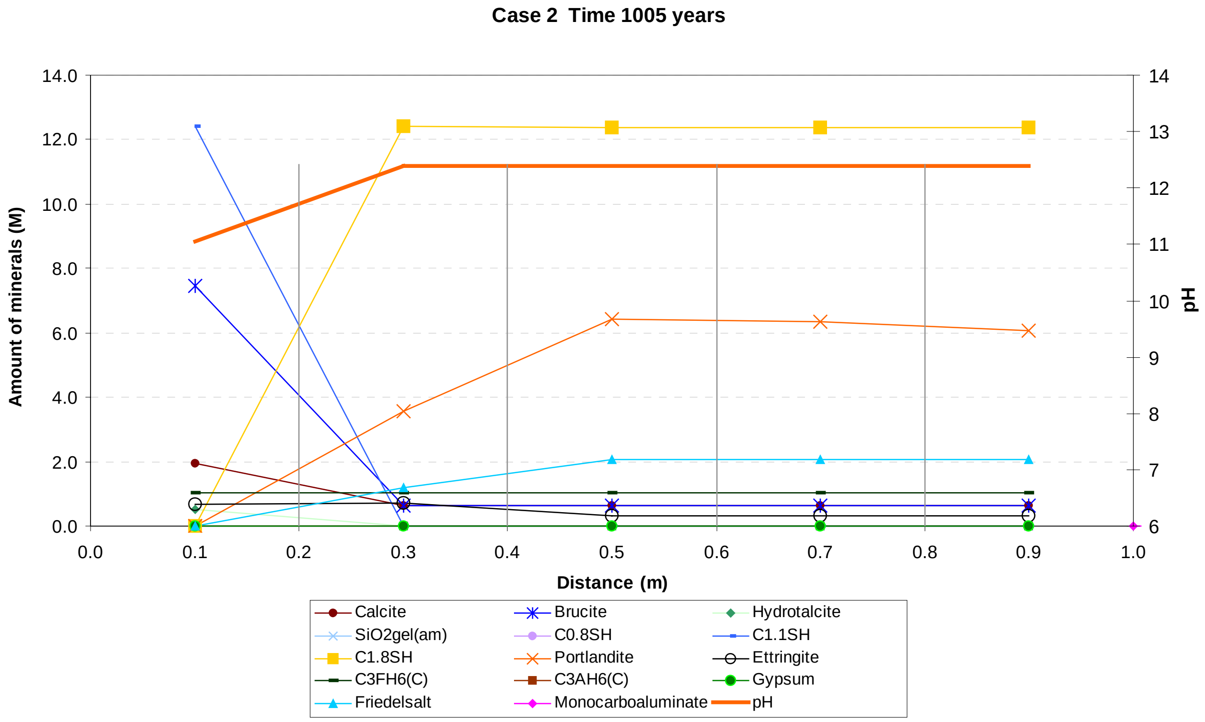

Figure 8.2c Results from leaching calculations for Case 2 after approximately 1000 years. Concentration profiles through a 1 m thick concrete slab percolated by ground-water flowing from the left to the right side. The positions of the markers refer to the centre in each cell. The vertical grey lines indicate the borders of the cells.

The gradual depletion of calcium continues at 1000 years. Portlandite, is fully depleted to a depth of 0.2 m and about half depleted to 0.3-0.4 m. Near the exposed surface at 0.1-0.2 m depth, a complete transformation of $C_{1.8}SH$ to $C_{1.1}SH$ has occurred, see Figure 8.2c. At a depth of 0-0.2 m, $C_{1.1}SH$ is the only *CSH*-phase present, whereas, at depths of more than 0.2 m $C_{1.8}SH$ remains unchanged.

A drop in pH to 11 has occurred in the first 0.2 m, but remains constant at 12.4 at depths of more than 0.2 m. The precipitation of brucite and calcite close to the exposed surface continues. A slight formation of the mineral hydrotalcite, $Mg_4Al_2O_7 \cdot 10H_2O$, has occurred near the exposed surface. Small amounts of ettringite is noticed to a depth of 0.3-0.4 m. Friedelsalt has been fully depleted to a depth of 0.2 m, and is partly depleted to a depth of 0.2-0.4 m.

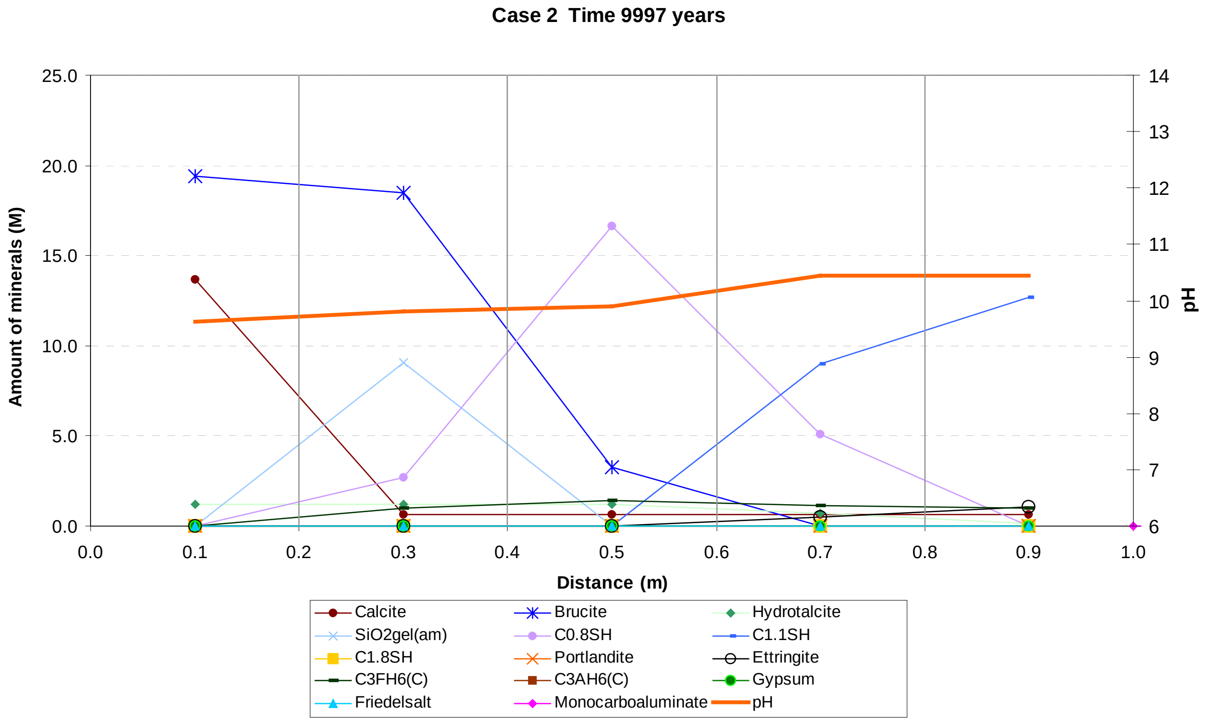

Figure 8.2d Results from leaching calculations for Case 2 after approximately 10000 years. Concentration profiles through a 1 m thick concrete slab percolated by groundwater flowing from the left to the right side. The positions of the markers refer to the centre in each cell. The vertical grey lines indicate the borders of the cells.

The $C_{1.8}SH$ has now been depleted throughout the 1 m slab. The $C_{1.1}SH$ has been completely transformed to $C_{0.8}SH$ to a depth of 0.5-0.6 m, and partly transformed to a depth of 0.7-0.8 m, see Figure 8.2d. At a depth of 0.2-0.4 m, $C_{0.8}SH$ is gradually replaced by SiO_2-gel. No SiO_2-gel is found in the 0-0.2 m close to the in-flow surface. A slight formation of hydrotalcite has also occurred to a depth of 0.7-0.8 m.

A drop in pH to slightly below 10 has occurred in the first 0.5-0.6 m. At depths more than 0.6 m the pH remains constant at 10.4, apparently buffered by the $C_{1.1}SH$–$C_{0.8}SH$ equilibrium. The precipitation of brucite and calcite continues. A significant precipitation of brucite is noticed to a depth of 0.5-0.6 m. Ettringite has been depleted to a depth of about 0.4 m.

8.2.2 Changes of aqueous composition and ion exchange species versus time in different cells - Case 2

During the initial period, sodium is introduced into the concrete from the groundwater. In the calculations, an ion exchange process for sodium, potassium and calcium has been assumed, presumably with the *CSH*-gel or the ballast providing the necessary ion exchange sites. The model has been calibrated with respect to the analytical (total) content of sodium and potassium, as well as measured pore water data reported by Lagerblad and Trägårdh (1995). Calibration was achieved by adjustment of the assumed amount of ion exchange sites. The relevance and applicability of this approach may certainly need further discussion from a scientific point of view, but never the less provides a feasible model to explain some aspects of the early leaching behaviour of concrete. Hence, it may prove feasible as a performance assessment model for the chemical long-term behaviour of concrete.

The calculated changes of the pore water composition for Case 2 are shown in Figures 8.2e-h. The initially high content of potassium in the concrete is released into the groundwater, whereas the sodium content is recharged by the groundwater. This exchange is rapid and is accompanied by a reduction in pH from about 13.1 to 12.4, where a plateau is reached (barely visible in the diagram for the displayed time scale). In Cell 1 (representing the 0.2 m concrete at the in-flow side for the groundwater), the exchange is completed in about 60 years, whereas in Cell 5 (0.8-1 m from the concrete surface) the time for exchange of potassium for sodium is estimated to about 500 years. As expected, equilibrium is rapidly reached with the concentrations in the groundwater for sodium and potassium.

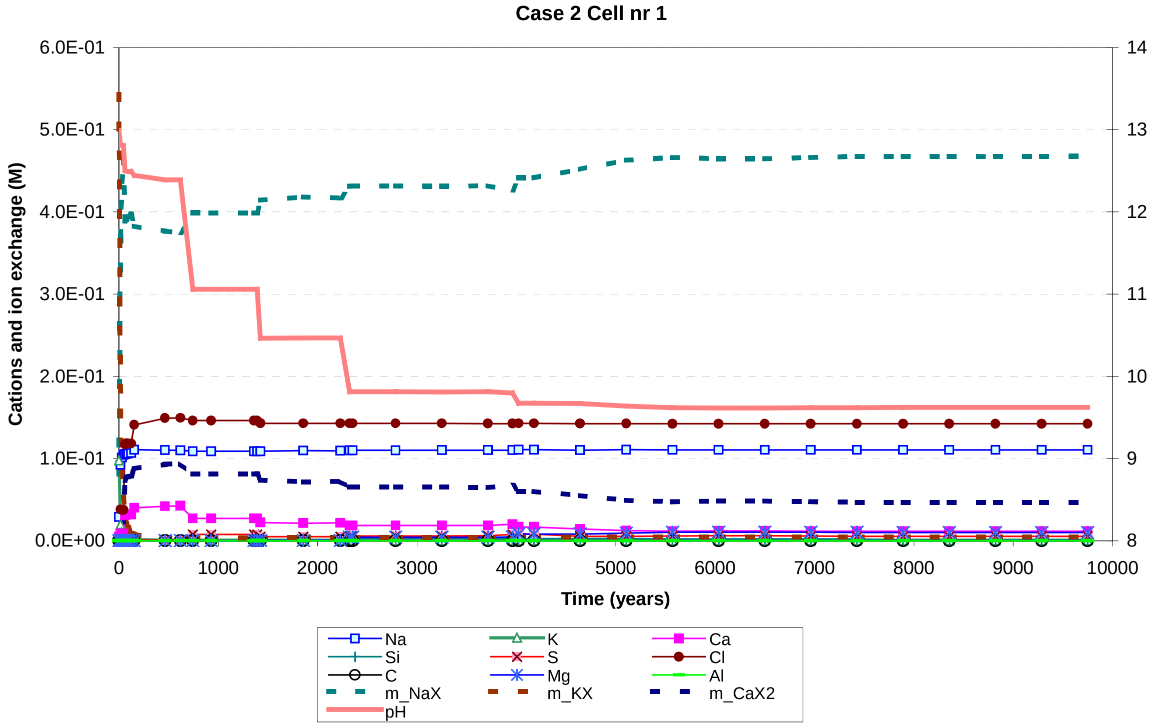

Figure 8.2e Results from leaching calculations for Case 2, Cell 1. The figure shows the development of aqueous concentrations and ion exchange species with time.

Comparing the recharge of sodium and chloride, both initially in higher concentrations in the SFR groundwater than in the concrete pore water, an interesting difference in the intrusion rate is observed. Sodium reaches its maximum concentration significantly faster than chloride. A comparison of e.g. Figure 8.2e (showing the aqueous concentrations in Cell 1) and Figure 8.2i (showing the amount of solid mineral phases in Cell 1) offers an explanation to this phenomenon. The chloride intrusion rate is retarded by the formation of a mineral phase, Friedelsalt, containing chloride. This means that chloride is consumed near the concrete surface as long as the chemical conditions are locally favourable for the formation of the Friedelsalt. The sodium is retarded by the assumed ion exchange process, but not as efficient as the uptake of chloride in the Friedelsalts. Therefore, chloride seemingly moves slower than sodium in the concrete. The same observation has been made in the results for Case 1.

A slight increase in sulphate concentration accompanies the drop in pH from 12.5 to 11 after about 1200 years. The magnesium concentration increases slightly after about 5500 years, marking the start of a pH regime where brucite will buffer the pore water.

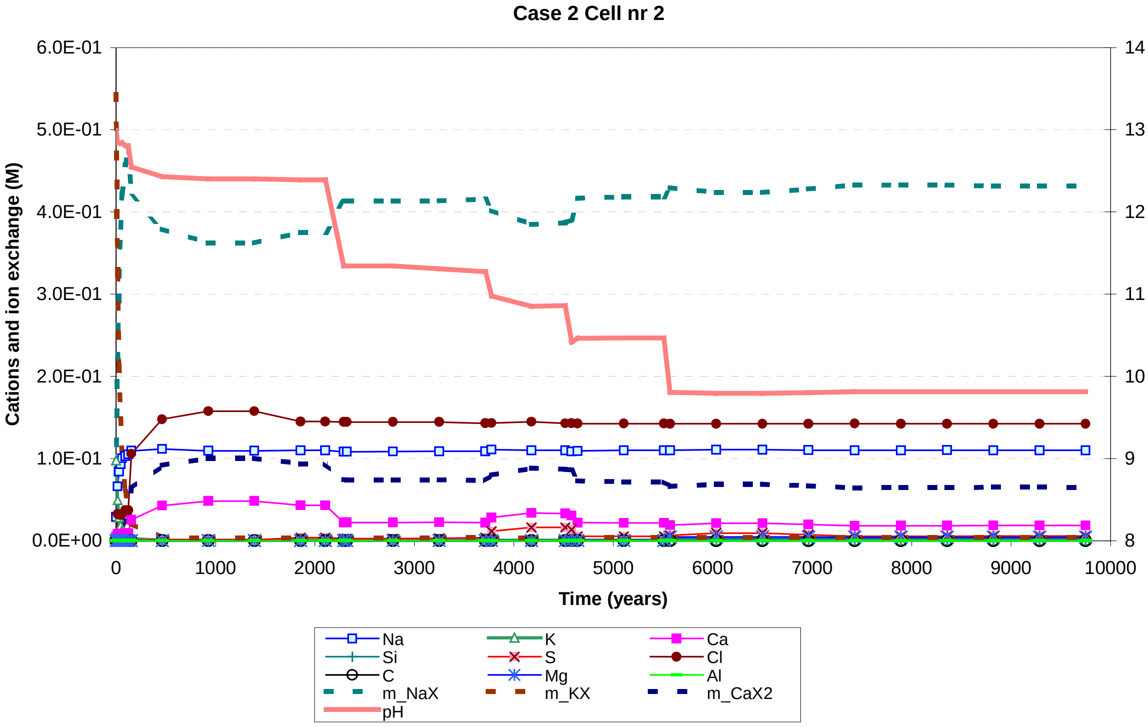

Figure 8.2f Results from leaching calculations for Case 2, Cell 2. The figure shows the development of aqueous concentrations and ion exchange species with time.

A rapid ion exchange occurs where potassium is replaced by sodium, a process that is mainly completed after about 50 years in Cell 2. The stepwise changes of pH follow the alterations of solid phase assembly, see comments in next section. As a consequence of transformations of the calcium silicate phase the calcium concentration in the pore water will change. Between 500 years and about 2000 years, the calcium concentration shows a maximum in Cell 2, see Figure 8.2f. In response to this, the amount of sodium bound in ion exchange complexes displays a minimum, while the ion exchanged calcium shows a maximum. After about 2500 years, the calcium concentration has dropped and the ion-exchanged sodium is again increased. It should be noted that in the calculations the ion exchange capacity is attributed to an arbitrary solid phase in the concrete, presumably the *CSH*-gel or the ballast. However, the calculations do not consider any effects of depleted or increased ion exchange capacity that may result from dissolution or precipitation of the minerals that presumably supply the necessary ion exchange sites.

At 2500 years a slight increase in sulphate and calcium concentrations is observed, again reflected in a decrease in ion-exchanged sodium and an increase in ion exchanged calcium. As shown in Figure 8.2k, this coincides with a depletion of ettringite when $C_{1.1}SH$ is transformed to $Ca_{0.8}SH$, and precipitation of hydrotalcite.

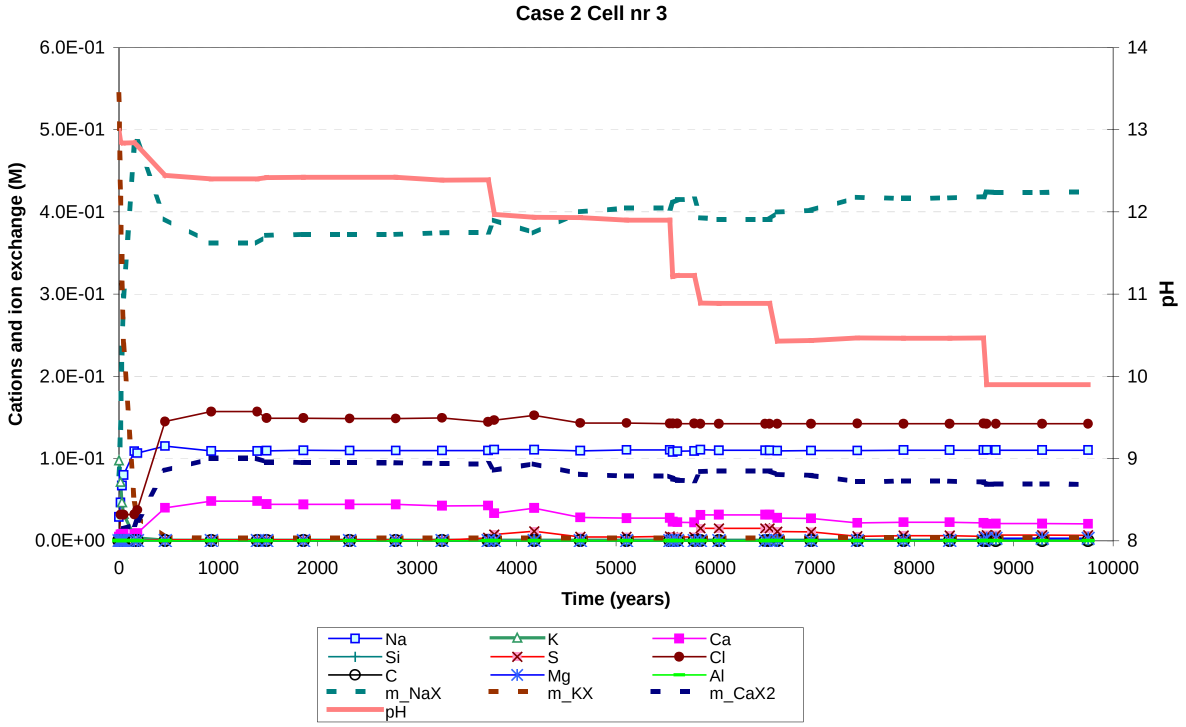

Figure 8.2g Results from leaching calculations for Case 2, Cell 3. The figure shows the development of aqueous concentrations and ion exchange species with time.

The rapid ion exchange between potassium and sodium dominated the early period up to about 80 years in Cell 3. Figure 8.1g shows very distinctive pH drops representing transformations between the predominant *CSH*-phases. Following the initial depletion of alkali hydroxides and portlandite, the first plateau at about pH 12.5 is reached where $C_{1.8}SH$ buffers the pH. After about 3000 years a transformation of $C_{1.8}SH$ to $C_{1.1}SH$ starts, which ends after 3800 years, marked by a stepwise change of pH to about 11.9. The next drop in pH occurs after about 5500 years, which follows an increased precipitation of $C_{1.1}SH$, ettringite, brucite, and the formation of hydrotalcite, c.f. Figure 8.2l. The next pH drop to 10.9 occurs after 5800 years when a slow dissolution of ettringite and an increased precipitation of hydrotalcite start. After 6500 years the pH drops to 10.4 due to depletion of brucite (magnesium instead precipitates as hydrotalcite) and the coinciding start of a transformation of $C_{1.1}SH$ to $C_{0.8}SH$. At 7200 years ettringite has been depleted and a slight transformation of hydrotalcite to brucite is indicated, cf. Figure 8.2l. The last major pH drop to 9.9 occurs after 8700 years as a result of depletion of $C_{1.1}SH$. At this late stage $C_{0.8}SH$ buffers the pH.

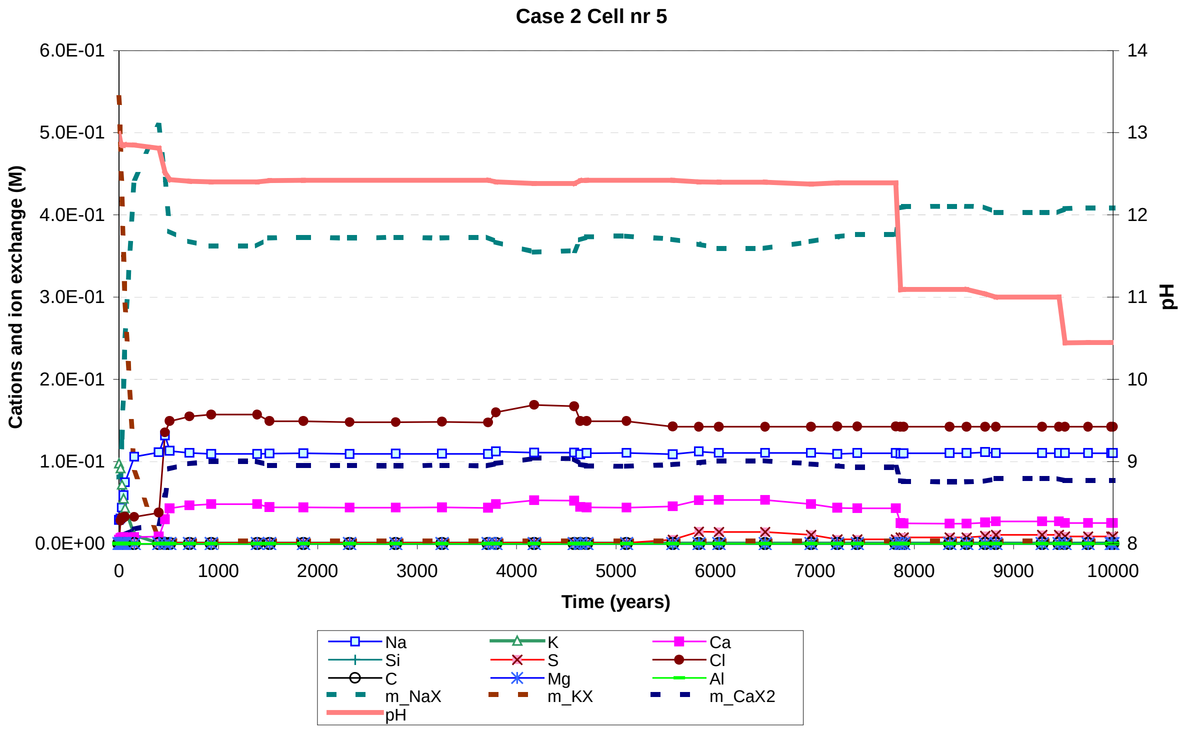

Figure 8.2h Results from leaching calculations for Case 2, Cell 5. The figure shows the development of aqueous concentrations and ion exchange species with time.

Also in Cell 5 the ion exchange between potassium and sodium is fairly rapid. The exchange is mainly completed after 120 years. Following the intrusion of chloride ions, the calcium concentration increases which causes an increase in the amount of ion exchanged calcium and a corresponding decrease in ion exchanged sodium, see Figure 8.2h.

The chemical changes in Cell 5 follow the same basic pattern as in Cells 1, 2 and 3, whereas the time scale is longer, compare Figures 8.2e-h. Hence the major pH drop from 12.4 to 11.1 resulting from depletion of $C_{1.8}SH$ occurs after 7800 years, as compared to 5500 years in Cell 3.

An increase in the sulphate concentration is indicated between 5800 and 7200 years resulting from an increased inflow of sulphate from Cell 4 ($C_{1.8}SH$ depleted in Cell 4 at 5800 years, which approximately destabilises the ettringite). Ettringite starts to dissolve in Cell 4 at 5800 years and is depleted after 7200 years. As a result, gypsum occurs, but is depleted after 6600 years and the sulphate concentration drops. A slight sulphate increase can be noticed at 7800 years resulting from dissolution of ettringite in Cell 4 (not shown in figures). At 8600 years the sulphate concentration increases again when ettringite starts to dissolve, which coincides with the formation of hydrotalcite. At 9500 years the sulphate drops following a stabilisation of ettringite and a slight dissolution of hydrotalcite in response to the depletion of brucite and precipitation of $C_{0.8}SH$ and accompanying drop in pH from 11 to 10.4.

8.2.3 Changes of mineral composition and ion exchange species versus time in different cells - Case 2

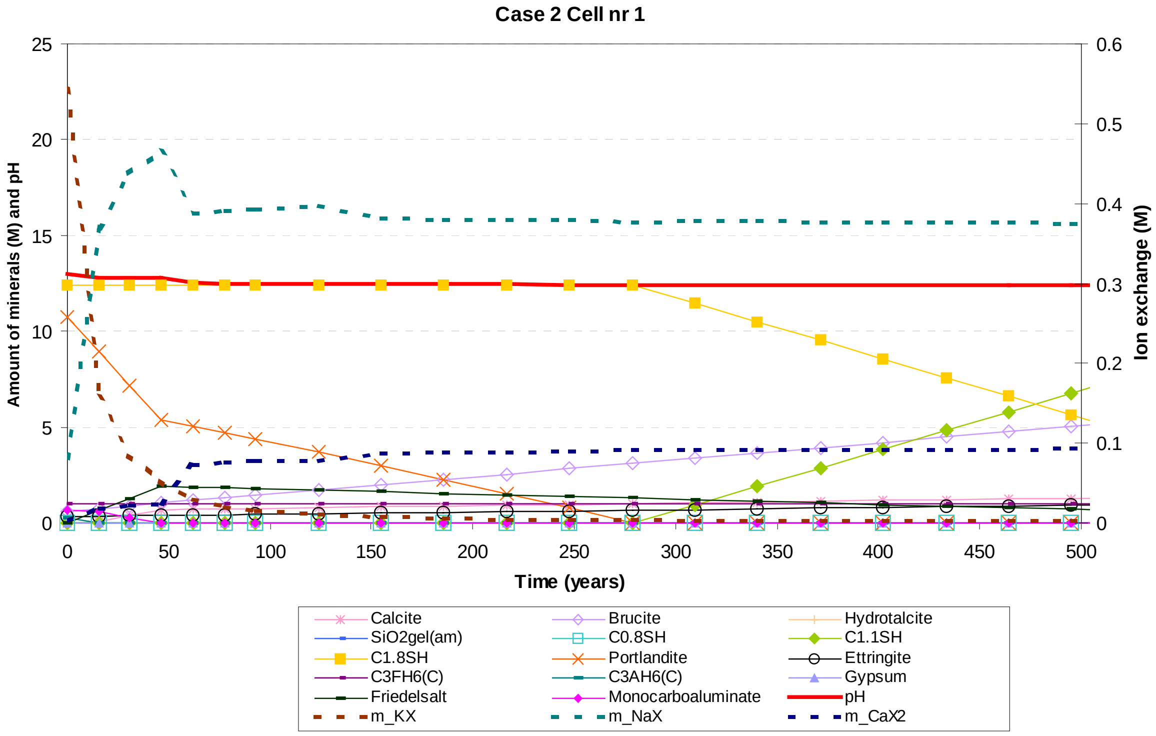

Figure 8.2i Assembly of different mineral phases in Case 2, Cell 1 during the first 500 years. The figure also shows the changes of ion exchange species with time.

The results for Case 2, Cell 1 representing a 0.2 m concrete layer near the surface exposed to groundwater, show that the available Portlandite is completely consumed during the first 280 years. Figure 8.2i displays the results with a more detailed time scale, 0 – 500 years, as compared to Figures 8.2j-m where the results are given for 0 – 10 000 years. When Portlandite is depleted the dissolution of the slightly less alkaline $C_{1.8}SH$-gel is initiated. After 500 years about half of the $C_{1.8}SH$-gel has been transformed into $C_{1.1}SH$-gel. In Figure 8.2j we can follow the transformation of $C_{1.8}SH$ to $C_{1.1}SH$ which is completed after 680 years.

Brucite is continuously formed by reaction between magnesium in the groundwater and the alkaline pore water. Calcite is initially transformed into monocarbo calcium aluminate by reaction with calcium aluminates, by which also ettringite is formed as well as a small amount of tricalcium aluminate hexahydrate (C_3AH_6).

Calcite is rapidly formed by reaction with both carbonate in the groundwater and carbonate released from a gradual depletion of monocarbo calcium aluminate. Simultaneously, Friedelsalt is formed by reaction between chloride ions in the groundwater and calcium aluminates. After an initial build-up of Friedelsalt during the first 50 years, a slow dissolution starts. After 700 years the Friedelsalt is depleted, see Figure 8.2j.

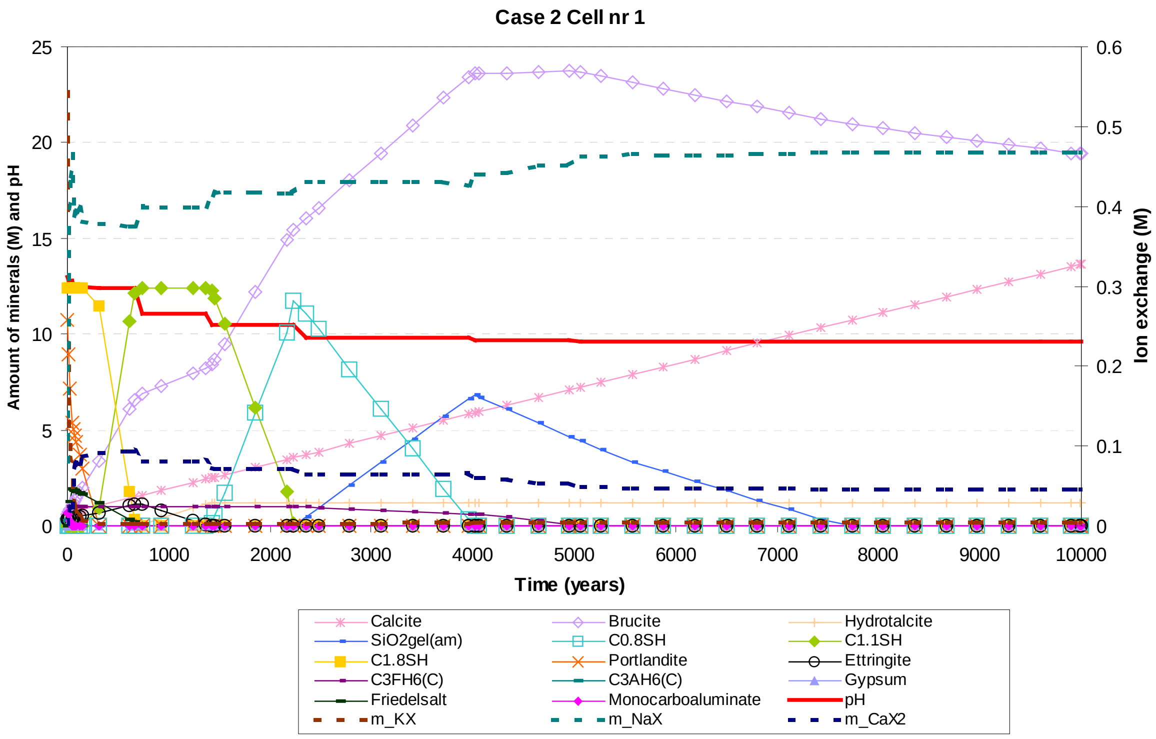

Figure 8.2j Assembly of different mineral phases in Case 2, Cell 1 during 10000 years. The figure also shows the changes of ion exchange species with time.

When $C_{1.8}SH$ has been depleted, hydrotalcite starts to precipitate. From Figure 8.2j, we can see that hydrotalcite increases at a steady rate between 680 years and 1400 years, gradually replacing ettringite which is depleted after 1400 years. Hydrotalcite remains stable throughout the 10 000 years considered in the calculation. When ettringite is depleted, $C_{0.8}SH$ starts to precipitate and gradually replaces $C_{1.1}SH$ which is depleted after 2200 years. The $C_{0.8}SH$-gel is in turn gradually dissolved and about 40% of the silica is transformed into SiO_2-gel, a process which is completed after 4000 years. The remaining silica is dissolved and is transported to the downstream Cell 2.

Following the gradual depletion of calcium in the pore water, C_3FH_6, a calcium ferrihydrate will start to dissolve and is depleted after 5000 years. In the calculations the C_3FH_6 has been assumed passive with respect to reactions with chloride, sulphate and carbonate. It can be expected that the calcium ferrihydrates react with these components in a similar way as the calcium aluminate hydrates. Thermodynamic data are, however unavailable and therefore these compounds cannot be considered in the calculations.

After 7600 years the SiO_2-gel has been completely dissolved. Calcite is continuously precipitated at a rate given by the carbonate content in the percolating groundwater. With decreasing calcium availability the calcite precipitation decreases slightly in Cell 1, resulting in a slight increase in the downstream Cell 2. The precipitation of brucite continues until 4000 years, when the pH drops below 9.7 and brucite starts to buffer the pH and is gradually dissolved. At 10 000 years significant amounts of brucite still remains.

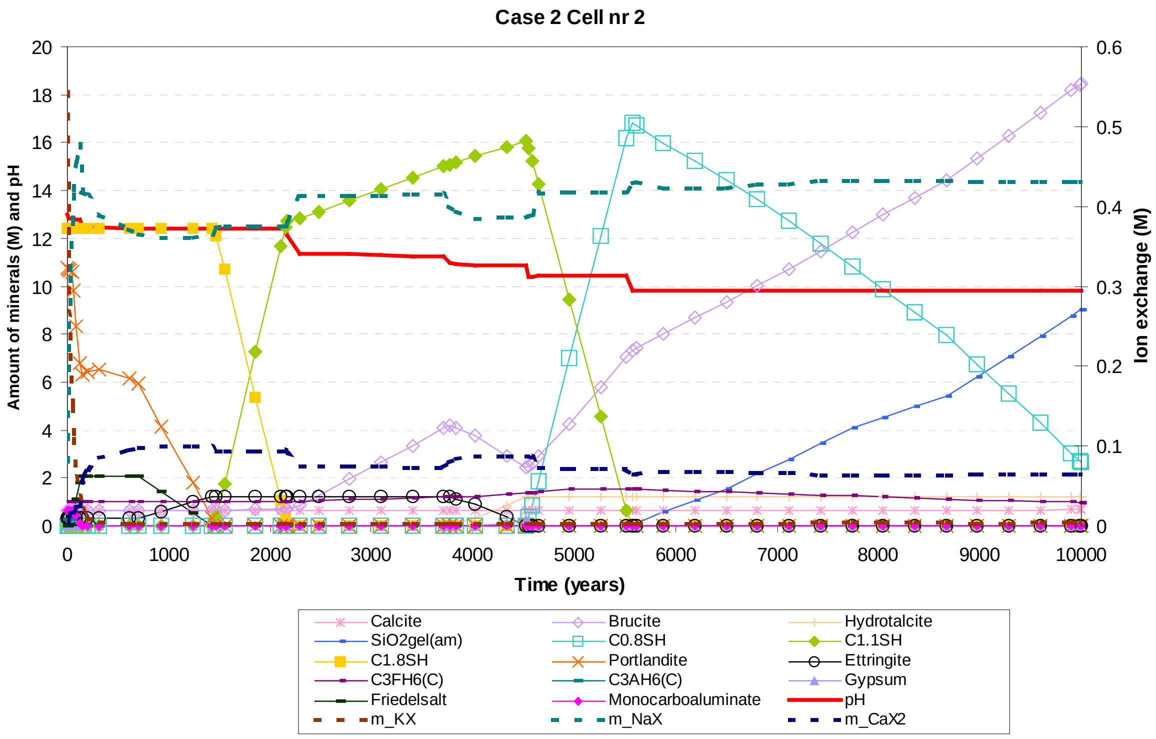

Figure 8.2k Assembly of different mineral phases in Case 2, Cell 2 during 10000 years. The figure also shows the changes of ion exchange species with time.

Figure 8.2k shows the results for Case 2, Cell 2 representing a 0.2 m layer of concrete 0.2 – 0.4 m from the inflow-side of the percolating groundwater. The same general pattern as in Cell 1 is repeated, but shifted in time. In addition, the components of the pore water in Cell 1 will flow into Cell 2 which will gradually change the chemical conditions. The chemical phenomena that remain fundamentally the same as for Cell 1 will not be repeated to full extent here.

The initially assumed calcite and monosulphate will react to form monocarbo calcium aluminate, ettringite and tricalcium aluminate hexahydrate (C_3AH_6). The monocarbo calcium aluminate and C_3AH_6 will react with chloride and sulphate in the percolating groundwater to form ettringite and Friedelsalt. The initially formed C_3AH_6 is depleted after 60 years and monocarbo calcium aluminate after 130 years. Following this the Friedelsalt starts to transform into ettringite by reaction with sulphate and is depleted after 1400 years. Ettringite remain stable in Cell 2 until 3800 years when the pH drops below 11 and ettringite starts to buffer the pore water.

The Portlandite is depleted after 1450 years, when the transformation from $C_{1.8}SH$ to $C_{1.1}SH$ starts, a process completed after 2100 years. From this time and up to 4500 years coexistence between $C_{1.1}SH$, ettringite, brucite and hydrotalcite is suggested by the results. When ettringite is eventually depleted, the $C_{1.1}SH$ starts to transform into $C_{0.8}SH$. Ettringite dissolves and brucite shows a slight tendency to dissolve, whereas hydrotalcite is precipitated. When ettringite has been depleted the formation of hydrotalcite stops and brucite is again formed by the magnesium in the percolating groundwater.

After 5500 years the $C_{1.1}SH$ has been exhausted and $C_{0.8}SH$ starts to form SiO_2-gel, a process which is only partially completed at 10 000 years. It is interesting to note that the amount of $C_{1.1}SH$ and $C_{0.8}SH$ at 4500 years and 5500 years respectively, are 30% and 35% greater than the initial amount of $C_{1.8}SH$ in Cell 2. The obvious explanation is that silica is released from Cell 1 and reacts with calcium in Cell 2 to precipitate more *CSH*-gel.

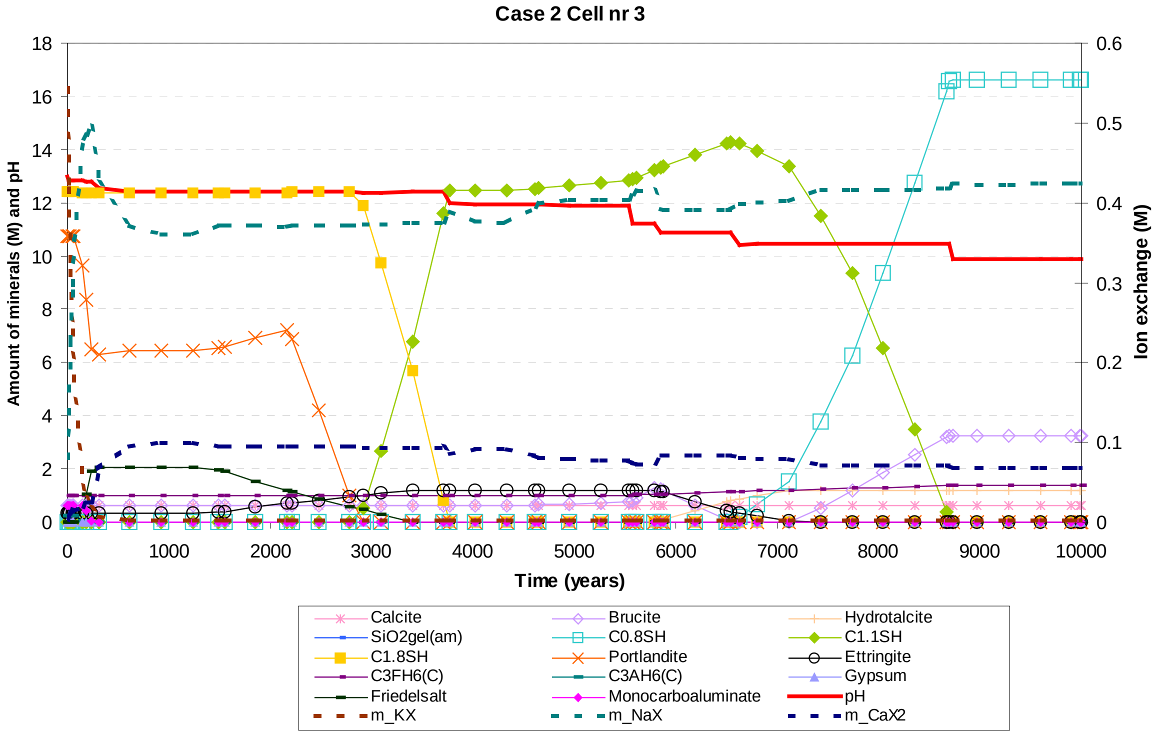

Figure 8.2l Assembly of different mineral phases in Case 2, Cell 3 during 10000 years. The figure also shows the changes of ion exchange species with time.

Figure 8.2l shows the results for Case 2, Cell 3 representing a 0.2 m concrete layer 0.4 – 0.6 m from the concrete surface exposed to groundwater. The reaction sequence is similar to that described for Case 2, Cell 2, but with a certain shift to later times.

A minor peculiarity is that after an initial reduction of Portlandite during the first 250 years, the amount starts to increase after 1400 years to a maximum after 2100 years. The reason for this is a slight destabilisation of Friedelsalt in Cell 3, in turn caused by depletion of Friedelsalt in the upstream Cell 2 which gives a slightly reduced chloride concentration. At 2100 years, Portlandite starts to dissolve and is depleted after 2900 years. This change reflects the exhaustion of $C_{1.8}SH$ in Cell 2 giving a reduced pH in the pore water flowing into Cell 3. In Cell 3, the pH decreases below 10 after about 8700 years.

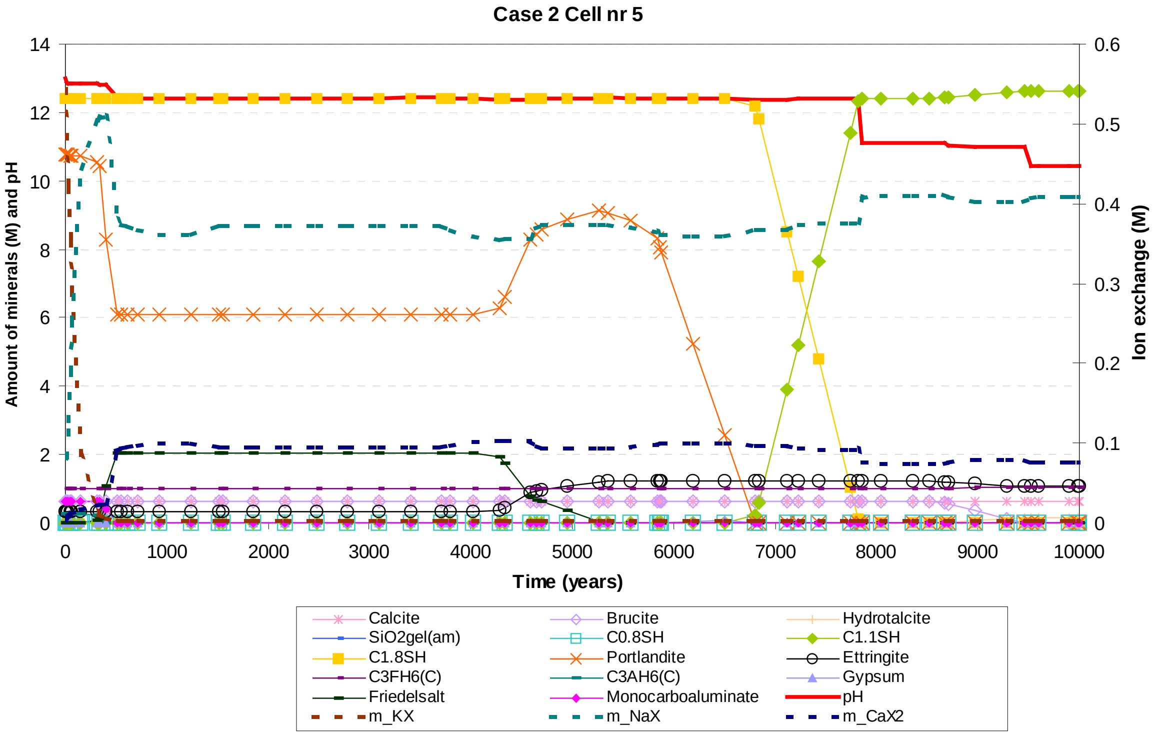

Figure 8.2m Assembly of different mineral phases in Case 2, Cell 5 during 10000 years. The figure also shows the changes of ion exchange species with time.

Figure 8.2m shows the results for Case 2, Cell 5 representing a 0.2 m concrete layer 0.8 – 1.0 m from the concrete surface where percolating groundwater is assumed to flow into the structure. The same pattern for the chemical transformations can be recognised as described for Cells 2 and 3, although shifted to later times. As in Cell 3, a build-up of Portlandite occurs, which is more pronounced in Cell 5. The pH does not drop below 10 during the 10 000 years considered.

8.2.4 Changes of porosity versus time in different cells - Case 2

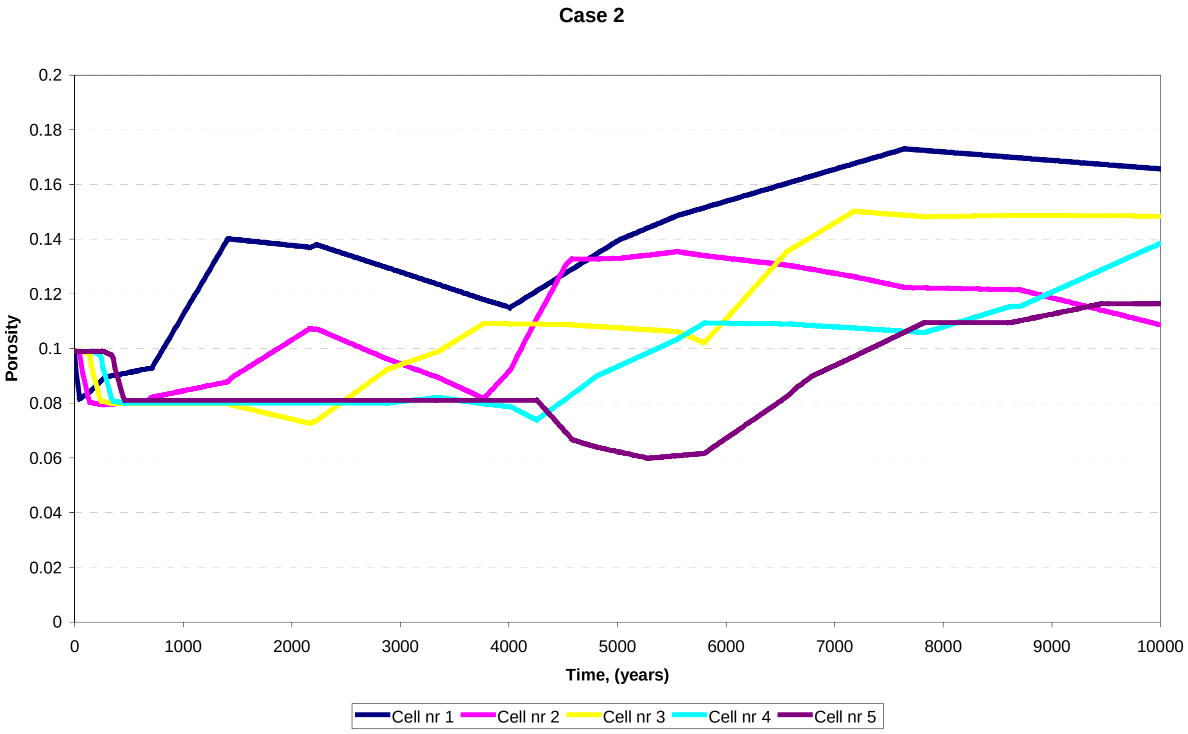

Figure 8.2n Compiled results for calculated changes of porosities in different cells in Case 2. The changes in porosity are shown as a function of time.

The changes of porosity in the five cells assumed in the model are presented in Figure 8.2n for the first 10 000 years. The initial porosity in the considered construction concrete is 0.099, a value calculated using a cement hydration model, see details in Chapter 5.

All cells show an initial reduction in porosity from 0.099 to about 0.08. The porosity change in Cell 1, which represents the 0.2 m close to the inflow surface for the percolating groundwater, is most rapid and will occur during the first 50 years. A similar change follows in a tight sequence also in Cells 2-5 after 150, 250, 350 and 450 years.

The cause of this porosity change is reaction of monocarbo calcium aluminate with chloride in the groundwater to form Friedelsalt. A slower reaction with sulphate in the groundwater then gradually transforms the Friedelsalt to ettringite, a reaction completed after 700 years in Cell 1. Other mineral transformations contribute to the complex porosity changes in Cell 1, such as formation of calcite and brucite (continues to 10 000 years), dissolution of Portlandite (completed after 280 years), transformation of $C_{1.8}SH$ to $C_{1.1}SH$ (from 280 to 680 years), dissolution of ettringite and precipitation of hydrotalcite (from 680 to 1400 years), transformation of $C_{1.1}SH$ to $C_{0.8}SH$ (from 1400 to 2200 years) followed by transformation of $C_{0.8}SH$ to SiO_2-gel (2200 to 4000 years), whereafter the SiO_2-gel gradually dissolves (depleted after 7600 years). After 7600 years calcite continues to precipitate, whereas brucite is slowly dissolved, hydrotalcite remain stable.

In Cell 2, representing 0.2 m concrete layer 0.2 – 0.4 m from the inflow surface for the percolating groundwater, the initial porosity reduction follows a transformation of monocarbo calcium aluminate and tricalcium aluminate hexahydrate, C_3AH_6, to Friedelsalt by reaction with chloride ions in the groundwater which is completed after 150 years. A minor precipitation of calcite occurs. Cell 2 enters a stagnant phase between 150 and 700 years. At 700 years, Friedelsalt is destabilised in Cell 2 and initiates a precipitation of ettringite by reaction with sulphate, a reaction that is completed after 1400 years, followed by a depletion of Portlandite at 1450 years. Between 1450 and 2100 years, $C_{1.8}SH$ transforms into $C_{1.1}SH$, followed by a short stagnant period to 2200 years when brucite precipitation intensifies accompanied by precipitation of $C_{1.1}SH$ which continues up to 3800 years. At this point ettringite is destabilised and starts to dissolve together with brucite, whereas hydrotalcite is formed. As a result of the sulphate released, gypsum is formed at 4000 years in Cell 2. At 4500 years ettringite has been depleted, gypsum rapidly dissolves, and $C_{1.1}SH$ starts to transform into $C_{0.8}SH$ until depleted at 5500 years, followed by transformation of $C_{0.8}SH$ to SiO_2-gel which is not completed at 10 000 years. From 4500 to 10 000 years, hydrotalcite remains stable, a minor precipitation of calcite occurs and brucite is steadily precipitated.

After an initial reaction sequence which is analogue to the description for Cell 2, the porosity in Cell 3 levels off at a constant value of 0.08 after 250 years. At 1400 years Friedelsalt starts to react with sulphate to form Portlandite and ettringite, which have larger molar volumes, visible in Figure 8.2n as a further reduction in porosity over the period 1400 – 2200 years. At 2200 years, Portlandite starts to redissolve causing the porosity to increase from a minimum value of 0.073. Portlandite is depleted after 2800 years, and a transformation of $C_{1.8}SH$ to $C_{1.1}SH$ starts. The Friedelsalt is depleted after 3400 years and $C_{1.8}SH$ after 3800 years. From 3800 to 5600 years the conditions are quite stable with only a minor precipitation of brucite. At 5600 years hydrotalcite appears and starts to increase at 5800 years when ettringite and brucite are destabilised. At 6500 years brucite has been depleted and $C_{1.1}SH$ starts to transform into $C_{0.8}SH$. Ettringite disappears after 7200 years and a slow precipitation of brucite starts once again. At 8600 years $C_{1.1}SH$ has been exhausted. An interesting detail is that $C_{0.8}SH$ remains stable from this point until 10 000 years. The porosity reaches a maximum value of about 0.15 after 7200 years, which is 0.02 lower than the maximum value in Cell 1, but 0.02 higher than for Cell 2.

Following the same sequence of reactions during the initial phase, the porosity in Cell 4, representing a 0.2 m concrete layer at 0.6 – 0.8 m from the concrete surface exposed to groundwater, a long period of fairly stagnant conditions is entered. The porosity levels off at 0.08 from 350 to 2900 years when Friedelsalt starts to form as a result of dissolution of Portlandite and ettringite and reaction with chloride ions, this process continues until 3400 years when it is reversed. This peculiar behaviour is explained by variations in the chemical composition of the percolating water, which reflect changes occurring in the upstream cells. At 4000 years the Friedelsalt is further destabilised resulting in depletion after 4200 years, accompanied by precipitation of ettringite. At this point, the porosity reaches a minimum value of 0.072. Dissolution of Portlandite leads to depletion after 4800 years, which again increases the porosity. Following this, $C_{1.8}SH$ transforms to $C_{1.1}SH$ during the period 4800 to 5800 years during which the porosity increases to 0.11. The conditions stabilise and remain almost unchanged until ettringite and brucite start to dissolve after 7800 years whereby hydrotalcite is formed. Brucite becomes exhausted and $C_{1.1}SH$ begins to transform into $C_{0.8}SH$, this reaction is not completed at 10 000 years. The porosity in Cell 4 is steadily increasing from 8000 years and is about 0.138 at 10 000 years.

Figure 8.2n shows that the chemical reactions in Cell 5 resemble those in Cells 1 – 4 during the early period. The porosity drops to 0.08 during the first 450 years due to transformation of monocarbo calcium aluminate and C_3AH_6 to Friedelsalt which is a result of chloride intrusion from the groundwater. During this period a part of the Portlandite is also consumed. A long period of invariant conditions follows. After 4200 years Friedelsalt starts to dissolve and ettringite and Portlandite are formed, this is clearly visible in Figure 8.2n as a reduction of the porosity that reaches a minimum value of 0.06 after 5300 years. After about 5700 years Portlandite starts to dissolve and is exhausted after 6500 years. At 5800 years a slight formation of gypsum occurs, reaches a maximum at 6500 years and disappears at 6600 years. After 6800 years, $C_{1.8}SH$ starts to transform into $C_{1.1}SH$ which is finalised at 7800 years. A new period of stagnant conditions follows that ends after 8600 years when hydrotalcite starts to precipitate, gradually replacing some of the ettringite and the brucite (exhausted after 9500 years). From 9500 to 10 000 years the conditions remain stable. The final porosity is 0.116.

To summarise the porosity changes in Case 2, the initial, maximum and minimum porosities calculated for the different cells are presented in Table 8.2.

Table 8.2 Initial maximum and minimum porosities for different cells in Case 2.

Cell	**Initial porosity**	**Maximum porosity**	**Minimum porosity**
1	0.099	0.173	0.082
2	0.099	0.135	0.079
3	0.099	0.150	0.073
4	0.099	0.140	0.074
5	0.099	0.116	0.06

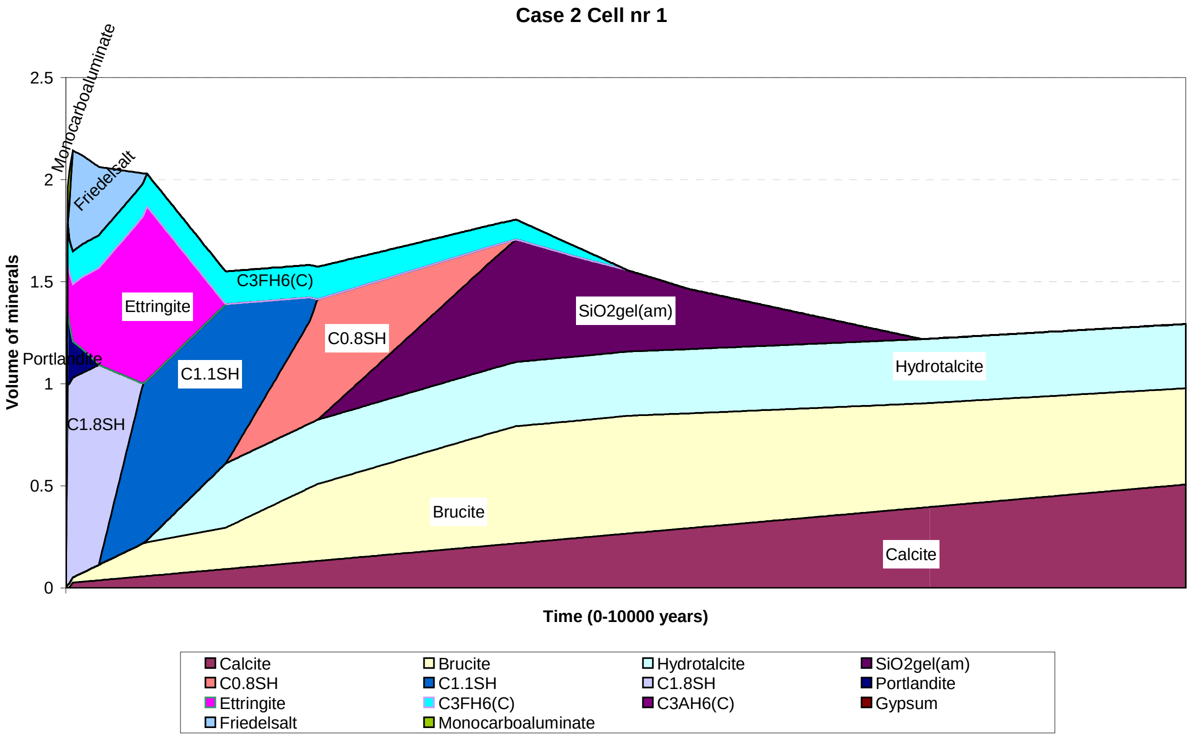

Figure 8.2o Contribution to the total volume of reactive minerals considered in the calculations for Case 2, Cell 1 for the period 0-10 000 years. The changes of the amounts of individual minerals have been used in the estimates of porosity changes. The total volume is expressed as (m^3 of reactive minerals per m^3 of initial pore volume of the material).

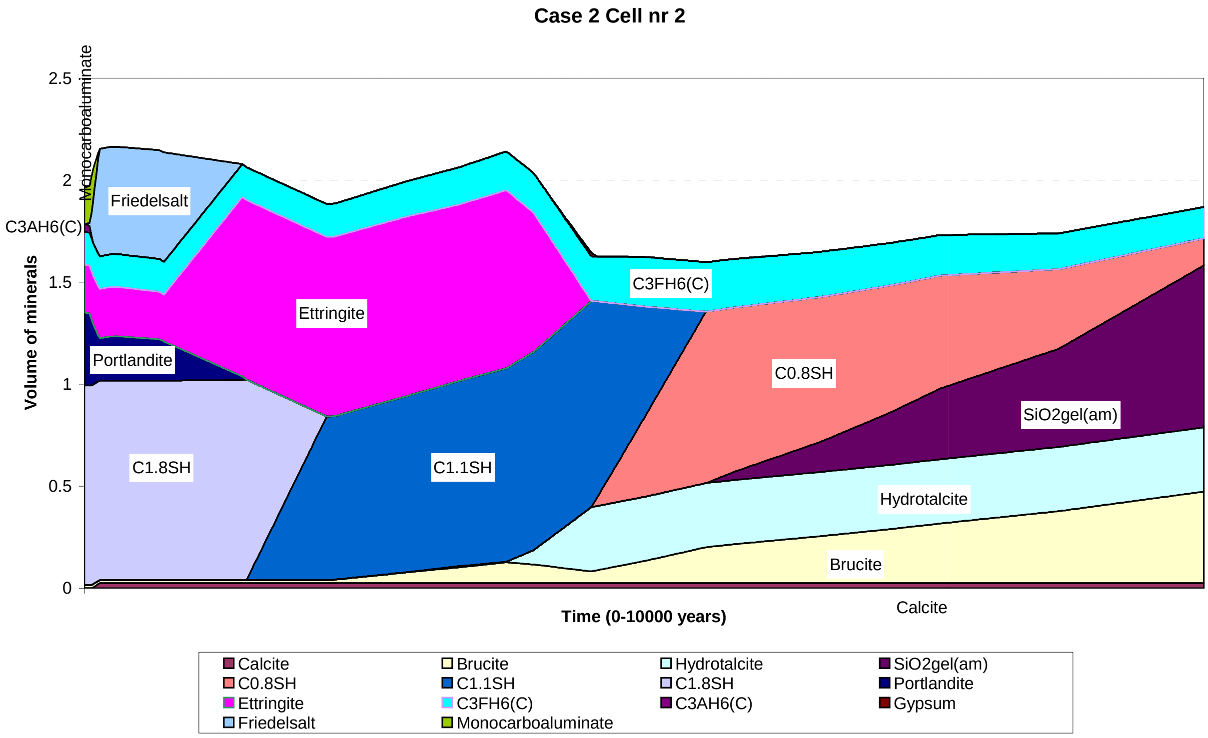

Figure 8.2p Contribution to the total volume of reactive minerals considered in the calculations for Case 2, Cell 2 for the period 0-10 000 years. The changes of the amounts of individual minerals have been used in the estimates of porosity changes. The total volume is expressed as (m^3 of reactive minerals per m^3 of initial pore volume of the material). The total volume is expressed as (m^3 of reactive minerals per m^3 of initial pore volume of the material).

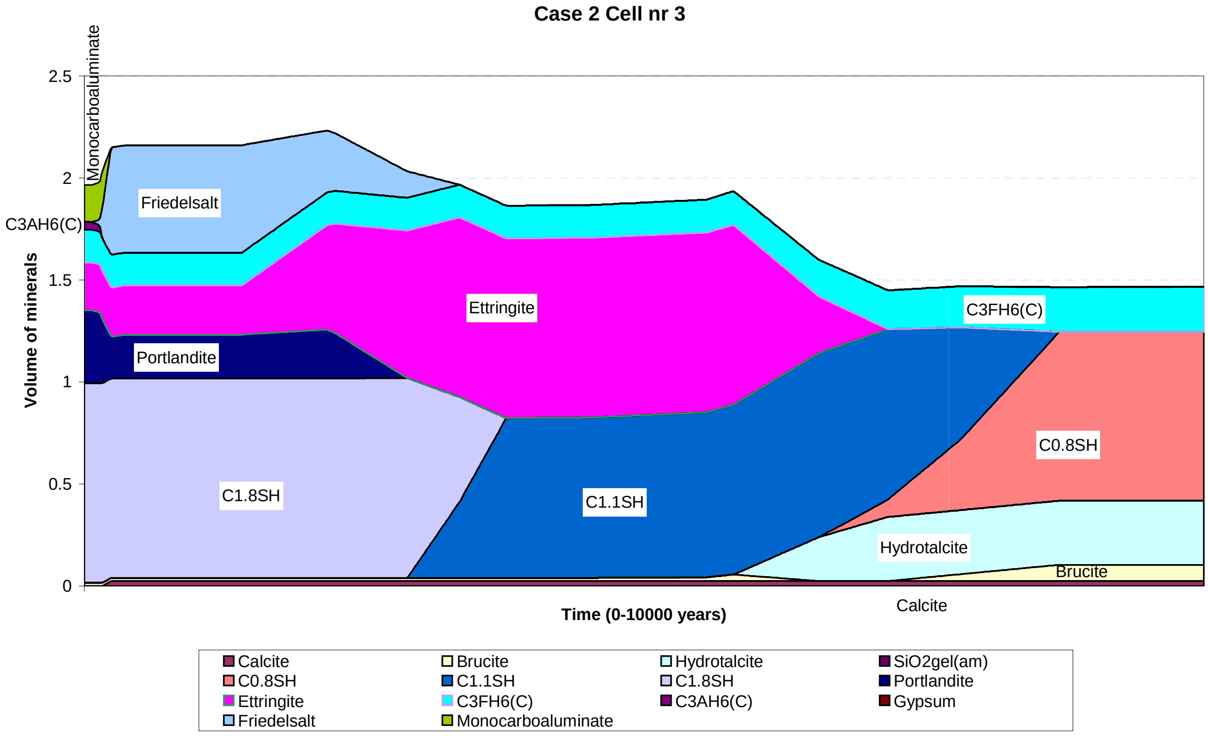

Figure 8.2q Contribution to the total volume of reactive minerals considered in the calculations for Case 2, Cell 3 for the period 0-10 000 years. The changes of the amounts of individual minerals have been used in the estimates of porosity changes. The total volume is expressed as (m^3 of reactive minerals per m^3 of initial pore volume of the material).

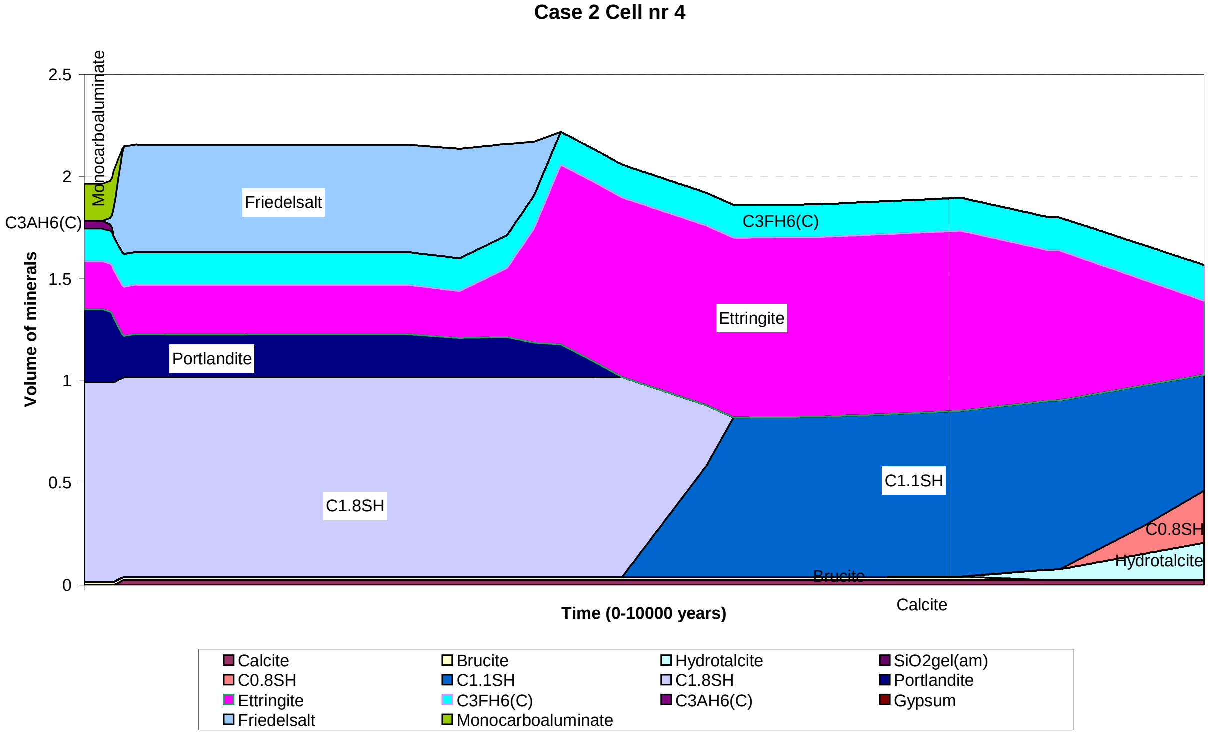

Figure 8.2r Contribution to the total volume of reactive minerals considered in the calculations for Case 2, Cell 4 for the period 0-10 000 years. The changes of the amounts of individual minerals have been used in the estimates of porosity changes. The total volume is expressed as (m^3 of reactive minerals per m^3 of initial pore volume of the material).

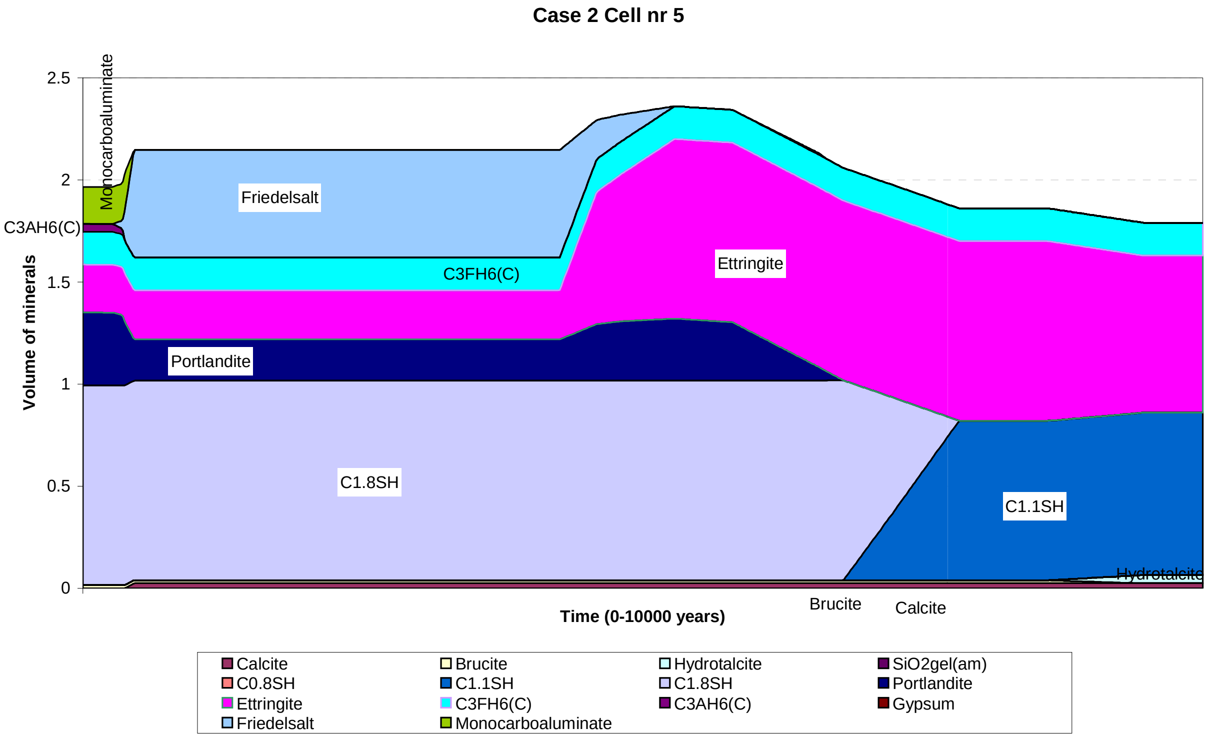

Figure 8.2s Contribution to the total volume of reactive minerals considered in the calculations for Case 2, Cell 5 for the period 0-10 000 years. The changes of the amounts of individual minerals have been used in the estimates of porosity changes. The total volume is expressed as (m^3 of reactive minerals per m^3 of initial pore volume of the material).

8.3 Case 3 - Diffusion through a sand/bentonite layer with constant groundwater composition as boundary condition

This case is a variation of Case 1, adding a sand/bentonite layer over the silo top. This calculation can be used to study the impact by the sand/bentonite layer as a transport barrier for the exchange of dissolved components between the groundwater and the concrete structures, as well as for introductory studies of the chemical interaction between bentonite and concrete. A possible future extension is to study the impact on the near-field rock by the leachate water leaving the repository. In Case 3 the ion exchange capacity of the sand/bentonite has been assumed to equal measured values for uncompacted material, e.g. values which could be expected in a slurry. Based on experimental data for compacted bentonite and sand/bentonite as compared to measurements in slurries, a reduction of the ion exchange capacity by a factor of 8.5 in the sand/bentonite barrier may be suggested (Torstenfelt et al, 1983; Torstenfelt and Allard, 1986; Albinsson et al 1993; Albinson 1993). The rationale for such a reduction would be that part of the ion exchange sites could become unavailable due to the compaction (Wanner et al, 1994). This has not been considered in the present study.

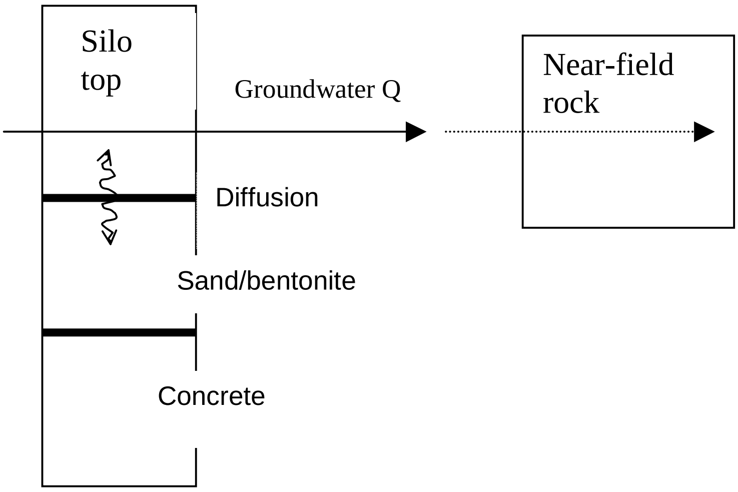

Figure 8.3 Simplified representation of leaching of a concrete barrier protected from direct contact with groundwater by a sand/bentonite layer at one side. Leaching is assumed to be governed by diffusion in the concrete and sand/bentonite layer. The groundwater composition is assumed to remain constant, which is representative for a situation where the groundwater renewal rate is fast compared to the diffusion of reactants through the sand/bentonite layer.

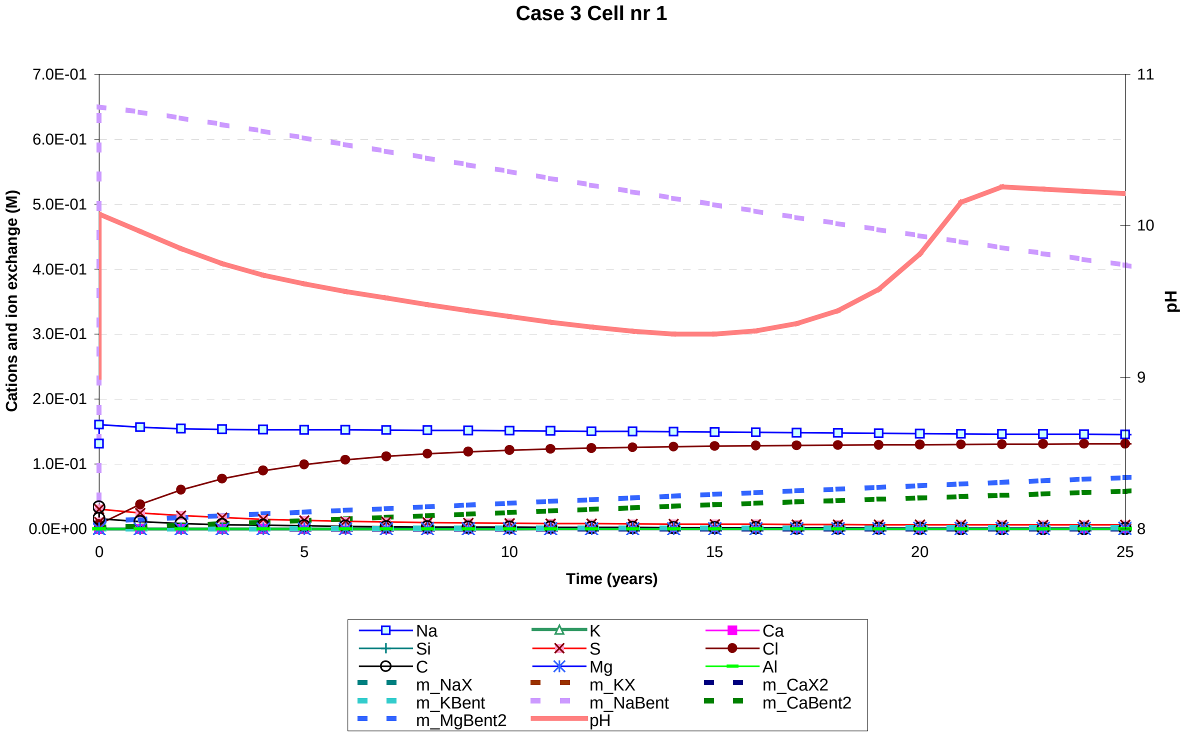

Figure 8.3a Results from leaching calculations for Case 3, Cell 1. The figure shows the development of aqueous concentrations and ion exchange species with time in a 0.32 m layer of the sand/bentonite barrier, in contact with the groundwater, situated 1.18 – 1.5 m from the interface between concrete and sand/bentonite.

The results in Figure 8.3a show that the pH, which is initially about 10, drops to a minimum value of 9.2 after 15 years in response to chloride intrusion from the groundwater. The ion exchange from sodium bentonite (denoted m_NaBent in the figure) to calcium and magnesium bentonite has started at this time due to intrusion of calcium and magnesium from the groundwater. Following this, the pH rapidly increases in response to alkaline components from the concrete to a maximum of 10.2 at 25 years, then decreasing again to reach a stable value of 9.6 after 100 years. At 25 years precipitation of brucite and hydrotalcite is started in addition to a slight precipitation of talc and calcite that started at an early time, c.f. Figure 8.3f. These precipitations continue to 10 000 years, with the exception for hydrotalcite which starts to decrease slightly after 1500 years. A continuous readjustment of the different ion exchange species occurs which is completed after 100 years. From this time on the chemical conditions in the pore water remain practically constant.

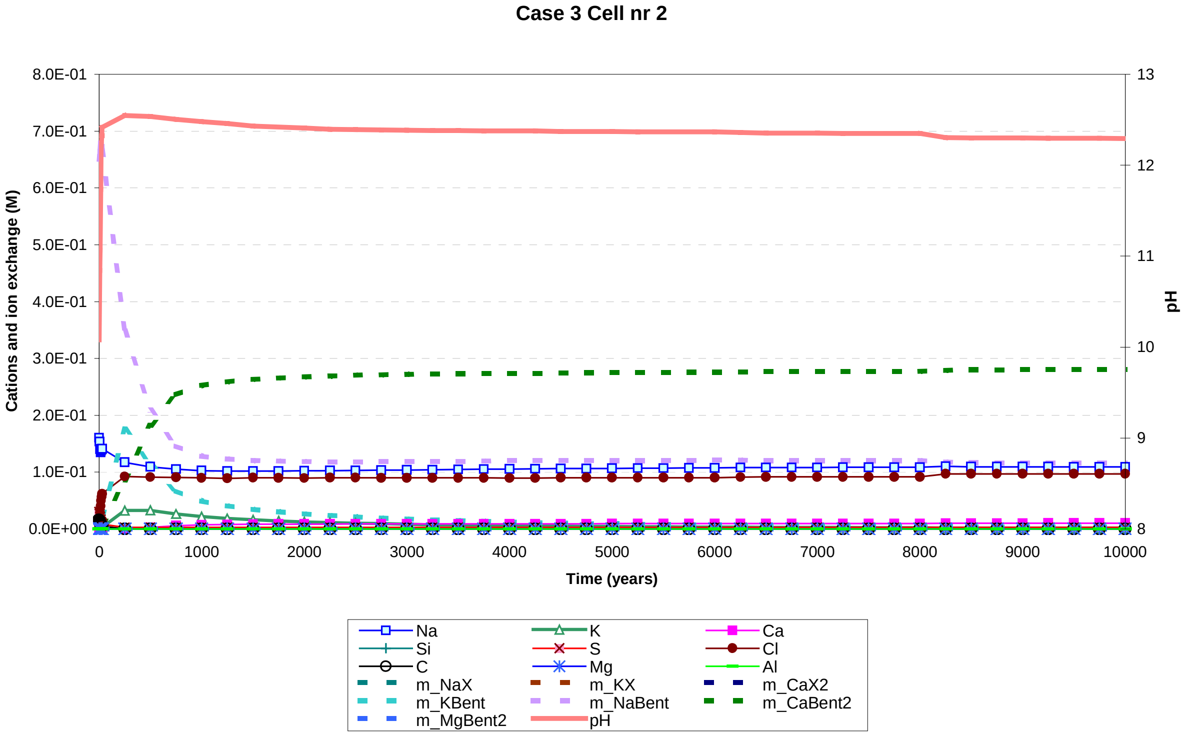

Figure 8.3b Results from leaching calculations for Case 3, Cell 2. The figure shows the development of aqueous concentrations and ion exchange species with time in a 0.87 m layer of the sand/bentonite barrier situated 0.32 – 1.18 m from the interface between concrete and sand/bentonite.

Figure 8.3b shows the results for Case 3, Cell 2, representing a 0.87 m layer of sand/bentonite 0.32 – 1.18 m from the interface with the concrete. In Cell 2 the influence by the concrete is more pronounced as clearly shown by a sharp increase in pH, reaching a practically steady value of about 12.5 after 40 years. The amount of sodium bentonite shows an initial increase due to sodium released from Cell 1 due to ion exchange with calcium and magnesium from the groundwater, and from Cell 3 due to ion exchange with potassium from the concrete. After 15 years the sodium bentonite steadily decreases, being gradually replaced first by potassium bentonite during the period 15 to 250 years, and then by calcium bentonite which will be the predominant form from 540 to 10 000 years. After about 1500 years the chemical conditions remain almost invariable. A slow but continuous precipitation of brucite occurs over the entire 10 000-year-period considered, c.f. Figure 8.3g. Calcite remains stable over time. A brief formation of talc and hydrotalcite is noted during the first 20 years.

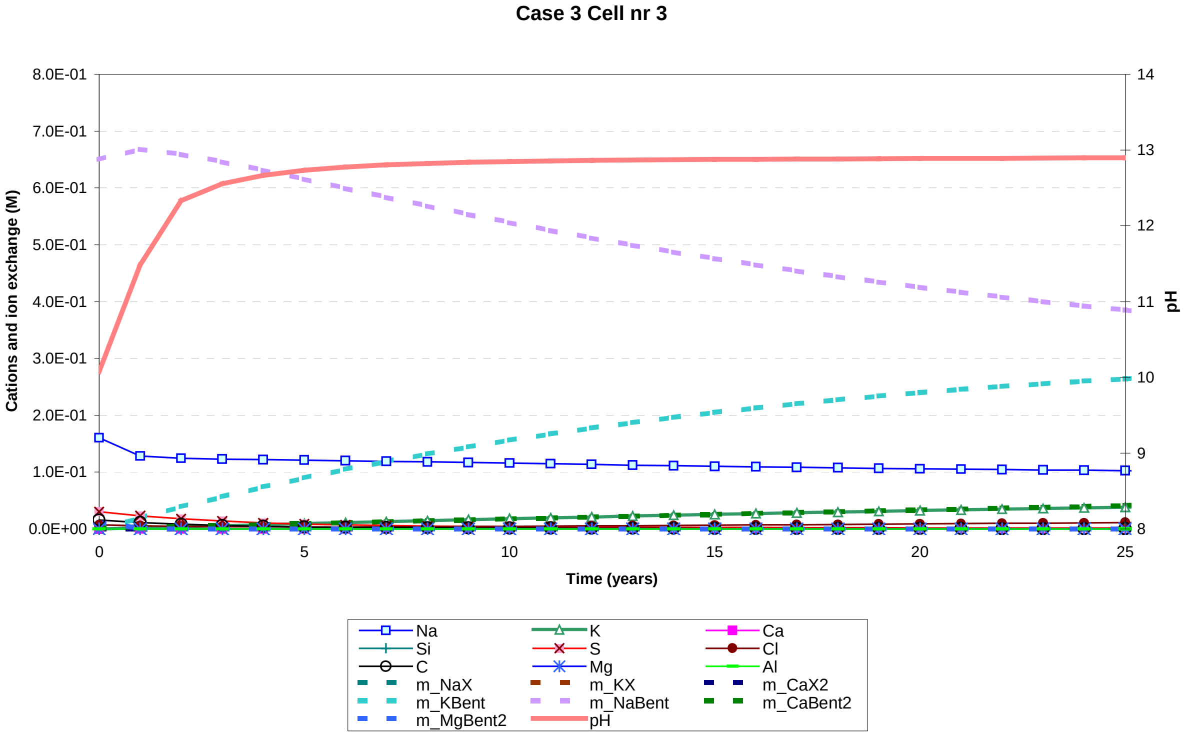

Figure 8.3c Results from leaching calculations for Case 3, Cell 3. The figure shows the development of aqueous concentrations and ion exchange species with time in a 0.32 m layer of the sand/bentonite barrier situated 0 – 0.32 m from the interface between concrete and sand/bentonite. A detailed time scale for the first 25 years is presented.

The chemical evolution in Case 3, Cell 3, representing a 0.32 m sand/bentonite layer at the interface to the concrete, is shown in Figure 8.3c. The chemical changes follow the sequence of events described for Cell 2, but occur at an earlier time. The pH stabilises at an almost constant value of 12.9 after 50 years (not shown in Figure 8.3c) due to interaction with the concrete. In Cell 3 the amount of calcium bentonite steadily increases throughout the considered 10 000 years in response to the calcium being released by the concrete. After 150 years, ettringite starts to precipitate which continues to 10 000 years, c.f. Figure 8.3h.

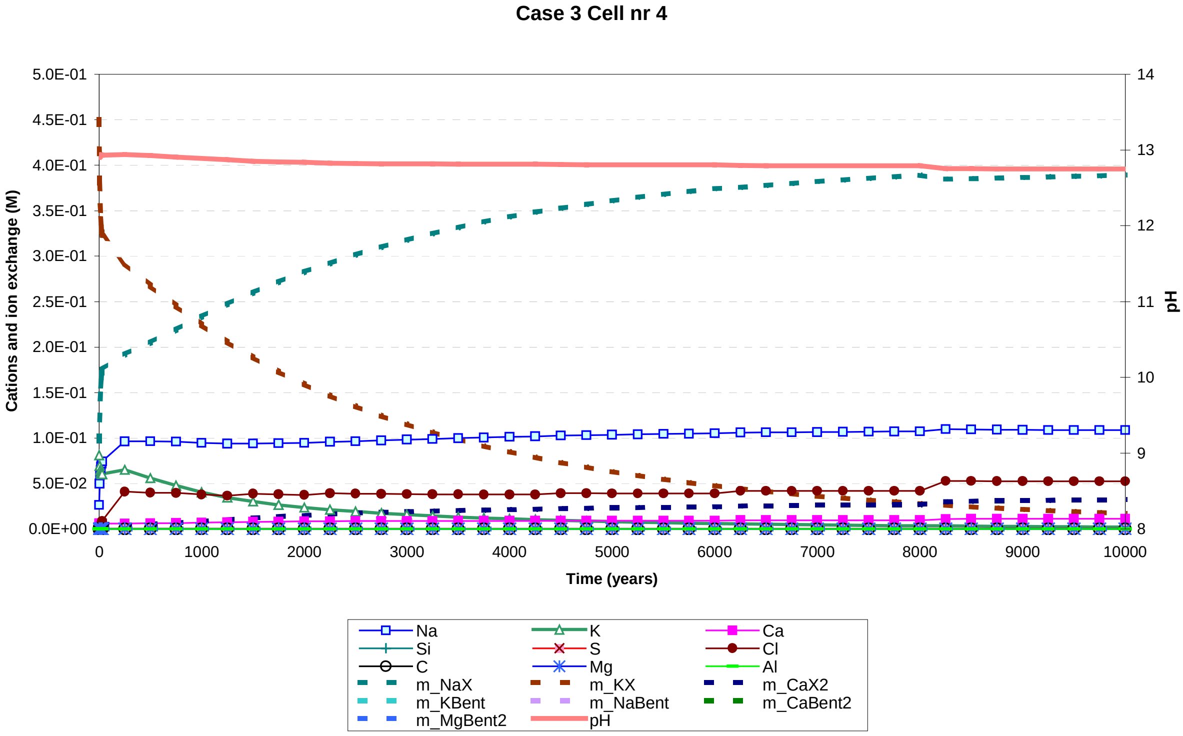

Figure 8.3d Results from leaching calculations for Case 3, Cell 4. The figure shows the development of aqueous concentrations and ion exchange species with time in a 0.05 m layer of the concrete situated 0 – 0.05 m from the interface between concrete and sand/bentonite.

Figure 8.3d shows the chemical changes in Case 3, Cell 4, which represent a 0.05 m layer of concrete in contact with the sand/bentonite. The pH is almost constant at 12.9 – 12.7 during 10 000 years. A gradual ion exchange of potassium for sodium occurs, at first rapid during 40 years and then at a low constant rate. After 940 years the amounts are equal and after 10 000 years the amount of ion exchanged sodium is about twice as high as the amount of ion exchanged potassium.

After 2000 years, calcite starts to precipitate in Cell 4 which continues to 4450 years and thereafter remains constant to 10 000 years. C_3AH_6 gradually dissolves and becomes depleted after 700 years. Portlandite also dissolves, whereas ettringite is precipitated. At 10 000 years about 35% of the Portlandite remains, c.f. Figure 8.3i.

Monocarbo calcium aluminate forms initially and increases slowly during the first 2000 years, thereafter slowly dissolves and becomes depleted after 4400 years. At 125 years, Friedelsalt starts to precipitate due to reaction with chloride from the groundwater. The precipitation of Friedelsalt continues until 700 years, marking the depletion of C_3AH_6 followed by a slow dissolution until 2000 years when the amount again starts to increase, a process which continues to 4400 years, thereafter slowly decreasing until 10 000 years.

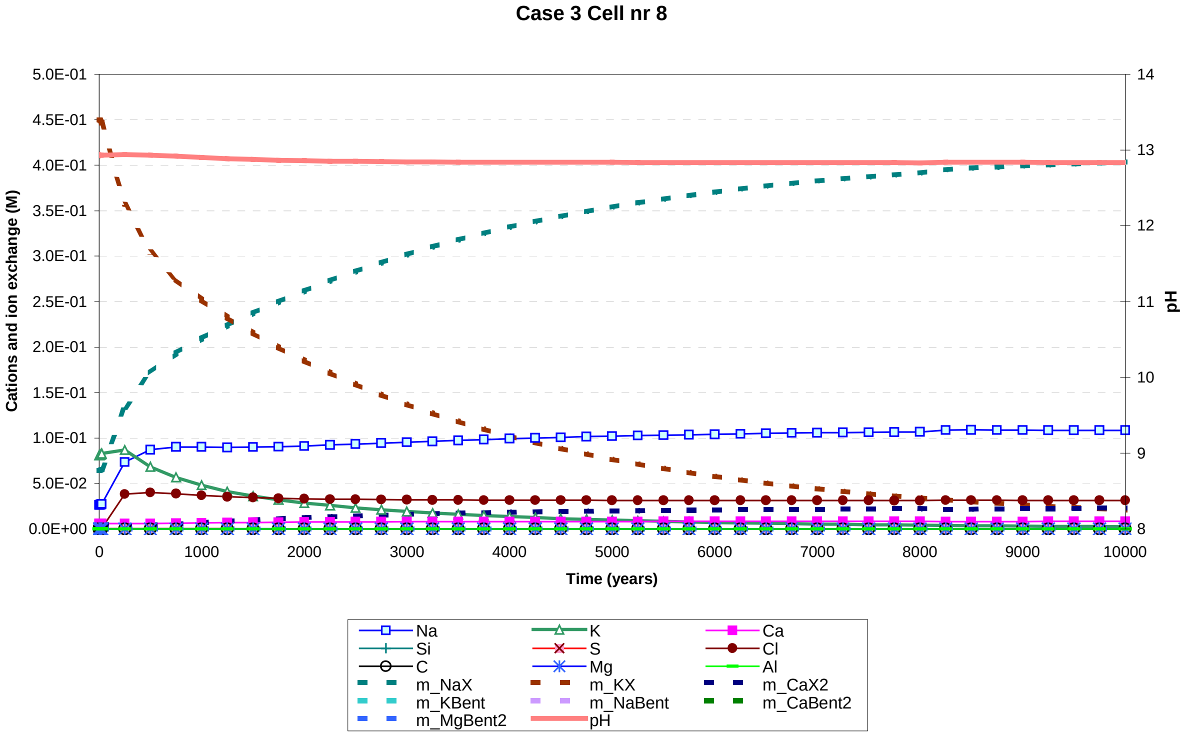

Figure 8.3e Results from leaching calculations for Case 3, Cell 8. The figure shows the development of aqueous concentrations and ion exchange species with time in a 0.6 m layer of the concrete situated 0.4 – 1.0 m from the interface between concrete and sand/bentonite.

The same pattern is repeated, at later times, for Cell 5, c.f. Figure 8.3j, Cells 6 – 7 (not shown in the figures) and in Cell 8 as shown in Figure 8.3e and 8.3k. The pH remains high, about 12.9 – 12.8, during the 10 000 years considered. The mineral assembly remains almost unchanged, with the following exceptions: Friedelsalt appears after 700 years in Cell 5, after 1300 years in Cell 6, after 2000 years in Cell 7, and after 3800 years in Cell 8. Calcite starts to precipitate after 4400 years in Cell 5, whereas monocarbo calcium aluminate is gradually depleted until 6200 years. About 92% of the initial content of Portlandite in Cell 8 remains after 10 000 years.

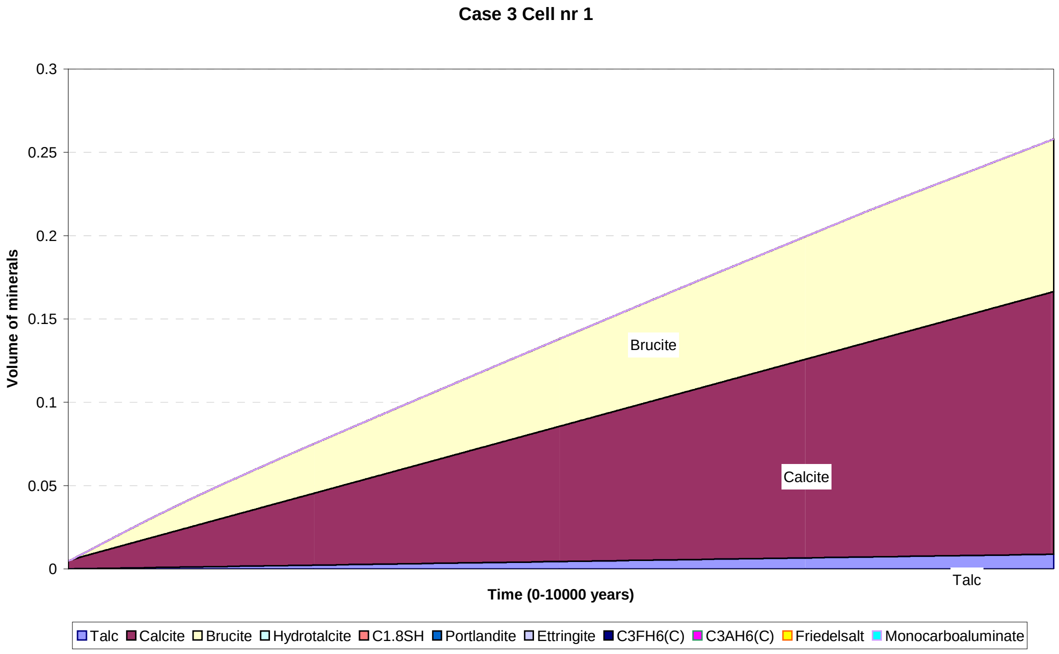

Figure 8.3f *Contribution to the total volume of reactive minerals considered in the calculations for Case 3, Cell 1 for the period 0-10 000 years. The changes of the amounts of individual minerals have been used in the estimates of porosity changes. The total volume is expressed as (m^3 of reactive minerals per m^3 of initial pore volume of the material).*

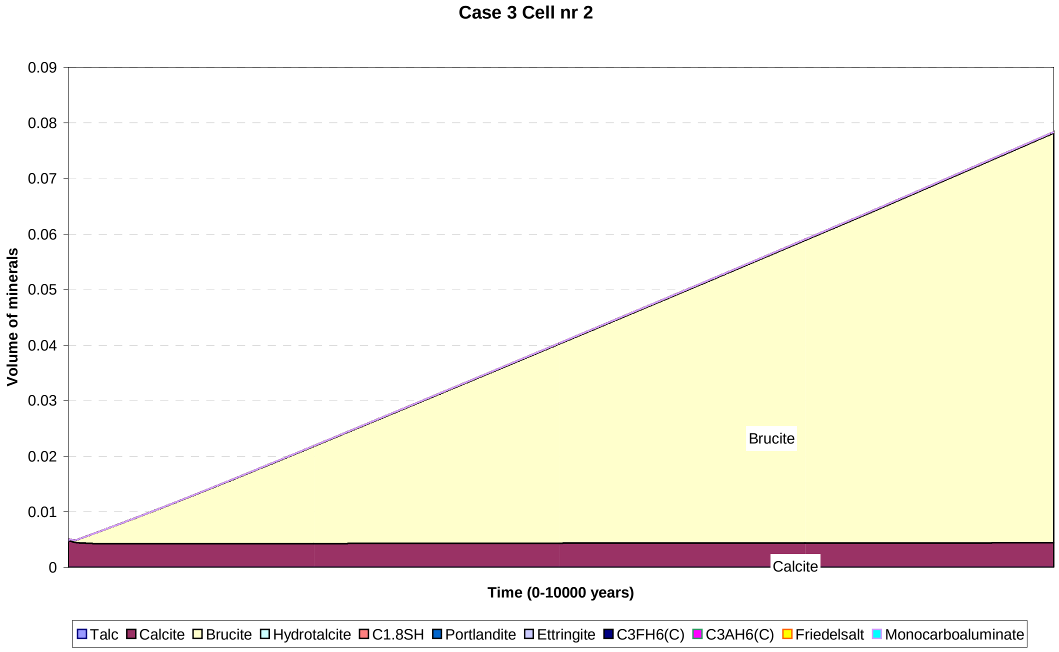

Figure 8.3g *Contribution to the total volume of reactive minerals considered in the calculations for Case 3, Cell 2 for the period 0-10 000 years. The changes of the amounts of individual minerals have been used in the estimates of porosity changes. The total volume is expressed as (m^3 of reactive minerals per m^3 of initial pore volume of the material).*

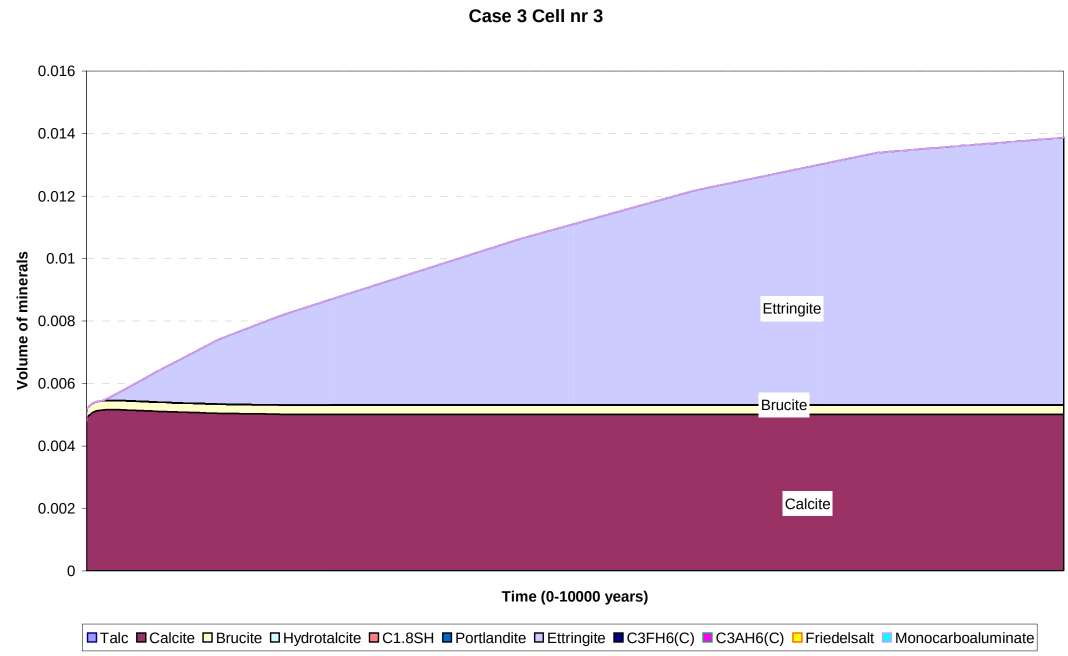

Figure 8.3h *Contribution to the total volume of reactive minerals considered in the calculations for Case 3, Cell 3 for the period 0-10 000 years. The changes of the amounts of individual minerals have been used in the estimates of porosity changes. The total volume is expressed as (m^3 of reactive minerals per m^3 of initial pore volume of the material).*

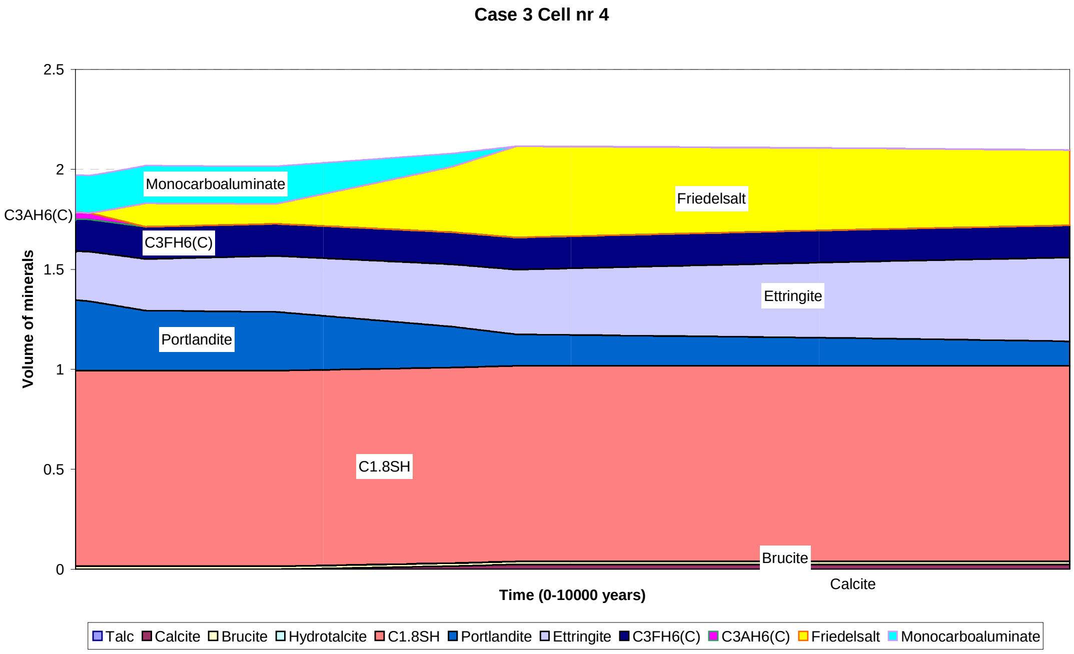

Figure 8.3i *Contribution to the total volume of reactive minerals considered in the calculations for Case 3, Cell 4 for the period 0-10 000 years. The changes of the amounts of individual minerals have been used in the estimates of porosity changes. The total volume is expressed as (m^3 of reactive minerals per m^3 of initial pore volume of the material).*

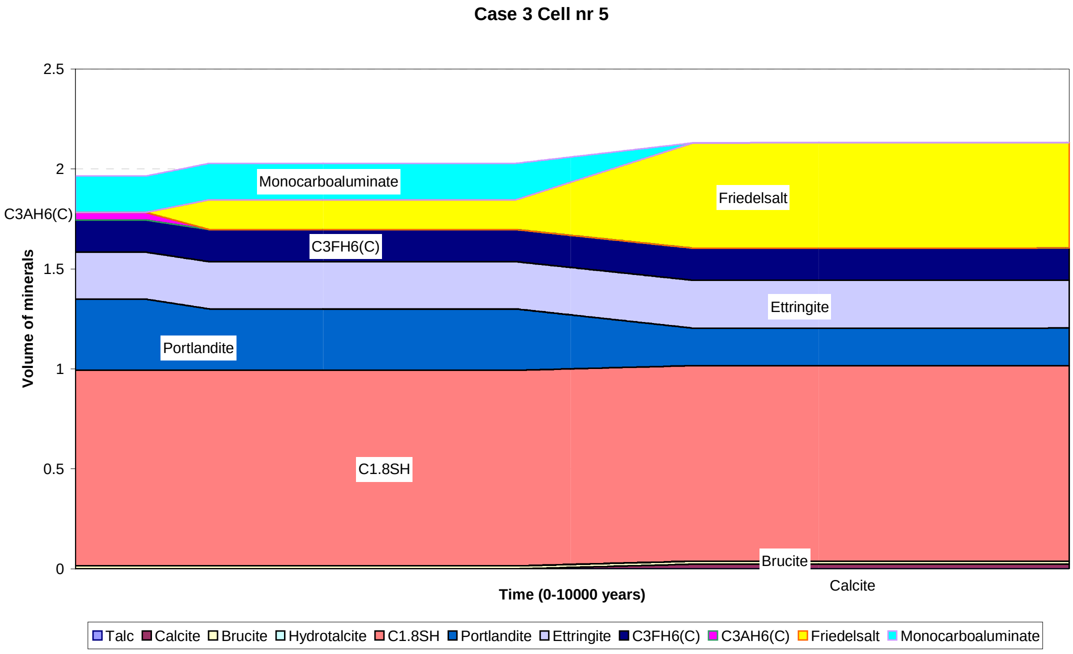

Figure 8.3j *Contribution to the total volume of reactive minerals considered in the calculations for Case 3, Cell 5 for the period 0-10 000 years. The changes of the amounts of individual minerals have been used in the estimates of porosity changes. The total volume is expressed as (m^3 of reactive minerals per m^3 of initial pore volume of the material).*

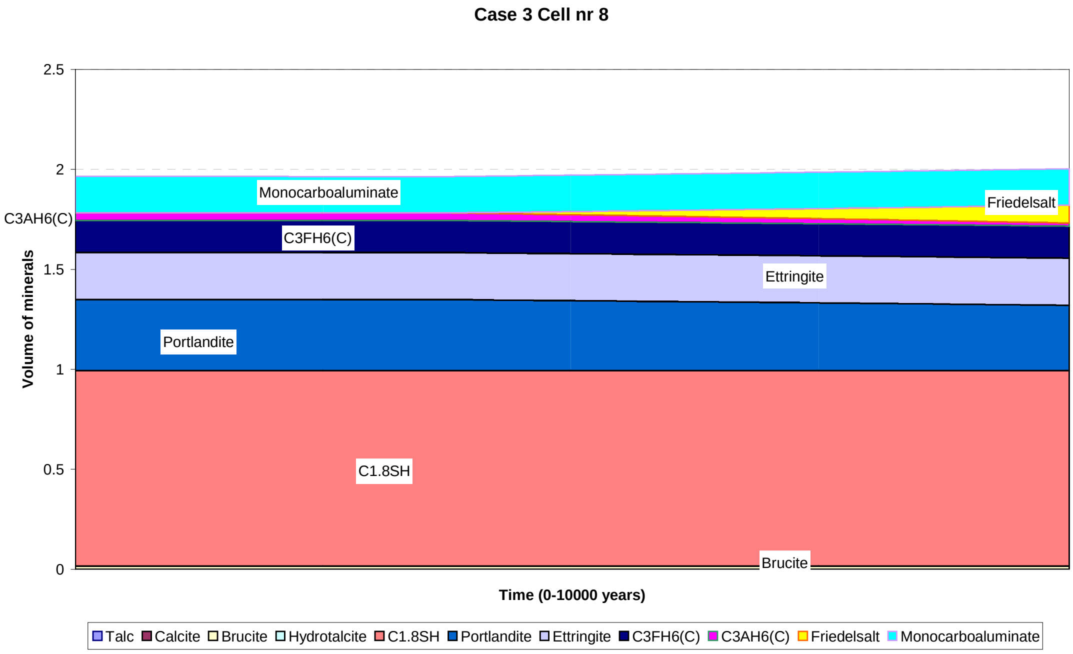

Figure 8.3k *Contribution to the total volume of reactive minerals considered in the calculations for Case 3, Cell 8 for the period 0-10 000 years. The changes of the amounts of individual minerals have been used in the estimates of porosity changes. The total volume is expressed as (m^3 of reactive minerals per m^3 of initial pore volume of the material).*

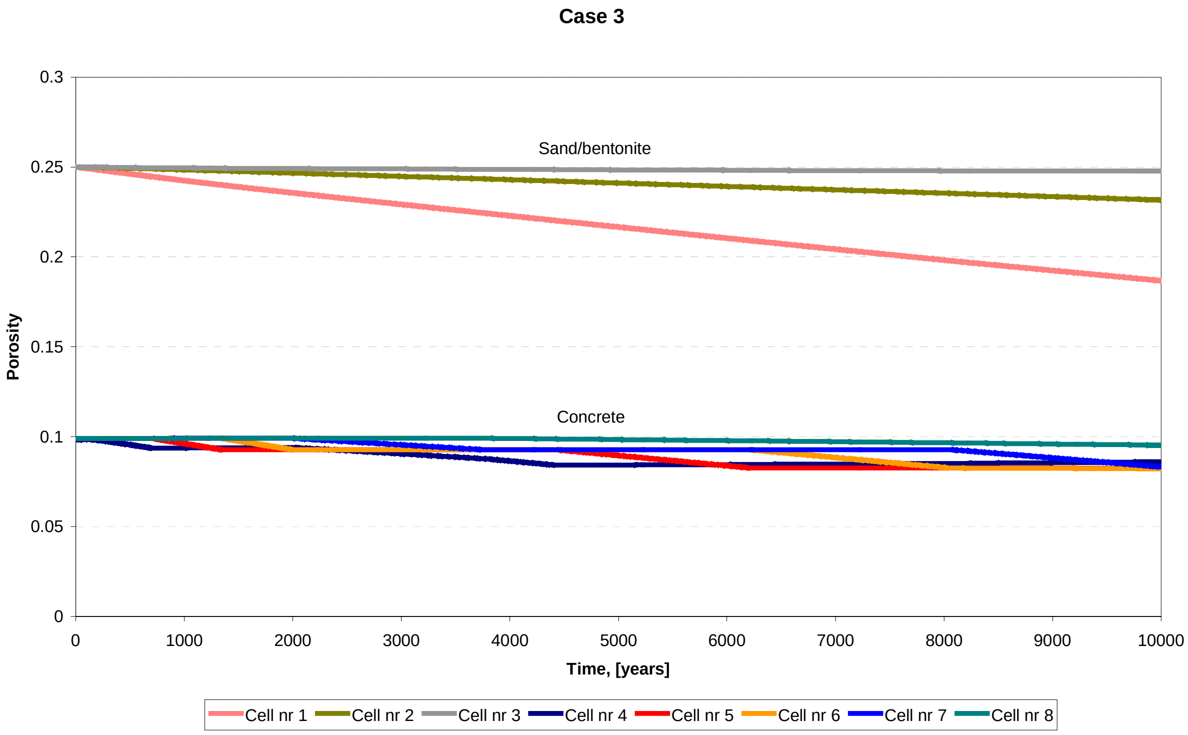

Figure 8.3l Calculated changes of porosity in Case 3 during the first 10 000 years in the different cells assumed in the model. The initial porosity in the construction concrete is 0.099 and in the sand/bentonite 0.25.

The calculations of porosity changes in different cells presented in Figure 8.3l show that very minor changes can be expected both in the sand/bentonite barrier and in the concrete. In Case 3, a decreasing porosity is expected in all cells. The largest porosity change is expected in the sand/bentonite barrier near the interface with the groundwater resulting from precipitation of calcite and brucite.

8.4 Applicability to specific conditions for the silo, BMA and BTF caverns.

Case 1 Can be used as estimates for all repository parts at least for early times when the diffusion depths do not exceed the thickness of the considered concrete structure.

Case 2 Can be used as estimates for all repository parts. The calculations have been adapted to the flow rates representative for the silo top. However, since the model in this case considers only porewater exchange cycles, the results can be scaled to another time scale representative for other parts of the repository.

Case 3 Applicable only to the silo top since a sand/bentonite layer is included in the calculations.

8.5 Comparison with analytical shrinking-core model

The results presented in the previous sections are based on fairly complex calculations and therefore difficult to assess in a simple way. As a comparison, a few calculations have been made with a simple shrinking-core model *(Levenspiel, 1972)* to put the results in perspective.

In the shrinking-core model it is assumed that a pseudo-steady-state condition is maintained for the diffusion of dissolved substances. In a slab this means that, at all times, a fully developed, linear concentration profile is maintained in the leached part of the concrete. A simple expression can be used for the calculations:

$$t = \frac{C^{0}_{bulk} \cdot x^{2}}{2 \cdot D_{e} \cdot C_{sol}}$$

where:

t = the time for the leaching front to reach a distance x (s)

x = the leaching depth (m)

C^0_{bulk} = the initial content of leached component (kmol/m^3)

D_e = the effective diffusivity (m^2/s)

C_{sol} = the solubility of the leached component in the pore water (kmol/m^3)

The calculations have been made for Portlandite with an initial content of 1.036 kmol/m^3 and a rough estimate of the solubility (since it varies with the leaching of several other components) of 0.04 kmol/m^3. The effective diffusivity is $1 \cdot 10^{-11}$ m^2/s. The results are presented in Table 8.3, the results for Case 1 are included for comparison.

Table 8.3 Calculated time to reach different leaching depths for Portlandite in concrete assuming a shrinking-core model as compared to the coupled model in Case 1.

Leaching depth (m)	Leaching time Shrinking-core model (years)	Leaching time Coupled model Case 1 (years)
0.05	103	95
0.1	411	520
0.2	1 645	1 645
0.4	6 578	5 850
1.0	41 100	>10 000

When comparing the results in Table 8.3, it must be stressed that the amount of Portlandite in Case 1 is influenced by different chemical reactions in the concrete system that cannot be considered in the analytical shrinking-core model. Considering this, the resemblance between the two models is quite satisfying. Additional tests not reported here, show a very close fit between results of the coupled model and the analytical model.

9 Summary and conclusions

Objective

The objective of this study is to quantify the impact on the properties of concrete by different chemical interactions between concrete, other barrier materials and groundwater. To achieve this, a conceptual model has been proposed which accounts for a variety of chemical processes that have been judged relevant for the conditions and time scales of interest in the SFR repository. To enable quantitative estimates of the chemical evolution in the concrete, complimentary thermodynamic data have been calculated from reported experimental investigations. The thermodynamic data has been assembled in a database which is used in the calculations.

The properties of barrier materials in the SFR repository are important from different aspects. The concrete barriers should supply e.g.:

- Mechanical strength in different constructions
- Radiation shielding for some waste types
- High pH to enhance sorption of many radionuclides
- Low hydraulic conductivity to reduce percolation
- Low diffusivity to reduce radionuclide mobility

This study focuses on estimates of the chemical conditions in the concrete and the effects of leaching on the diffusivity. The results also give information on the long-term pH evolution in the concrete.

Conceptual model

The conceptual model accounts for reactions involving the most alkaline components of the cement, i.e. the alkali hydroxides (K and Na), three end-member components of calcium silicate hydrate[5] ($C_{1.8}SH$, $C_{1.1}SH$ and $C_{0.8}SH$) and different calcium aluminate hydrates. In addition, ion exchange processes have been assumed to occur for potassium, sodium and calcium. Ion exchange may offer an explanation for the observed differences between the total content and the pore water concentrations of alkali hydroxides. The necessary ion exchange sites are presumably supplied by the calcium silicate hydrate gels or other solid phases such as the ballast. The calcium aluminate hydrates include an assembly of different reaction products with sulphate, chloride and carbonate ions. Calcium aluminate silicate hydrates have not been considered in the present study. For the interaction with the groundwater the formation of brucite, hydrotalcite and calcite are also important features included in the conceptual model.

Considered cases

Calculations have been made for a 1 m thick concrete wall considering three limiting cases based on the conceptual model:

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[5] An abbreviated notation common in cement literature is used for many of the calcium minerals, see explanation for abbreviations in Table 3.1 and chemical formula for different minerals in Table 7.1.

- In Case 1, the concrete barrier is in direct contact with the groundwater and the masstransfer is governed by diffusion in the concrete ($D_e=1\cdot10^{-11}$ m^2/s), whereas the groundwater composition has been assumed constant. Case 1 may be representative for an unfractured concrete structure in contact with groundwater with high turnover rate. Case 1 may be used for estimates for concrete barriers both in the silo (neglecting the influence by the sand/bentonite barrier) and in the BMA/BTF vaults (relevant for early times until the leaching depth exceeds the thickness of the compartment walls).

- Case 2 considers a situation where the groundwater flow percolates an initially fractured concrete structure at a constant rate. The groundwater flow rate has been assumed to resemble the calculated flow through the silo repository (3.8 m^3/year, equal to a pore water turnover time of 15.5 years) for steady-state conditions during the saltwater period. Case 2 may be representative for a concrete structure with a high degree of initial fracturing. Case 2 may be used for estimates for concrete barriers both in the silo (neglecting the influence by the sand/bentonite barrier) and in the BMA/BTF vaults (relevant for early times until the leaching depth exceeds the thickness of the compartment walls).

- Case 3 resembles the situation in Case 1, but a 1.5 m sand/bentonite barrier has been considered which restricts the direct interaction between concrete and groundwater. The masstransfer has been assumed to be governed by diffusion in the sand/bentonite ($D_e=1\cdot10^{-10}$ m^2/s) and in the concrete ($D_e=1\cdot10^{-11}$ m^2/s). Case 3 may be representative for the situation in the silo top where the influence of the sand/bentonite barrier is considered.

Brief summary of results

In Case 1, the leaching is slow, governed by diffusion. The calculations show that even after 10 000 years the calcium silicates of the concrete remain essentially intact at depths larger than about 0.4 m. Formation of Friedelsalt and an accompanying reduction of the amount of Portlandite are observed throughout the concrete due to chloride intrusion from the groundwater. Close to the surface, however, significant chemical changes have occurred in the concrete. For Case 1, the porosity is initially about 10%, reaching a minimum value of 7.4 % and subsequently a maximum value of about 19% within the first 0.1 m from the exposed surface. At larger depth, the porosity ranges from 7.6 % to 13 %.

In Case 2, the leaching is faster than in Case 1 (except for the initial leaching close to the surface), governed by percolation of groundwater. The calculations show that after 10 000 years the calcium silicates of the concrete are almost depleted to a depth of about 0.3-0.4 m and significant mineral transformations are indicated by the calculations to occur throughout the considered 1 m slab. Formation of Friedelsalt and an accompanying reduction of the amount of Portlandite are observed throughout the whole thickness in less than 500 years due to chloride intrusion from the groundwater. After 10 000 years, significant chemical changes have occurred in the concrete, as an example the pH is in the range of 9.7 – 10.4 in different parts of the concrete. For Case 2, the porosity is initially about 10%, reaching a minimum value of 8% in most cells, but as low as 6% in the cell situated 0.8-1.0 m from the inflow surface for groundwater, and subsequently a maximum value of about 17%.

In Case 3, the leaching is very slow, governed by diffusion in both the sand/bentonite barrier and in the concrete. The calculations show that even after 10 000 years the calcium silicates of the concrete remain intact at all depths. Formation of Friedelsalt and an accompanying reduction of the amount of Portlandite are observed throughout the concrete due to chloride intrusion from the groundwater, in the inner parts this occurs after about 3800 years. Even close to the concrete surface, i.e. near the interface between concrete and sand/bentonite, only minor chemical changes has occurred in the concrete. For Case 3, the concrete porosity is initially about 10%, slowly decreasing with time to a minimum value of 8%, and in the sand/bentonite, decreasing from an initial porosity of 25% to a minimum value of about 19%.

Discussion of critical processes

Ion exchange processes have been shown rapid. The ion exchange will nevertheless retard the estimated leaching of alkali hydroxides during the initial period compared to when the alkali hydroxides are assumed to be dissolved in the pore water. The counter effects of ions, e.g. sodium, in the groundwater also contribute to decrease the rate of leaching of alkali hydroxides. An effect of the assumed ion exchange is that the initial estimates of pH in the concrete pore water are slightly lower than for a case when alkali hydroxides are assumed fully soluble. However, the drop in pH as a result of leaching is slower when ion exchange is considered. The slow drop of the pore water pH also slows the leaching of Portlandite and calcium silicates.

In the different calculations, the gradual transformation of the initially present monocarbo calcium aluminate to Friedelsalt has been observed. This reaction occurs as a result of intrusion of chloride from the groundwater. The reaction also consumes some Portlandite. Hence, the chloride intrusion is predicted to result in both a phase transformation and in a partial depletion of Portlandite. Subsequently, sulphate will enter the concrete and react with Friedelsalt to form ettringite. A special feature is that ettringite has been proposed to form by a direct reaction with the solid phase of calcium aluminates, i.e. an alternative way to the more common dissolution-precipitation reactions. A possible consequence of this is the development of high swelling pressures. In laboratory experiments, a swelling pressure of 350 MPa has been reported (Mather, 1969). Different aspects on this phenomenon are discussed in Höglund (1992).

Leaching gradually depletes portlandite and when consumed, the transformation of calcium silicate hydrate gels from more alkaline to less alkaline phases will start by means of incongruent leaching of calcium. As a consequence of this, the pH will gradually drop. These processes are important since the calcium silicate hydrates are the primary binding phases in the cement. This general behaviour of the leaching has also been described in a recent study by Holgersson (2000).

Near the concrete surface precipitation of brucite and calcite will occur. The amounts of these components gradually increase with time, governed by the rate of supply from the groundwater. Following the complete transformation of $C_{1.8}SH$ to $C_{1.1}SH$, a gradual reaction between ettringite and brucite to form hydrotalcite will take place.

The ion exchange properties of the sand/bentonite barrier have been investigated and the results show that this factor has only limited impact on the leaching behaviour of the concrete. However, the effect of the reduced interaction with the groundwater by the presence of a sand/bentonite barrier is significant. In their review for SKI, Savage et al. (2000) concludes that the cation exchange reactions with suitable minerals in the engineered barriers, in particular the bentonite, will be relatively fast. A certain precipitation of ettringite is observed in the sand/bentonite barrier near the interface with the concrete, and precipitation of brucite, calcite and talc occur near the interface with the groundwater.

Implications for the chemical conditions

The calculations show that alkaline conditions will be maintained in the concrete during the entire period of 10 000 years. This will contribute to a sustained sorption capacity in the concrete barriers for the radionuclides. The initially high pH may act to restrict the sorption of caesium and strontium in the concrete since they may be retarded mainly by ion exchange processes. Following the initial leaching and ion exchange of potassium for sodium, the sorption capacity for caesium and strontium may therefore increase provided that they are not leached together with the potassium.

The calculations show that even for the most degraded parts of the concrete in Case 2, the pH does not drop below 9.7 during the 10 000 years considered. In Case 1, the pH drops below 11 after 840 to 6100 years in the 0.2 m closest to the surface of the concrete, and slowly decreases to a value of 12.4 at 10 000 years in the inner parts of the concrete wall.

The alkaline leachate water will react with the groundwater by which brucite and calcite will precipitate. In the long-term, this may result in blocking of concrete surfaces which would then become impermeable. This could have a positive effect on the release of radionuclides. However, owing to the difficulties to estimate such effect it is advised not to consider this in the present performance assessment.

It can be concluded that the chemical conditions in the concrete will remain alkaline over extended periods of time. The chemical changes can be expected to be gradual and slow. The ion exchange between potassium and sodium is the most rapid chemical process according to the calculations. Also the intrusion of chloride from the groundwater and the subsequent reaction with different calcium aluminates in the cement has been found to occur rapidly.

Implications for the barrier properties

The calculated initial porosity of the fully hydrated concrete is 9.9% (equivalent to a total porosity of the hydrated cement phase of 35.9%). In the performance assessment calculations a porosity of 15% has been suggested for the construction concrete. The calculated porosity, considering the various chemical transformations, is well below this value, the only exceptions are the most degraded cells in the diffusion case (Case 1) and the percolation case (Case 2) where the maximum porosity reaches a peak values of 18.9 % and 17.3 % respectively. Over the considered 10 000 year period, the calculated porosities in the different cases range from 6% to 17.3% (Case 2), 7.4 % (6.2 % at the surface) to 18.9 % (Case 1) and with smaller changes in Case 3. The porosity of the sand/bentonite barrier in Case 3 has been estimated to decrease from 25% to about 19% near the interface with the groundwater.

The change of porosity directly influences the effective diffusivity of soluble species in the concrete, which in turn has an impact on the radionuclide release rates. The effective diffusivity is a linear function of the porosity if the pore structure would otherwise remain the same. A general relationship between the effective diffusivity and the porosity is:

$$D_e = D_0 \cdot \varepsilon \cdot \delta/\tau^2$$

where:

D_e = effective diffusivity	[m^2/s]
D_0 = diffusivity in free water (assumed to $2 \cdot 10^{-9}$)	[m^2/s]

ε	= porosity	$[m^3/m^3]$
δ	= constrictivity factor	[-]
τ^2	= tortuosity factor	[-]

The constrictivity is a measure of the number of bottlenecks along the diffusion path. The tortuosity is a measure of the diffusion length in the winding pores of a porous slab compared to the geometrical length of the slab. The components of the quotient δ/τ^2 are difficult to distinguish in experiments and are usually lumped together.

First, we consider only the changes of the porosity. In the performance assessment, the effective diffusivity of concrete with a porosity of 15% has been estimated to $1 \cdot 10^{-11}$ m^2/s. For the calculated changes of porosity the range of effective diffusivities would be between $7 \cdot 10^{-12}$ and $1.6 \cdot 10^{-11}$ m^2/s.

If instead a relative change of the diffusivity is calculated assuming that the value $1 \cdot 10^{-11}$ m^2/s is representative for the best estimated porosity of 9.9%, we would for the present estimates of porosity changes find that the effective diffusivity may vary between $6 \cdot 10^{-12}$ and $1.9 \cdot 10^{-11}$ m^2/s.

Second, we consider the possible impact of leaching on the pore structure, i.e. on the quotient δ/τ^2. For the proposed values of the porosity and effective diffusivity (15% and $1 \cdot 10^{-11}$ m^2/s) we can calculate the initial value of the quotient δ/τ^2 to $3.3 \cdot 10^{-2}$. The leaching of different components in the cement is likely to effect the pore structure differently. It may be expected that significant leaching of the calcium silicate hydrate gels would change the pore structure to a high degree, at least in late stages. If we would like to make an extreme estimate for the most degraded parts of the concrete (the first cells in Case 1 and Case 2) the quotient δ/τ^2 may be assumed to approach a maximum value of 0.5 (expected in a bed of sand which may resemble the remaining ballast material after complete leaching), i.e. an increase by a factor of 15. This would result in an effective diffusivity (locally) within the range of $1.1 \cdot 10^{-10}$ and $2.3 \cdot 10^{-10}$ m^2/s. It should be noted that such drastic degradation is only observed in the calculations for the most degraded part of the concrete in the most pessimistic cases: In Case 1, 0.1 m (after about 3500-6000 years) to 0.2 m (after about 9000- 10 000 years) closest to the exposed surface, and in Case 2, 0.2 m (after about 2000 – 3500 years) to 0.4 m (after about 5500 – 10 000 years) closest to the inflow side for percolating groundwater, assuming an initially fractured concrete with high hydraulic conductivity.

To conclude, the calculations show that fairly small changes of the porosity can be expected. Only for pessimistic assumptions the porosity will locally (i.e. within the the first 0.1 – 0.2 m from the exposed surface) exceed the value 15% proposed for the performance assessment calculations. The recommendation is therefore to use this value for the radionuclide release calculations. The effect by leaching on the pore structure is more difficult to assess, but for unfavourable assumptions the diffusivity may increase by a factor of 30 (i.e. about a factor of 2 with respect to maximum porosity increase and a factor of 15 with respect to maximum changes in the pore structure) in the most exposed parts of the concrete. It would therefore seem appropriate to include a variation case with increased effective diffusivity in the most degraded parts of the concrete, however, this does not imply that the entire thickness of the concrete would be fully degraded within the 10 000 years considered.

Uncertainties

The conceptual understanding of the rather complex chemical system of concrete in contact with groundwater is not complete. The present model estimates are based on a proposed conceptual model that accounts for a number of chemical processes that have been judged relevant for the expected conditions. This is, of course, not a complete representation of the real system and the potential effects of unresolved conceptual uncertainties are difficult to estimate.

The assembled thermodynamic data originate from different experimental studies and may therefore be subjected to systematic differences due to the used experimental strategies, methods for chemical analyses and the way they have been interpreted. A systematic approach has been used in the present study to interpret thermodynamic stability constants which may be a way to facilitate comparison of data from different investigations. However, it is recognised that the results from the different experimental investigations give a certain spread in the estimated stability constants. Hence, when applying stability constants calculated from one set of experiments to another set of experimental data, supersaturation is in some cases indicated for minerals not reported to be present in the experiments. As an example of this type of complication, the solubility data for so called Kuzel´s salt (Glasser et al., 1999) display supersaturation with respect to several other solid phases, e.g. Monosulphate, C_3AH_6 and ettringite. Glasser et al. (1999) discusses the inherent difficulties in the experimental investigations of these complex systems and points out that Monosulphate, although not thermodynamically stable with respect to ettringite at 20^0C, may persist as a metastable phase due to slow kinetics. Reviewing by and discussion with relevant expertise to improve the quality of the used thermodynamic database is, therefore, welcome.

Due to lack of thermodynamic data, calcium ferri hydrates have been neglected in the calculations. The calcium ferri hydrates are expected to show some similarities with the calcium aluminate hydrates, and would possibly react with chloride, sulphate and carbonate in a similar way. The consequence of this would be an increased amount of reactive minerals in the concrete, possibly leading to larger porosity changes in the long-term. However, lacking relevant data make any attempts to quantitative estimates questionable.

The geometrical model representations of the studied cases are idealised and may differ to some extent from the real system. However, it is expected that the range of results represented by the different limiting cases would encompass the most likely outcome.

In the present study, only groundwater representing the salt water period (i.e. approximately the first 1000 years) has been considered. This water has been judged more aggressive to the concrete than the fresh water owing to the high chloride content. The calculations are therefore not fully representative for the fresh water period.

A direct comparison of the results from the present model calculations with experimental studies is not straightforward. However, an experimental study conducted at Chalmers University of Technology, as reported in Wiborgh (ed.) (1995), show similar results. The experiments were conducted with crushed samples of pure cement paste (Degerhamn Anläggningscement) that were leached in so called NASK water (a synthetic saline groundwater defined in a collaborative research project between Nagra and SKB). The chemical conditions in the leachate were followed and the results show that a fairly constant pH of 12.5 was maintained during about 40 steps of leaching, comparable to about 800-900 pore water exchange cycles, whereafter the pH drops rapidly. In the model calculations, the same behaviour is observed. A comparison with Case 2, see e.g. Figure 8.2h, reveals that the pH drops below 12.5 after about 8000 years, corresponding to about 500 pore water exchange cycles. In the model calculations a saline water representative for the SFR area have been assumed. Hence, the model results compare reasonably well with the experimental results considering the differences in conditions. Berner (1990) reports calculations showing a similar leaching behaviour with a drop of pH below 12.5 after approximately 1000 pore water exchange cycles, however, using other types of cement and other groundwaters than in the present study.

The results for Case 1 are similar to the results presented in section 8.5 for the analytical shrinking-core model. In Case 1, the Portlandite is depleted to a depth of 0.05 m after 95 years compared to 103 year in the shrinking-core model. The corresponding times to a depth of 0.1 m are 520 years (Case 1) and 411 years (shrinking core), 0.2 m 1645 years (Case 1) and 1645 years (shrinking-core), 0.4 m 5850 years (Case 1) and 6580 years (shrinking-core). Both models predict >10 000 years for depletion to the full depth of 1.0 m considered in the calculations.

The possible chemical effects of the alkaline concrete pore water on the stability of montmorillonite in the sand/bentonite barrier have been neglected in the present calculations. It has been suggested that alkaline hydrolysis may occur of the montmorillonite at a low rate governed by reaction kinetics, see e.g. Bauer and Berger (1998). The reaction between christobalite and alkaline components has not been considered in the present study. Christobalite would be expected to react with alkaline concrete pore water to precipitate additional *CSH*-gel, although this has not been demonstrated in the present study.

10 References

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Appendix A

Details of thermodynamic calculations

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Reading data base.
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SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
SOLUTION_SPECIES
PHASES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
END
------------------------------------
Reading input data for simulation 1.
------------------------------------

TITLE Calculation of thermodynamical stability constants for the cement system
PRINT
species False # When False, the details of the aqueous speciation are not shown
SOLUTION 1  Silikagel
        units   mmol/kgw
        pH      6.38
        density 1.0
        temp    25.0
        Ca              0.
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              1.41
        Cl              0.
        S(6)            0.
SOLUTION 2  Silikagel + CSH_0.8
        units   mmol/kgw
        pH      10.17
        density 1.0
        temp    25.0
        Ca              1.52
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              4.18
        Cl              0.
        S(6)            0.
SOLUTION 3  CSH_0.8
        units   mmol/kgw
        pH      10.88
        density 1.0
        temp    25.0
        Ca              1.23
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              1.55
        Cl              0.
        S(6)            0.
SOLUTION 4  CSH_0.8 + CSH_1.1
        units   mmol/kgw
        pH      10.91
        density 1.0
        temp    25.0
        Ca              1.25
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              1.47
        Cl              0.
        S(6)            0.
```

```
SOLUTION 5  CSH_1.1
        units   mmol/kgw
        pH      11.03
        density 1.0
        temp    25.0
        Ca              1.23
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              1.12
        Cl              0.
        S(6)            0.
SOLUTION 6  CSH_1.1 + CSH_1.8
        units   mmol/kgw
        pH      12.43
        density 1.0
        temp    25.0
        Ca             19.3
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              2.45e-2
        Cl              0.
        S(6)            0.
SOLUTION 7  CSH_1.8 + CH
        units   mmol/kgw
        pH      12.53
        density 1.0
        temp    25.0
        Ca             22.0
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              1.90e-2
        Cl              0.
        S(6)            0.
SOLUTION 8  CH
        units   mmol/kgw
        pH      12.52
        density 1.0
        temp    25.0
        Ca             21.9
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              0.
        Cl              0.
        S(6)            0.
END
```

```
-----
TITLE
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 Calculation of thermodynamical stability constants for the cement system

-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.Silikagel

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

Elements           Molality       Moles

Si                1.410e-03   1.410e-03

----------------------------Description of solution----------------------------

                                       pH  =   6.380
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   4.199e-07
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   5.429e-09
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -5.429e-09
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.65
                               Iterations  =   2
                                  Total H  = 1.110181e+02
                                  Total O  = 5.551186e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

Chalcedony        0.67   -2.85   -3.52  SiO2
Cristobalite      0.74   -2.85   -3.59  SiO2
O2(g)           -41.60   41.52   83.12  O2
Quartz            1.16   -2.85   -4.01  SiO2
SiO2(a)           0.17   -2.85   -3.02  SiO2
SiO2(am)         -0.14   -2.85   -2.71  SiO2
SiO2gel(am)      -0.00   -2.85   -2.85  SiO2

Initial solution 2.Silikagel + CSH_0.8

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

Elements           Molality       Moles

Ca                1.520e-03   1.520e-03
Si                4.180e-03   4.180e-03

----------------------------Description of solution----------------------------

                                       pH  =  10.170
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   4.643e-03
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   3.026e-03
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =   1.423e-05
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.23
                               Iterations  =   4
                                  Total H  = 1.110265e+02
                                  Total O  = 5.552310e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

Ca-Olivine       -5.70   31.95   37.65  Ca2SiO4
Ca3SiO5         -24.52   49.35   73.87  Ca3SiO5
CH               -5.50   17.40   22.90  Ca(OH)2
Chalcedony        0.68   -2.85   -3.52  SiO2
Cristobalite      0.74   -2.85   -3.59  SiO2
CSH_0.8          -0.01   11.07   11.08  Ca0.8SiO2.8:H2O
CSH_1.1          -0.43   16.29   16.72  Ca1.1SiO3.1:H2O
CSH_1.8          -4.23   28.47   32.70  Ca1.8SiO3.8:H2O
Larnite          -7.19   31.95   39.14  Ca2SiO4
```

```
Lime             -15.40   17.40   32.80  CaO
O2(g)            -26.44   56.68   83.12  O2
P-Wollstanite      0.71   14.55   13.85  CaSiO3
Portlandite       -5.28   17.40   22.68  Ca(OH)2
Quartz             1.16   -2.85   -4.01  SiO2
SiO2(a)            0.17   -2.85   -3.02  SiO2
SiO2(am)          -0.14   -2.85   -2.71  SiO2
SiO2gel(am)        0.00   -2.85   -2.85  SiO2
Tob                3.93   69.91   65.98  Ca5Si6O17:5H2O
Wollastonite       1.56   14.55   13.00  CaSiO3

Initial solution 3.CSH_0.8

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

Elements           Molality       Moles

Ca                1.230e-03   1.230e-03
Si                1.550e-03   1.550e-03

----------------------------Description of solution----------------------------

                                       pH  =  10.880
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   3.892e-03
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   2.486e-03
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -2.630e-05
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.54
                               Iterations  =   4
                                  Total H  = 1.110178e+02
                                  Total O  = 5.551325e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

Ca-Olivine        -4.09   33.56   37.65  Ca2SiO4
Ca3SiO5          -21.58   52.29   73.87  Ca3SiO5
CH                -4.17   18.73   22.90  Ca(OH)2
Chalcedony        -0.38   -3.90   -3.52  SiO2
Cristobalite      -0.31   -3.90   -3.59  SiO2
CSH_0.8            0.00   11.08   11.08  Ca0.8SiO2.8:H2O
CSH_1.1           -0.02   16.70   16.72  Ca1.1SiO3.1:H2O
CSH_1.8           -2.89   29.81   32.70  Ca1.8SiO3.8:H2O
Larnite           -5.58   33.56   39.14  Ca2SiO4
Lime             -14.07   18.73   32.80  CaO
O2(g)            -23.60   59.52   83.12  O2
P-Wollstanite      0.98   14.83   13.85  CaSiO3
Portlandite       -3.94   18.73   22.68  Ca(OH)2
Quartz             0.10   -3.90   -4.01  SiO2
SiO2(a)           -0.88   -3.90   -3.02  SiO2
SiO2(am)          -1.19   -3.90   -2.71  SiO2
SiO2gel(am)       -1.05   -3.90   -2.85  SiO2
Tob                4.26   70.24   65.98  Ca5Si6O17:5H2O
Wollastonite       1.83   14.83   13.00  CaSiO3

Initial solution 4.CSH_0.8 + CSH_1.1

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

Elements           Molality       Moles

Ca                1.250e-03   1.250e-03
Si                1.470e-03   1.470e-03

----------------------------Description of solution----------------------------

                                       pH  =  10.910
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   3.930e-03
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   2.484e-03
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =   1.573e-05
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.32
                               Iterations  =   4
                                  Total H  = 1.110176e+02
                                  Total O  = 5.551299e+01
```

```
------------------------------Saturation indices------------------------------

Phase               SI log IAP  log KT

Ca-Olivine       -4.01   33.64   37.65  Ca2SiO4
Ca3SiO5         -21.43   52.43   73.87  Ca3SiO5
CH               -4.10   18.80   22.90  Ca(OH)2
Chalcedony       -0.43   -3.96   -3.52  SiO2
Cristobalite     -0.37   -3.96   -3.59  SiO2
CSH_0.8           0.00   11.08   11.08  Ca0.8SiO2.8:H2O
CSH_1.1          -0.00   16.72   16.72  Ca1.1SiO3.1:H2O
CSH_1.8          -2.82   29.88   32.70  Ca1.8SiO3.8:H2O
Larnite          -5.51   33.64   39.14  Ca2SiO4
Lime            -14.00   18.80   32.80  CaO
O2(g)           -23.48   59.64   83.12  O2
P-Wollstanite     0.99   14.84   13.85  CaSiO3
Portlandite      -3.88   18.80   22.68  Ca(OH)2
Quartz            0.05   -3.96   -4.01  SiO2
SiO2(a)          -0.94   -3.96   -3.02  SiO2
SiO2(am)         -1.25   -3.96   -2.71  SiO2
SiO2gel(am)      -1.11   -3.96   -2.85  SiO2
Tob               4.26   70.24   65.98  Ca5Si6O17:5H2O
Wollastonite      1.84   14.84   13.00  CaSiO3

Initial solution 5.CSH_1.1

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

Elements           Molality       Moles

Ca                1.230e-03   1.230e-03
Si                1.120e-03   1.120e-03

----------------------------Description of solution----------------------------

                                       pH  =  11.030
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   3.859e-03
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   2.460e-03
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -8.366e-08
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   4
                                  Total H  = 1.110168e+02
                                  Total O  = 5.551188e+01

------------------------------Saturation indices------------------------------

Phase               SI log IAP  log KT

Ca-Olivine       -3.80   33.85   37.65  Ca2SiO4
Ca3SiO5         -20.99   52.88   73.87  Ca3SiO5
CH               -3.87   19.03   22.90  Ca(OH)2
Chalcedony       -0.69   -4.21   -3.52  SiO2
Cristobalite     -0.62   -4.21   -3.59  SiO2
CSH_0.8          -0.07   11.01   11.08  Ca0.8SiO2.8:H2O
CSH_1.1           0.00   16.72   16.72  Ca1.1SiO3.1:H2O
CSH_1.8          -2.66   30.04   32.70  Ca1.8SiO3.8:H2O
Larnite          -5.29   33.85   39.14  Ca2SiO4
Lime            -13.77   19.03   32.80  CaO
O2(g)           -23.00   60.12   83.12  O2
P-Wollstanite     0.97   14.82   13.85  CaSiO3
Portlandite      -3.65   19.03   22.68  Ca(OH)2
Quartz           -0.20   -4.21   -4.01  SiO2
SiO2(a)          -1.19   -4.21   -3.02  SiO2
SiO2(am)         -1.50   -4.21   -2.71  SiO2
SiO2gel(am)      -1.36   -4.21   -2.85  SiO2
Tob               3.91   69.89   65.98  Ca5Si6O17:5H2O
Wollastonite      1.82   14.82   13.00  CaSiO3

Initial solution 6.CSH_1.1 + CSH_1.8

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

Elements           Molality       Moles

Ca                1.930e-02   1.930e-02
Si                2.450e-05   2.450e-05
```

```
----------------------------Description of solution----------------------------

                                       pH  =  12.430
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   4.685e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   3.872e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -1.154e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.17
                               Iterations  =   4
                                  Total H  = 1.110512e+02
                                  Total O  = 5.554498e+01

------------------------------Saturation indices------------------------------

Phase               SI  log IAP  log KT

Ca-Olivine       -0.47   37.18   37.65  Ca2SiO4
Ca3SiO5         -13.99   59.87   73.87  Ca3SiO5
CH               -0.20   22.70   22.90  Ca(OH)2
Chalcedony       -4.69   -8.22   -3.52  SiO2
Cristobalite     -4.63   -8.22   -3.59  SiO2
CSH_0.8          -1.14    9.94   11.08  Ca0.8SiO2.8:H2O
CSH_1.1           0.03   16.75   16.72  Ca1.1SiO3.1:H2O
CSH_1.8          -0.06   32.64   32.70  Ca1.8SiO3.8:H2O
Larnite          -1.96   37.18   39.14  Ca2SiO4
Lime            -10.10   22.70   32.80  CaO
O2(g)           -17.40   65.72   83.12  O2
P-Wollstanite     0.63   14.48   13.85  CaSiO3
Portlandite       0.02   22.70   22.68  Ca(OH)2
Quartz           -4.21   -8.22   -4.01  SiO2
SiO2(a)          -5.20   -8.22   -3.02  SiO2
SiO2(am)         -5.51   -8.22   -2.71  SiO2
SiO2gel(am)      -5.37   -8.22   -2.85  SiO2
Tob              -1.79   64.19   65.98  Ca5Si6O17:5H2O
Wollastonite      1.48   14.48   13.00  CaSiO3

Initial solution 7.CSH_1.8 + CH

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

Elements           Molality       Moles

Ca                2.200e-02   2.200e-02
Si                1.900e-05   1.900e-05

----------------------------Description of solution----------------------------

                                       pH  =  12.530
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   5.416e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   4.952e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -5.518e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -6.99
                               Iterations  =   4
                                  Total H  = 1.110620e+02
                                  Total O  = 5.555577e+01
```

```
------------------------------Saturation indices-------------------------------

Phase               SI  log IAP  log KT

Ca-Olivine       -0.36   37.29   37.65  Ca2SiO4
Ca3SiO5         -13.67   60.20   73.87  Ca3SiO5
CH                0.01   22.91   22.90  Ca(OH)2
Chalcedony       -5.01   -8.53   -3.52  SiO2
Cristobalite     -4.95   -8.53   -3.59  SiO2
CSH_0.8          -1.28    9.80   11.08  Ca0.8SiO2.8:H2O
CSH_1.1          -0.05   16.67   16.72  Ca1.1SiO3.1:H2O
CSH_1.8           0.01   32.71   32.70  Ca1.8SiO3.8:H2O
Larnite          -1.85   37.29   39.14  Ca2SiO4
Lime             -9.89   22.91   32.80  CaO
O2(g)           -17.00   66.12   83.12  O2
P-Wollstanite     0.53   14.38   13.85  CaSiO3
Portlandite       0.24   22.91   22.68  Ca(OH)2
Quartz           -4.53   -8.53   -4.01  SiO2
SiO2(a)          -5.51   -8.53   -3.02  SiO2
SiO2(am)         -5.82   -8.53   -2.71  SiO2
SiO2gel(am)      -5.68   -8.53   -2.85  SiO2
Tob              -2.63   63.35   65.98  Ca5Si6O17:5H2O
Wollastonite      1.38   14.38   13.00  CaSiO3

Initial solution 8.CH

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

Elements           Molality       Moles

Ca                2.190e-02   2.190e-02

----------------------------Description of solution----------------------------

                                       pH  =  12.520
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   5.363e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   4.835e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -4.551e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -5.85
                               Iterations  =   4
                                  Total H  = 1.110608e+02
                                  Total O  = 5.555457e+01

------------------------------Saturation indices-------------------------------

Phase               SI  log IAP  log KT

CH               -0.01   22.89   22.90  Ca(OH)2
Lime             -9.90   22.89   32.80  CaO
O2(g)           -17.04   66.08   83.12  O2
Portlandite       0.22   22.89   22.68  Ca(OH)2

------------------
End of simulation.
------------------
```

```
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Reading input data for simulation 2.
-----------------------------------

TITLE  The System CaO-Al2O3-CaCl2-H2O
       Ref: Birnin-Yauri, Glasser, Cement and Concrete Research, 1998,
       Vol 28, No 12, 1713-1723
SOLUTION 9  Friedelsalt - mean values
        units   mmol/kgw
        pH      12.118
        density 1.0
        temp    20.0
        Ca              9.03
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              0.
        Al              4.87 as Al(OH)4-
        Cl              4.92
        S(6)            0.
SOLUTION 10  Friedelsalt - Dispersion 1
        units   mmol/kgw
        pH      12.106
        density 1.0
        temp    20.0
        Ca              9.17
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              0.
        Al              4.40 as Al(OH)4-
        Cl              6.03
        S(6)            0.
SOLUTION 11  Friedelsalt - Dispersion 2
        units   mmol/kgw
        pH      12.106
        density 1.0
        temp    20.0
        Ca              9.48
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              0.
        Al              5.04 as Al(OH)4-
        Cl              4.80
        S(6)            0.
SOLUTION 12  Friedelsalt - Dispersion 3
        units   mmol/kgw
        pH      12.145
        density 1.0
        temp    20.0
        Ca              9.11
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              0.
        Al              4.89 as Al(OH)4-
        Cl              4.89
        S(6)            0.
SOLUTION 13  Friedelsalt - Dispersion 4
        units   mmol/kgw
        pH      12.084
        density 1.0
        temp    20.0
        Ca              8.67
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              0.
        Al              4.97 as Al(OH)4-
        Cl              4.40
        S(6)            0.
```

```
SOLUTION 14  Friedelsalt - Dispersion 5
        units   mmol/kgw
        pH      12.107
        density 1.0
        temp    20.0
        Ca              8.73
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              0.
        Al              5.07 as Al(OH)4-
        Cl              4.49
        S(6)            0.
SOLUTION 15  Friedelsalt - C4AH13 x=0
        units   mmol/kgw
        pH      12.409
        density 1.0
        temp    20.0
        Ca             38.05
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              0.
        Al              1.30 as Al(OH)4-
        Cl             64.17
        S(6)            0.
SOLUTION 16  Friedelsalt - C4AH13 x=0.1
        units   mmol/kgw
        pH      12.452
        density 1.0
        temp    20.0
        Ca             26.20
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              0.
        Al              0.69 as Al(OH)4-
        Cl             14.46
        S(6)            0.
SOLUTION 17  Friedelsalt - C4AH13 x=0.2
        units   mmol/kgw
        pH      12.637
        density 1.0
        temp    20.0
        Ca             24.82
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              0.
        Al              0.70 as Al(OH)4-
        Cl             13.94
        S(6)            0.
SOLUTION 18  Friedelsalt - C4AH13 x=0.3
        units   mmol/kgw
        pH      12.655
        density 1.0
        temp    20.0
        Ca             23.45
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              0.
        Al              0.72 as Al(OH)4-
        Cl             13.40
        S(6)            0.
```

```
SOLUTION 19  Friedelsalt - C4AH13 x=0.4
        units   mmol/kgw
        pH      12.669
        density 1.0
        temp    20.0
        Ca             22.20
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              0.
        Al              0.75 as Al(OH)4-
        Cl              8.82
        S(6)            0.
SOLUTION 20  Friedelsalt - C4AH13 x=0.5
        units   mmol/kgw
        pH      12.682
        density 1.0
        temp    20.0
        Ca             20.96
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              0.
        Al              0.75 as Al(OH)4-
        Cl              4.23
        S(6)            0.
SOLUTION 21  Friedelsalt - C4AH13 x=0.6
        units   mmol/kgw
        pH      12.713
        density 1.0
        temp    20.0
        Ca             20.21
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              0.
        Al              0.70 as Al(OH)4-
        Cl              2.33
        S(6)            0.
SOLUTION 22  Friedelsalt - C4AH13 x=0.7
        units   mmol/kgw
        pH      12.733
        density 1.0
        temp    20.0
        Ca             19.96
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              0.
        Al              0.66 as Al(OH)4-
        Cl              2.07
        S(6)            0.
SOLUTION 23  Friedelsalt - C4AH13 x=0.8
        units   mmol/kgw
        pH      12.734
        density 1.0
        temp    20.0
        Ca             19.21
        Mg              0.
        Na              0.
        K               0.
        Fe              0.
        Mn              0.
        Si              0.
        Al              0.67 as Al(OH)4-
        Cl              1.90
        S(6)            0.
END
```

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TITLE
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  The System CaO-Al2O3-CaCl2-H2O
       Ref: Birnin-Yauri, Glasser, Cement and Concrete Research, 1998,
       Vol 28, No 12, 1713-1723

-------------------------------------------
Beginning of initial solution calculations.
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Initial solution 9.Friedelsalt - mean values

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

Elements           Molality       Moles

Al                4.870e-03   4.870e-03
Ca                9.030e-03   9.030e-03
Cl                4.920e-03   4.920e-03

----------------------------Description of solution----------------------------

                                       pH  =  12.118
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   2.652e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   3.114e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  20.000
                  Electrical balance (eq)  =  -3.386e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -9.09
                               Iterations  =   4
                                  Total H  = 1.110436e+02
                                  Total O  = 5.553735e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

(CaO)3CaCl2:15H2O -97.68   58.56  156.24  (CaO)3CaCl2:15H2O
Al(OH)3(a)       -1.66    9.05   10.72  Al(OH)3
Al2O3            -4.87   18.11   22.98  Al2O3
Boehmite          0.12    9.05    8.93  AlOOH
C3AH6            -1.13   83.77   84.91  Ca3Al2(OH)12
C3AH6(C)          2.55   83.77   81.22  Ca3Al2(OH)12
CaCl2:6H20       -9.56   -7.11    2.45  CaCl2:6H2O
CaOCaCl2:2H2O   -39.04   14.78   53.82  CaOCaCl2:2H2O
CH               -1.40   21.89   23.28  Ca(OH)2
Diaspore          1.87    9.05    7.18  AlOOH
Fried0.86Al5.14OH  -2.27   66.35   68.62  Ca4Al0.86Cl2(OH)8.58
Fried0.88Al5.12OH  -2.72   66.53   69.25  Ca4Al0.88Cl2(OH)8.64
Fried1.04Al4.96OH  -3.16   67.98   71.14  Ca4Al1.04Cl2(OH)9.12
Fried1.34Al4.66OH  -3.10   70.69   73.80  Ca4Al1.34Cl2(OH)10.02
Fried1.42Al4.58OH  -3.02   71.42   74.44  Ca4Al1.42Cl2(OH)10.26
Fried1.96Al4.04OH  -1.84   76.31   78.14  Ca4Al1.96Cl2(OH)11.88
Friedelsalt      -0.00   76.67   76.67  Ca4Al2Cl2(OH)12
Gibbsite(C)      -0.00    9.05    9.06  Al(OH)3
Lime            -11.49   21.89   33.38  CaO
O2(g)           -20.32   64.47   84.79  O2
Portlandite      -1.17   21.89   23.06  Ca(OH)2

Initial solution 10.Friedelsalt - Dispersion 1

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

Elements           Molality       Moles

Al                4.400e-03   4.400e-03
Ca                9.170e-03   9.170e-03
Cl                6.030e-03   6.030e-03

----------------------------Description of solution----------------------------

                                       pH  =  12.106
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   2.700e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   2.897e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  20.000
```

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                  Electrical balance (eq)  =  -3.459e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -9.13
                               Iterations  =   4
                                  Total H  = 1.110414e+02
                                  Total O  = 5.553519e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

(CaO)3CaCl2:15H2O -97.55   58.69  156.24  (CaO)3CaCl2:15H2O
Al(OH)3(a)       -1.70    9.02   10.72  Al(OH)3
Al2O3            -4.94   18.04   22.98  Al2O3
Boehmite          0.09    9.02    8.93  AlOOH
C3AH6            -1.25   83.66   84.91  Ca3Al2(OH)12
C3AH6(C)          2.44   83.66   81.22  Ca3Al2(OH)12
CaCl2:6H20       -9.37   -6.92    2.45  CaCl2:6H2O
CaOCaCl2:2H2O   -38.87   14.95   53.82  CaOCaCl2:2H2O
CH               -1.41   21.87   23.28  Ca(OH)2
Diaspore          1.84    9.02    7.18  AlOOH
Fried0.86Al5.14OH  -2.17   66.45   68.62  Ca4Al0.86Cl2(OH)8.58
Fried0.88Al5.12OH  -2.62   66.63   69.25  Ca4Al0.88Cl2(OH)8.64
Fried1.04Al4.96OH  -3.07   68.07   71.14  Ca4Al1.04Cl2(OH)9.12
Fried1.34Al4.66OH  -3.02   70.78   73.80  Ca4Al1.34Cl2(OH)10.02
Fried1.42Al4.58OH  -2.94   71.50   74.44  Ca4Al1.42Cl2(OH)10.26
Fried1.96Al4.04OH  -1.77   76.37   78.14  Ca4Al1.96Cl2(OH)11.88
Friedelsalt       0.06   76.73   76.67  Ca4Al2Cl2(OH)12
Gibbsite(C)      -0.03    9.02    9.06  Al(OH)3
Lime            -11.50   21.87   33.38  CaO
O2(g)           -20.37   64.42   84.79  O2
Portlandite      -1.19   21.87   23.06  Ca(OH)2

Initial solution 11.Friedelsalt - Dispersion 2

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

Elements           Molality       Moles

Al                5.040e-03   5.040e-03
Ca                9.480e-03   9.480e-03
Cl                4.800e-03   4.800e-03

----------------------------Description of solution----------------------------

                                       pH  =  12.106
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   2.728e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   3.157e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  20.000
                  Electrical balance (eq)  =  -2.292e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -6.05
                               Iterations  =   4
                                  Total H  = 1.110440e+02
                                  Total O  = 5.553779e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

(CaO)3CaCl2:15H2O -97.70   58.54  156.24  (CaO)3CaCl2:15H2O
Al(OH)3(a)       -1.64    9.08   10.72  Al(OH)3
Al2O3            -4.82   18.16   22.98  Al2O3
Boehmite          0.15    9.08    8.93  AlOOH
C3AH6            -1.09   83.81   84.91  Ca3Al2(OH)12
C3AH6(C)          2.59   83.81   81.22  Ca3Al2(OH)12
CaCl2:6H20       -9.56   -7.11    2.45  CaCl2:6H2O
CaOCaCl2:2H2O   -39.04   14.78   53.82  CaOCaCl2:2H2O
CH               -1.40   21.88   23.28  Ca(OH)2
Diaspore          1.90    9.08    7.18  AlOOH
Fried0.86Al5.14OH  -2.26   66.36   68.62  Ca4Al0.86Cl2(OH)8.58
Fried0.88Al5.12OH  -2.71   66.54   69.25  Ca4Al0.88Cl2(OH)8.64
Fried1.04Al4.96OH  -3.15   67.99   71.14  Ca4Al1.04Cl2(OH)9.12
Fried1.34Al4.66OH  -3.08   70.71   73.80  Ca4Al1.34Cl2(OH)10.02
Fried1.42Al4.58OH  -3.00   71.44   74.44  Ca4Al1.42Cl2(OH)10.26
Fried1.96Al4.04OH  -1.80   76.34   78.14  Ca4Al1.96Cl2(OH)11.88
Friedelsalt       0.04   76.71   76.67  Ca4Al2Cl2(OH)12
Gibbsite(C)       0.03    9.08    9.06  Al(OH)3
Lime            -11.49   21.88   33.38  CaO
O2(g)           -20.37   64.42   84.79  O2
Portlandite      -1.17   21.88   23.06  Ca(OH)2
```

```
Initial solution 12.Friedelsalt - Dispersion 3

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

Elements           Molality       Moles

Al                4.890e-03   4.890e-03
Ca                9.110e-03   9.110e-03
Cl                4.890e-03   4.890e-03

----------------------------Description of solution----------------------------

                                       pH  =  12.145
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   2.691e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   3.197e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  20.000
                  Electrical balance (eq)  =  -3.973e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -10.45
                               Iterations  =   4
                                  Total H  = 1.110444e+02
                                  Total O  = 5.553819e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

(CaO)3CaCl2:15H2O -97.53   58.71  156.24  (CaO)3CaCl2:15H2O
Al(OH)3(a)       -1.69    9.03   10.72  Al(OH)3
Al2O3            -4.92   18.06   22.98  Al2O3
Boehmite          0.10    9.03    8.93  AlOOH
C3AH6            -1.03   83.88   84.91  Ca3Al2(OH)12
C3AH6(C)          2.66   83.88   81.22  Ca3Al2(OH)12
CaCl2:6H20       -9.56   -7.11    2.45  CaCl2:6H2O
CaOCaCl2:2H2O   -38.99   14.83   53.82  CaOCaCl2:2H2O
CH               -1.34   21.94   23.28  Ca(OH)2
Diaspore          1.85    9.03    7.18  AlOOH
Fried0.86Al5.14OH  -2.14   66.48   68.62  Ca4Al0.86Cl2(OH)8.58
Fried0.88Al5.12OH  -2.59   66.66   69.25  Ca4Al0.88Cl2(OH)8.64
Fried1.04Al4.96OH  -3.04   68.10   71.14  Ca4Al1.04Cl2(OH)9.12
Fried1.34Al4.66OH  -2.98   70.81   73.80  Ca4Al1.34Cl2(OH)10.02
Fried1.42Al4.58OH  -2.91   71.53   74.44  Ca4Al1.42Cl2(OH)10.26
Fried1.96Al4.04OH  -1.73   76.41   78.14  Ca4Al1.96Cl2(OH)11.88
Friedelsalt       0.10   76.77   76.67  Ca4Al2Cl2(OH)12
Gibbsite(C)      -0.03    9.03    9.06  Al(OH)3
Lime            -11.43   21.94   33.38  CaO
O2(g)           -20.21   64.58   84.79  O2
Portlandite      -1.12   21.94   23.06  Ca(OH)2

Initial solution 13.Friedelsalt - Dispersion 4

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

Elements           Molality       Moles

Al                4.970e-03   4.970e-03
Ca                8.670e-03   8.670e-03
Cl                4.400e-03   4.400e-03

----------------------------Description of solution----------------------------

                                       pH  =  12.084
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   2.535e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   3.060e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  20.000
                  Electrical balance (eq)  =  -2.753e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -7.78
                               Iterations  =   4
                                  Total H  = 1.110430e+02
                                  Total O  = 5.553682e+01
```

```
------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

(CaO)3CaCl2:15H2O -98.02   58.22  156.24  (CaO)3CaCl2:15H2O
Al(OH)3(a)       -1.62    9.10   10.72  Al(OH)3
Al2O3            -4.78   18.20   22.98  Al2O3
Boehmite          0.17    9.10    8.93  AlOOH
C3AH6            -1.28   83.63   84.91  Ca3Al2(OH)12
C3AH6(C)          2.41   83.63   81.22  Ca3Al2(OH)12
CaCl2:6H20       -9.66   -7.21    2.45  CaCl2:6H2O
CaOCaCl2:2H2O   -39.22   14.60   53.82  CaOCaCl2:2H2O
CH               -1.47   21.81   23.28  Ca(OH)2
Diaspore          1.92    9.10    7.18  AlOOH
Fried0.86Al5.14OH  -2.57   66.05   68.62  Ca4Al0.86Cl2(OH)8.58
Fried0.88Al5.12OH  -3.02   66.23   69.25  Ca4Al0.88Cl2(OH)8.64
Fried1.04Al4.96OH  -3.45   67.69   71.14  Ca4Al1.04Cl2(OH)9.12
Fried1.34Al4.66OH  -3.38   70.41   73.80  Ca4Al1.34Cl2(OH)10.02
Fried1.42Al4.58OH  -3.30   71.14   74.44  Ca4Al1.42Cl2(OH)10.26
Fried1.96Al4.04OH  -2.09   76.06   78.14  Ca4Al1.96Cl2(OH)11.88
Friedelsalt      -0.25   76.42   76.67  Ca4Al2Cl2(OH)12
Gibbsite(C)       0.04    9.10    9.06  Al(OH)3
Lime            -11.56   21.81   33.38  CaO
O2(g)           -20.46   64.34   84.79  O2
Portlandite      -1.25   21.81   23.06  Ca(OH)2

Initial solution 14.Friedelsalt - Dispersion 5

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

Elements           Molality       Moles

Al                5.070e-03   5.070e-03
Ca                8.730e-03   8.730e-03
Cl                4.490e-03   4.490e-03

----------------------------Description of solution----------------------------

                                       pH  =  12.107
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   2.575e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   3.160e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  20.000
                  Electrical balance (eq)  =  -3.415e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -9.44
                               Iterations  =   4
                                  Total H  = 1.110440e+02
                                  Total O  = 5.553781e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

(CaO)3CaCl2:15H2O -97.87   58.37  156.24  (CaO)3CaCl2:15H2O
Al(OH)3(a)       -1.63    9.08   10.72  Al(OH)3
Al2O3            -4.81   18.17   22.98  Al2O3
Boehmite          0.15    9.08    8.93  AlOOH
C3AH6            -1.17   83.73   84.91  Ca3Al2(OH)12
C3AH6(C)          2.51   83.73   81.22  Ca3Al2(OH)12
CaCl2:6H20       -9.64   -7.19    2.45  CaCl2:6H2O
CaOCaCl2:2H2O   -39.16   14.66   53.82  CaOCaCl2:2H2O
CH               -1.43   21.86   23.28  Ca(OH)2
Diaspore          1.90    9.08    7.18  AlOOH
Fried0.86Al5.14OH  -2.43   66.19   68.62  Ca4Al0.86Cl2(OH)8.58
Fried0.88Al5.12OH  -2.88   66.37   69.25  Ca4Al0.88Cl2(OH)8.64
Fried1.04Al4.96OH  -3.32   67.82   71.14  Ca4Al1.04Cl2(OH)9.12
Fried1.34Al4.66OH  -3.25   70.55   73.80  Ca4Al1.34Cl2(OH)10.02
Fried1.42Al4.58OH  -3.17   71.27   74.44  Ca4Al1.42Cl2(OH)10.26
Fried1.96Al4.04OH  -1.97   76.18   78.14  Ca4Al1.96Cl2(OH)11.88
Friedelsalt      -0.13   76.54   76.67  Ca4Al2Cl2(OH)12
Gibbsite(C)       0.03    9.08    9.06  Al(OH)3
Lime            -11.52   21.86   33.38  CaO
O2(g)           -20.37   64.43   84.79  O2
Portlandite      -1.20   21.86   23.06  Ca(OH)2
```

```
Initial solution 15.Friedelsalt - C4AH13 x=0

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

Elements           Molality       Moles

Al                1.300e-03   1.300e-03
Ca                3.805e-02   3.805e-02
Cl                6.417e-02   6.417e-02


----------------------------Description of solution----------------------------

                                       pH  =  12.409
                                       pe  =   4.000
                        Activity of water  =   0.998
                           Ionic strength  =   1.101e-01
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   3.521e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  20.000
                  Electrical balance (eq)  =  -1.938e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -12.28
                               Iterations  =   4
                                  Total H  = 1.110476e+02
                                  Total O  = 5.554143e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

(CaO)3CaCl2:15H2O -92.01   64.23  156.24  (CaO)3CaCl2:15H2O
Al(OH)3(a)       -2.57    8.14   10.72  Al(OH)3
Al2O3            -6.69   16.29   22.98  Al2O3
Boehmite         -0.78    8.15    8.93  AlOOH
C3AH6             0.15   85.06   84.91  Ca3Al2(OH)12
C3AH6(C)          3.83   85.06   81.22  Ca3Al2(OH)12
CaCl2:6H20       -6.98   -4.53    2.45  CaCl2:6H2O
CaOCaCl2:2H2O   -35.43   18.39   53.82  CaOCaCl2:2H2O
CH               -0.36   22.92   23.28  Ca(OH)2
Diaspore          0.96    8.15    7.18  AlOOH
Fried0.86Al5.14OH   2.63   71.24   68.62  Ca4Al0.86Cl2(OH)8.58
Fried0.88Al5.12OH   2.16   71.41   69.25  Ca4Al0.88Cl2(OH)8.64
Fried1.04Al4.96OH   1.57   72.71   71.14  Ca4Al1.04Cl2(OH)9.12
Fried1.34Al4.66OH   1.36   75.15   73.80  Ca4Al1.34Cl2(OH)10.02
Fried1.42Al4.58OH   1.36   75.80   74.44  Ca4Al1.42Cl2(OH)10.26
Fried1.96Al4.04OH   2.06   80.20   78.14  Ca4Al1.96Cl2(OH)11.88
Friedelsalt       3.86   80.53   76.67  Ca4Al2Cl2(OH)12
Gibbsite(C)      -0.91    8.14    9.06  Al(OH)3
Lime            -10.45   22.92   33.38  CaO
O2(g)           -19.16   65.63   84.79  O2
Portlandite      -0.14   22.92   23.06  Ca(OH)2

Initial solution 16.Friedelsalt - C4AH13 x=0.1

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

Elements           Molality       Moles

Al                6.900e-04   6.900e-04
Ca                2.620e-02   2.620e-02
Cl                1.446e-02   1.446e-02

----------------------------Description of solution----------------------------

                                       pH  =  12.452
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   6.384e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   3.258e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  20.000
                  Electrical balance (eq)  =   7.427e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   8.60
                               Iterations  =   4
                                  Total H  = 1.110450e+02
                                  Total O  = 5.553880e+01
```

```
------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

(CaO)3CaCl2:15H2O -93.48   62.76  156.24  (CaO)3CaCl2:15H2O
Al(OH)3(a)       -2.87    7.85   10.72  Al(OH)3
Al2O3            -7.29   15.69   22.98  Al2O3
Boehmite         -1.08    7.85    8.93  AlOOH
C3AH6            -0.55   84.35   84.91  Ca3Al2(OH)12
C3AH6(C)          3.13   84.35   81.22  Ca3Al2(OH)12
CaCl2:6H20       -8.35   -5.90    2.45  CaCl2:6H2O
CaOCaCl2:2H2O   -36.83   16.99   53.82  CaOCaCl2:2H2O
CH               -0.40   22.89   23.28  Ca(OH)2
Diaspore          0.66    7.85    7.18  AlOOH
Fried0.86Al5.14OH   0.90   69.51   68.62  Ca4Al0.86Cl2(OH)8.58
Fried0.88Al5.12OH   0.42   69.67   69.25  Ca4Al0.88Cl2(OH)8.64
Fried1.04Al4.96OH  -0.21   70.93   71.14  Ca4Al1.04Cl2(OH)9.12
Fried1.34Al4.66OH  -0.52   73.28   73.80  Ca4Al1.34Cl2(OH)10.02
Fried1.42Al4.58OH  -0.54   73.91   74.44  Ca4Al1.42Cl2(OH)10.26
Fried1.96Al4.04OH  -0.00   78.14   78.14  Ca4Al1.96Cl2(OH)11.88
Friedelsalt       1.79   78.46   76.67  Ca4Al2Cl2(OH)12
Gibbsite(C)      -1.21    7.85    9.06  Al(OH)3
Lime            -10.49   22.89   33.38  CaO
O2(g)           -18.99   65.81   84.79  O2
Portlandite      -0.17   22.89   23.06  Ca(OH)2

Initial solution 17.Friedelsalt - C4AH13 x=0.2

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

Elements           Molality       Moles

Al                7.000e-04   7.000e-04
Ca                2.482e-02   2.482e-02
Cl                1.394e-02   1.394e-02

----------------------------Description of solution----------------------------

                                       pH  =  12.637
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   6.480e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   4.724e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  20.000
                  Electrical balance (eq)  =  -9.438e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -10.00
                               Iterations  =   4
                                  Total H  = 1.110597e+02
                                  Total O  = 5.555345e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

(CaO)3CaCl2:15H2O -92.69   63.55  156.24  (CaO)3CaCl2:15H2O
Al(OH)3(a)       -3.05    7.67   10.72  Al(OH)3
Al2O3            -7.65   15.33   22.98  Al2O3
Boehmite         -1.26    7.67    8.93  AlOOH
C3AH6            -0.01   84.89   84.91  Ca3Al2(OH)12
C3AH6(C)          3.67   84.89   81.22  Ca3Al2(OH)12
CaCl2:6H20       -8.45   -6.00    2.45  CaCl2:6H2O
CaOCaCl2:2H2O   -36.63   17.19   53.82  CaOCaCl2:2H2O
CH               -0.10   23.19   23.28  Ca(OH)2
Diaspore          0.49    7.67    7.18  AlOOH
Fried0.86Al5.14OH   1.54   70.15   68.62  Ca4Al0.86Cl2(OH)8.58
Fried0.88Al5.12OH   1.06   70.31   69.25  Ca4Al0.88Cl2(OH)8.64
Fried1.04Al4.96OH   0.39   71.53   71.14  Ca4Al1.04Cl2(OH)9.12
Fried1.34Al4.66OH   0.04   73.83   73.80  Ca4Al1.34Cl2(OH)10.02
Fried1.42Al4.58OH   0.00   74.45   74.44  Ca4Al1.42Cl2(OH)10.26
Fried1.96Al4.04OH   0.44   78.59   78.14  Ca4Al1.96Cl2(OH)11.88
Friedelsalt       2.22   78.89   76.67  Ca4Al2Cl2(OH)12
Gibbsite(C)      -1.39    7.67    9.06  Al(OH)3
Lime            -10.19   23.19   33.38  CaO
O2(g)           -18.25   66.55   84.79  O2
Portlandite       0.13   23.19   23.06  Ca(OH)2
```

```
Initial solution 18.Friedelsalt - C4AH13 x=0.3

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

Elements           Molality       Moles

Al                7.200e-04   7.200e-04
Ca                2.345e-02   2.345e-02
Cl                1.340e-02   1.340e-02

----------------------------Description of solution----------------------------

                                       pH  =  12.655
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   6.279e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   4.862e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  20.000
                  Electrical balance (eq)  =  -1.296e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -13.98
                               Iterations  =   4
                                  Total H  = 1.110611e+02
                                  Total O  = 5.555484e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

(CaO)3CaCl2:15H2O -92.72   63.52  156.24  (CaO)3CaCl2:15H2O
Al(OH)3(a)       -3.06    7.66   10.72  Al(OH)3
Al2O3            -7.66   15.32   22.98  Al2O3
Boehmite         -1.27    7.66    8.93  AlOOH
C3AH6             0.00   84.91   84.91  Ca3Al2(OH)12
C3AH6(C)          3.69   84.91   81.22  Ca3Al2(OH)12
CaCl2:6H20       -8.51   -6.06    2.45  CaCl2:6H2O
CaOCaCl2:2H2O   -36.68   17.13   53.82  CaOCaCl2:2H2O
CH               -0.09   23.20   23.28  Ca(OH)2
Diaspore          0.48    7.66    7.18  AlOOH
Fried0.86Al5.14OH   1.50   70.12   68.62  Ca4Al0.86Cl2(OH)8.58
Fried0.88Al5.12OH   1.02   70.27   69.25  Ca4Al0.88Cl2(OH)8.64
Fried1.04Al4.96OH   0.35   71.49   71.14  Ca4Al1.04Cl2(OH)9.12
Fried1.34Al4.66OH  -0.00   73.79   73.80  Ca4Al1.34Cl2(OH)10.02
Fried1.42Al4.58OH  -0.04   74.41   74.44  Ca4Al1.42Cl2(OH)10.26
Fried1.96Al4.04OH   0.40   78.54   78.14  Ca4Al1.96Cl2(OH)11.88
Friedelsalt       2.18   78.85   76.67  Ca4Al2Cl2(OH)12
Gibbsite(C)      -1.39    7.66    9.06  Al(OH)3
Lime            -10.18   23.20   33.38  CaO
O2(g)           -18.17   66.62   84.79  O2
Portlandite       0.14   23.20   23.06  Ca(OH)2

Initial solution 19.Friedelsalt - C4AH13 x=0.4

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

Elements           Molality       Moles

Al                7.500e-04   7.500e-04
Ca                2.220e-02   2.220e-02
Cl                8.820e-03   8.820e-03

----------------------------Description of solution----------------------------

                                       pH  =  12.669
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   5.879e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   4.961e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  20.000
                  Electrical balance (eq)  =  -1.178e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -13.56
                               Iterations  =   4
                                  Total H  = 1.110620e+02
                                  Total O  = 5.555583e+01
```

```
------------------------------Saturation indices------------------------------

Phase               SI log IAP  log KT

(CaO)3CaCl2:15H2O -93.08   63.16  156.24  (CaO)3CaCl2:15H2O
Al(OH)3(a)       -3.05    7.67   10.72  Al(OH)3
Al2O3            -7.64   15.34   22.98  Al2O3
Boehmite         -1.26    7.67    8.93  AlOOH
C3AH6             0.03   84.94   84.91  Ca3Al2(OH)12
C3AH6(C)          3.72   84.94   81.22  Ca3Al2(OH)12
CaCl2:6H20       -8.89   -6.44    2.45  CaCl2:6H2O
CaOCaCl2:2H2O   -37.06   16.76   53.82  CaOCaCl2:2H2O
CH               -0.08   23.20   23.28  Ca(OH)2
Diaspore          0.49    7.67    7.18  AlOOH
Fried0.86Al5.14OH   1.14   69.76   68.62  Ca4Al0.86Cl2(OH)8.58
Fried0.88Al5.12OH   0.66   69.91   69.25  Ca4Al0.88Cl2(OH)8.64
Fried1.04Al4.96OH  -0.00   71.14   71.14  Ca4Al1.04Cl2(OH)9.12
Fried1.34Al4.66OH  -0.36   73.44   73.80  Ca4Al1.34Cl2(OH)10.02
Fried1.42Al4.58OH  -0.39   74.05   74.44  Ca4Al1.42Cl2(OH)10.26
Fried1.96Al4.04OH   0.05   78.19   78.14  Ca4Al1.96Cl2(OH)11.88
Friedelsalt       1.83   78.50   76.67  Ca4Al2Cl2(OH)12
Gibbsite(C)      -1.39    7.67    9.06  Al(OH)3
Lime            -10.17   23.20   33.38  CaO
O2(g)           -18.12   66.67   84.79  O2
Portlandite       0.14   23.20   23.06  Ca(OH)2


Initial solution 20.Friedelsalt - C4AH13 x=0.5

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

Elements           Molality       Moles

Al                7.500e-04   7.500e-04
Ca                2.096e-02   2.096e-02
Cl                4.230e-03   4.230e-03

----------------------------Description of solution---------------------------

                                       pH  =  12.682
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   5.479e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   5.038e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  20.000
                  Electrical balance (eq)  =  -1.044e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -12.90
                               Iterations  =   4
                                  Total H  = 1.110628e+02
                                  Total O  = 5.555660e+01

------------------------------Saturation indices------------------------------

Phase               SI log IAP  log KT

(CaO)3CaCl2:15H2O -93.73   62.51  156.24  (CaO)3CaCl2:15H2O
Al(OH)3(a)       -3.06    7.66   10.72  Al(OH)3
Al2O3            -7.67   15.31   22.98  Al2O3
Boehmite         -1.27    7.66    8.93  AlOOH
C3AH6             0.02   84.92   84.91  Ca3Al2(OH)12
C3AH6(C)          3.70   84.92   81.22  Ca3Al2(OH)12
CaCl2:6H20       -9.55   -7.10    2.45  CaCl2:6H2O
CaOCaCl2:2H2O   -37.71   16.11   53.82  CaOCaCl2:2H2O
CH               -0.08   23.20   23.28  Ca(OH)2
Diaspore          0.48    7.66    7.18  AlOOH
Fried0.86Al5.14OH   0.48   69.10   68.62  Ca4Al0.86Cl2(OH)8.58
Fried0.88Al5.12OH   0.00   69.25   69.25  Ca4Al0.88Cl2(OH)8.64
Fried1.04Al4.96OH  -0.66   70.48   71.14  Ca4Al1.04Cl2(OH)9.12
Fried1.34Al4.66OH  -1.02   72.77   73.80  Ca4Al1.34Cl2(OH)10.02
Fried1.42Al4.58OH  -1.06   73.39   74.44  Ca4Al1.42Cl2(OH)10.26
Fried1.96Al4.04OH  -0.62   77.52   78.14  Ca4Al1.96Cl2(OH)11.88
Friedelsalt       1.16   77.83   76.67  Ca4Al2Cl2(OH)12
Gibbsite(C)      -1.40    7.66    9.06  Al(OH)3
Lime            -10.17   23.20   33.38  CaO
O2(g)           -18.07   66.73   84.79  O2
Portlandite       0.14   23.20   23.06  Ca(OH)2
```

```
Initial solution 21.Friedelsalt - C4AH13 x=0.6

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

Elements           Molality       Moles

Al                7.000e-04   7.000e-04
Ca                2.021e-02   2.021e-02
Cl                2.330e-03   2.330e-03

----------------------------Description of solution----------------------------

                                       pH  =  12.713
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   5.364e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   5.321e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  20.000
                  Electrical balance (eq)  =  -1.302e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -16.21
                               Iterations  =   4
                                  Total H  = 1.110656e+02
                                  Total O  = 5.555943e+01


------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

(CaO)3CaCl2:15H2O -94.16   62.08  156.24  (CaO)3CaCl2:15H2O
Al(OH)3(a)       -3.12    7.60   10.72  Al(OH)3
Al2O3            -7.79   15.19   22.98  Al2O3
Boehmite         -1.33    7.60    8.93  AlOOH
C3AH6             0.01   84.92   84.91  Ca3Al2(OH)12
C3AH6(C)          3.70   84.92   81.22  Ca3Al2(OH)12
CaCl2:6H20      -10.09   -7.64    2.45  CaCl2:6H2O
CaOCaCl2:2H2O   -38.22   15.60   53.82  CaOCaCl2:2H2O
CH               -0.04   23.24   23.28  Ca(OH)2
Diaspore          0.42    7.60    7.18  AlOOH
Fried0.86Al5.14OH   0.00   68.62   68.62  Ca4Al0.86Cl2(OH)8.58
Fried0.88Al5.12OH  -0.48   68.77   69.25  Ca4Al0.88Cl2(OH)8.64
Fried1.04Al4.96OH  -1.15   69.99   71.14  Ca4Al1.04Cl2(OH)9.12
Fried1.34Al4.66OH  -1.53   72.26   73.80  Ca4Al1.34Cl2(OH)10.02
Fried1.42Al4.58OH  -1.57   72.87   74.44  Ca4Al1.42Cl2(OH)10.26
Fried1.96Al4.04OH  -1.17   76.97   78.14  Ca4Al1.96Cl2(OH)11.88
Friedelsalt       0.61   77.28   76.67  Ca4Al2Cl2(OH)12
Gibbsite(C)      -1.46    7.60    9.06  Al(OH)3
Lime            -10.13   23.24   33.38  CaO
O2(g)           -17.94   66.85   84.79  O2
Portlandite       0.18   23.24   23.06  Ca(OH)2

Initial solution 22.Friedelsalt - C4AH13 x=0.7

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

Elements           Molality       Moles

Al                6.600e-04   6.600e-04
Ca                1.996e-02   1.996e-02
Cl                2.070e-03   2.070e-03

----------------------------Description of solution----------------------------

                                       pH  =  12.733
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   5.384e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   5.525e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  20.000
                  Electrical balance (eq)  =  -1.542e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -18.91
                               Iterations  =   4
                                  Total H  = 1.110677e+02
                                  Total O  = 5.556146e+01
```

```
------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

(CaO)3CaCl2:15H2O -94.19   62.05  156.24  (CaO)3CaCl2:15H2O
Al(OH)3(a)       -3.17    7.55   10.72  Al(OH)3
Al2O3            -7.88   15.10   22.98  Al2O3
Boehmite         -1.38    7.55    8.93  AlOOH
C3AH6            -0.00   84.91   84.91  Ca3Al2(OH)12
C3AH6(C)          3.69   84.91   81.22  Ca3Al2(OH)12
CaCl2:6H20      -10.21   -7.76    2.45  CaCl2:6H2O
CaOCaCl2:2H2O   -38.30   15.51   53.82  CaOCaCl2:2H2O
CH               -0.01   23.27   23.28  Ca(OH)2
Diaspore          0.37    7.55    7.18  AlOOH
Fried0.86Al5.14OH  -0.07   68.55   68.62  Ca4Al0.86Cl2(OH)8.58
Fried0.88Al5.12OH  -0.55   68.70   69.25  Ca4Al0.88Cl2(OH)8.64
Fried1.04Al4.96OH  -1.23   69.91   71.14  Ca4Al1.04Cl2(OH)9.12
Fried1.34Al4.66OH  -1.62   72.17   73.80  Ca4Al1.34Cl2(OH)10.02
Fried1.42Al4.58OH  -1.67   72.77   74.44  Ca4Al1.42Cl2(OH)10.26
Fried1.96Al4.04OH  -1.29   76.85   78.14  Ca4Al1.96Cl2(OH)11.88
Friedelsalt       0.48   77.15   76.67  Ca4Al2Cl2(OH)12
Gibbsite(C)      -1.50    7.55    9.06  Al(OH)3
Lime            -10.11   23.27   33.38  CaO
O2(g)           -17.86   66.93   84.79  O2
Portlandite       0.21   23.27   23.06  Ca(OH)2


Initial solution 23.Friedelsalt - C4AH13 x=0.8

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

Elements           Molality       Moles

Al                6.700e-04   6.700e-04
Ca                1.921e-02   1.921e-02
Cl                1.900e-03   1.900e-03

----------------------------Description of solution----------------------------

                                       pH  =  12.734
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   5.262e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   5.507e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  20.000
                  Electrical balance (eq)  =  -1.654e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -20.65
                               Iterations  =   4
                                  Total H  = 1.110675e+02
                                  Total O  = 5.556129e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

(CaO)3CaCl2:15H2O -94.32   61.92  156.24  (CaO)3CaCl2:15H2O
Al(OH)3(a)       -3.16    7.56   10.72  Al(OH)3
Al2O3            -7.86   15.12   22.98  Al2O3
Boehmite         -1.37    7.56    8.93  AlOOH
C3AH6            -0.03   84.88   84.91  Ca3Al2(OH)12
C3AH6(C)          3.66   84.88   81.22  Ca3Al2(OH)12
CaCl2:6H20      -10.29   -7.84    2.45  CaCl2:6H2O
CaOCaCl2:2H2O   -38.41   15.41   53.82  CaOCaCl2:2H2O
CH               -0.03   23.26   23.28  Ca(OH)2
Diaspore          0.38    7.56    7.18  AlOOH
Fried0.86Al5.14OH  -0.19   68.42   68.62  Ca4Al0.86Cl2(OH)8.58
Fried0.88Al5.12OH  -0.67   68.58   69.25  Ca4Al0.88Cl2(OH)8.64
Fried1.04Al4.96OH  -1.36   69.78   71.14  Ca4Al1.04Cl2(OH)9.12
Fried1.34Al4.66OH  -1.74   72.05   73.80  Ca4Al1.34Cl2(OH)10.02
Fried1.42Al4.58OH  -1.79   72.66   74.44  Ca4Al1.42Cl2(OH)10.26
Fried1.96Al4.04OH  -1.41   76.74   78.14  Ca4Al1.96Cl2(OH)11.88
Friedelsalt       0.37   77.04   76.67  Ca4Al2Cl2(OH)12
Gibbsite(C)      -1.50    7.56    9.06  Al(OH)3
Lime            -10.12   23.26   33.38  CaO
O2(g)           -17.86   66.94   84.79  O2
Portlandite       0.20   23.26   23.06  Ca(OH)2

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End of simulation.
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Reading input data for simulation 3.
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TITLE  The System CaO-Al2O3-CaSO4-H2O
       Ref: Damidot, Atkins, Kindness, Glasser, Cement and Concrete Research, 1992,
       Vol 22, No 2/3, 229-234
SOLUTION 24  AFt Exp 1
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              0.351
        Al              2.035
        S(6)            4.084
        Na            997.5
SOLUTION 25  AFt Exp 2
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              0.55
        Al              0.451
        S(6)            2.20
        Na            503.8
SOLUTION 26  AFt Exp 3
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              0.5425
        Al              0.37
        S(6)            1.124
        Na            248.3
SOLUTION 27  AFt Exp 4
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              0.602
        Al              0.326
        S(6)            1.10
        Na             95.65
SOLUTION 28  AFt Exp 5
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              0.6175
        Al              0.311
        S(6)            0.91
        Na             53.48
SOLUTION 29  AFt Exp 6
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              0.515
        Al              0.443
        S(6)            1.196
        Na             27.82
SOLUTION 30  AFt Exp 7
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              0.8075
        Al              0.323
        S(6)            0.806
        Na            16.52
SOLUTION 31  AFt Exp 8
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              0.935
        Al              0.342
        S(6)            0.676
        Na              9.78
```

```
SOLUTION 32  AFt Exp 9
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              1.175
        Al              0.457
        S(6)            0.819
        Na              5.65
SOLUTION 33  AFt Exp 10
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              1.395
        Al              0.431
        S(6)            0.728
        Na              3.
SOLUTION 34  AFt Exp 11
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              1.68
        Al              0.513
        S(6)            0.81
        Na              1.87
SOLUTION 35  AFt Exp 12
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              1.65
        Al              0.649
        S(6)            0.884
        Na              1.26
SOLUTION 36  AFt Exp 13
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              0.825
        Al              0.777
        S(6)          122.5
        Na            249.2
SOLUTION 37  AFt Exp 14
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              1.15
        Al              0.629
        S(6)           49.2
        Na             99.3
SOLUTION 38  AFt Exp 15
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              1.50
        Al              0.592
        S(6)           26.0
        Na             50.8
SOLUTION 39  AFt Exp 16
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              1.995
        Al              0.552
        S(6)            0.81
        Na              0.
SOLUTION 40  Calculated Invariant point G (C3AH6 - AFt - CH)
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca             20.74
        Al              0.074
        S(6)            0.034
        Na              0.
```

```
SOLUTION 41  Calculated Invariant point H2 (C3AH6 - AFt - AH3)
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              7.6
        Al              1.174
        S(6)            0.074
        Na              0.
SOLUTION 42  Calculated Invariant point F (CH - AFt - Gypsum)
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca             32.13
        Al              0.0003
        S(6)           12.24
        Na              0.
SOLUTION 43  Calculated Invariant point E2 (AH3 - AFt - Gypsum)
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca             15.34
        Al              0.0178
        S(6)           15.20
        Na              0.
SOLUTION 44  Jones Invariant point G(J) (C3AH6 - AFt - CH)
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca             19.17
        Al              0.01
        S(6)            0.18
        Na              0.
SOLUTION 45  Jones Invariant point H2(J) (C3AH6 - AFt - AH3)
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              3.495
        Al              0.09
        S(6)            0.375
        Na              0.
SOLUTION 46  Jones Invariant point F(J) (CH - AFt - Gypsum)
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca             31.56
        Al              0.06
        S(6)           12.33
        Na              0.
SOLUTION 47  Jones Invariant point E2(J) (AH3 - AFt - Gypsum)
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca             15.645
        Al              0.025
        S(6)           14.97
        Na              0.
SOLUTION 48  D'Ans and Eick Invariant point G(E) (C3AH6 - AFt - CH)
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    20.0
        Ca             21.46
        Al              0.025
        S(6)            0.107
        Na              0.
SOLUTION 49  D'Ans and Eick Invariant point H2(E) (C3AH6 - AFt - AH3)
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    20.0
        Ca              3.103
        Al              0.158
        S(6)            0.263
        Na              0.
```

```
SOLUTION 50  D'Ans and Eick Invariant point F(E) (CH - AFt - Gypsum)
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    20.0
        Ca             32.8
        Al              0.027
        S(6)           12.2
        Na              0.
SOLUTION 51  D'Ans and Eick Invariant point E2(E) (AH3 - AFt - Gypsum)
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    20.0
        Ca             15.136
        Al              0.09
        S(6)           14.82
        Na              0.
SOLUTION 52  Jones Invariant point G(J) (C3AH6 - AFt - CH)
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca             1.62
        Al              0.085
        S(6)            0.93
        Na            250.
SOLUTION 53  Jones Invariant point H2(J) (C3AH6 - AFt - AH3)
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              0.001
        Al             16.8
        S(6)           60.6
        Na            250.
SOLUTION 54  Jones Invariant point F(J) (CH - AFt - Gypsum)
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca             15.39
        Al              0.025
        S(6)           93.9
        Na            250.
SOLUTION 55  Jones Invariant point E2(J) (AH3 - AFt - Gypsum)
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca             10.17
        Al              0.14
        S(6)          134.7
        Na            250.
END
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TITLE
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  The System CaO-Al2O3-CaSO4-H2O
       Ref: Damidot, Atkins, Kindness, Glasser, Cement and Concrete Research, 1992,
       Vol 22, No 2/3, 229-234

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Beginning of initial solution calculations.
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Initial solution 24.AFt Exp 1

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

Elements           Molality       Moles

Al                2.035e-03   2.035e-03
Ca                3.510e-04   3.510e-04
Na                9.975e-01   9.975e-01
S(6)              4.084e-03   4.084e-03

----------------------------Description of solution----------------------------

                                       pH  =  13.771      Charge balance
                                       pe  =   4.000
                        Activity of water  =   0.966
                           Ionic strength  =   9.988e-01
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   9.961e-01
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -3.086e-10
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   6
                                  Total H  = 1.120086e+02
                                  Total O  = 5.651869e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm              -0.34   72.22   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -2.27   55.17   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -4.03    6.35   10.38  Al(OH)3
Al2O3           -10.24   12.74   22.98  Al2O3
Al4(OH)10SO4    -28.35   -5.65   22.70  Al4(OH)10SO4
AlOHSO4         -21.46  -24.69   -3.23  AlOHSO4
Anhydrite        -3.74   -8.38   -4.64  CaSO4
Boehmite         -2.22    6.36    8.58  AlOOH
C3AH6            -2.22   80.69   82.91  Ca3Al2(OH)12
C3AH6(C)          1.23   80.69   79.45  Ca3Al2(OH)12
CH               -0.24   22.66   22.90  Ca(OH)2
Diaspore         -0.51    6.36    6.87  AlOOH
Ettr_GCA         -1.92   55.17   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -2.42    6.35    8.77  Al(OH)3
Gypsum           -3.56   -8.41   -4.85  CaSO4:2H2O
Gypsum_Cem       -3.81   -8.41   -4.60  CaSO4:2H2O
Lime            -10.12   22.68   32.80  CaO
Mirabilite       -2.86   -3.97   -1.11  Na2SO4:10H2O
O2(g)           -12.07   71.05   83.12  O2
Portlandite      -0.01   22.66   22.68  Ca(OH)2
Thenardite       -3.64   -3.82   -0.18  Na2SO4

Initial solution 25.AFt Exp 2

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

Elements           Molality       Moles

Al                4.510e-04   4.510e-04
Ca                5.500e-04   5.500e-04
Na                5.038e-01   5.038e-01
S(6)              2.200e-03   2.200e-03

----------------------------Description of solution----------------------------

                                       pH  =  13.505      Charge balance
                                       pe  =   4.000
                        Activity of water  =   0.983
                           Ionic strength  =   5.055e-01
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   5.019e-01
                    Total carbon (mol/kg)  =   0.000e+00
```

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                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =   1.755e-13
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                               Iterations  =   5
                                  Total H  = 1.115143e+02
                                  Total O  = 5.601687e+01

------------------------------Saturation indices-------------------------------
Phase               SI log IAP  log KT

AFm              -0.94    71.62    72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -1.99    55.45    57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -4.40     5.98    10.38  Al(OH)3
Al2O3           -11.00    11.98    22.98  Al2O3
Al4(OH)10SO4    -29.36    -6.66    22.70  Al4(OH)10SO4
AlOHSO4         -21.37   -24.60    -3.23  AlOHSO4
Anhydrite        -3.37    -8.01    -4.64  CaSO4
Boehmite         -2.59     5.99     8.58  AlOOH
C3AH6            -3.23    79.67    82.91  Ca3Al2(OH)12
C3AH6(C)          0.22    79.67    79.45  Ca3Al2(OH)12
CH               -0.33    22.57    22.90  Ca(OH)2
Diaspore         -0.89     5.99     6.87  AlOOH
Ettr_GCA         -1.64    55.45    57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -2.79     5.98     8.77  Al(OH)3
Gypsum           -3.18    -8.02    -4.85  CaSO4:2H2O
Gypsum_Cem       -3.42    -8.02    -4.60  CaSO4:2H2O
Lime            -10.22    22.58    32.80  CaO
Mirabilite       -3.44    -4.56    -1.11  Na2SO4:10H2O
O2(g)           -13.12    70.00    83.12  O2
Portlandite      -0.10    22.57    22.68  Ca(OH)2
Thenardite       -4.30    -4.48    -0.18  Na2SO4

Initial solution 26.AFt Exp 3

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

Elements           Molality       Moles

Al                3.700e-04   3.700e-04
Ca                5.425e-04   5.425e-04
Na                2.483e-01   2.483e-01
S(6)              1.124e-03   1.124e-03

----------------------------Description of solution----------------------------

                                       pH  =  13.232      Charge balance
                                       pe  =   4.000
                        Activity of water  =   0.992
                           Ionic strength  =   2.498e-01
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   2.482e-01
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -1.853e-13
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   5
                                  Total H  = 1.112607e+02
                                  Total O  = 5.575896e+01

------------------------------Saturation indices-------------------------------
Phase               SI log IAP  log KT

AFm              -1.34    71.22    72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -2.08    55.36    57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -4.19     6.19    10.38  Al(OH)3
Al2O3           -10.58    12.40    22.98  Al2O3
Al4(OH)10SO4    -28.07    -5.37    22.70  Al4(OH)10SO4
AlOHSO4         -20.72   -23.95    -3.23  AlOHSO4
Anhydrite        -3.26    -7.89    -4.64  CaSO4
Boehmite         -2.38     6.20     8.58  AlOOH
C3AH6            -3.77    79.13    82.91  Ca3Al2(OH)12
C3AH6(C)         -0.32    79.13    79.45  Ca3Al2(OH)12
CH               -0.65    22.25    22.90  Ca(OH)2
Diaspore         -0.68     6.20     6.87  AlOOH
Ettr_GCA         -1.73    55.36    57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -2.58     6.19     8.77  Al(OH)3
Gypsum           -3.05    -7.90    -4.85  CaSO4:2H2O
Gypsum_Cem       -3.30    -7.90    -4.60  CaSO4:2H2O
Lime            -10.54    22.25    32.80  CaO
Mirabilite       -4.09    -5.20    -1.11  Na2SO4:10H2O
O2(g)           -14.20    68.92    83.12  O2
Portlandite      -0.43    22.25    22.68  Ca(OH)2
Thenardite       -4.99    -5.17    -0.18  Na2SO4
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Initial solution 27.AFt Exp 4

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

Elements           Molality       Moles

Al                3.260e-04   3.260e-04
Ca                6.020e-04   6.020e-04
Na                9.565e-02   9.565e-02
S(6)              1.100e-03   1.100e-03

----------------------------Description of solution----------------------------

                                       pH  =  12.856      Charge balance
                                       pe  =   4.000
                        Activity of water  =   0.997
                           Ionic strength  =   9.763e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   9.563e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =   1.053e-14
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                               Iterations  =   4
                                  Total H  = 1.111081e+02
                                  Total O  = 5.560625e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm              -1.40   71.16   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -1.07   56.37   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -3.83    6.55   10.38  Al(OH)3
Al2O3            -9.88   13.10   22.98  Al2O3
Al4(OH)10SO4    -25.69   -2.99   22.70  Al4(OH)10SO4
AlOHSO4         -19.41  -22.64   -3.23  AlOHSO4
Anhydrite        -2.74   -7.38   -4.64  CaSO4
Boehmite         -2.03    6.55    8.58  AlOOH
C3AH6            -4.36   78.54   82.91  Ca3Al2(OH)12
C3AH6(C)         -0.91   78.54   79.45  Ca3Al2(OH)12
CH               -1.09   21.81   22.90  Ca(OH)2
Diaspore         -0.32    6.55    6.87  AlOOH
Ettr_GCA         -0.72   56.37   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -2.22    6.55    8.77  Al(OH)3
Gypsum           -2.53   -7.38   -4.85  CaSO4:2H2O
Gypsum_Cem       -2.78   -7.38   -4.60  CaSO4:2H2O
Lime            -10.98   21.82   32.80  CaO
Mirabilite       -4.64   -5.75   -1.11  Na2SO4:10H2O
O2(g)           -15.70   67.42   83.12  O2
Portlandite      -0.86   21.81   22.68  Ca(OH)2
Thenardite       -5.56   -5.74   -0.18  Na2SO4

Initial solution 28.AFt Exp 5

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

Elements           Molality       Moles

Al                3.110e-04   3.110e-04
Ca                6.175e-04   6.175e-04
Na                5.348e-02   5.348e-02
S(6)              9.100e-04   9.100e-04

----------------------------Description of solution----------------------------

                                       pH  =  12.623      Charge balance
                                       pe  =   4.000
                        Activity of water  =   0.998
                           Ionic strength  =   5.555e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   5.383e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -1.318e-14
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   4
                                  Total H  = 1.110663e+02
                                  Total O  = 5.556368e+01
```

```
------------------------------Saturation indices-------------------------------


Phase               SI log IAP  log KT

AFm              -1.71   70.85   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -1.02   56.42   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -3.60    6.78   10.38  Al(OH)3
Al2O3            -9.42   13.56   22.98  Al2O3
Al4(OH)10SO4    -24.28   -1.58   22.70  Al4(OH)10SO4
AlOHSO4         -18.70  -21.93   -3.23  AlOHSO4
Anhydrite        -2.57   -7.21   -4.64  CaSO4
Boehmite         -1.80    6.78    8.58  AlOOH
C3AH6            -4.84   78.06   82.91  Ca3Al2(OH)12
C3AH6(C)         -1.39   78.06   79.45  Ca3Al2(OH)12
CH               -1.40   21.50   22.90  Ca(OH)2
Diaspore         -0.09    6.78    6.87  AlOOH
Ettr_GCA         -0.67   56.42   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -1.99    6.78    8.77  Al(OH)3
Gypsum           -2.36   -7.21   -4.85  CaSO4:2H2O
Gypsum_Cem       -2.61   -7.21   -4.60  CaSO4:2H2O
Lime            -11.30   21.50   32.80  CaO
Mirabilite       -5.08   -6.19   -1.11  Na2SO4:10H2O
O2(g)           -16.63   66.49   83.12  O2
Portlandite      -1.17   21.50   22.68  Ca(OH)2
Thenardite       -6.00   -6.18   -0.18  Na2SO4

Initial solution 29.AFt Exp 6

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

Elements           Molality       Moles

Al                4.430e-04   4.430e-04
Ca                5.150e-04   5.150e-04
Na                2.782e-02   2.782e-02
S(6)              1.196e-03   1.196e-03

----------------------------Description of solution----------------------------

                                       pH  =  12.338      Charge balance
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   3.006e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   2.779e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -2.849e-15
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   5
                                  Total H  = 1.110402e+02
                                  Total O  = 5.553879e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm              -2.10   70.46   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -0.88   56.56   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -3.14    7.24   10.38  Al(OH)3
Al2O3            -8.50   14.48   22.98  Al2O3
Al4(OH)10SO4    -21.67    1.03   22.70  Al4(OH)10SO4
AlOHSO4         -17.46  -20.69   -3.23  AlOHSO4
Anhydrite        -2.31   -6.95   -4.64  CaSO4
Boehmite         -1.34    7.24    8.58  AlOOH
C3AH6            -5.50   77.41   82.91  Ca3Al2(OH)12
C3AH6(C)         -2.04   77.41   79.45  Ca3Al2(OH)12
CH               -1.92   20.98   22.90  Ca(OH)2
Diaspore          0.37    7.24    6.87  AlOOH
Ettr_GCA         -0.53   56.56   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -1.53    7.24    8.77  Al(OH)3
Gypsum           -2.10   -6.95   -4.85  CaSO4:2H2O
Gypsum_Cem       -2.35   -6.95   -4.60  CaSO4:2H2O
Lime            -11.82   20.98   32.80  CaO
Mirabilite       -5.39   -6.51   -1.11  Na2SO4:10H2O
O2(g)           -17.77   65.35   83.12  O2
Portlandite      -1.70   20.98   22.68  Ca(OH)2
Thenardite       -6.32   -6.50   -0.18  Na2SO4
```

```
Initial solution 30.AFt Exp 7

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

Elements           Molality       Moles

Al                3.230e-04   3.230e-04
Ca                8.075e-04   8.075e-04
Na                1.652e-02   1.652e-02
S(6)              8.060e-04   8.060e-04

----------------------------Description of solution----------------------------

                                       pH  =  12.143      Charge balance
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   1.925e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   1.749e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -5.852e-11
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   5
                                  Total H  = 1.110299e+02
                                  Total O  = 5.552693e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm              -2.16   70.41   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -0.63   56.81   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -3.07    7.31   10.38  Al(OH)3
Al2O3            -8.36   14.62   22.98  Al2O3
Al4(OH)10SO4    -21.12    1.58   22.70  Al4(OH)10SO4
AlOHSO4         -17.12  -20.35   -3.23  AlOHSO4
Anhydrite        -2.16   -6.79   -4.64  CaSO4
Boehmite         -1.27    7.31    8.58  AlOOH
C3AH6            -5.70   77.20   82.91  Ca3Al2(OH)12
C3AH6(C)         -2.25   77.20   79.45  Ca3Al2(OH)12
CH               -2.04   20.86   22.90  Ca(OH)2
Diaspore          0.44    7.31    6.87  AlOOH
Ettr_GCA         -0.28   56.81   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -1.46    7.31    8.77  Al(OH)3
Gypsum           -1.95   -6.80   -4.85  CaSO4:2H2O
Gypsum_Cem       -2.20   -6.80   -4.60  CaSO4:2H2O
Lime            -11.93   20.86   32.80  CaO
Mirabilite       -5.94   -7.06   -1.11  Na2SO4:10H2O
O2(g)           -18.55   64.57   83.12  O2
Portlandite      -1.81   20.86   22.68  Ca(OH)2
Thenardite       -6.87   -7.05   -0.18  Na2SO4

Initial solution 31.AFt Exp 8

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

Elements           Molality       Moles

Al                3.420e-04   3.420e-04
Ca                9.350e-04   9.350e-04
Na                9.780e-03   9.780e-03
S(6)              6.760e-04   6.760e-04

----------------------------Description of solution----------------------------

                                       pH  =  11.940      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   1.282e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   1.132e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -1.975e-14
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   6
                                  Total H  = 1.110238e+02
                                  Total O  = 5.552024e+01
```

```
------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm              -2.44   70.12   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -0.74   56.70   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -2.84    7.54   10.38  Al(OH)3
Al2O3            -7.89   15.09   22.98  Al2O3
Al4(OH)10SO4    -19.81    2.89   22.70  Al4(OH)10SO4
AlOHSO4         -16.52  -19.75   -3.23  AlOHSO4
Anhydrite        -2.07   -6.71   -4.64  CaSO4
Boehmite         -1.03    7.55    8.58  AlOOH
C3AH6            -6.07   76.83   82.91  Ca3Al2(OH)12
C3AH6(C)         -2.62   76.83   79.45  Ca3Al2(OH)12
CH               -2.32   20.58   22.90  Ca(OH)2
Diaspore          0.67    7.55    6.87  AlOOH
Ettr_GCA         -0.39   56.70   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -1.23    7.54    8.77  Al(OH)3
Gypsum           -1.86   -6.71   -4.85  CaSO4:2H2O
Gypsum_Cem       -2.11   -6.71   -4.60  CaSO4:2H2O
Lime            -12.22   20.58   32.80  CaO
Mirabilite       -6.42   -7.53   -1.11  Na2SO4:10H2O
O2(g)           -19.36   63.76   83.12  O2
Portlandite      -2.09   20.58   22.68  Ca(OH)2
Thenardite       -7.35   -7.53   -0.18  Na2SO4

Initial solution 32.AFt Exp 9

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

Elements           Molality       Moles

Al                4.570e-04   4.570e-04
Ca                1.175e-03   1.175e-03
Na                5.650e-03   5.650e-03
S(6)              8.190e-04   8.190e-04

----------------------------Description of solution----------------------------

                                       pH  =  11.717      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   9.492e-03
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   7.733e-03
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -8.162e-11
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   6
                                  Total H  = 1.110202e+02
                                  Total O  = 5.551723e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm              -2.42   70.14   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -0.24   57.20   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -2.48    7.90   10.38  Al(OH)3
Al2O3            -7.18   15.80   22.98  Al2O3
Al4(OH)10SO4    -17.85    4.85   22.70  Al4(OH)10SO4
AlOHSO4         -15.61  -18.84   -3.23  AlOHSO4
Anhydrite        -1.83   -6.47   -4.64  CaSO4
Boehmite         -0.68    7.90    8.58  AlOOH
C3AH6            -6.29   76.62   82.91  Ca3Al2(OH)12
C3AH6(C)         -2.84   76.62   79.45  Ca3Al2(OH)12
CH               -2.63   20.27   22.90  Ca(OH)2
Diaspore          1.03    7.90    6.87  AlOOH
Ettr_GCA          0.11   57.20   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -0.87    7.90    8.77  Al(OH)3
Gypsum           -1.62   -6.47   -4.85  CaSO4:2H2O
Gypsum_Cem       -1.87   -6.47   -4.60  CaSO4:2H2O
Lime            -12.52   20.27   32.80  CaO
Mirabilite       -6.78   -7.89   -1.11  Na2SO4:10H2O
O2(g)           -20.25   62.87   83.12  O2
Portlandite      -2.40   20.27   22.68  Ca(OH)2
Thenardite       -7.71   -7.89   -0.18  Na2SO4
```

```
Initial solution 33.AFt Exp 10

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

Elements           Molality       Moles

Al                4.310e-04   4.310e-04
Ca                1.395e-03   1.395e-03
Na                3.000e-03   3.000e-03
S(6)              7.280e-04   7.280e-04

----------------------------Description of solution----------------------------

                                       pH  =  11.540      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   7.415e-03
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   5.627e-03
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -5.719e-15
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   7
                                  Total H  = 1.110181e+02
                                  Total O  = 5.551476e+01

------------------------------Saturation indices-------------------------------

Phase               SI  log IAP  log KT

AFm              -2.79   69.77   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -0.49   56.95   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -2.32    8.06   10.38  Al(OH)3
Al2O3            -6.87   16.11   22.98  Al2O3
Al4(OH)10SO4    -16.91    5.79   22.70  Al4(OH)10SO4
AlOHSO4         -15.15  -18.38   -3.23  AlOHSO4
Anhydrite        -1.77   -6.41   -4.64  CaSO4
Boehmite         -0.52    8.06    8.58  AlOOH
C3AH6            -6.73   76.18   82.91  Ca3Al2(OH)12
C3AH6(C)         -3.27   76.18   79.45  Ca3Al2(OH)12
CH               -2.88   20.02   22.90  Ca(OH)2
Diaspore          1.18    8.06    6.87  AlOOH
Ettr_GCA         -0.14   56.95   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -0.71    8.06    8.77  Al(OH)3
Gypsum           -1.56   -6.41   -4.85  CaSO4:2H2O
Gypsum_Cem       -1.81   -6.41   -4.60  CaSO4:2H2O
Lime            -12.77   20.02   32.80  CaO
Mirabilite       -7.36   -8.48   -1.11  Na2SO4:10H2O
O2(g)           -20.96   62.16   83.12  O2
Portlandite      -2.65   20.02   22.68  Ca(OH)2
Thenardite       -8.30   -8.48   -0.18  Na2SO4

Initial solution 34.AFt Exp 11

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

Elements           Molality       Moles

Al                5.130e-04   5.130e-04
Ca                1.680e-03   1.680e-03
Na                1.870e-03   1.870e-03
S(6)              8.100e-04   8.100e-04

----------------------------Description of solution----------------------------

                                       pH  =  11.438      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   7.126e-03
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   5.149e-03
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -3.230e-13
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   7
                                  Total H  = 1.110176e+02
                                  Total O  = 5.551461e+01
```

```
------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm              -2.66   69.90   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -0.11   57.33   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -2.15    8.23   10.38  Al(OH)3
Al2O3            -6.51   16.47   22.98  Al2O3
Al4(OH)10SO4    -15.95    6.75   22.70  Al4(OH)10SO4
AlOHSO4         -14.72  -17.95   -3.23  AlOHSO4
Anhydrite        -1.65   -6.28   -4.64  CaSO4
Boehmite         -0.34    8.23    8.58  AlOOH
C3AH6            -6.73   76.18   82.91  Ca3Al2(OH)12
C3AH6(C)         -3.27   76.18   79.45  Ca3Al2(OH)12
CH               -3.00   19.90   22.90  Ca(OH)2
Diaspore          1.36    8.23    6.87  AlOOH
Ettr_GCA          0.24   57.33   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -0.54    8.23    8.77  Al(OH)3
Gypsum           -1.43   -6.28   -4.85  CaSO4:2H2O
Gypsum_Cem       -1.68   -6.28   -4.60  CaSO4:2H2O
Lime            -12.89   19.90   32.80  CaO
Mirabilite       -7.73   -8.85   -1.11  Na2SO4:10H2O
O2(g)           -21.37   61.75   83.12  O2
Portlandite      -2.77   19.90   22.68  Ca(OH)2
Thenardite       -8.67   -8.85   -0.18  Na2SO4

Initial solution 35.AFt Exp 12

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

Elements           Molality       Moles

Al                6.490e-04   6.490e-04
Ca                1.650e-03   1.650e-03
Na                1.260e-03   1.260e-03
S(6)              8.840e-04   8.840e-04

----------------------------Description of solution----------------------------

                                       pH  =  11.280      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   6.505e-03
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   4.739e-03
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -5.021e-11
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   7
                                  Total H  = 1.110172e+02
                                  Total O  = 5.551449e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm              -3.04   69.52   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -0.40   57.04   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -1.88    8.50   10.38  Al(OH)3
Al2O3            -5.99   16.99   22.98  Al2O3
Al4(OH)10SO4    -14.54    8.16   22.70  Al4(OH)10SO4
AlOHSO4         -14.10  -17.33   -3.23  AlOHSO4
Anhydrite        -1.60   -6.24   -4.64  CaSO4
Boehmite         -0.08    8.50    8.58  AlOOH
C3AH6            -7.15   75.76   82.91  Ca3Al2(OH)12
C3AH6(C)         -3.70   75.76   79.45  Ca3Al2(OH)12
CH               -3.31   19.59   22.90  Ca(OH)2
Diaspore          1.62    8.50    6.87  AlOOH
Ettr_GCA         -0.05   57.04   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -0.27    8.50    8.77  Al(OH)3
Gypsum           -1.39   -6.24   -4.85  CaSO4:2H2O
Gypsum_Cem       -1.64   -6.24   -4.60  CaSO4:2H2O
Lime            -13.21   19.59   32.80  CaO
Mirabilite       -8.03   -9.14   -1.11  Na2SO4:10H2O
O2(g)           -22.00   61.12   83.12  O2
Portlandite      -3.09   19.59   22.68  Ca(OH)2
Thenardite       -8.96   -9.14   -0.18  Na2SO4
```

```
Initial solution 36.AFt Exp 13

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

Elements           Molality       Moles

Al                7.770e-04   7.770e-04
Ca                8.250e-04   8.250e-04
Na                2.492e-01   2.492e-01
S(6)              1.225e-01   1.225e-01

----------------------------Description of solution----------------------------

                                       pH  =  11.529      Charge balance
                                       pe  =   4.000
                        Activity of water  =   0.994
                           Ionic strength  =   3.252e-01
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   8.181e-03
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =   3.886e-16
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                               Iterations  =   9
                                  Total H  = 1.110206e+02
                                  Total O  = 5.600440e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm              -4.44   68.12   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -0.62   56.83   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -2.17    8.21   10.38  Al(OH)3
Al2O3            -6.56   16.42   22.98  Al2O3
Al4(OH)10SO4    -14.61    8.09   22.70  Al4(OH)10SO4
AlOHSO4         -13.30  -16.53   -3.23  AlOHSO4
Anhydrite        -0.98   -5.62   -4.64  CaSO4
Boehmite         -0.37    8.21    8.58  AlOOH
C3AH6            -9.15   73.76   82.91  Ca3Al2(OH)12
C3AH6(C)         -5.69   73.76   79.45  Ca3Al2(OH)12
CH               -3.78   19.12   22.90  Ca(OH)2
Diaspore          1.34    8.21    6.87  AlOOH
Ettr_GCA         -0.27   56.83   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -0.56    8.21    8.77  Al(OH)3
Gypsum           -0.78   -5.63   -4.85  CaSO4:2H2O
Gypsum_Cem       -1.03   -5.63   -4.60  CaSO4:2H2O
Lime            -13.68   19.12   32.80  CaO
Mirabilite       -2.17   -3.29   -1.11  Na2SO4:10H2O
O2(g)           -21.01   62.11   83.12  O2
Portlandite      -3.56   19.12   22.68  Ca(OH)2
Thenardite       -3.08   -3.26   -0.18  Na2SO4

Initial solution 37.AFt Exp 14

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

Elements           Molality       Moles

Al                6.290e-04   6.290e-04
Ca                1.150e-03   1.150e-03
Na                9.930e-02   9.930e-02
S(6)              4.920e-02   4.920e-02

----------------------------Description of solution----------------------------

                                       pH  =  11.274      Charge balance
                                       pe  =   4.000
                        Activity of water  =   0.998
                           Ionic strength  =   1.375e-01
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   5.087e-03
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -3.319e-11
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   7
                                  Total H  = 1.110175e+02
                                  Total O  = 5.570810e+01
```

```
------------------------------Saturation indices-------------------------------
Phase               SI log IAP  log KT

AFm              -4.64   67.92   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -0.62   56.82   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -1.98    8.40   10.38  Al(OH)3
Al2O3            -6.17   16.81   22.98  Al2O3
Al4(OH)10SO4    -13.52    9.18   22.70  Al4(OH)10SO4
AlOHSO4         -12.80  -16.03   -3.23  AlOHSO4
Anhydrite        -0.91   -5.54   -4.64  CaSO4
Boehmite         -0.17    8.40    8.58  AlOOH
C3AH6            -9.43   73.47   82.91  Ca3Al2(OH)12
C3AH6(C)         -5.98   73.47   79.45  Ca3Al2(OH)12
CH               -4.01   18.89   22.90  Ca(OH)2
Diaspore          1.53    8.40    6.87  AlOOH
Ettr_GCA         -0.27   56.82   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -0.37    8.40    8.77  Al(OH)3
Gypsum           -0.70   -5.54   -4.85  CaSO4:2H2O
Gypsum_Cem       -0.94   -5.54   -4.60  CaSO4:2H2O
Lime            -13.91   18.89   32.80  CaO
Mirabilite       -3.08   -4.19   -1.11  Na2SO4:10H2O
O2(g)           -22.02   61.10   83.12  O2
Portlandite      -3.79   18.89   22.68  Ca(OH)2
Thenardite       -4.00   -4.18   -0.18  Na2SO4

Initial solution 38.AFt Exp 15

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

Elements           Molality       Moles

Al                5.920e-04   5.920e-04
Ca                1.500e-03   1.500e-03
Na                5.080e-02   5.080e-02
S(6)              2.600e-02   2.600e-02

----------------------------Description of solution----------------------------

                                       pH  =  10.971      Charge balance
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   7.428e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   3.576e-03
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -4.311e-13
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   8
                                  Total H  = 1.110160e+02
                                  Total O  = 5.561379e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm              -5.11   67.45   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -0.96   56.48   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -1.68    8.70   10.38  Al(OH)3
Al2O3            -5.57   17.41   22.98  Al2O3
Al4(OH)10SO4    -11.88   10.82   22.70  Al4(OH)10SO4
AlOHSO4         -12.06  -15.29   -3.23  AlOHSO4
Anhydrite        -0.84   -5.48   -4.64  CaSO4
Boehmite          0.13    8.70    8.58  AlOOH
C3AH6            -9.97   72.93   82.91  Ca3Al2(OH)12
C3AH6(C)         -6.52   72.93   79.45  Ca3Al2(OH)12
CH               -4.39   18.51   22.90  Ca(OH)2
Diaspore          1.83    8.70    6.87  AlOOH
Ettr_GCA         -0.61   56.48   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -0.07    8.70    8.77  Al(OH)3
Gypsum           -0.63   -5.48   -4.85  CaSO4:2H2O
Gypsum_Cem       -0.88   -5.48   -4.60  CaSO4:2H2O
Lime            -14.29   18.51   32.80  CaO
Mirabilite       -3.76   -4.87   -1.11  Na2SO4:10H2O
O2(g)           -23.24   59.88   83.12  O2
Portlandite      -4.17   18.51   22.68  Ca(OH)2
Thenardite       -4.69   -4.87   -0.18  Na2SO4
```

```
Initial solution 39.AFt Exp 16

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

Elements           Molality       Moles

Al                5.520e-04   5.520e-04
Ca                1.995e-03   1.995e-03
S(6)              8.100e-04   8.100e-04

----------------------------Description of solution----------------------------

                                       pH  =  11.207      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   6.158e-03
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   4.026e-03
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -2.385e-17
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   8
                                  Total H  = 1.110165e+02
                                  Total O  = 5.551348e+01

------------------------------Saturation indices-------------------------------


Phase               SI log IAP  log KT

AFm              -3.16   69.40   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -0.43   57.02   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -1.88    8.50   10.38  Al(OH)3
Al2O3            -5.98   17.00   22.98  Al2O3
Al4(OH)10SO4    -14.43    8.27   22.70  Al4(OH)10SO4
AlOHSO4         -14.00  -17.23   -3.23  AlOHSO4
Anhydrite        -1.56   -6.19   -4.64  CaSO4
Boehmite         -0.08    8.50    8.58  AlOOH
C3AH6            -7.31   75.60   82.91  Ca3Al2(OH)12
C3AH6(C)         -3.85   75.60   79.45  Ca3Al2(OH)12
CH               -3.37   19.53   22.90  Ca(OH)2
Diaspore          1.63    8.50    6.87  AlOOH
Ettr_GCA         -0.08   57.02   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -0.27    8.50    8.77  Al(OH)3
Gypsum           -1.35   -6.19   -4.85  CaSO4:2H2O
Gypsum_Cem       -1.59   -6.19   -4.60  CaSO4:2H2O
Lime            -13.26   19.53   32.80  CaO
O2(g)           -22.29   60.83   83.12  O2
Portlandite      -3.14   19.53   22.68  Ca(OH)2

Initial solution 40.Calculated Invariant point G (C3AH6 - AFt - CH)

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

Elements           Molality       Moles

Al                7.400e-05   7.400e-05
Ca                2.074e-02   2.074e-02
S(6)              3.400e-05   3.400e-05

----------------------------Description of solution----------------------------

                                       pH  =  12.454      Charge balance
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   4.987e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   4.163e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =   1.388e-10
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                               Iterations  =   4
                                  Total H  = 1.110541e+02
                                  Total O  = 5.554799e+01
```

```
------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm               1.20   73.76   72.56  Ca4Al2SO4(OH)12:6H2O
AFt               1.95   59.39   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -4.05    6.33   10.38  Al(OH)3
Al2O3           -10.32   12.66   22.98  Al2O3
Al4(OH)10SO4    -27.32   -4.62   22.70  Al4(OH)10SO4
AlOHSO4         -20.38  -23.61   -3.23  AlOHSO4
Anhydrite        -2.54   -7.18   -4.64  CaSO4
Boehmite         -2.25    6.33    8.58  AlOOH
C3AH6            -1.96   80.95   82.91  Ca3Al2(OH)12
C3AH6(C)          1.50   80.95   79.45  Ca3Al2(OH)12
CH               -0.14   22.76   22.90  Ca(OH)2
Diaspore         -0.54    6.33    6.87  AlOOH
Ettr_GCA          2.30   59.39   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -2.44    6.33    8.77  Al(OH)3
Gypsum           -2.33   -7.18   -4.85  CaSO4:2H2O
Gypsum_Cem       -2.58   -7.18   -4.60  CaSO4:2H2O
Lime            -10.03   22.76   32.80  CaO
O2(g)           -17.30   65.82   83.12  O2
Portlandite       0.09   22.76   22.68  Ca(OH)2


Initial solution 41.Calculated Invariant point H2 (C3AH6 - AFt - AH3)

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

Elements           Molality       Moles

Al                1.174e-03   1.174e-03
Ca                7.600e-03   7.600e-03
S(6)              7.400e-05   7.400e-05

----------------------------Description of solution----------------------------

                                       pH  =  12.039      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   2.039e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   1.857e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -1.659e-16
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   6
                                  Total H  = 1.110310e+02
                                  Total O  = 5.552509e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm               1.40   73.96   72.56  Ca4Al2SO4(OH)12:6H2O
AFt               2.61   60.05   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -2.41    7.97   10.38  Al(OH)3
Al2O3            -7.04   15.94   22.98  Al2O3
Al4(OH)10SO4    -19.43    3.27   22.70  Al4(OH)10SO4
AlOHSO4         -17.41  -20.64   -3.23  AlOHSO4
Anhydrite        -2.32   -6.95   -4.64  CaSO4
Boehmite         -0.61    7.97    8.58  AlOOH
C3AH6            -1.99   80.92   82.91  Ca3Al2(OH)12
C3AH6(C)          1.47   80.92   79.45  Ca3Al2(OH)12
CH               -1.24   21.66   22.90  Ca(OH)2
Diaspore          1.10    7.97    6.87  AlOOH
Ettr_GCA          2.96   60.05   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -0.80    7.97    8.77  Al(OH)3
Gypsum           -2.11   -6.95   -4.85  CaSO4:2H2O
Gypsum_Cem       -2.35   -6.95   -4.60  CaSO4:2H2O
Lime            -11.14   21.66   32.80  CaO
O2(g)           -18.97   64.15   83.12  O2
Portlandite      -1.02   21.66   22.68  Ca(OH)2

Initial solution 42.Calculated Invariant point F (CH - AFt - Gypsum)

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

Elements           Molality       Moles

Al                3.000e-07   3.000e-07
Ca                3.213e-02   3.213e-02
S(6)              1.224e-02   1.224e-02
```

```
----------------------------Description of solution----------------------------

                                       pH  =  12.407      Charge balance
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   7.437e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   3.978e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -1.749e-12
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   5
                                  Total H  = 1.110522e+02
                                  Total O  = 5.559496e+01


------------------------------Saturation indices------------------------------

Phase               SI log IAP  log KT

AFm              -0.93   71.63   72.56  Ca4Al2SO4(OH)12:6H2O
AFt               4.98   62.42   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -6.41    3.97   10.38  Al(OH)3
Al2O3           -15.04    7.94   22.98  Al2O3
Al4(OH)10SO4    -34.18  -11.48   22.70  Al4(OH)10SO4
AlOHSO4         -20.16  -23.39   -3.23  AlOHSO4
Anhydrite         0.04   -4.60   -4.64  CaSO4
Boehmite         -4.61    3.97    8.58  AlOOH
C3AH6            -6.67   76.24   82.91  Ca3Al2(OH)12
C3AH6(C)         -3.21   76.24   79.45  Ca3Al2(OH)12
CH               -0.13   22.77   22.90  Ca(OH)2
Diaspore         -2.90    3.97    6.87  AlOOH
Ettr_GCA          5.33   62.42   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -4.80    3.97    8.77  Al(OH)3
Gypsum            0.25   -4.60   -4.85  CaSO4:2H2O
Gypsum_Cem       -0.00   -4.60   -4.60  CaSO4:2H2O
Lime            -10.03   22.77   32.80  CaO
O2(g)           -17.49   65.63   83.12  O2
Portlandite       0.09   22.77   22.68  Ca(OH)2

Initial solution 43.Calculated Invariant point E2 (AH3 - AFt - Gypsum)

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

Elements           Molality       Moles

Al                1.780e-05   1.780e-05
Ca                1.534e-02   1.534e-02
S(6)              1.520e-02   1.520e-02

----------------------------Description of solution----------------------------

                                       pH  =  10.280      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   4.086e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   3.334e-04
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -1.177e-10
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   9
                                  Total H  = 1.110128e+02
                                  Total O  = 5.556735e+01
```

```
------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm              -6.53   66.03   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -0.62   56.83   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -2.49    7.89   10.38  Al(OH)3
Al2O3            -7.20   15.78   22.98  Al2O3
Al4(OH)10SO4    -14.02    8.68   22.70  Al4(OH)10SO4
AlOHSO4         -11.76  -14.99   -3.23  AlOHSO4
Anhydrite         0.04   -4.60   -4.64  CaSO4
Boehmite         -0.69    7.89    8.58  AlOOH
C3AH6           -12.28   70.63   82.91  Ca3Al2(OH)12
C3AH6(C)         -8.82   70.63   79.45  Ca3Al2(OH)12
CH               -4.62   18.28   22.90  Ca(OH)2
Diaspore          1.02    7.89    6.87  AlOOH
Ettr_GCA         -0.27   56.83   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -0.88    7.89    8.77  Al(OH)3
Gypsum            0.25   -4.60   -4.85  CaSO4:2H2O
Gypsum_Cem        0.00   -4.60   -4.60  CaSO4:2H2O
Lime            -14.51   18.28   32.80  CaO
O2(g)           -26.00   57.12   83.12  O2
Portlandite      -4.39   18.28   22.68  Ca(OH)2

Initial solution 44.Jones Invariant point G(J) (C3AH6 - AFt - CH)

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

Elements           Molality       Moles

Al                1.000e-05   1.000e-05
Ca                1.917e-02   1.917e-02
S(6)              1.800e-04   1.800e-04


----------------------------Description of solution----------------------------

                                       pH  =  12.423      Charge balance
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   4.653e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   3.801e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =   2.242e-10
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                               Iterations  =   4
                                  Total H  = 1.110504e+02
                                  Total O  = 5.554495e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm              -0.00   72.56   72.56  Ca4Al2SO4(OH)12:6H2O
AFt               2.18   59.62   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -4.89    5.49   10.38  Al(OH)3
Al2O3           -11.99   10.99   22.98  Al2O3
Al4(OH)10SO4    -29.87   -7.17   22.70  Al4(OH)10SO4
AlOHSO4         -20.42  -23.65   -3.23  AlOHSO4
Anhydrite        -1.83   -6.46   -4.64  CaSO4
Boehmite         -3.08    5.49    8.58  AlOOH
C3AH6            -3.88   79.03   82.91  Ca3Al2(OH)12
C3AH6(C)         -0.43   79.03   79.45  Ca3Al2(OH)12
CH               -0.22   22.68   22.90  Ca(OH)2
Diaspore         -1.38    5.49    6.87  AlOOH
Ettr_GCA          2.53   59.62   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -3.28    5.49    8.77  Al(OH)3
Gypsum           -1.62   -6.47   -4.85  CaSO4:2H2O
Gypsum_Cem       -1.87   -6.47   -4.60  CaSO4:2H2O
Lime            -10.12   22.68   32.80  CaO
O2(g)           -17.43   65.69   83.12  O2
Portlandite       0.00   22.68   22.68  Ca(OH)2
```

```
Initial solution 45.Jones Invariant point H2(J) (C3AH6 - AFt - AH3)

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

Elements           Molality       Moles

Al                9.000e-05   9.000e-05
Ca                3.495e-03   3.495e-03
S(6)              3.750e-04   3.750e-04

----------------------------Description of solution----------------------------

                                       pH  =  11.719      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   9.914e-03
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   6.510e-03
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -4.909e-11
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   6
                                  Total H  = 1.110189e+02
                                  Total O  = 5.551423e+01

------------------------------Saturation indices-------------------------------

Phase               SI  log IAP  log KT

AFm              -2.28   70.28   72.56  Ca4Al2SO4(OH)12:6H2O
AFt               0.05   57.50   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -3.19    7.19   10.38  Al(OH)3
Al2O3            -8.60   14.38   22.98  Al2O3
Al4(OH)10SO4    -21.09    1.61   22.70  Al4(OH)10SO4
AlOHSO4         -16.73  -19.96   -3.23  AlOHSO4
Anhydrite        -1.75   -6.39   -4.64  CaSO4
Boehmite         -1.39    7.19    8.58  AlOOH
C3AH6            -6.24   76.67   82.91  Ca3Al2(OH)12
C3AH6(C)         -2.78   76.67   79.45  Ca3Al2(OH)12
CH               -2.14   20.76   22.90  Ca(OH)2
Diaspore          0.32    7.19    6.87  AlOOH
Ettr_GCA          0.40   57.50   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -1.58    7.19    8.77  Al(OH)3
Gypsum           -1.54   -6.39   -4.85  CaSO4:2H2O
Gypsum_Cem       -1.79   -6.39   -4.60  CaSO4:2H2O
Lime            -12.03   20.76   32.80  CaO
O2(g)           -20.24   62.88   83.12  O2
Portlandite      -1.91   20.76   22.68  Ca(OH)2

Initial solution 46.Jones Invariant point F(J) (CH - AFt - Gypsum)

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

Elements           Molality       Moles

Al                6.000e-05   6.000e-05
Ca                3.156e-02   3.156e-02
S(6)              1.233e-02   1.233e-02

----------------------------Description of solution----------------------------

                                       pH  =  12.393      Charge balance
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   7.327e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   3.864e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -2.756e-12
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   5
                                  Total H  = 1.110511e+02
                                  Total O  = 5.559418e+01
```

```
------------------------------Saturation indices-------------------------------

Phase               SI  log IAP  log KT

AFm               3.61   76.17   72.56  Ca4Al2SO4(OH)12:6H2O
AFt               9.52   66.96   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -4.09    6.29   10.38  Al(OH)3
Al2O3           -10.40   12.58   22.98  Al2O3
Al4(OH)10SO4    -24.88   -2.18   22.70  Al4(OH)10SO4
AlOHSO4         -17.82  -21.05   -3.23  AlOHSO4
Anhydrite         0.04   -4.60   -4.64  CaSO4
Boehmite         -2.29    6.29    8.58  AlOOH
C3AH6            -2.13   80.77   82.91  Ca3Al2(OH)12
C3AH6(C)          1.32   80.77   79.45  Ca3Al2(OH)12
CH               -0.17   22.73   22.90  Ca(OH)2
Diaspore         -0.59    6.29    6.87  AlOOH
Ettr_GCA          9.87   66.96   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -2.48    6.29    8.77  Al(OH)3
Gypsum            0.25   -4.60   -4.85  CaSO4:2H2O
Gypsum_Cem       -0.00   -4.60   -4.60  CaSO4:2H2O
Lime            -10.06   22.73   32.80  CaO
O2(g)           -17.55   65.57   83.12  O2
Portlandite       0.06   22.73   22.68  Ca(OH)2

Initial solution 47.Jones Invariant point E2(J) (AH3 - AFt - Gypsum)

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

Elements           Molality       Moles

Al                2.500e-05   2.500e-05
Ca                1.565e-02   1.565e-02
S(6)              1.497e-02   1.497e-02

----------------------------Description of solution----------------------------

                                       pH  =  10.983      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   4.142e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   1.425e-03
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -1.626e-13
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   8
                                  Total H  = 1.110139e+02
                                  Total O  = 5.556752e+01


------------------------------Saturation indices-------------------------------

Phase               SI  log IAP  log KT

AFm              -3.41   69.15   72.56  Ca4Al2SO4(OH)12:6H2O
AFt               2.50   59.94   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -3.04    7.34   10.38  Al(OH)3
Al2O3            -8.31   14.67   22.98  Al2O3
Al4(OH)10SO4    -17.65    5.05   22.70  Al4(OH)10SO4
AlOHSO4         -13.73  -16.96   -3.23  AlOHSO4
Anhydrite         0.03   -4.60   -4.64  CaSO4
Boehmite         -1.24    7.34    8.58  AlOOH
C3AH6            -9.15   73.76   82.91  Ca3Al2(OH)12
C3AH6(C)         -5.70   73.76   79.45  Ca3Al2(OH)12
CH               -3.21   19.69   22.90  Ca(OH)2
Diaspore          0.46    7.34    6.87  AlOOH
Ettr_GCA          2.85   59.94   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -1.43    7.34    8.77  Al(OH)3
Gypsum            0.25   -4.60   -4.85  CaSO4:2H2O
Gypsum_Cem       -0.00   -4.60   -4.60  CaSO4:2H2O
Lime            -13.10   19.69   32.80  CaO
O2(g)           -23.19   59.93   83.12  O2
Portlandite      -2.98   19.69   22.68  Ca(OH)2
```

```
Initial solution 48.D'Ans and Eick Invariant point G(E) (C3AH6 - AFt - CH)

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

Elements           Molality       Moles

Al                2.500e-05   2.500e-05
Ca                2.146e-02   2.146e-02
S(6)              1.070e-04   1.070e-04

----------------------------Description of solution----------------------------

                                       pH  =  12.634      Charge balance
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   5.162e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   4.278e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  20.000
                  Electrical balance (eq)  =   1.565e-11
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                               Iterations  =   4
                                  Total H  = 1.110552e+02
                                  Total O  = 5.554943e+01

------------------------------Saturation indices-------------------------------

Phase               SI  log IAP  log KT

AFm               0.87   75.20   74.33  Ca4Al2SO4(OH)12:6H2O
AFt               2.64   61.85   59.21  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -4.49    6.23   10.72  Al(OH)3
Al2O3           -10.52   12.46   22.98  Al2O3
Al4(OH)10SO4    -27.59   -4.89   22.70  Al4(OH)10SO4
AlOHSO4         -20.35  -23.58   -3.23  AlOHSO4
Anhydrite        -2.08   -6.67   -4.59  CaSO4
Boehmite         -2.70    6.23    8.93  AlOOH
C3AH6            -3.04   81.87   84.91  Ca3Al2(OH)12
C3AH6(C)          0.65   81.87   81.22  Ca3Al2(OH)12
CH               -0.15   23.14   23.28  Ca(OH)2
Diaspore         -0.95    6.23    7.18  AlOOH
Ettr_GCA          3.60   61.85   58.25  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -2.83    6.23    9.06  Al(OH)3
Gypsum           -1.82   -6.67   -4.85  CaSO4:2H2O
Gypsum_Cem       -2.07   -6.67   -4.60  CaSO4:2H2O
Lime            -10.24   23.14   33.38  CaO
O2(g)           -18.26   66.54   84.79  O2
Portlandite       0.08   23.14   23.06  Ca(OH)2


Initial solution 49.D'Ans and Eick Invariant point H2(E) (C3AH6 - AFt - AH3)

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

Elements           Molality       Moles

Al                1.580e-04   1.580e-04
Ca                3.103e-03   3.103e-03
S(6)              2.630e-04   2.630e-04

----------------------------Description of solution----------------------------

                                       pH  =  11.844      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   8.863e-03
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   6.154e-03
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  20.000
                  Electrical balance (eq)  =  -4.361e-13
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   6
                                  Total H  = 1.110186e+02
                                  Total O  = 5.551342e+01
```

```
------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm              -2.23   72.10   74.33  Ca4Al2SO4(OH)12:6H2O
AFt              -0.24   58.97   59.21  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -2.85    7.86   10.72  Al(OH)3
Al2O3            -7.25   15.73   22.98  Al2O3
Al4(OH)10SO4    -18.78    3.92   22.70  Al4(OH)10SO4
AlOHSO4         -16.44  -19.67   -3.23  AlOHSO4
Anhydrite        -1.97   -6.56   -4.59  CaSO4
Boehmite         -1.07    7.86    8.93  AlOOH
C3AH6            -6.25   78.66   84.91  Ca3Al2(OH)12
C3AH6(C)         -2.56   78.66   81.22  Ca3Al2(OH)12
CH               -2.31   20.98   23.28  Ca(OH)2
Diaspore          0.68    7.86    7.18  AlOOH
Ettr_GCA          0.72   58.97   58.25  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -1.19    7.86    9.06  Al(OH)3
Gypsum           -1.71   -6.56   -4.85  CaSO4:2H2O
Gypsum_Cem       -1.96   -6.56   -4.60  CaSO4:2H2O
Lime            -12.40   20.98   33.38  CaO
O2(g)           -21.42   63.38   84.79  O2
Portlandite      -2.08   20.98   23.06  Ca(OH)2

Initial solution 50.D'Ans and Eick Invariant point F(E) (CH - AFt - Gypsum)

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

Elements           Molality       Moles

Al                2.700e-05   2.700e-05
Ca                3.280e-02   3.280e-02
S(6)              1.220e-02   1.220e-02

----------------------------Description of solution----------------------------

                                       pH  =  12.589      Charge balance
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   7.620e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   4.128e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  20.000
                  Electrical balance (eq)  =  -4.256e-13
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   5
                                  Total H  = 1.110537e+02
                                  Total O  = 5.559630e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm               3.09   77.42   74.33  Ca4Al2SO4(OH)12:6H2O
AFt               9.02   68.23   59.21  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -4.42    6.29   10.72  Al(OH)3
Al2O3           -10.39   12.59   22.98  Al2O3
Al4(OH)10SO4    -25.25   -2.55   22.70  Al4(OH)10SO4
AlOHSO4         -18.21  -21.44   -3.23  AlOHSO4
Anhydrite         0.00   -4.59   -4.59  CaSO4
Boehmite         -2.63    6.29    8.93  AlOOH
C3AH6            -2.90   82.01   84.91  Ca3Al2(OH)12
C3AH6(C)          0.79   82.01   81.22  Ca3Al2(OH)12
CH               -0.14   23.14   23.28  Ca(OH)2
Diaspore         -0.89    6.29    7.18  AlOOH
Ettr_GCA          9.98   68.23   58.25  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -2.76    6.29    9.06  Al(OH)3
Gypsum            0.26   -4.59   -4.85  CaSO4:2H2O
Gypsum_Cem        0.01   -4.59   -4.60  CaSO4:2H2O
Lime            -10.23   23.14   33.38  CaO
O2(g)           -18.44   66.36   84.79  O2
Portlandite       0.08   23.14   23.06  Ca(OH)2

Initial solution 51.D'Ans and Eick Invariant point E2(E) (AH3 - AFt - Gypsum)

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

Elements           Molality       Moles

Al                9.000e-05   9.000e-05
Ca                1.514e-02   1.514e-02
S(6)              1.482e-02   1.482e-02
```

```
----------------------------Description of solution----------------------------

                                       pH  =  10.765      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   4.071e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   9.020e-04
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  20.000
                  Electrical balance (eq)  =  -6.227e-11
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   8
                                  Total H  = 1.110133e+02
                                  Total O  = 5.556640e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm              -3.85   70.48   74.33  Ca4Al2SO4(OH)12:6H2O
AFt               2.07   61.28   59.21  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -2.06    8.66   10.72  Al(OH)3
Al2O3            -5.66   17.32   22.98  Al2O3
Al4(OH)10SO4    -11.91   10.79   22.70  Al4(OH)10SO4
AlOHSO4         -11.96  -15.19   -3.23  AlOHSO4
Anhydrite        -0.01   -4.60   -4.59  CaSO4
Boehmite         -0.27    8.66    8.93  AlOOH
C3AH6            -9.82   75.08   84.91  Ca3Al2(OH)12
C3AH6(C)         -6.14   75.08   81.22  Ca3Al2(OH)12
CH               -4.03   19.25   23.28  Ca(OH)2
Diaspore          1.48    8.66    7.18  AlOOH
Ettr_GCA          3.03   61.28   58.25  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -0.39    8.66    9.06  Al(OH)3
Gypsum            0.25   -4.60   -4.85  CaSO4:2H2O
Gypsum_Cem        0.00   -4.60   -4.60  CaSO4:2H2O
Lime            -14.12   19.25   33.38  CaO
O2(g)           -25.73   59.06   84.79  O2
Portlandite      -3.80   19.25   23.06  Ca(OH)2

Initial solution 52.Jones Invariant point G(J) (C3AH6 - AFt - CH)

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

Elements           Molality       Moles

Al                8.500e-05   8.500e-05
Ca                1.620e-03   1.620e-03
Na                2.500e-01   2.500e-01
S(6)              9.300e-04   9.300e-04

----------------------------Description of solution----------------------------

                                       pH  =  13.238      Charge balance
                                       pe  =   4.000
                        Activity of water  =   0.991
                           Ionic strength  =   2.532e-01
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   2.516e-01
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -3.233e-13
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   5
                                  Total H  = 1.112641e+02
                                  Total O  = 5.576157e+01
```

```
------------------------------Saturation indices-------------------------------

Phase               SI  log IAP  log KT

AFm              -0.80   71.76   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -0.78   56.67   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -4.83    5.55   10.38  Al(OH)3
Al2O3           -11.87   11.11   22.98  Al2O3
Al4(OH)10SO4    -30.75   -8.05   22.70  Al4(OH)10SO4
AlOHSO4         -21.46  -24.69   -3.23  AlOHSO4
Anhydrite        -2.87   -7.51   -4.64  CaSO4
Boehmite         -3.03    5.55    8.58  AlOOH
C3AH6            -3.61   79.29   82.91  Ca3Al2(OH)12
C3AH6(C)         -0.16   79.29   79.45  Ca3Al2(OH)12
CH               -0.17   22.73   22.90  Ca(OH)2
Diaspore         -1.32    5.55    6.87  AlOOH
Ettr_GCA         -0.43   56.67   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -3.22    5.55    8.77  Al(OH)3
Gypsum           -2.67   -7.52   -4.85  CaSO4:2H2O
Gypsum_Cem       -2.92   -7.52   -4.60  CaSO4:2H2O
Lime            -10.06   22.74   32.80  CaO
Mirabilite       -4.17   -5.29   -1.11  Na2SO4:10H2O
O2(g)           -14.18   68.94   83.12  O2
Portlandite       0.06   22.73   22.68  Ca(OH)2
Thenardite       -5.07   -5.25   -0.18  Na2SO4

Initial solution 53.Jones Invariant point H2(J) (C3AH6 - AFt - AH3)

-----------------------------Solution composition------------------------------
Elements           Molality       Moles

Al                1.680e-02   1.680e-02
Ca                1.000e-06   1.000e-06
Na                2.500e-01   2.500e-01
S(6)              6.060e-02   6.060e-02

----------------------------Description of solution----------------------------

                                       pH  =  12.882      Charge balance
                                       pe  =   4.000
                        Activity of water  =   0.993
                           Ionic strength  =   2.851e-01
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   1.792e-01
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -7.643e-13
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   6
                                  Total H  = 1.111916e+02
                                  Total O  = 5.592782e+01

------------------------------Saturation indices-------------------------------
Phase               SI  log IAP  log KT

AFm              -8.43   64.13   72.56  Ca4Al2SO4(OH)12:6H2O
AFt             -11.08   46.36   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -2.19    8.19   10.38  Al(OH)3
Al2O3            -6.58   16.40   22.98  Al2O3
Al4(OH)10SO4    -17.65    5.05   22.70  Al4(OH)10SO4
AlOHSO4         -16.30  -19.53   -3.23  AlOHSO4
Anhydrite        -4.22   -8.86   -4.64  CaSO4
Boehmite         -0.38    8.20    8.58  AlOOH
C3AH6            -9.90   73.01   82.91  Ca3Al2(OH)12
C3AH6(C)         -6.45   73.01   79.45  Ca3Al2(OH)12
CH               -4.03   18.87   22.90  Ca(OH)2
Diaspore          1.32    8.20    6.87  AlOOH
Ettr_GCA        -10.73   46.36   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -0.58    8.19    8.77  Al(OH)3
Gypsum           -4.01   -8.86   -4.85  CaSO4:2H2O
Gypsum_Cem       -4.26   -8.86   -4.60  CaSO4:2H2O
Lime            -13.92   18.88   32.80  CaO
Mirabilite       -2.42   -3.53   -1.11  Na2SO4:10H2O
O2(g)           -15.60   67.52   83.12  O2
Portlandite      -3.80   18.87   22.68  Ca(OH)2
Thenardite       -3.32   -3.50   -0.18  Na2SO4
```

```
Initial solution 54.Jones Invariant point F(J) (CH - AFt - Gypsum)

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

Elements           Molality       Moles

Al                2.500e-05   2.500e-05
Ca                1.539e-02   1.539e-02
Na                2.500e-01   2.500e-01
S(6)              9.390e-02   9.390e-02

----------------------------Description of solution-----------------------------

                                       pH  =  12.775      Charge balance
                                       pe  =   4.000
                        Activity of water  =   0.993
                           Ionic strength  =   3.255e-01
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   9.305e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =   1.531e-13
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                               Iterations  =   6
                                  Total H  = 1.111055e+02
                                  Total O  = 5.597487e+01

------------------------------Saturation indices--------------------------------

Phase               SI log IAP  log KT

AFm               2.30   74.86   72.56  Ca4Al2SO4(OH)12:6H2O
AFt               8.28   65.72   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -4.91    5.47   10.38  Al(OH)3
Al2O3           -12.03   10.95   22.98  Al2O3
Al4(OH)10SO4    -28.20   -5.50   22.70  Al4(OH)10SO4
AlOHSO4         -18.67  -21.90   -3.23  AlOHSO4
Anhydrite         0.10   -4.54   -4.64  CaSO4
Boehmite         -3.11    5.47    8.58  AlOOH
C3AH6            -3.48   79.42   82.91  Ca3Al2(OH)12
C3AH6(C)         -0.03   79.42   79.45  Ca3Al2(OH)12
CH               -0.07   22.83   22.90  Ca(OH)2
Diaspore         -1.40    5.47    6.87  AlOOH
Ettr_GCA          8.63   65.72   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -3.30    5.47    8.77  Al(OH)3
Gypsum            0.30   -4.55   -4.85  CaSO4:2H2O
Gypsum_Cem        0.05   -4.55   -4.60  CaSO4:2H2O
Lime             -9.96   22.83   32.80  CaO
Mirabilite       -2.29   -3.41   -1.11  Na2SO4:10H2O
O2(g)           -16.03   67.09   83.12  O2
Portlandite       0.15   22.83   22.68  Ca(OH)2
Thenardite       -3.20   -3.38   -0.18  Na2SO4

Initial solution 55.Jones Invariant point E2(J) (AH3 - AFt - Gypsum)

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

Elements           Molality       Moles

Al                1.400e-04   1.400e-04
Ca                1.017e-02   1.017e-02
Na                2.500e-01   2.500e-01
S(6)              1.347e-01   1.347e-01

----------------------------Description of solution-----------------------------

                                       pH  =  10.712      Charge balance
                                       pe  =   4.000
                        Activity of water  =   0.994
                           Ionic strength  =   3.435e-01
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   1.360e-03
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -2.011e-09
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   8
                                  Total H  = 1.110138e+02
                                  Total O  = 5.604638e+01
```

```
------------------------------Saturation indices-------------------------------

Phase               SI  log IAP  log KT

AFm              -4.84   67.72   72.56  Ca4Al2SO4(OH)12:6H2O
AFt               1.19   58.63   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -2.10    8.28   10.38  Al(OH)3
Al2O3            -6.42   16.56   22.98  Al2O3
Al4(OH)10SO4    -12.68   10.02   22.70  Al4(OH)10SO4
AlOHSO4         -11.58  -14.81   -3.23  AlOHSO4
Anhydrite         0.12   -4.52   -4.64  CaSO4
Boehmite         -0.30    8.28    8.58  AlOOH
C3AH6           -10.65   72.26   82.91  Ca3Al2(OH)12
C3AH6(C)         -7.19   72.26   79.45  Ca3Al2(OH)12
CH               -4.33   18.57   22.90  Ca(OH)2
Diaspore          1.41    8.28    6.87  AlOOH
Ettr_GCA          1.54   58.63   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -0.49    8.28    8.77  Al(OH)3
Gypsum            0.32   -4.52   -4.85  CaSO4:2H2O
Gypsum_Cem        0.08   -4.52   -4.60  CaSO4:2H2O
Lime            -14.23   18.57   32.80  CaO
Mirabilite       -2.16   -3.28   -1.11  Na2SO4:10H2O
O2(g)           -24.28   58.84   83.12  O2
Portlandite      -4.11   18.57   22.68  Ca(OH)2
Thenardite       -3.07   -3.25   -0.18  Na2SO4

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End of simulation.
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```

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Reading input data for simulation 4.
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TITLE  The System CaO-Al2O3-CaSO4-H2O-SiO2-MgO
       Ref: Atkins, Glasser, Kindness, Cement and Concrete Research, 1992,
       Vol 22, No 2/3, 241-246
SOLUTION 56  AFt
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              1.47
        Si              0.0
        Al              0.45
        S(6)            1.00
        Mg              0.0
SOLUTION 57  Hydrogarnet, HG = C3AH6
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              6.14
        Si              0.0
        Al              4.57
        S(6)            0.0
        Mg              0.0
SOLUTION 58  AFm Dispersion 2
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              6.84
        Si              0.0
        Al              3.52
        S(6)            0.01
        Mg              0.0
SOLUTION 59  AFm Dispersion 5
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              5.05
        Si              0.0
        Al              2.70
        S(6)            0.018
        Mg              0.0
SOLUTION 60  Gehlenite GH Dispersion 1
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              2.00
        Si              0.01
        Al              0.97
        S(6)            0.0
        Mg              0.0
SOLUTION 61  Gehlenite GH Dispersion 6
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              0.91
        Si              0.027
        Al              0.61
        S(6)            0.0
        Mg              0.0
SOLUTION 62  Tobermorite Tob Dispersion 2
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              1.01
        Si              0.343
        Al              0.0
        S(6)            0.0
        Mg              0.0
```

```
SOLUTION 63  Tobermorite Tob Dispersion 7
        units   mmol/kgw
        pH      12.734 -charge
        density 1.0
        temp    25.0
        Ca              0.48
        Si              0.393
        Al              0.0
        S(6)            0.0
        Mg              0.0
SOLUTION 64  Hydrotalcite HT Dispersion 3 Tentative Ksp = -119.3 for M4AH10
        units   mmol/kgw
        pH      9.3
        density 1.0
        temp    25.0
        Ca              0.0
        Si              0.0
        Al              0.014
        S(6)            0.0
        Mg              0.033
SOLUTION 65  Hydrotalcite HT Dispersion 5
        units   mmol/kgw
        pH      9.3 -charge
        density 1.0
        temp    25.0
        Ca              0.0
        Si              0.0
        Al              0.008
        S(6)            0.0
        Mg              0.060
SOLUTION 66  CSH 0.9
        units   mmol/kgw
        pH      12.6 -charge
        density 1.0
        temp    25.0
        Ca              1.67
        Si              0.135
        Al              0.0
        S(6)            0.0
        Mg              0.0
SOLUTION 67  CSH 1.3
        units   mmol/kgw
        pH      12.6 -charge
        density 1.0
        temp    25.0
        Ca              9.75
        Si              0.012
        Al              0.0
        S(6)            0.0
        Mg              0.0
SOLUTION 68  CSH 1.7
        units   mmol/kgw
        pH      12.6 -charge
        density 1.0
        temp    25.0
        Ca             20.34
        Si              0.006
        Al              0.0
        S(6)            0.0
        Mg              0.0
END
```

```
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TITLE
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  The System CaO-Al2O3-CaSO4-H2O-SiO2-MgO
       Ref: Atkins, Glasser, Kindness, Cement and Concrete Research, 1992,
       Vol 22, No 2/3, 241-246

-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 56.AFt

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

Elements           Molality       Moles

Al                4.500e-04   4.500e-04
Ca                1.470e-03   1.470e-03
S(6)              1.000e-03   1.000e-03

----------------------------Description of solution----------------------------

                                       pH  =  10.645      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   4.863e-03
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   2.290e-03
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -4.484e-15
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   9
                                  Total H  = 1.110147e+02
                                  Total O  = 5.551251e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm              -5.94   66.62   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -3.20   54.24   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -1.40    8.98   10.38  Al(OH)3
Al2O3            -5.03   17.95   22.98  Al2O3
Al4(OH)10SO4    -11.28   11.42   22.70  Al4(OH)10SO4
AlOHSO4         -12.27  -15.50   -3.23  AlOHSO4
Anhydrite        -1.56   -6.19   -4.64  CaSO4
Boehmite          0.40    8.98    8.58  AlOOH
C3AH6           -10.09   72.82   82.91  Ca3Al2(OH)12
C3AH6(C)         -6.63   72.82   79.45  Ca3Al2(OH)12
CH               -4.61   18.29   22.90  Ca(OH)2
Diaspore          2.10    8.98    6.87  AlOOH
Ettr_GCA         -2.85   54.24   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)       0.21    8.98    8.77  Al(OH)3
Gypsum           -1.34   -6.19   -4.85  CaSO4:2H2O
Gypsum_Cem       -1.59   -6.19   -4.60  CaSO4:2H2O
Lime            -14.51   18.29   32.80  CaO
O2(g)           -24.54   58.58   83.12  O2
Portlandite      -4.39   18.29   22.68  Ca(OH)2

Initial solution 57.Hydrogarnet, HG = C3AH6

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

Elements           Molality       Moles

Al                4.570e-03   4.570e-03
Ca                6.140e-03   6.140e-03

----------------------------Description of solution----------------------------

                                       pH  =  11.792      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   1.721e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   2.599e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -3.043e-12
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   6
```

```
                                  Total H  = 1.110384e+02
                                  Total O  = 5.553221e+01

------------------------------Saturation indices------------------------------

Phase               SI log IAP  log KT

Al(OH)3(a)       -1.57    8.81   10.38  Al(OH)3
Al2O3            -5.35   17.63   22.98  Al2O3
Boehmite          0.23    8.81    8.58  AlOOH
C3AH6            -1.93   80.98   82.91  Ca3Al2(OH)12
C3AH6(C)          1.52   80.98   79.45  Ca3Al2(OH)12
CH               -1.78   21.12   22.90  Ca(OH)2
Diaspore          1.94    8.81    6.87  AlOOH
Gibbsite(C)       0.04    8.81    8.77  Al(OH)3
Lime            -11.68   21.12   32.80  CaO
O2(g)           -19.95   63.17   83.12  O2
Portlandite      -1.56   21.12   22.68  Ca(OH)2

Initial solution 58.AFm Dispersion 2

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

Elements           Molality       Moles

Al                3.520e-03   3.520e-03
Ca                6.840e-03   6.840e-03
S(6)              1.000e-05   1.000e-05

----------------------------Description of solution----------------------------

                                       pH  =  11.906      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   1.884e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   2.422e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -3.270e-14
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   6
                                  Total H  = 1.110367e+02
                                  Total O  = 5.553048e+01

------------------------------Saturation indices------------------------------

Phase               SI log IAP  log KT

AFm               0.89   73.45   72.56  Ca4Al2SO4(OH)12:6H2O
AFt               0.35   57.79   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -1.80    8.58   10.38  Al(OH)3
Al2O3            -5.81   17.17   22.98  Al2O3
Al4(OH)10SO4    -17.58    5.12   22.70  Al4(OH)10SO4
AlOHSO4         -17.39  -20.62   -3.23  AlOHSO4
Anhydrite        -3.19   -7.83   -4.64  CaSO4
Boehmite          0.00    8.58    8.58  AlOOH
C3AH6            -1.62   81.28   82.91  Ca3Al2(OH)12
C3AH6(C)          1.83   81.28   79.45  Ca3Al2(OH)12
CH               -1.53   21.37   22.90  Ca(OH)2
Diaspore          1.71    8.58    6.87  AlOOH
Ettr_GCA          0.70   57.79   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -0.19    8.58    8.77  Al(OH)3
Gypsum           -2.98   -7.83   -4.85  CaSO4:2H2O
Gypsum_Cem       -3.23   -7.83   -4.60  CaSO4:2H2O
Lime            -11.42   21.37   32.80  CaO
O2(g)           -19.50   63.62   83.12  O2
Portlandite      -1.30   21.37   22.68  Ca(OH)2
```

```
Initial solution 59.AFm Dispersion 5

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

Elements           Molality       Moles

Al                2.700e-03   2.700e-03
Ca                5.050e-03   5.050e-03
S(6)              1.800e-05   1.800e-05


----------------------------Description of solution----------------------------

                                       pH  =  11.782      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   1.415e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   1.816e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -4.982e-12
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   6
                                  Total H  = 1.110306e+02
                                  Total O  = 5.552445e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm               0.09   72.65   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -0.05   57.40   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -1.78    8.60   10.38  Al(OH)3
Al2O3            -5.78   17.20   22.98  Al2O3
Al4(OH)10SO4    -16.96    5.74   22.70  Al4(OH)10SO4
AlOHSO4         -16.82  -20.05   -3.23  AlOHSO4
Anhydrite        -2.99   -7.63   -4.64  CaSO4
Boehmite          0.02    8.60    8.58  AlOOH
C3AH6            -2.63   80.28   82.91  Ca3Al2(OH)12
C3AH6(C)          0.82   80.28   79.45  Ca3Al2(OH)12
CH               -1.87   21.03   22.90  Ca(OH)2
Diaspore          1.73    8.60    6.87  AlOOH
Ettr_GCA          0.30   57.40   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -0.17    8.60    8.77  Al(OH)3
Gypsum           -2.78   -7.63   -4.85  CaSO4:2H2O
Gypsum_Cem       -3.03   -7.63   -4.60  CaSO4:2H2O
Lime            -11.77   21.03   32.80  CaO
O2(g)           -19.99   63.13   83.12  O2
Portlandite      -1.65   21.03   22.68  Ca(OH)2

Initial solution 60.Gehlenite GH Dispersion 1

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

Elements           Molality       Moles

Al                9.700e-04   9.700e-04
Ca                2.000e-03   2.000e-03
Si                1.000e-05   1.000e-05

----------------------------Description of solution----------------------------

                                       pH  =  11.427      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   5.801e-03
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   6.910e-03
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -3.872e-13
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   7
                                  Total H  = 1.110194e+02
                                  Total O  = 5.551315e+01
```

```
-----------------------------Saturation indices------------------------------

Phase               SI log IAP  log KT

Al(OH)3(a)       -1.86    8.52   10.38  Al(OH)3
Al2O3            -5.93   17.05   22.98  Al2O3
Anorthite        -1.92   23.51   25.43  CaAl2Si2O8
Boehmite         -0.05    8.53    8.58  AlOOH
C3AH6            -5.86   77.04   82.91  Ca3Al2(OH)12
C3AH6(C)         -2.41   77.04   79.45  Ca3Al2(OH)12
Ca-Olivine       -4.42   33.23   37.65  Ca2SiO4
Ca3SiO5         -20.64   53.23   73.87  Ca3SiO5
CH               -2.90   20.00   22.90  Ca(OH)2
Chalcedony       -3.25   -6.77   -3.52  SiO2
Cristobalite     -3.18   -6.77   -3.59  SiO2
CSH_0.8          -1.85    9.23   11.08  Ca0.8SiO2.8:H2O
CSH_1.1          -1.49   15.23   16.72  Ca1.1SiO3.1:H2O
CSH_1.8          -3.47   29.23   32.70  Ca1.8SiO3.8:H2O
Diaspore          1.65    8.53    6.87  AlOOH
Gehlenite        -6.54   50.28   56.82  Ca2Al2SiO7
Gibbsite(C)      -0.25    8.52    8.77  Al(OH)3
Halloysite       -5.48    3.51    8.99  Al2Si2O5(OH)4
Kaolinite        -2.21    3.51    5.73  Al2Si2O5(OH)4
Larnite          -5.91   33.23   39.14  Ca2SiO4
Laumontite       -4.49    9.97   14.46  CaAl2Si4O12:4H2O
Leonhardite       3.45   19.94   16.49  Ca2Al4Si8O24:7H2O
Lime            -12.80   20.00   32.80  CaO
O2(g)           -21.41   61.71   83.12  O2
P-Wollstanite    -0.62   13.23   13.85  CaSiO3
Portlandite      -2.68   20.00   22.68  Ca(OH)2
Pyrophyllite     -8.43  -10.03   -1.60  Al2Si4O10(OH)2
Quartz           -2.76   -6.77   -4.01  SiO2
SiO2(a)          -3.75   -6.77   -3.02  SiO2
SiO2(am)         -4.06   -6.77   -2.71  SiO2
SiO2gel(am)      -3.92   -6.77   -2.85  SiO2
Tob              -6.60   59.38   65.98  Ca5Si6O17:5H2O
Wairakite        -8.90    9.97   18.87  CaAl2Si4O12:2H2O
Wollastonite      0.23   13.23   13.00  CaSiO3

Initial solution 61.Gehlenite GH Dispersion 6

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

Elements           Molality       Moles

Al                6.100e-04   6.100e-04
Ca                9.100e-04   9.100e-04
Si                2.700e-05   2.700e-05

----------------------------Description of solution----------------------------

                                       pH  =  11.037      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   2.694e-03
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   3.650e-03
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -4.848e-14
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   8
                                  Total H  = 1.110161e+02
                                  Total O  = 5.550994e+01
```

```
------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

Al(OH)3(a)       -1.66    8.72   10.38  Al(OH)3
Al2O3            -5.53   17.45   22.98  Al2O3
Anorthite        -0.71   24.72   25.43  CaAl2Si2O8
Boehmite          0.15    8.72    8.58  AlOOH
C3AH6            -8.68   74.23   82.91  Ca3Al2(OH)12
C3AH6(C)         -5.22   74.23   79.45  Ca3Al2(OH)12
Ca-Olivine       -5.62   32.03   37.65  Ca2SiO4
Ca3SiO5         -22.91   50.95   73.87  Ca3SiO5
CH               -3.97   18.93   22.90  Ca(OH)2
Chalcedony       -2.30   -5.83   -3.52  SiO2
Cristobalite     -2.24   -5.83   -3.59  SiO2
CSH_0.8          -1.77    9.31   11.08  Ca0.8SiO2.8:H2O
CSH_1.1          -1.73   14.99   16.72  Ca1.1SiO3.1:H2O
CSH_1.8          -4.46   28.24   32.70  Ca1.8SiO3.8:H2O
Diaspore          1.85    8.72    6.87  AlOOH
Gehlenite        -7.35   49.48   56.82  Ca2Al2SiO7
Gibbsite(C)      -0.05    8.72    8.77  Al(OH)3
Halloysite       -3.20    5.79    8.99  Al2Si2O5(OH)4
Kaolinite         0.07    5.79    5.73  Al2Si2O5(OH)4
Larnite          -7.11   32.03   39.14  Ca2SiO4
Laumontite       -1.39   13.07   14.46  CaAl2Si4O12:4H2O
Leonhardite       9.64   26.13   16.49  Ca2Al4Si8O24:7H2O
Lime            -13.87   18.93   32.80  CaO
O2(g)           -22.97   60.15   83.12  O2
P-Wollstanite    -0.75   13.10   13.85  CaSiO3
Portlandite      -3.75   18.93   22.68  Ca(OH)2
Pyrophyllite     -4.26   -5.86   -1.60  Al2Si4O10(OH)2
Quartz           -1.82   -5.83   -4.01  SiO2
SiO2(a)          -2.81   -5.83   -3.02  SiO2
SiO2(am)         -3.12   -5.83   -2.71  SiO2
SiO2gel(am)      -2.98   -5.83   -2.85  SiO2
Tob              -6.31   59.67   65.98  Ca5Si6O17:5H2O
Wairakite        -5.80   13.07   18.87  CaAl2Si4O12:2H2O
Wollastonite      0.10   13.10   13.00  CaSiO3

Initial solution 62.Tobermorite Tob Dispersion 2

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

Elements           Molality       Moles

Ca                1.010e-03   1.010e-03
Si                3.430e-04   3.430e-04

----------------------------Description of solution----------------------------

                                       pH  =  11.168      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   3.056e-03
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   2.020e-03
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =   7.026e-17
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                               Iterations  =   8
                                  Total H  = 1.110150e+02
                                  Total O  = 5.550919e+01
```

```
-----------------------------Saturation indices------------------------------

Phase               SI  log IAP  log KT

Ca-Olivine       -4.08   33.57   37.65  Ca2SiO4
Ca3SiO5         -21.07   52.80   73.87  Ca3SiO5
CH               -3.67   19.23   22.90  Ca(OH)2
Chalcedony       -1.36   -4.88   -3.52  SiO2
Cristobalite     -1.29   -4.88   -3.59  SiO2
CSH_0.8          -0.58   10.50   11.08  Ca0.8SiO2.8:H2O
CSH_1.1          -0.45   16.27   16.72  Ca1.1SiO3.1:H2O
CSH_1.8          -2.97   29.73   32.70  Ca1.8SiO3.8:H2O
Larnite          -5.57   33.57   39.14  Ca2SiO4
Lime            -13.57   19.23   32.80  CaO
O2(g)           -22.45   60.67   83.12  O2
P-Wollstanite     0.50   14.35   13.85  CaSiO3
Portlandite      -3.45   19.23   22.68  Ca(OH)2
Quartz           -0.87   -4.88   -4.01  SiO2
SiO2(a)          -1.86   -4.88   -3.02  SiO2
SiO2(am)         -2.17   -4.88   -2.71  SiO2
SiO2gel(am)      -2.03   -4.88   -2.85  SiO2
Tob               0.87   66.85   65.98  Ca5Si6O17:5H2O
Wollastonite      1.35   14.35   13.00  CaSiO3

Initial solution 63.Tobermorite Tob Dispersion 7

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

Elements           Molality       Moles

Ca                4.800e-04   4.800e-04
Si                3.930e-04   3.930e-04

---------------------------Description of solution---------------------------

                                       pH  =  10.734      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   1.467e-03
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   9.600e-04
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =   7.676e-17
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                               Iterations  =   9
                                  Total H  = 1.110142e+02
                                  Total O  = 5.550836e+01

-----------------------------Saturation indices------------------------------

Phase               SI  log IAP  log KT

Ca-Olivine       -5.84   31.81   37.65  Ca2SiO4
Ca3SiO5         -23.99   49.88   73.87  Ca3SiO5
CH               -4.83   18.07   22.90  Ca(OH)2
Chalcedony       -0.81   -4.34   -3.52  SiO2
Cristobalite     -0.75   -4.34   -3.59  SiO2
CSH_0.8          -0.96   10.12   11.08  Ca0.8SiO2.8:H2O
CSH_1.1          -1.18   15.54   16.72  Ca1.1SiO3.1:H2O
CSH_1.8          -4.51   28.19   32.70  Ca1.8SiO3.8:H2O
Larnite          -7.33   31.81   39.14  Ca2SiO4
Lime            -14.72   18.07   32.80  CaO
O2(g)           -24.18   58.94   83.12  O2
P-Wollstanite    -0.11   13.74   13.85  CaSiO3
Portlandite      -4.60   18.07   22.68  Ca(OH)2
Quartz           -0.33   -4.34   -4.01  SiO2
SiO2(a)          -1.32   -4.34   -3.02  SiO2
SiO2(am)         -1.63   -4.34   -2.71  SiO2
SiO2gel(am)      -1.49   -4.34   -2.85  SiO2
Tob              -1.63   64.35   65.98  Ca5Si6O17:5H2O
Wollastonite      0.74   13.74   13.00  CaSiO3

Initial solution 64.Hydrotalcite HT Dispersion 3 Tentative Ksp = -119.3 for M4AH10

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

Elements           Molality       Moles

Al                1.400e-05   1.400e-05
Mg                3.300e-05   3.300e-05
```

```
----------------------------Description of solution----------------------------

                                       pH  =   9.300
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   8.294e-05
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   7.629e-05
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =   3.171e-05
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  31.68
                               Iterations  =   3
                                  Total H  = 1.110125e+02
                                  Total O  = 5.550629e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

Al(OH)3(a)       -1.54    8.84   10.38  Al(OH)3
Al2O3            -5.30   17.68   22.98  Al2O3
Boehmite          0.26    8.84    8.58  AlOOH
Brucite          -2.69   14.10   16.79  Mg(OH)2
Diaspore          1.97    8.84    6.87  AlOOH
Gibbsite(C)       0.07    8.84    8.77  Al(OH)3
HT               -4.91   74.07   78.98  Mg4Al2O7:10H2O
O2(g)           -29.92   53.20   83.12  O2
Periclase        -7.41   14.10   21.51  MgO
Spinel           -4.56   31.78   36.33  MgAl2O4

Initial solution 65.Hydrotalcite HT Dispersion 5

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

Elements           Molality       Moles

Al                8.000e-06   8.000e-06
Mg                6.000e-05   6.000e-05

----------------------------Description of solution----------------------------

                                       pH  =  10.037      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   1.780e-04
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   1.440e-04
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =   2.711e-19
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                               Iterations  =   5
                                  Total H  = 1.110126e+02
                                  Total O  = 5.550636e+01


------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

Al(OH)3(a)       -2.52    7.86   10.38  Al(OH)3
Al2O3            -7.26   15.72   22.98  Al2O3
Boehmite         -0.72    7.86    8.58  AlOOH
Brucite          -0.97   15.82   16.79  Mg(OH)2
Diaspore          0.99    7.86    6.87  AlOOH
Gibbsite(C)      -0.91    7.86    8.77  Al(OH)3
HT                0.01   78.99   78.98  Mg4Al2O7:10H2O
O2(g)           -26.97   56.15   83.12  O2
Periclase        -5.69   15.82   21.51  MgO
Spinel           -4.80   31.54   36.33  MgAl2O4

Initial solution 66.CSH 0.9

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

Elements           Molality       Moles

Ca                1.670e-03   1.670e-03
Si                1.350e-04   1.350e-04
```

```
----------------------------Description of solution----------------------------

                                       pH  =  11.451      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   4.884e-03
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   3.340e-03
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -1.613e-16
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   7
                                  Total H  = 1.110159e+02
                                  Total O  = 5.550991e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

Ca-Olivine       -3.36   34.29   37.65  Ca2SiO4
Ca3SiO5         -19.61   54.26   73.87  Ca3SiO5
CH               -2.92   19.98   22.90  Ca(OH)2
Chalcedony       -2.14   -5.67   -3.52  SiO2
Cristobalite     -2.08   -5.67   -3.59  SiO2
CSH_0.8          -0.77   10.31   11.08  Ca0.8SiO2.8:H2O
CSH_1.1          -0.41   16.31   16.72  Ca1.1SiO3.1:H2O
CSH_1.8          -2.41   30.29   32.70  Ca1.8SiO3.8:H2O
Larnite          -4.86   34.29   39.14  Ca2SiO4
Lime            -12.82   19.98   32.80  CaO
O2(g)           -21.32   61.80   83.12  O2
P-Wollstanite     0.46   14.31   13.85  CaSiO3
Portlandite      -2.70   19.98   22.68  Ca(OH)2
Quartz           -1.66   -5.67   -4.01  SiO2
SiO2(a)          -2.65   -5.67   -3.02  SiO2
SiO2(am)         -2.96   -5.67   -2.71  SiO2
SiO2gel(am)      -2.82   -5.67   -2.85  SiO2
Tob              -0.10   65.88   65.98  Ca5Si6O17:5H2O
Wollastonite      1.31   14.31   13.00  CaSiO3


Initial solution 67.CSH 1.3

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

Elements           Molality       Moles

Ca                9.750e-03   9.750e-03
Si                1.200e-05   1.200e-05

----------------------------Description of solution----------------------------

                                       pH  =  12.174      Charge balance
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   2.539e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   1.950e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -8.296e-14
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =   5
                                  Total H  = 1.110319e+02
                                  Total O  = 5.552574e+01
```

```
------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

Ca-Olivine       -1.64   36.01   37.65  Ca2SiO4
Ca3SiO5         -15.86   58.00   73.87  Ca3SiO5
CH               -0.90   22.00   22.90  Ca(OH)2
Chalcedony       -4.46   -7.99   -3.52  SiO2
Cristobalite     -4.40   -7.99   -3.59  SiO2
CSH_0.8          -1.47    9.61   11.08  Ca0.8SiO2.8:H2O
CSH_1.1          -0.51   16.21   16.72  Ca1.1SiO3.1:H2O
CSH_1.8          -1.09   31.61   32.70  Ca1.8SiO3.8:H2O
Larnite          -3.13   36.01   39.14  Ca2SiO4
Lime            -10.80   22.00   32.80  CaO
O2(g)           -18.43   64.69   83.12  O2
P-Wollstanite     0.16   14.01   13.85  CaSiO3
Portlandite      -0.68   22.00   22.68  Ca(OH)2
Quartz           -3.98   -7.99   -4.01  SiO2
SiO2(a)          -4.97   -7.99   -3.02  SiO2
SiO2(am)         -5.28   -7.99   -2.71  SiO2
SiO2gel(am)      -5.14   -7.99   -2.85  SiO2
Tob              -3.92   62.06   65.98  Ca5Si6O17:5H2O
Wollastonite      1.01   14.01   13.00  CaSiO3

Initial solution 68.CSH 1.7

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

Elements           Molality       Moles

Ca               2.034e-02   2.034e-02
Si               6.000e-06   6.000e-06

----------------------------Description of solution----------------------------

                                       pH  =  12.448      Charge balance
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   4.901e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   4.068e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =   1.286e-12
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                               Iterations  =   4
                                  Total H  = 1.110531e+02
                                  Total O  = 5.554691e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

Ca-Olivine       -1.02   36.63   37.65  Ca2SiO4
Ca3SiO5         -14.49   59.37   73.87  Ca3SiO5
CH               -0.15   22.75   22.90  Ca(OH)2
Chalcedony       -5.34   -8.87   -3.52  SiO2
Cristobalite     -5.28   -8.87   -3.59  SiO2
CSH_0.8          -1.75    9.33   11.08  Ca0.8SiO2.8:H2O
CSH_1.1          -0.57   16.15   16.72  Ca1.1SiO3.1:H2O
CSH_1.8          -0.62   32.08   32.70  Ca1.8SiO3.8:H2O
Larnite          -2.51   36.63   39.14  Ca2SiO4
Lime            -10.05   22.75   32.80  CaO
O2(g)           -17.33   65.79   83.12  O2
P-Wollstanite     0.03   13.88   13.85  CaSiO3
Portlandite       0.07   22.75   22.68  Ca(OH)2
Quartz           -4.86   -8.87   -4.01  SiO2
SiO2(a)          -5.85   -8.87   -3.02  SiO2
SiO2(am)         -6.16   -8.87   -2.71  SiO2
SiO2gel(am)      -6.02   -8.87   -2.85  SiO2
Tob              -5.45   60.53   65.98  Ca5Si6O17:5H2O
Wollastonite      0.88   13.88   13.00  CaSiO3

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End of simulation.
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Reading input data for simulation 5.
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SOLUTION 69  Invariant point G (C3AH6 - AFt - CH)
        units   mmol/kgw
        pH      12.52
        density 1.0
        temp    25.0
        Ca             21.25
        Al              0.01
        S(6)            0.015
        Na              0.
SOLUTION 70  Invariant point H2 (C3AH6 - AFt - AH3)
        units   mmol/kgw
        pH      11.92
        density 1.0
        temp    25.0
        Ca              5.04
        Al              0.386
        S(6)            0.03
        Na              0.
SOLUTION 71  Invariant point F (CH - AFt - Gypsum)
        units   mmol/kgw
        pH      12.47
        density 1.0
        temp    25.0
        Ca             31.3
        Al              0.0003
        S(6)           11.4
        Na              0.
SOLUTION 72  Invariant point E2 (AH3 - AFt - Gypsum)
        units   mmol/kgw
        pH      10.66
        density 1.0
        temp    25.0
        Ca             11.12
        Al              0.0143
        S(6)           35.8
        Na              50.
SOLUTION 80  Invariant point E2 (AH3 - AFt - Gypsum)
        units   mmol/kgw
        pH      10.43
        density 1.0
        temp    20.0
        Ca             15.17
        Al              0.001
        S(6)           15.
        Na              0.
END
```

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Beginning of initial solution calculations.
-------------------------------------------

Initial solution 69.Invariant point G (C3AH6 - AFt - CH)

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

Elements           Molality       Moles

Al                1.000e-05   1.000e-05
Ca                2.125e-02   2.125e-02
S(6)              1.500e-05   1.500e-05

----------------------------Description of solution----------------------------

                                       pH  =  12.520
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   5.261e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   4.813e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -5.626e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -7.34
                               Iterations  =   4
                                  Total H  = 1.110606e+02
                                  Total O  = 5.555440e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm              -0.69   71.87   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -0.68   56.77   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -4.99    5.39   10.38  Al(OH)3
Al2O3           -12.19   10.79   22.98  Al2O3
Al4(OH)10SO4    -31.56   -8.86   22.70  Al4(OH)10SO4
AlOHSO4         -21.81  -25.04   -3.23  AlOHSO4
Anhydrite        -2.91   -7.55   -4.64  CaSO4
Boehmite         -3.18    5.39    8.58  AlOOH
C3AH6            -3.48   79.43   82.91  Ca3Al2(OH)12
C3AH6(C)         -0.02   79.43   79.45  Ca3Al2(OH)12
CH               -0.02   22.88   22.90  Ca(OH)2
Diaspore         -1.48    5.39    6.87  AlOOH
Ettr_GCA         -0.33   56.77   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -3.38    5.39    8.77  Al(OH)3
Gypsum           -2.70   -7.55   -4.85  CaSO4:2H2O
Gypsum_Cem       -2.95   -7.55   -4.60  CaSO4:2H2O
Lime             -9.92   22.88   32.80  CaO
O2(g)           -17.04   66.08   83.12  O2
Portlandite       0.21   22.88   22.68  Ca(OH)2


Initial solution 70.Invariant point H2 (C3AH6 - AFt - AH3)

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

Elements           Molality       Moles

Al                3.860e-04   3.860e-04
Ca                5.040e-03   5.040e-03
S(6)              3.000e-05   3.000e-05

----------------------------Description of solution----------------------------

                                       pH  =  11.920
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   1.403e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   1.164e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -4.647e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -2.41
                               Iterations  =   4
                                  Total H  = 1.110241e+02
                                  Total O  = 5.551798e+01
```

```
------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm              -0.89   71.68   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -0.60   56.84   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -2.76    7.62   10.38  Al(OH)3
Al2O3            -7.75   15.23   22.98  Al2O3
Al4(OH)10SO4    -20.94    1.76   22.70  Al4(OH)10SO4
AlOHSO4         -17.86  -21.09   -3.23  AlOHSO4
Anhydrite        -2.78   -7.42   -4.64  CaSO4
Boehmite         -0.96    7.62    8.58  AlOOH
C3AH6            -3.81   79.09   82.91  Ca3Al2(OH)12
C3AH6(C)         -0.36   79.09   79.45  Ca3Al2(OH)12
CH               -1.61   21.29   22.90  Ca(OH)2
Diaspore          0.74    7.62    6.87  AlOOH
Ettr_GCA         -0.25   56.84   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -1.15    7.62    8.77  Al(OH)3
Gypsum           -2.57   -7.42   -4.85  CaSO4:2H2O
Gypsum_Cem       -2.82   -7.42   -4.60  CaSO4:2H2O
Lime            -11.51   21.29   32.80  CaO
O2(g)           -19.44   63.68   83.12  O2
Portlandite      -1.39   21.29   22.68  Ca(OH)2

Initial solution 71.Invariant point F (CH - AFt - Gypsum)

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

Elements           Molality       Moles

Al                3.000e-07   3.000e-07
Ca                3.130e-02   3.130e-02
S(6)              1.140e-02   1.140e-02

----------------------------Description of solution----------------------------

                                       pH  =  12.470
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   7.452e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   4.556e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -5.763e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -5.92
                               Iterations  =   5
                                  Total H  = 1.110580e+02
                                  Total O  = 5.559738e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm              -0.79   71.77   72.56  Ca4Al2SO4(OH)12:6H2O
AFt               5.03   62.47   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -6.47    3.91   10.38  Al(OH)3
Al2O3           -15.16    7.82   22.98  Al2O3
Al4(OH)10SO4    -34.58  -11.88   22.70  Al4(OH)10SO4
AlOHSO4         -20.38  -23.61   -3.23  AlOHSO4
Anhydrite        -0.01   -4.65   -4.64  CaSO4
Boehmite         -4.67    3.91    8.58  AlOOH
C3AH6            -6.48   76.42   82.91  Ca3Al2(OH)12
C3AH6(C)         -3.03   76.42   79.45  Ca3Al2(OH)12
CH               -0.03   22.87   22.90  Ca(OH)2
Diaspore         -2.96    3.91    6.87  AlOOH
Ettr_GCA          5.38   62.47   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -4.86    3.91    8.77  Al(OH)3
Gypsum            0.20   -4.65   -4.85  CaSO4:2H2O
Gypsum_Cem       -0.05   -4.65   -4.60  CaSO4:2H2O
Lime             -9.93   22.87   32.80  CaO
O2(g)           -17.24   65.88   83.12  O2
Portlandite       0.19   22.87   22.68  Ca(OH)2
```

```
Initial solution 72.Invariant point E2 (AH3 - AFt - Gypsum)

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

Elements           Molality       Moles

Al                1.430e-05   1.430e-05
Ca                1.112e-02   1.112e-02
Na                5.000e-02   5.000e-02
S(6)              3.580e-02   3.580e-02

----------------------------Description of solution----------------------------

                                       pH  =  10.660
                                       pe  =   4.000
                        Activity of water  =   0.998
                           Ionic strength  =   9.396e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   6.918e-04
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -8.938e-06
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.01
                               Iterations  =   5
                                  Total H  = 1.110131e+02
                                  Total O  = 5.565011e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm              -6.21   66.35   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -0.29   57.15   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -2.99    7.39   10.38  Al(OH)3
Al2O3            -8.20   14.78   22.98  Al2O3
Al4(OH)10SO4    -16.46    6.24   22.70  Al4(OH)10SO4
AlOHSO4         -12.70  -15.93   -3.23  AlOHSO4
Anhydrite         0.04   -4.59   -4.64  CaSO4
Boehmite         -1.19    7.39    8.58  AlOOH
C3AH6           -11.96   70.94   82.91  Ca3Al2(OH)12
C3AH6(C)         -8.51   70.94   79.45  Ca3Al2(OH)12
CH               -4.18   18.72   22.90  Ca(OH)2
Diaspore          0.52    7.39    6.87  AlOOH
Ettr_GCA          0.06   57.15   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -1.38    7.39    8.77  Al(OH)3
Gypsum            0.25   -4.59   -4.85  CaSO4:2H2O
Gypsum_Cem        0.01   -4.59   -4.60  CaSO4:2H2O
Lime            -14.07   18.72   32.80  CaO
Mirabilite       -3.74   -4.86   -1.11  Na2SO4:10H2O
O2(g)           -24.48   58.64   83.12  O2
Portlandite      -3.95   18.72   22.68  Ca(OH)2
Thenardite       -4.67   -4.85   -0.18  Na2SO4

Initial solution 80.Invariant point E2 (AH3 - AFt - Gypsum)

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

Elements           Molality       Moles

Al                1.000e-06   1.000e-06
Ca                1.517e-02   1.517e-02
S(6)              1.500e-02   1.500e-02

----------------------------Description of solution----------------------------

                                       pH  =  10.430
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   4.078e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   2.548e-04
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  20.000
                  Electrical balance (eq)  =   8.822e-05
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.22
                               Iterations  =   5
                                  Total H  = 1.110127e+02
                                  Total O  = 5.556647e+01
```

```
------------------------------Saturation indices-------------------------------

Phase               SI  log IAP  log KT

AFm              -9.09   65.24   74.33  Ca4Al2SO4(OH)12:6H2O
AFt              -3.17   56.05   59.21  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -3.68    7.04   10.72  Al(OH)3
Al2O3            -8.90   14.08   22.98  Al2O3
Al4(OH)10SO4    -17.71    4.99   22.70  Al4(OH)10SO4
AlOHSO4         -12.91  -16.14   -3.23  AlOHSO4
Anhydrite        -0.01   -4.60   -4.59  CaSO4
Boehmite         -1.89    7.04    8.93  AlOOH
C3AH6           -15.07   69.84   84.91  Ca3Al2(OH)12
C3AH6(C)        -11.38   69.84   81.22  Ca3Al2(OH)12
CH               -4.70   18.58   23.28  Ca(OH)2
Diaspore         -0.14    7.04    7.18  AlOOH
Ettr_GCA         -2.20   56.05   58.25  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -2.01    7.04    9.06  Al(OH)3
Gypsum            0.26   -4.60   -4.85  CaSO4:2H2O
Gypsum_Cem        0.01   -4.60   -4.60  CaSO4:2H2O
Lime            -14.79   18.58   33.38  CaO
O2(g)           -27.07   57.72   84.79  O2
Portlandite      -4.47   18.58   23.06  Ca(OH)2

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End of simulation.
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Reading input data for simulation 6.
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SOLUTION 81  Damidot and Glasser Invariant point lambda-eta-alfa-delta (CH-Ettr-C3AH6-hcA)
        units   mmol/kgw
        pH      12.52
        density 1.0
        temp    25.0
        Ca             21.9
        Al              0.00759
        S(6)            0.0076
        C(4)            0.00162
        Na              0.
SOLUTION 82  Damidot and Glasser Invariant point eta-alfa-delta-phi (Ettr-C3AH6-hcA-mcA)
        units   mmol/kgw
        pH      12.43
        density 1.0
        temp    25.0
        Ca             17.3
        Al              0.00141
        S(6)            0.0078
        C(4)            0.00285
        Na              0.
SOLUTION 83  Damidot and Glasser Invariant point kappa-eta-alfa-phi (Gibbsite-Ettr-C3AH6-mcA)
        units   mmol/kgw
        pH      11.97
        density 1.0
        temp    25.0
        Ca              5.62
        Al              0.347
        S(6)            0.0103
        C(4)            0.00313
        Na              0.
SOLUTION 84  Damidot and Glasser Invariant point lambda-delta-phi-eta (CH-hcA-mcA-Ettr)
        units   mmol/kgw
        pH      12.52
        density 1.0
        temp    25.0
        Ca             21.9
        Al              0.00574
        S(6)            0.00915
        C(4)            0.00495
        Na              0.
SOLUTION 85  Damidot and Glasser Invariant point xsi-lambda-phi-eta (Cc-CH-mcA-Ettr)
        units   mmol/kgw
        pH      12.52
        density 1.0
        temp    25.0
        Ca             21.9
        Al              0.00485
        S(6)            0.0102
        C(4)            0.00693
        Na              0.
SOLUTION 86  Damidot and Glasser Invariant point my-eta-lambda-xsi (Gypsum-Ettr-CH-Cc)
        units   mmol/kgw
        pH      12.49
        density 1.0
        temp    25.0
        Ca             33.9
        Al              1.01e-7
        S(6)           12.4
        C(4)            0.00694
        Na              0.
SOLUTION 87  Damidot and Glasser Invariant point kappa-xsi-eta-phi (Gibbsite-Cc-Ettr-mcA)
        units   mmol/kgw
        pH      11.92
        density 1.0
        temp    25.0
        Ca              5.02
        Al              0.310
        S(6)            0.0146
        C(4)            0.00782
        Na              0.
SOLUTION 88  Damidot and Glasser Invariant point my-kappa-xsi-eta (Gypsum-Gibbsite-Cc-Ettr)
        units   mmol/kgw
        pH      10.25
        density 1.0
        temp    25.0
        Ca             15.3
        Al              0.00703
        S(6)           15.2
        C(4)            0.00839
        Na              0.
END
```

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Beginning of initial solution calculations.
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Initial solution 81.Damidot and Glasser Invariant point lambda-eta-alfa-delta (CH-Ettr-C3AH6-hcA)

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

Elements           Molality       Moles

Al                7.590e-06   7.590e-06
C(4)              1.620e-06   1.620e-06
Ca                2.190e-02   2.190e-02
S(6)              7.600e-06   7.600e-06
----------------------------Description of solution----------------------------

                                       pH  =  12.520
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   5.364e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   4.838e-02
                       Total CO2 (mol/kg)  =   1.620e-06
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -4.576e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -5.88
                               Iterations  =   6
                                  Total H  = 1.110608e+02
                                  Total O  = 5.555463e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm              -1.18   71.38   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -1.75   55.69   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -5.11    5.27   10.38  Al(OH)3
Al2O3           -12.43   10.55   22.98  Al2O3
Al4(OH)10SO4    -32.34   -9.64   22.70  Al4(OH)10SO4
AlOHSO4         -22.23  -25.46   -3.23  AlOHSO4
Anhydrite        -3.20   -7.84   -4.64  CaSO4
Aragonite        -0.69   -9.02   -8.34  CaCO3
Boehmite         -3.30    5.27    8.58  AlOOH
C3AH6            -3.68   79.22   82.91  Ca3Al2(OH)12
C3AH6(C)         -0.23   79.22   79.45  Ca3Al2(OH)12
Calcite          -0.55   -9.02   -8.47  CaCO3
CH               -0.01   22.89   22.90  Ca(OH)2
CH4(g)         -123.97 -164.07  -40.10  CH4
CO2(g)          -13.76  -31.92  -18.16  CO2
Diaspore         -1.60    5.27    6.87  AlOOH
Ettr_GCA         -1.40   55.69   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -3.50    5.27    8.77  Al(OH)3
Gypsum           -2.99   -7.84   -4.85  CaSO4:2H2O
Gypsum_Cem       -3.24   -7.84   -4.60  CaSO4:2H2O
Hemicarboaluminat  -2.29   63.26   65.55  Ca3Al2O6.5C0.5(OH):11.5H2O
Lime             -9.90   22.89   32.80  CaO
Monocarboaluminat  -0.30   70.20   70.49  (CaO)3Al2O3CaCO3:11H2O
O2(g)           -17.04   66.08   83.12  O2
Portlandite       0.22   22.89   22.68  Ca(OH)2

Initial solution 82.Damidot and Glasser Invariant point eta-alfa-delta-phi (Ettr-C3AH6-hcA-mcA)

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

Elements           Molality       Moles

Al                1.410e-06   1.410e-06
C(4)              2.850e-06   2.850e-06
Ca                1.730e-02   1.730e-02
S(6)              7.800e-06   7.800e-06

----------------------------Description of solution----------------------------

                                       pH  =  12.430
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   4.351e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   3.795e-02
                       Total CO2 (mol/kg)  =   2.850e-06
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -3.363e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -5.38
                               Iterations  =   5
                                  Total H  = 1.110504e+02
                                  Total O  = 5.554420e+01
```

```
------------------------------Saturation indices------------------------------
Phase                SI log IAP  log KT

AFm              -3.17   69.39   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -3.76   53.69   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -5.74    4.64   10.38  Al(OH)3
Al2O3           -13.70    9.28   22.98  Al2O3
Al4(OH)10SO4    -34.65  -11.95   22.70  Al4(OH)10SO4
AlOHSO4         -22.63  -25.86   -3.23  AlOHSO4
Anhydrite        -3.21   -7.85   -4.64  CaSO4
Aragonite        -0.45   -8.78   -8.34  CaCO3
Boehmite         -3.94    4.64    8.58  AlOOH
C3AH6            -5.67   77.24   82.91  Ca3Al2(OH)12
C3AH6(C)         -2.21   77.24   79.45  Ca3Al2(OH)12
Calcite          -0.31   -8.78   -8.47  CaCO3
CH               -0.25   22.65   22.90  Ca(OH)2
CH4(g)         -122.78 -162.88  -40.10  CH4
CO2(g)          -13.28  -31.44  -18.16  CO2
Diaspore         -2.23    4.64    6.87  AlOOH
Ettr_GCA         -3.41   53.69   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -4.13    4.64    8.77  Al(OH)3
Gypsum           -3.00   -7.85   -4.85  CaSO4:2H2O
Gypsum_Cem       -3.25   -7.85   -4.60  CaSO4:2H2O
Hemicarboaluminat  -4.04   61.52   65.55  Ca3Al2O6.5C0.5(OH):11.5H2O
Lime            -10.14   22.65   32.80  CaO
Monocarboaluminat  -2.04   68.45   70.49  (CaO)3Al2O3CaCO3:11H2O
O2(g)           -17.40   65.72   83.12  O2
Portlandite      -0.02   22.65   22.68  Ca(OH)2

Initial solution 83.Damidot and Glasser Invariant point kappa-eta-alfa-phi (Gibbsite-Ettr-C3AH6-mcA)

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

Elements           Molality       Moles

Al                3.470e-04   3.470e-04
C(4)              3.130e-06   3.130e-06
Ca                5.620e-03   5.620e-03
S(6)              1.030e-05   1.030e-05

----------------------------Description of solution----------------------------

                                       pH  =  11.970
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   1.554e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   1.285e-02
                       Total CO2 (mol/kg)  =   3.130e-06
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -5.871e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -2.74
                               Iterations  =   4
                                  Total H  = 1.110253e+02
                                  Total O  = 5.551911e+01

------------------------------Saturation indices------------------------------
Phase                SI log IAP  log KT

AFm              -1.13   71.43   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -1.74   55.71   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -2.86    7.52   10.38  Al(OH)3
Al2O3            -7.95   15.03   22.98  Al2O3
Al4(OH)10SO4    -21.92    0.78   22.70  Al4(OH)10SO4
AlOHSO4         -18.54  -21.77   -3.23  AlOHSO4
Anhydrite        -3.23   -7.86   -4.64  CaSO4
Aragonite        -0.46   -8.80   -8.34  CaCO3
Boehmite         -1.06    7.52    8.58  AlOOH
C3AH6            -3.61   79.30   82.91  Ca3Al2(OH)12
C3AH6(C)         -0.16   79.30   79.45  Ca3Al2(OH)12
Calcite          -0.32   -8.80   -8.47  CaCO3
CH               -1.48   21.42   22.90  Ca(OH)2
CH4(g)         -117.88 -157.98  -40.10  CH4
CO2(g)          -12.06  -30.22  -18.16  CO2
Diaspore          0.64    7.52    6.87  AlOOH
Ettr_GCA         -1.39   55.71   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -1.25    7.52    8.77  Al(OH)3
Gypsum           -3.01   -7.86   -4.85  CaSO4:2H2O
Gypsum_Cem       -3.26   -7.86   -4.60  CaSO4:2H2O
Hemicarboaluminat  -1.37   64.19   65.55  Ca3Al2O6.5C0.5(OH):11.5H2O
Lime            -11.38   21.42   32.80  CaO
Monocarboaluminat   0.01   70.50   70.49  (CaO)3Al2O3CaCO3:11H2O
O2(g)           -19.24   63.88   83.12  O2
Portlandite      -1.25   21.42   22.68  Ca(OH)2
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Initial solution 84.Damidot and Glasser Invariant point lambda-delta-phi-eta (CH-hcA-mcA-Ettr)

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

Elements           Molality       Moles

Al                5.740e-06   5.740e-06
C(4)              4.950e-06   4.950e-06
Ca                2.190e-02   2.190e-02
S(6)              9.150e-06   9.150e-06

----------------------------Description of solution----------------------------

                                       pH  =  12.520
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   5.364e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   4.838e-02
                       Total CO2 (mol/kg)  =   4.950e-06
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -4.583e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -5.89
                               Iterations  =   6
                                  Total H  = 1.110608e+02
                                  Total O  = 5.555464e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm              -1.35   71.22   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -1.75   55.69   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -5.23    5.15   10.38  Al(OH)3
Al2O3           -12.68   10.30   22.98  Al2O3
Al4(OH)10SO4    -32.75  -10.05   22.70  Al4(OH)10SO4
AlOHSO4         -22.27  -25.50   -3.23  AlOHSO4
Anhydrite        -3.12   -7.76   -4.64  CaSO4
Aragonite        -0.20   -8.54   -8.34  CaCO3
Boehmite         -3.43    5.15    8.58  AlOOH
C3AH6            -3.93   78.98   82.91  Ca3Al2(OH)12
C3AH6(C)         -0.47   78.98   79.45  Ca3Al2(OH)12
Calcite          -0.06   -8.54   -8.47  CaCO3
CH               -0.01   22.89   22.90  Ca(OH)2
CH4(g)         -123.49 -163.59  -40.10  CH4
CO2(g)          -13.27  -31.43  -18.16  CO2
Diaspore         -1.72    5.15    6.87  AlOOH
Ettr_GCA         -1.40   55.69   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -3.62    5.15    8.77  Al(OH)3
Gypsum           -2.91   -7.76   -4.85  CaSO4:2H2O
Gypsum_Cem       -3.16   -7.76   -4.60  CaSO4:2H2O
Hemicarboaluminat  -2.29   63.26   65.55  Ca3Al2O6.5C0.5(OH):11.5H2O
Lime             -9.90   22.89   32.80  CaO
Monocarboaluminat  -0.05   70.44   70.49  (CaO)3Al2O3CaCO3:11H2O
O2(g)           -17.04   66.08   83.12  O2
Portlandite       0.22   22.89   22.68  Ca(OH)2

Initial solution 85.Damidot and Glasser Invariant point xsi-lambda-phi-eta (Cc-CH-mcA-Ettr)

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

Elements           Molality       Moles

Al                4.850e-06   4.850e-06
C(4)              6.930e-06   6.930e-06
Ca                2.190e-02   2.190e-02
S(6)              1.020e-05   1.020e-05

----------------------------Description of solution----------------------------

                                       pH  =  12.520
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   5.364e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   4.838e-02
                       Total CO2 (mol/kg)  =   6.930e-06
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -4.588e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -5.90
                               Iterations  =   6
                                  Total H  = 1.110608e+02
                                  Total O  = 5.555465e+01
```

```
-----------------------------Saturation indices------------------------------

Phase               SI log IAP  log KT

AFm              -1.44   71.12   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -1.76   55.68   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -5.30    5.08   10.38  Al(OH)3
Al2O3           -12.82   10.16   22.98  Al2O3
Al4(OH)10SO4    -32.99  -10.29   22.70  Al4(OH)10SO4
AlOHSO4         -22.30  -25.53   -3.23  AlOHSO4
Anhydrite        -3.08   -7.71   -4.64  CaSO4
Aragonite        -0.06   -8.39   -8.34  CaCO3
Boehmite         -3.50    5.08    8.58  AlOOH
C3AH6            -4.07   78.83   82.91  Ca3Al2(OH)12
C3AH6(C)         -0.62   78.83   79.45  Ca3Al2(OH)12
Calcite           0.08   -8.39   -8.47  CaCO3
CH               -0.01   22.89   22.90  Ca(OH)2
CH4(g)         -123.34 -163.44  -40.10  CH4
CO2(g)          -13.12  -31.28  -18.16  CO2
Diaspore         -1.79    5.08    6.87  AlOOH
Ettr_GCA         -1.41   55.68   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -3.69    5.08    8.77  Al(OH)3
Gypsum           -2.86   -7.71   -4.85  CaSO4:2H2O
Gypsum_Cem       -3.11   -7.71   -4.60  CaSO4:2H2O
Hemicarboaluminat  -2.37   63.19   65.55  Ca3Al2O6.5C0.5(OH):11.5H2O
Lime             -9.90   22.89   32.80  CaO
Monocarboaluminat  -0.05   70.44   70.49  (CaO)3Al2O3CaCO3:11H2O
O2(g)           -17.04   66.08   83.12  O2
Portlandite       0.22   22.89   22.68  Ca(OH)2

Initial solution 86.Damidot and Glasser Invariant point my-eta-lambda-xsi (Gypsum-Ettr-CH-Cc)

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

Elements           Molality       Moles

Al                1.010e-10   1.010e-10
C(4)              6.940e-06   6.940e-06
Ca                3.390e-02   3.390e-02
S(6)              1.240e-02   1.240e-02

----------------------------Description of solution----------------------------

                                       pH  =  12.490
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   7.959e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   4.842e-02
                       Total CO2 (mol/kg)  =   6.940e-06
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -5.421e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -5.22
                               Iterations  =   7
                                  Total H  = 1.110608e+02
                                  Total O  = 5.560425e+01

-----------------------------Saturation indices------------------------------

Phase               SI log IAP  log KT

AFm              -7.55   65.01   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -1.65   55.79   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -9.97    0.41   10.38  Al(OH)3
Al2O3           -22.15    0.83   22.98  Al2O3
Al4(OH)10SO4    -48.58  -25.88   22.70  Al4(OH)10SO4
AlOHSO4         -23.89  -27.12   -3.23  AlOHSO4
Anhydrite         0.03   -4.60   -4.64  CaSO4
Aragonite        -0.04   -8.38   -8.34  CaCO3
Boehmite         -8.16    0.41    8.58  AlOOH
C3AH6           -13.29   69.62   82.91  Ca3Al2(OH)12
C3AH6(C)         -9.84   69.62   79.45  Ca3Al2(OH)12
Calcite           0.09   -8.38   -8.47  CaCO3
CH                0.03   22.93   22.90  Ca(OH)2
CH4(g)         -123.13 -163.23  -40.10  CH4
CO2(g)          -13.15  -31.31  -18.16  CO2
Diaspore         -6.46    0.41    6.87  AlOOH
Ettr_GCA         -1.30   55.79   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -8.36    0.41    8.77  Al(OH)3
Gypsum            0.24   -4.60   -4.85  CaSO4:2H2O
Gypsum_Cem       -0.00   -4.60   -4.60  CaSO4:2H2O
Hemicarboaluminat -11.60   53.96   65.55  Ca3Al2O6.5C0.5(OH):11.5H2O
Lime             -9.87   22.93   32.80  CaO
Monocarboaluminat  -9.26   61.23   70.49  (CaO)3Al2O3CaCO3:11H2O
O2(g)           -17.16   65.96   83.12  O2
Portlandite       0.25   22.93   22.68  Ca(OH)2
```

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Initial solution 87.Damidot and Glasser Invariant point kappa-xsi-eta-phi (Gibbsite-Cc-Ettr-mcA)

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

Elements           Molality       Moles

Al                3.100e-04   3.100e-04
C(4)              7.820e-06   7.820e-06
Ca                5.020e-03   5.020e-03
S(6)              1.460e-05   1.460e-05

----------------------------Description of solution----------------------------

                                       pH  =  11.920
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   1.394e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   1.135e-02
                       Total CO2 (mol/kg)  =   7.820e-06
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -4.077e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -2.13
                               Iterations  =   4
                                  Total H  = 1.110238e+02
                                  Total O  = 5.551763e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm              -1.39   71.17   72.56  Ca4Al2SO4(OH)12:6H2O
AFt              -1.73   55.71   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -2.86    7.52   10.38  Al(OH)3
Al2O3            -7.94   15.04   22.98  Al2O3
Al4(OH)10SO4    -21.63    1.07   22.70  Al4(OH)10SO4
AlOHSO4         -18.26  -21.49   -3.23  AlOHSO4
Anhydrite        -3.09   -7.73   -4.64  CaSO4
Aragonite        -0.07   -8.41   -8.34  CaCO3
Boehmite         -1.06    7.52    8.58  AlOOH
C3AH6            -4.01   78.90   82.91  Ca3Al2(OH)12
C3AH6(C)         -0.55   78.90   79.45  Ca3Al2(OH)12
Calcite           0.07   -8.41   -8.47  CaCO3
CH               -1.61   21.29   22.90  Ca(OH)2
CH4(g)         -116.95 -157.05  -40.10  CH4
CO2(g)          -11.53  -29.69  -18.16  CO2
Diaspore          0.65    7.52    6.87  AlOOH
Ettr_GCA         -1.38   55.71   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)      -1.25    7.52    8.77  Al(OH)3
Gypsum           -2.88   -7.73   -4.85  CaSO4:2H2O
Gypsum_Cem       -3.13   -7.73   -4.60  CaSO4:2H2O
Hemicarboaluminat  -1.50   64.05   65.55  Ca3Al2O6.5C0.5(OH):11.5H2O
Lime            -11.51   21.29   32.80  CaO
Monocarboaluminat  -0.00   70.49   70.49  (CaO)3Al2O3CaCO3:11H2O
O2(g)           -19.44   63.68   83.12  O2
Portlandite      -1.39   21.29   22.68  Ca(OH)2

Initial solution 88.Damidot and Glasser Invariant point my-kappa-xsi-eta (Gypsum-Gibbsite-Cc-Ettr)

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

Elements           Molality       Moles

Al                7.030e-06   7.030e-06
C(4)              8.390e-06   8.390e-06
Ca                1.530e-02   1.530e-02
S(6)              1.520e-02   1.520e-02

----------------------------Description of solution----------------------------

                                       pH  =  10.250
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   4.079e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   2.881e-04
                       Total CO2 (mol/kg)  =   8.390e-06
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -6.702e-05
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.16
                               Iterations  =   6
                                  Total H  = 1.110127e+02
                                  Total O  = 5.556731e+01
```

```
------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

AFm             -7.47   65.10   72.56  Ca4Al2SO4(OH)12:6H2O
AFt             -1.55   55.89   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)      -2.86    7.52   10.38  Al(OH)3
Al2O3           -7.94   15.04   22.98  Al2O3
Al4(OH)10SO4   -15.45    7.25   22.70  Al4(OH)10SO4
AlOHSO4        -12.07  -15.30   -3.23  AlOHSO4
Anhydrite        0.04   -4.60   -4.64  CaSO4
Aragonite       -0.06   -8.39   -8.34  CaCO3
Boehmite        -1.06    7.52    8.58  AlOOH
C3AH6          -13.21   69.70   82.91  Ca3Al2(OH)12
C3AH6(C)        -9.75   69.70   79.45  Ca3Al2(OH)12
Calcite          0.08   -8.39   -8.47  CaCO3
CH              -4.68   18.22   22.90  Ca(OH)2
CH4(g)        -100.51 -140.61  -40.10  CH4
CO2(g)          -8.45  -26.61  -18.16  CO2
Diaspore         0.64    7.52    6.87  AlOOH
Ettr_GCA        -1.20   55.89   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Gibbsite(C)     -1.25    7.52    8.77  Al(OH)3
Gypsum           0.25   -4.60   -4.85  CaSO4:2H2O
Gypsum_Cem      -0.00   -4.60   -4.60  CaSO4:2H2O
Hemicarboaluminat  -9.17   56.39   65.55  Ca3Al2O6.5C0.5(OH):11.5H2O
Lime           -14.58   18.22   32.80  CaO
Monocarboaluminat  -9.19   61.30   70.49  (CaO)3Al2O3CaCO3:11H2O
O2(g)          -26.12   57.00   83.12  O2
Portlandite     -4.45   18.22   22.68  Ca(OH)2

------------------
End of simulation.
------------------
```

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Reading input data for simulation 7.
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SOLUTION 89  Damidot D., Stronach S., Kindness M., Atkins M., Glasser F. P. (1994)
        units   mmol/kgw
        pH      11.62
        density 1.0
        temp    25.0
        Ca              4.22
        Al              2.02
        C(4)            0.72
SOLUTION 90  Damidot D., Stronach S., Kindness M., Atkins M., Glasser F. P. (1994)
        units   mmol/kgw
        pH      11.30
        density 1.0
        temp    25.0
        Ca              2.72
        Al              1.39
        C(4)            0.90
END
```

```
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 89.Damidot D., Stronach S., Kindness M., Atkins M., Glasser F. P. (1994)

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

Elements           Molality       Moles

Al                2.020e-03   2.020e-03
C(4)              7.200e-04   7.200e-04
Ca                4.220e-03   4.220e-03

----------------------------Description of solution----------------------------

                                       pH  =  11.620
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   1.086e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   1.445e-02
                       Total CO2 (mol/kg)  =   7.200e-04
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =   4.892e-05
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.34
                               Iterations  =   5
                                  Total H  = 1.110255e+02
                                  Total O  = 5.552140e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

Al(OH)3(a)       -1.74    8.64   10.38  Al(OH)3
Al2O3            -5.70   17.28   22.98  Al2O3
Aragonite         1.87   -6.46   -8.34  CaCO3
Boehmite          0.06    8.64    8.58  AlOOH
C3AH6            -3.81   79.09   82.91  Ca3Al2(OH)12
C3AH6(C)         -0.36   79.09   79.45  Ca3Al2(OH)12
Calcite           2.01   -6.46   -8.47  CaCO3
CH               -2.30   20.60   22.90  Ca(OH)2
CH4(g)         -111.93 -152.03  -40.10  CH4
CO2(g)           -8.91  -27.07  -18.16  CO2
Diaspore          1.77    8.64    6.87  AlOOH
Gibbsite(C)      -0.13    8.64    8.77  Al(OH)3
Hemicarboaluminat   0.00   65.56   65.55  Ca3Al2O6.5C0.5(OH):11.5H2O
Lime            -12.19   20.61   32.80  CaO
Monocarboaluminat   2.14   72.63   70.49  (CaO)3Al2O3CaCO3:11H2O
O2(g)           -20.64   62.48   83.12  O2
Portlandite      -2.07   20.60   22.68  Ca(OH)2

Initial solution 90.Damidot D., Stronach S., Kindness M., Atkins M., Glasser F. P. (1994)

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

Elements           Molality       Moles

Al                1.390e-03   1.390e-03
C(4)              9.000e-04   9.000e-04
Ca                2.720e-03   2.720e-03

----------------------------Description of solution----------------------------

                                       pH  =  11.300
                                       pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   6.749e-03
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   9.603e-03
                       Total CO2 (mol/kg)  =   9.000e-04
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =   7.387e-06
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.09
                               Iterations  =   4
                                  Total H  = 1.110203e+02
                                  Total O  = 5.551675e+01
```

```
------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

Al(OH)3(a)       -1.57    8.81   10.38  Al(OH)3
Al2O3            -5.37   17.61   22.98  Al2O3
Aragonite         1.91   -6.43   -8.34  CaCO3
Boehmite          0.23    8.81    8.58  AlOOH
C3AH6            -5.95   76.95   82.91  Ca3Al2(OH)12
C3AH6(C)         -2.50   76.95   79.45  Ca3Al2(OH)12
Calcite           2.05   -6.43   -8.47  CaCO3
CH               -3.12   19.78   22.90  Ca(OH)2
CH4(g)         -108.51 -148.61  -40.10  CH4
CO2(g)           -8.05  -26.21  -18.16  CO2
Diaspore          1.93    8.81    6.87  AlOOH
Gibbsite(C)       0.04    8.81    8.77  Al(OH)3
Hemicarboaluminat  -1.71   63.85   65.55  Ca3Al2O6.5C0.5(OH):11.5H2O
Lime            -13.02   19.78   32.80  CaO
Monocarboaluminat   0.03   70.52   70.49  (CaO)3Al2O3CaCO3:11H2O
O2(g)           -21.92   61.20   83.12  O2
Portlandite      -2.89   19.78   22.68  Ca(OH)2

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End of simulation.
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```

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Reading input data for simulation 8.
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Solution 92 Data for Kuzel´s salt Glasser, Kindness, Stonach (1999) Cem&Concr Res 29, 861-866
        units   mmol/l
        pH      12.20
        density 1.0
        temp    25.0
        Ca              7.73
        Al              4.61
        Cl              3.96
        S(6)            0.007
END
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 92.Data for Kuzel´s salt Glasser, Kindness, Stonach (1999) Cem&Concr Res 29, 861-866

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

Elements           Molality       Moles

Al                4.613e-03   4.613e-03
Ca                7.734e-03   7.734e-03
Cl                3.962e-03   3.962e-03
S(6)              7.004e-06   7.004e-06

----------------------------Description of solution----------------------------

                                       pH  =  12.200
                                       pe  =   4.000
                        Activity of water  =   0.999
                           Ionic strength  =   2.671e-02
                       Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   3.875e-02
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                      Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  -1.342e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -32.62
                               Iterations  =   6
                                  Total H  = 1.110512e+02
                                  Total O  = 5.554500e+01

------------------------------Saturation indices-------------------------------

Phase               SI log IAP  log KT

(CaO)3CaCl2:15H2O -96.83   58.41  155.24  (CaO)3CaCl2:15H2O
AFm               2.02   74.58   72.56  Ca4Al2SO4(OH)12:6H2O
AFt               1.08   58.52   57.44  Ca6Al2(SO4)3(OH)12:26H2O
Al(OH)3(a)       -1.98    8.40   10.38  Al(OH)3
Al2O3            -6.18   16.80   22.98  Al2O3
Al4(OH)10SO4    -19.08    3.62   22.70  Al4(OH)10SO4
AlOHSO4         -18.34  -21.57   -3.23  AlOHSO4
Anhydrite        -3.39   -8.03   -4.64  CaSO4
Boehmite         -0.18    8.40    8.58  AlOOH
C3AH6            -0.29   82.61   82.91  Ca3Al2(OH)12
C3AH6(C)          3.16   82.61   79.45  Ca3Al2(OH)12
CaCl2:6H20       -9.86   -7.41    2.45  CaCl2:6H2O
CaOCaCl2:2H2O   -38.95   14.53   53.49  CaOCaCl2:2H2O
CH               -0.96   21.94   22.90  Ca(OH)2
Diaspore          1.52    8.40    6.87  AlOOH
Ettr_GCA          1.43   58.52   57.09  Ca6Al2(SO4)3(OH)12:26H2O
Fried0.86Al5.14OH  -1.65   65.63   67.28  Ca4Al0.86Cl2(OH)8.58
Fried0.88Al5.12OH  -2.11   65.80   67.91  Ca4Al0.88Cl2(OH)8.64
Fried1.04Al4.96OH  -2.59   67.14   69.74  Ca4Al1.04Cl2(OH)9.12
Fried1.34Al4.66OH  -2.62   69.66   72.28  Ca4Al1.34Cl2(OH)10.02
Fried1.42Al4.58OH  -2.56   70.34   72.90  Ca4Al1.42Cl2(OH)10.26
Fried1.96Al4.04OH  -1.52   74.87   76.39  Ca4Al1.96Cl2(OH)11.88
Friedelsalt       0.30   75.21   74.90  Ca4Al2Cl2(OH)12
Gibbsite(C)      -0.37    8.40    8.77  Al(OH)3
Gypsum           -3.18   -8.03   -4.85  CaSO4:2H2O
Gypsum_Cem       -3.43   -8.03   -4.60  CaSO4:2H2O
Kuzelsalt         0.00   74.89   74.89  Ca4Al2(SO4)0.5Cl(OH)12:6H2O
Lime            -10.86   21.94   32.80  CaO
O2(g)           -18.32   64.80   83.12  O2
Portlandite      -0.74   21.94   22.68  Ca(OH)2
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End of simulation.
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Reading input data for simulation 9.
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```

No memory leaks