Test calculations

Title	Solubilities and activities in solutions of metastable and stable cement phase assemblages
Interaction model	Pitzer
Elements	Na, K, Mg, Ca, Cl, S, C, Al, Si
Benchmark number	6
Editor(s)	Stefan Wilhelm, Helge Moog, Frank Bok, Christiane Bube
Main-editor	Stefan Wilhelm
Reviewer	Anke Richter
Revision	1.0
Date	2013-06-28

Change Log

Rev 0.5 (2013-02-02)
(x) final draft version for review
Rev 0.6 (2013-02-02)
(x) addition of cases 10a-c for CHEMAPP and EG3/6
Rev 0.7 (2013-06-13)
(x) various small changes

Pending changes

(x)

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1 Description

These test cases cover a number of single calculations for metastable and stable hydrated cement phase assemblages at 298.15 °C. The choice of the assemblages was only motivated by trying to cover the complete chemical system. The individual assemblages do not claim for being representative or substantial for cement systems.

Metastable as well as stable assemblages are chosen. Thus, depending on the respective model code (e.g. GWB) certain stable minerals have to be suppressed during individual calculations. This especially concerns Gibbsite that is more stable with respect to $Al(OH)_3$(mcr) and α-Quartz that is stable with respect to SiO_2(am).

Cases 1a-c and 2 describe different stable and metastable assemblages in the pure CaO-Al_2O_3-H_2O system. Cases 3, 4, 6 and 7 describe stable and metastable assemblages in CaO-Al_2O_3-H_2O systems enhanced by one or more additional components, e.g. Cl<->, CO_3<2->, SO_4<2->, $Si(OH)_4$<0>. In cases 5 and 9 Mg replaces Ca and thus describe assemblages in MgO-Al_2O_3-H_2O and MgO-SiO_2-H_2O system, respectively. The solution composition in the CaO-SiO_2-H_2O system presence of different CSH-phases – and SiO_2(am) or portlandite - is described by the cases 8a-d. Finally, the solubility of SiO_2(am) in $MgCl_2$-solutions of different concentration is covered by cases 10a – c.

The results are presented in terms of molal concentrations of relevant aqueous species and pH defined as log activity H<+>.

2 CHEMAPP

2.1 Classification

Version	
Date when parameter file was built	07.01.2013
Editor for test calculations with CHEMAPP	Helge Moog

2.2 Synopsis

1.	Add 1 kg H_2O(l)
2.	Set: T = 298.15 K, p = 100000 Pa
3.	Eliminate: gas phase
4.	Set dormant: any other solid phase as appropriate for the particular calculation
5.	Set activity of two mineral phases to unity as appropriate for the particular calculation

The resulting streams for all calculations are given below.

Number	Stream
(all streams)	T = 298.15000000 K P = 1.00000E+05 Pa STREAM CONSTITUENT H2O/AQUEOUS/ AMOUNT/mol = 5.55084391000000E+01 ELIMINATED PHASES: GAS
1a	Stable assemblage of Portlandite and Hydrogarnet
	Hydrogarnet ACTIVITY = 1.00000000000000E+00 Portlandite ACTIVITY = 1.00000000000000E+00
1b	Stable assemblage of Gibbsite and Hydrogarnet
	Gibbsite ACTIVITY = 1.00000000000000E+00 Hydrogarnet ACTIVITY = 1.00000000000000E+00
1c	Metastable assemblage of Al(OH)3(mcr) and Hydrogarnet
	Al(OH)3(mcr) ACTIVITY = 1.00000000000000E+00

Number	Stream
	Hydrogarnet ACTIVITY = 1.00000000000000E+00 DORMANT PHASES: Gibbsite
2	Metastable assemblage of C2AH8 and C4AH13
	C2AH8 ACTIVITY = 1.00000000000000E+00 C4AH13 ACTIVITY = 1.00000000000000E+00 DORMANT PHASES: Al(OH)3(mcr) Gibbsite Hydrogarnet Portlandite
3	Metastable assemblage of Al(OH)3(mcr)and Ettringite
	Al(OH)3(mcr) ACTIVITY = 1.00000000000000E+00 Ettringite ACTIVITY = 1.00000000000000E+00
4	Metastable assemblage of Calcite and Monocarbonate
	Calcite ACTIVITY = 1.00000000000000E+00 Monocarbonate ACTIVITY = 1.00000000000000E+00 DORMANT PHASES: Al(OH)3(mcr) Gibbsite
5	Stable assemblage of Brucite and Hydrotalcite
	Brucite ACTIVITY = 1.00000000000000E+00 Hydrotalcite ACTIVITY = 1.00000000000000E+00
6	Metastable assemblage of Ca4Cl2(OH)6:13H2O(cr)and Friedel’s salt
	Ca4Cl2(OH)6:13H2O(cr) ACTIVITY = 1.00000000000000E+00 Friedels_salt ACTIVITY = 1.00000000000000E+00 DORMANT PHASES: Portlandite
7	Stable assemblage of Si-Hydrogarnet and Gibbsite
	Gibbsite

Number	Stream
	ACTIVITY = 1.00000000000000E+00 Si-Hydrogarnet ACTIVITY = 1.00000000000000E+00
8a	Stable assemblage of Portlandite and CSH(1.8)
	CSH(1.8) ACTIVITY = 1.00000000000000E+00 Portlandite ACTIVITY = 1.00000000000000E+00
8b	Stable assemblage of CSH(1.8) and CSH(1.1)
	CSH(1.1) ACTIVITY = 1.00000000000000E+00 CSH(1.8) ACTIVITY = 1.00000000000000E+00
8c	Stable assemblage of CSH(1.1) and CSH(0.8)
	CSH(0.8) ACTIVITY = 1.00000000000000E+00 CSH(1.1) ACTIVITY = 1.00000000000000E+00
8d	Metastable assemblage of CSH(0.8) and SiO2(am)
	CSH(0.8) ACTIVITY = 1.00000000000000E+00 SiO2(am) ACTIVITY = 1.00000000000000E+00
9	Metastable assemblage of Kerolite and SiO2(am)
	Kerolite ACTIVITY = 1.00000000000000E+00 SiO2(am) ACTIVITY = 1.00000000000000E+00 ELIMINATED PHASES: Sepiolite SiO2_alpha_Qtz(cr)
10a	Solubility of SiO2(am) in 0.1 molal MgCl2 solution
	H2O/AQUEOUS/ AMOUNT/mol = 5.55084391000000E+01 Cl<->/AQUEOUS/ AMOUNT/mol = 2.00000000000000E-01 Mg<2+>/AQUEOUS/ AMOUNT/mol = 1.00000000000000E-01 SiO2(am) ACTIVITY = 1.00000000000000E+00 ELIMINATED PHASES: GAS SiO2_alpha_Qtz(cr)
10b	Solubility of SiO2(am) in 3 molal MgCl2 solution

Number	Stream
	STREAM CONSTITUENT H2O/AQUEOUS/ AMOUNT/mol = 5.55084391000000E+01 Cl<->/AQUEOUS/ AMOUNT/mol = 6.00000000000000E+00 Mg<2+>/AQUEOUS/ AMOUNT/mol = 3.00000000000000E+00 SiO2(am) ACTIVITY = 1.00000000000000E+00 ELIMINATED PHASES: GAS SiO2_alpha_Qtz(cr)
10c	Solubility of SiO2(am) in 5 molal MgCl2 solution
	STREAM CONSTITUENT H2O/AQUEOUS/ AMOUNT/mol = 5.55084391000000E+01 Cl<->/AQUEOUS/ AMOUNT/mol = 1.00000000000000E+01 Mg<2+>/AQUEOUS/ AMOUNT/mol = 5.00000000000000E+00 SiO2(am) ACTIVITY = 1.00000000000000E+00 ELIMINATED PHASES: GAS SiO2_alpha_Qtz(cr)

2.3 Remarks

Setting a phase "dormant" causes CHEMAPP to calculate the activity of this phase. At the same time, the phase is not allowed to be formed at runtime.

"Streams" are concepts in CHEMAPP to define a set of boundary conditions. Prior to calculation one can retrieve streams from CHEMAPP to make sure, that the code interpreted the settings for the calculation correctly. It is used here as a means of documenting the benchmark calculation.

Some calculations represent metastable phases. Thus, other phases which otherwise would precipitate as thermodynamically stable phases had to be set dormant.

3 PHREEQC

3.1 Classification

Version	2.18.3.5570
Date when parameter file was built	07.01.2013
Editor for test calculations with PHREEQC	Stefan Wilhelm

3.2 Synopsis

1.	SOLUTION > General: leave all properties as default, T = 25°C
1.b	Set charge balance to pH for calculations 10 a-c
2.	SOLUTION > Individual Element Input (as required by the considered phases)
3	EQUILIBRIUM_PHASES > Set sat. index = 0 and amount of moles = 10 for required solid phases and force them to equality
4.	Set PITZER option MacInnes = false
5.	Set PITZER use-etheta = true

The resulting scripts for all calculations are given below.

Number	PHREEQC script
1a	`Stable assemblage of Portlandite and Hydrogarnet`

	`SOLUTION 1`
	`    temp      25`
	`    pH        7`
	`    pe        4`
	`    redox     pe`
	`    units     mmol/kgw`
	`    density   1`
	`    Ca        0`
	`    Al        0`
	`    -water    1 # kg`
	
	`EQUILIBRIUM_PHASES 1`
	`    Portlandite 0 10`
	`        -force_equality`
	`    Hydrogarnet 0 10`
	`        -force_equality`

1b	`Stable assemblage of Gibbsite and Hydrogarnet`

Number	PHREEQC script
	SOLUTION 1 temp 25 pH 7 pe 4 redox pe units mmol/kgw density 1 Ca 0 Al 0 -water 1 # kg EQUILIBRIUM_PHASES 1 Hydrogarnet 0 10 -force_equality Gibbsite 0 10 -force_equality
1c	Metastable assemblage of Al(OH)3(mcr) and Hydrogarnet
	SOLUTION 1 temp 25 pH 7 pe 4 redox pe units mmol/kgw density 1 Ca 0 Al 0 -water 1 # kg EQUILIBRIUM_PHASES 1 Hydrogarnet 0 10 -force_equality Al(OH)3(mcr) 0 10 -force_equality
2	Metastable assemblage of C2AH8 and C4AH13
	SOLUTION 1 temp 25 pH 7 pe 4 redox pe units mmol/kgw density 1 Ca 0 Al 0 -water 1 # kg EQUILIBRIUM_PHASES 1 C2AH8 0 10 -force_equality C4AH13 0 10 -force_equality
3	Metastable assemblage of Al(OH)3(mcr)and Ettringite

Number	PHREEQC script
	SOLUTION 1 temp 25 pH 7 pe 4 redox pe units mmol/kgw density 1 Ca 0 Al 0 S(6) 0 -water 1 # kg EQUILIBRIUM_PHASES 1 Al(OH)3(mcr) 0 10 -force_equality Ettringite 0 10 -force_equality
4	Metastable assemblage of Calcite and Monocarbonate
	SOLUTION 1 temp 25 pH 7 pe 4 redox pe units mmol/kgw density 1 Ca 0 Al 0 C(4) 0 -water 1 # kg EQUILIBRIUM_PHASES 1 Calcite 0 10 -force_equality Monocarbonate 0 10 -force_equality
5	Stable assemblage of Brucite and Hydrotalcite
	SOLUTION 1 temp 25 pH 7 pe 4 redox pe units mmol/kgw density 1 Al 0 Mg(2) 0 -water 1 # kg EQUILIBRIUM_PHASES 1 Brucite 0 10 -force_equality Hydrotalcite 0 10 -force_equality

Number	PHREEQC script
6	Metastable assemblage of Ca4Cl2(OH)6:13H2O(cr)and Friedel's salt
	SOLUTION 1 temp 25 pH 7 pe 4 redox pe units mmol/kgw density 1 Ca 0 Al 0 Cl(-1) 0 S(6) 0 -water 1 # kg EQUILIBRIUM_PHASES 1 Ca4Cl2(OH)6:13H2O(cr) 0 10 -force_equality Friedels_salt 0 10 -force_equality
7	Stable assemblage of Si-Hydrogarnet and Gibbsite
	SOLUTION 1 temp 25 pH 7 pe 4 redox pe units mmol/kgw density 1 Al 0 Si(4) 0 Ca(2) 0 -water 1 # kg EQUILIBRIUM_PHASES 1 Si-Hydrogarnet 0 10 -force_equality Gibbsite 0 10 -force_equality
8a	Stable assemblage of Portlandite and CSH(1.8)

Number	PHREEQC script
	SOLUTION 1 temp 25 pH 7 pe 4 redox pe units mmol/kgw density 1 Si(4) 0 Ca(2) 0 -water 1 # kg EQUILIBRIUM_PHASES 1 Portlandite 0 10 -force_equality CSH(1.8) 0 10 -force_equality
8b	Stable assemblage of CSH(1.8) and CSH(1.1)
	SOLUTION 1 temp 25 pH 7 pe 4 redox pe units mmol/kgw density 1 Si(4) 0 Ca(2) 0 -water 1 # kg EQUILIBRIUM_PHASES 1 CSH(1.1) 0 10 -force_equality CSH(1.8) 0 10 -force_equality
8c	Stable assemblage of CSH(1.1) and CSH(0.8)
	SOLUTION 1 temp 25 pH 7 pe 4 redox pe units mmol/kgw density 1 Si(4) 0 Ca(2) 0 -water 1 # kg EQUILIBRIUM_PHASES 1 CSH(0.8) 0 10 -force_equality CSH(1.1) 0 10 -force_equality
8d	Metastable assemblage of CSH(0.8) and SiO2(am)

Number	PHREEQC script
	SOLUTION 1 temp 25 pH 7 pe 4 redox pe units mmol/kgw density 1 Si(4) 0 Ca(2) 0 -water 1 # kg EQUILIBRIUM_PHASES 1 CSH(0.8) 0 10 -force_equality SiO2(am) 0 10 -force_equality
9	Metastable assemblage of Kerolite and SiO2(am)
	SOLUTION 1 temp 25 pH 7 pe 4 redox pe units mmol/kgw density 1 Al(3) 0 Mg(2) 0 Si(4) 0 -water 1 # kg EQUILIBRIUM_PHASES 1 Kerolite 0 10 -force_equality SiO2(am) 0 10 -force_equality
10a	Solubility of SiO2(am) in 0.1 molal MgCl2 solution
	SOLUTION 1 temp 25 pH 7 charge pe 4 redox pe units mol/kgw density 1 Mg(2) 0.1 Cl(-1) 0.2 Si(4) 0 -water 1 # kg EQUILIBRIUM_PHASES 1 SiO2(am) 0 10 -force_equality
10b	Solubility of SiO2(am) in 3 molal MgCl2 solution

Number	PHREEQC script
	SOLUTION 1 temp 25 pH 7 charge pe 4 redox pe units mol/kgw density 1 Mg(2) 3 Cl(-1) 6 Si(4) 0 -water 1 # kg EQUILIBRIUM_PHASES 1 SiO2(am) 0 10 -force_equality
10c	Solubility of SiO2(am) in 5 molal MgCl2 solution
	SOLUTION 1 temp 25 pH 7 charge pe 4 redox pe units mol/kgw density 1 Mg(2) 5 Cl(-1) 10 Si(4) 0 -water 1 # kg EQUILIBRIUM_PHASES 1 SiO2(am) 0 10 -force_equality
All calculations	PITZER -MacInnes false -use_etheta true -redox false END

3.3 Remarks

- One can start the calculation without setting values for density, redox and pe in the "SOLUTION 1" block. This does not have an influence on the calculation (for the above described test cases). However, if one uses the GUI, these lines are added with default values by PHREEQC even if the proposed values in the GUI are deleted.

- Unfortunately, there is no way in PHREEQC to define all phases as possible equilibrium phases by default. Thus, one has to check the result for a possible oversaturation. Phases with positive SI that shall be considered have to be defined as EQUILIBRIUM PHASE, either with a sufficient amount of mols or with 0.0 mols for phases forming during reaction. In this benchmark setting, the amount of mole for equilibrium phase to 10 has turned out to be sufficient.

- PHREEQC offers two scaling conventions for individual-ion activity coefficients. By default the MacInnes [MAC1919] convention is used, where $\gamma_{KCl}^{\pm} = \gamma_{K^+} = \gamma_{Cl^-}$. However, the MacInnes convention cannot be relied on to deliver accurate individual ion activity coefficients at high solute concentrations as those considered in the above described ternary systems. Thus, one has to unselect this option ("-MacInnes false") so that no scaling is performed. With this measure, the concentrations and activity coefficients calculated with PHREEQC are in good agreement to those calculated by CHEMAPP.

- PHREEQC offers two scaling conventions for treating non-symmetric mixing terms – cation/cation and anion/anion of different charge [PIT1987]. If the flag – use-etheta is true, the terms are included; if false these terms are excluded from all equations. The default is true.

- As the test cases do not include redox reactions the redox convention within the "PITZER" block can be set to "false".

4 Geochemist's Workbench (GWB)

4.1 Classification

Version	9.0.3
Date when parameter file was built	07.01.2013
Editor for test calculations with GWB	Frank Bok

4.2 Synopsis

1.	Set Basis General: leave all properties as default
	Set Basis Individual Element Input: select necessary basis species with initial concentrations ≈ 1 mmol / kg (watch out for charge balanced initial solution)
	Set "balance off"
1a.	Calculations No. 10a-c only: Set initial concentrations of Mg<2+> and Cl<-> to given ionic strength
1b.	For metastable assemblages only: Suppress all minerals ("suppress ALL") Unsuppress required minerals ("unsuppress …")
2.	Set Reactants by selecting the first mineral with a sufficient amount (1 mol), run calculation, then pickup entire system, selecting the second mineral with a sufficient amount (1 mol)
3	Enter "go", click Run or press Ctrl+G

The resulting scripts for all calculations are given below.

Number	Geochemist's Workbench script

all	`data = .\THEREDA_PIT_GWB_r06.dat verify`
	`temperature = 25`
	`H2O = 1 free kg`
	`pH = 7`
	`balance off`

	`Stable assemblage of Portlandite and Hydrogarnet`

1a	`Ca++ = 1 umol/kg`
	`Al(OH)4- = 2 umol/kg`
	`react 1 mol Hydrogarnet`
	`go`
	`pickup entire`
	`react 1 mol Portlandite`
	`printout species = long`
	`suffix _R-06_01a`
	`go`

Number	Geochemist's Workbench script
	Stable assemblage of Gibbsite and Hydrogarnet
1b	Ca++ = 1 umol/kg Al(OH)4- = 2 umol/kg react 1 mol Hydrogarnet go pickup entire react 1 mol Gibbsite printout species = long suffix _R-06_01b go
	Metastable assemblage of Al(OH)3(mcr) and Hydrogarnet
1c	Ca++ = 1 umol/kg Al(OH)4- = 2 umol/kg suppress ALL unsuppress Al(OH)3(mcr) Hydrogarnet react 1 mol Hydrogarnet go pickup entire react 1 mol Al(OH)3(mcr) printout species = long suffix _R-06_01c go
	Metastable assemblage of C2AH8 and C4AH13
2	Ca++ = 1 umol/kg Al(OH)4- = 1 umol/kg suppress ALL unsuppress C2AH8 C4AH13 react 1 mol C2AH8 go pickup entire react 1 mol C4AH13 printout species = long suffix _R-06_02 go
	Metastable assemblage of Al(OH)3(mcr)and Ettringite

Number	Geochemist's Workbench script
3	Ca++ = 1.5 umol/kg Al(OH)4- = 1 umol/kg SO4-- = 1 umol/kg suppress ALL unsuppress Al(OH)3(mcr) Ettringite react 1 mol Al(OH)3(mcr) go pickup entire react 1 mol Ettringite printout species = long suffix _R-06_03 go
	Metastable assemblage of Calcite and Monocarbonate
4	Ca++ = 1.5 umol/kg Al(OH)4- = 1 umol/kg CO3-- = 1 umol/kg suppress ALL unsuppress Calcite Monocarbonate react 1 mol Calcite go pickup entire react 1 mol Monocarbonate printout species = long suffix _R-06_04 go
	Stable assemblage of Brucite and Hydrotalcite
5	Mg++ = 1 umol/kg Al(OH)4- = 2 umol/kg react 1 mol Brucite go pickup entire react 1 mol Hydrotalcite printout species = long suffix _R-06_05 go
	Metastable assemblage of Ca4Cl2(OH)6:13H2O(cr)and Friedel's salt

Number	Geochemist's Workbench script
6	Ca++ = 1 umol/kg Al(OH)4- = 1 umol/kg Cl- = 1 umol/kg suppress ALL unsuppress Ca4Cl2(OH)6:13H2O(cr) Friedels_salt react 1 mol Ca4Cl2(OH)6:13H2O(cr) go pickup entire react 1 mol Friedels_salt printout species = long suffix _R-06_06 go
	Stable assemblage of Si-Hydrogarnet and Gibbsite
7	Ca++ = 1 umol/kg Al(OH)4- = 2 umol/kg Si(OH)4 = 1 umol/kg suppress ALL unsuppress Gibbsite Si-Hydrogarnet react 1 mol Gibbsite go pickup entire react 1 mol Si-Hydrogarnet printout species = long suffix _R-06_07 go
	Stable assemblage of Portlandite and CSH(1.8)
8a	Ca++ = 1 umol/kg Si(OH)4 = 1 umol/kg react 1 mol Portlandite go pickup entire react 1 mol CSH(1.8) printout species = long suffix _R-06_08a go
	Stable assemblage of CSH(1.8) and CSH(1.1)
8b	Ca++ = 1 umol/kg Si(OH)4 = 1 umol/kg react 1 mol CSH(1.8) go pickup entire react 1 mol CSH(1.1) printout species = long suffix _R-06_08b go

Number	Geochemist's Workbench script
	Stable assemblage of CSH(1.1) and CSH(0.8)
8c	Ca++ = 1 umol/kg Si(OH)4 = 1 umol/kg react 1 mol CSH(1.1) go pickup entire react 1 mol CSH(0.8) printout species = long suffix _R-06_08c go
	Metastable assemblage of CSH(0.8) and SiO2(am)
8d	Ca++ = 1 umol/kg Si(OH)4 = 1 umol/kg suppress ALL unsuppress SiO2(am) CSH(0.8) react 1 mol SiO2(am) go pickup entire react 1 mol CSH(0.8) printout species = long suffix _R-06_08d go
	Metastable assemblage of Kerolite and SiO2(am)
9	Mg++ = 1 umol/kg Al(OH)4- = 2 umol/kg Si(OH)4 = 1 umol/kg suppress ALL unsuppress Kerolite SiO2(am) react 1 mol SiO2(am) go pickup entire react 1 mol Kerolite printout species = long suffix _R-06_09 go
	Solubility of SiO2(am) in 0.1 molal MgCl2 solution
10a	Mg++ = 0.1 molal Cl- = 0.2 molal Si(OH)4 = 1 umol/kg suppress ALL unsuppress SiO2(am) react 1 mol SiO2(am) printout species = long suffix _R-06_10a go

Number	Geochemist's Workbench script
	Solubility of SiO2(am) in 3 molal MgCl2 solution
10b	Mg++ = 3 molal Cl- = 6 molal Si(OH)4 = 1 umol/kg suppress ALL unsuppress SiO2(am) react 1 mol SiO2(am) printout species = long suffix _R-06_10b go
	Solubility of SiO2(am) in 5 molal MgCl2 solution
10c	Mg++ = 5 molal Cl- = 10 molal Si(OH)4 = 1 umol/kg suppress ALL unsuppress SiO2(am) react 1 mol SiO2(am) printout species = long suffix _R-06_10c go

4.3 Remarks

Charge balancing has to be disabled or calculations No. 8a-d will not work.

5 EQ3/6

5.1 Classification

Code version	8.0a
Date when parameter file was built	07.01.2013
Editor for test calculations with EQ3/6	Christiane Bube

5.2 Synopsis

1.	Compile THEREDA parameter file using EQPT
2.	Set-up EQ3 input file leaving all values default except for “internal” pH scale, T = 25°C, charge balance turned off (except for calculations No. 4 and 10 a-c)
3.	Set molalities of all species to very low value ~10^{-20}
4.	Run EQ3
5.	Add minerals in EQ6 input file

The resulting streams for all calculations are given below.

Number	Excerpt of input file

All EQ3 files (except no. 4)	`|Temperature (C) | 2.50000E+01| (tempc) |`
	`|---|`
	`|Pressure option (jpres3): |`
	`| [x] ( 0) Data file reference curve value |`
	`| [ ] ( 1) 1.013-bar/steam-saturation curve value |`
	`| [ ] ( 2) Value (bars) | 0.00000E+00| (press) |`
	`|---|`
	`|Density (g/cm3) | 1.00000E+00| (rho) |`
	`|---|`
	`|Total dissolved solutes option (itdsf3): |`
	`| [x] ( 0) Value (mg/kg.sol) | 0.00000E+00| (tdspkg) |`
	`| [ ] ( 1) Value (mg/L) | 0.00000E+00| (tdspl) |`
	`|---|`
	`|Electrical balancing option (iebal3): |`
	`| [x] ( 0) No balancing is done |`
	`| [ ] ( 1) Balance on species | | (uebal) |`
	`|---|`
	`|Default redox constraint (irdxc3): |`
	`| [ ] (-3) Use O2(g) line in the aqueous basis species block |`
	`| [x] (-2) pe (pe units) | 4.00000E+00| (pei) |`
	`| [ ] (-1) Eh (volts) | 0.00000E+00| (ehi) |`
	`| [ ] ( 0) Log fO2 (log bars) | 0.00000E+00| (fo2lgi) |`
	`| [ ] ( 1) Couple (aux. sp.) |None | (uredox) |`

EQ3 input file no.4	`|Electrical balancing option (iebal3): |`
	`| [ ] ( 0) No balancing is done |`
	`| [x] ( 1) Balance on species |H+ | (uebal) |`

Reactant options used in all EQ6 files	`|->|Surface area option (nsk(n)): |` **`|->| [x] ( 0) Constant surface area: |`** **`|->| Value (cm2) | 0.00000E+00| (sfcar(n)) |`** **`|->| [ ] ( 1) Constant specific surface area: |`** **`|->| Value (cm2/g) | 0.00000E+00| (ssfcar(n)) |`** **`|->| [ ] ( 2) n**2/3 growth law- current surface area: |`** **`|->| Value (cm2) | 0.00000E+00| (sfcar(n)) |`** **`|---|`**

Number	Excerpt of input file
	|->|Surface area factor | 0.00000E+00| (fkrc(n))
	|----------|
	|->|Forward rate law |Relative rate equation | (urcnrk(nrk(1,n)))
	|----------|
	|--->|dXi(n)/dXi (mol/mol) | 1.00000E+01| (rkb(1,1,n))
	|----------|
	|--->|d2Xi(n)/dXi2 (mol/mol2) | 0.00000E+00| (rkb(2,1,n))
	|----------|
	|--->|d3Xi(n)/dXi3 (mol/mol3) | 0.00000E+00| (rkb(3,1,n))
	|----------|
	|->|Backward rate law |Partial equilibrium | (urcnrk(nrk(2,n)))
1a	Stable assemblage of Portlandite and Hydrogarnet
Excerpt of EQ3-input file	|Ca++ | 1.00000E-20|Molality | |Al(OH)4- | 1.00000E-20|Molality | |H+ | 1.00000E-07|Molality |
Excerpts of EQ6-input file	|Reactant |Portlandite | (ureac(n)) | |----------| |->|Type |Pure mineral | (urcjco(jcode(n))) | |----------| |->|Status |Reacting | (urcjre(jreac(n))) | |----------| |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) | |----------| |->|Amount destroyed (moles) | 0.00000E+00| (modr(n)) |
	|Reactant |Hydrogarnet | (ureac(n)) | |----------| |->|Type |Pure mineral | (urcjco(jcode(n))) | |----------| |->|Status |Reacting | (urcjre(jreac(n))) | |----------| |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) | |----------| |->|Amount destroyed (moles) | 0.00000E+00| (modr(n)) |
1b	Stable assemblage of Gibbsite and Hydrogarnet
Excerpt of EQ3-input file	|Ca++ | 1.00000E-20|Molality | |Al(OH)4- | 1.00000E-20|Molality | |H+ | 1.00000E-07|Molality |
Excerpts of EQ6-input file	|Reactant |Gibbsite | (ureac(n)) | |----------| |->|Type |Pure mineral | (urcjco(jcode(n))) | |----------| |->|Status |Reacting | (urcjre(jreac(n))) | |----------| |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) | |----------| |->|Amount destroyed (moles) | 0.00000E+00| (modr(n)) |
	|Reactant |Hydrogarnet | (ureac(n)) | |----------| |->|Type |Pure mineral | (urcjco(jcode(n))) | |----------| |->|Status |Reacting | (urcjre(jreac(n))) | |----------| |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) | |----------| |->|Amount destroyed (moles) | 0.00000E+00| (modr(n)) |
1c	Metastable assemblage of Al(OH)3(mcr) and Hydrogarnet
Excerpts of EQ3-input file	|Ca++ | 1.00000E-20|Molality | |Al(OH)4- | 1.00000E-20|Molality | |H+ | 1.00000E-07|Molality |
	|Alter/Suppress Options | (nxmod) | |----------| |Species |Option |Alter value | | (uxmod(n)) |(ukxm(kxmod(n)))| (xlkmod(n))| |----------| |Gibbsite |Suppress | |
Excerpts of EQ6-input	|Reactant |Al(OH)3(mcr) | (ureac(n)) | |----------| |->|Type |Pure mineral | (urcjco(jcode(n))) |

Number	Excerpt of input file
file	|----------| |->|Status |Reacting | (urcjre(jreac(n))) |----------| |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) |----------| |->|Amount destroyed (moles) | 0.00000E+00| (modr(n))
	|Reactant |Hydrogarnet | (ureac(n)) |----------| |->|Type |Pure mineral | (urcjco(jcode(n))) |----------| |->|Status |Reacting | (urcjre(jreac(n))) |----------| |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) |----------| |->|Amount destroyed (moles) | 0.00000E+00| (modr(n))
2	Metastable assemblage of C2AH8 and C4AH13
Excerpts of EQ3-input file	|Ca++ | 1.00000E-20|Molality | |Al(OH)4- | 1.00000E-20|Molality | |H+ | 1.00000E-07|Molality |
	|Alter/Suppress Options | (nxmod) |----------| |Species |Option |Alter value | | (uxmod(n)) |(ukxm(kxmod(n)))| (xlkmod(n))| |----------| |Gibbsite |Suppress | | |Al(OH)3(mcr) |Suppress | | |Hydrogarnet |Suppress | |
Excerpts of EQ6-input file	|Reactant |C2AH8 | (ureac(n)) |----------| |->|Type |Pure mineral | (urcjco(jcode(n))) |----------| |->|Status |Reacting | (urcjre(jreac(n))) |----------| |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) |----------| |->|Amount destroyed (moles) | 0.00000E+00| (modr(n))
	|Reactant |C4AH13 | (ureac(n)) |----------| |->|Type |Pure mineral | (urcjco(jcode(n))) |----------| |->|Status |Reacting | (urcjre(jreac(n))) |----------| |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) |----------| |->|Amount destroyed (moles) | 0.00000E+00| (modr(n))
3	Metastable assemblage of Al(OH)3(mcr)and Ettringite
Excerpts of EQ3-input file	|Ca++ | 1.00000E-20|Molality | |Al(OH)4- | 1.00000E-20|Molality | |SO4-- | 1.00000E-20|Molality | |H+ | 1.00000E-07|Molality |
	|Alter/Suppress Options | (nxmod) |----------| |Species |Option |Alter value | | (uxmod(n)) |(ukxm(kxmod(n)))| (xlkmod(n))| |----------| |Gibbsite |Suppress | | |Hydrogarnet |Suppress | |
Excerpts of EQ6-input file	|Reactant |Al(OH)3(mcr) | (ureac(n)) |----------| |->|Type |Pure mineral | (urcjco(jcode(n))) |----------| |->|Status |Reacting | (urcjre(jreac(n))) |----------| |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) |----------| |->|Amount destroyed (moles) | 0.00000E+00| (modr(n))
	|Reactant |Ettringite | (ureac(n)) |----------| |->|Type |Pure mineral | (urcjco(jcode(n)))

Number	Excerpt of input file
	|----------| |->|Status |Reacting | (urcjre(jreac(n))) |----------| |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) |----------| |->|Amount destroyed (moles) | 0.00000E+00| (modr(n))
4	Metastable assemblage of Calcite and Monocarbonate
Excerpts of EQ3-input file	|Ca++ | 1.00000E-20|Molality |Al(OH)4- | 1.00000E-20|Molality |CO3-- | 1.00000E-20|Molality |H+ | 1.00000E-07|Molality
	|Alter/Suppress Options | (nxmod) |----------| |Species |Option |Alter value | | (uxmod(n)) |(ukxm(kxmod(n)))| (xlkmod(n))| |----------| |Gibbsite |Suppress | | |Al(OH)3(mcr) |Suppress | |
Excerpts of EQ6-input file	|Reactant |Calcite | (ureac(n)) |----------| |->|Type |Pure mineral | (urcjco(jcode(n))) |----------| |->|Status |Reacting | (urcjre(jreac(n))) |----------| |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) |----------| |->|Amount destroyed (moles) | 0.00000E+00| (modr(n))
	|Reactant |Monocarbonate | (ureac(n)) |----------| |->|Type |Pure mineral | (urcjco(jcode(n))) |----------| |->|Status |Reacting | (urcjre(jreac(n))) |----------| |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) |----------| |->|Amount destroyed (moles) | 0.00000E+00| (modr(n))
5	Stable assemblage of Brucite and Hydrotalcite
Excerpt of EQ3-input file	|Mg++ | 1.00000E-20|Molality |Al(OH)4- | 1.00000E-20|Molality |H+ | 1.00000E-07|Molality
Excerpts of EQ6-input file	|Reactant |Brucite | (ureac(n)) |----------| |->|Type |Pure mineral | (urcjco(jcode(n))) |----------| |->|Status |Reacting | (urcjre(jreac(n))) |----------| |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) |----------| |->|Amount destroyed (moles) | 0.00000E+00| (modr(n))
	|Reactant |Hydrotalcite | (ureac(n)) |----------| |->|Type |Pure mineral | (urcjco(jcode(n))) |----------| |->|Status |Reacting | (urcjre(jreac(n))) |----------| |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) |----------| |->|Amount destroyed (moles) | 0.00000E+00| (modr(n))
6	Metastable assemblage of Ca4Cl2(OH)6:13H2O(cr)and Friedel’s salt
Excerpts of EQ3-input file	|Ca++ | 1.00000E-20|Molality |Al(OH)4- | 1.00000E-20|Molality |Cl- | 1.00000E-20|Molality |SO4-- | 1.00000E-20|Molality |H+ | 1.00000E-07|Molality
	|Alter/Suppress Options | (nxmod) |----------|

Number	Excerpt of input file
	|Species | (uxmod(n)) |Option |(ukxm(kxmod(n))) |Alter value | (xlkmod(n)) | |Portlandite |Suppress | |
Excerpts of EQ6-input file	|Reactant |Ca4Cl2(OH)6.13H2O(cr) | (ureac(n)) | |->|Type |Pure mineral | (urcjco(jcode(n))) | |->|Status |Reacting | (urcjre(jreac(n))) | |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) | |->|Amount destroyed (moles) | 0.00000E+00| (modr(n)) |
	|Reactant |Friedels_salt | (ureac(n)) | |->|Type |Pure mineral | (urcjco(jcode(n))) | |->|Status |Reacting | (urcjre(jreac(n))) | |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) | |->|Amount destroyed (moles) | 0.00000E+00| (modr(n)) |
7	Stable assemblage of Si-Hydrogarnet and Gibbsite
Excerpt of EQ3-input file	|Ca++ | 1.00000E-20|Molality | |Al(OH)4- | 1.00000E-20|Molality | |Si(OH)4(aq) | 1.00000E-20|Molality | |H+ | 1.00000E-07|Molality |
Excerpts of EQ6-input file	|Reactant |Si-Hydrogarnet | (ureac(n)) | |->|Type |Pure mineral | (urcjco(jcode(n))) | |->|Status |Reacting | (urcjre(jreac(n))) | |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) | |->|Amount destroyed (moles) | 0.00000E+00| (modr(n)) |
	|Reactant |Gibbsite | (ureac(n)) | |->|Type |Pure mineral | (urcjco(jcode(n))) | |->|Status |Reacting | (urcjre(jreac(n))) | |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) | |->|Amount destroyed (moles) | 0.00000E+00| (modr(n)) |
8a	Stable assemblage of Portlandite and CSH(1.8)
Excerpt of EQ3-input file	|Ca++ | 1.00000E-20|Molality | |Si(OH)4(aq) | 1.00000E-20|Molality | |H+ | 1.00000E-07|Molality |
Excerpts of EQ6-input file	|Reactant |Portlandite | (ureac(n)) | |->|Type |Pure mineral | (urcjco(jcode(n))) | |->|Status |Reacting | (urcjre(jreac(n))) | |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) | |->|Amount destroyed (moles) | 0.00000E+00| (modr(n)) |
	|Reactant |CSH(1.8) | (ureac(n)) | |->|Type |Pure mineral | (urcjco(jcode(n))) | |->|Status |Reacting | (urcjre(jreac(n))) | |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) | |->|Amount destroyed (moles) | 0.00000E+00| (modr(n)) |
8b	Stable assemblage of CSH(1.8) and CSH(1.1)

Number	Excerpt of input file
Excerpt of EQ3-input file	|Ca++ | 1.00000E-20|Molality | |Si(OH)4(aq) | 1.00000E-20|Molality | |H+ | 1.00000E-07|Molality |
Excerpts of EQ6-input file	|Reactant |CSH(1.1) | (ureac(n)) | |->|Type |Pure mineral | (urcjco(jcode(n))) | |->|Status |Reacting | (urcjre(jreac(n))) | |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) | |->|Amount destroyed (moles) | 0.00000E+00| (modr(n)) |
	|Reactant |CSH(1.8) | (ureac(n)) | |->|Type |Pure mineral | (urcjco(jcode(n))) | |->|Status |Reacting | (urcjre(jreac(n))) | |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) | |->|Amount destroyed (moles) | 0.00000E+00| (modr(n)) |
8c	Stable assemblage of CSH(1.1) and CSH(0.8)
Excerpt of EQ3-input file	|Ca++ | 1.00000E-20|Molality | |Si(OH)4(aq) | 1.00000E-20|Molality | |H+ | 1.00000E-07|Molality |
Excerpts of EQ6-input file	|Reactant |CSH(1.1) | (ureac(n)) | |->|Type |Pure mineral | (urcjco(jcode(n))) | |->|Status |Reacting | (urcjre(jreac(n))) | |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) | |->|Amount destroyed (moles) | 0.00000E+00| (modr(n)) |
	|Reactant |CSH(0.8) | (ureac(n)) | |->|Type |Pure mineral | (urcjco(jcode(n))) | |->|Status |Reacting | (urcjre(jreac(n))) | |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) | |->|Amount destroyed (moles) | 0.00000E+00| (modr(n)) |
8d	Metastable assemblage of CSH(0.8) and SiO2(am)
Excerpts of EQ3-input file	|Ca++ | 1.00000E-20|Molality | |Si(OH)4(aq) | 1.00000E-20|Molality | |H+ | 1.00000E-07|Molality |
	|Alter/Suppress Options | (nxmod) | |Species |Option |Alter value | | (uxmod(n)) |(ukxm(kxmod(n)))| (xlkmod(n))| |SiO2_alpha_Qtz(cr) |Suppress | |
Excerpts of EQ6-input file	|Reactant |SiO2(am) | (ureac(n)) | |->|Type |Pure mineral | (urcjco(jcode(n))) | |->|Status |Reacting | (urcjre(jreac(n))) | |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) | |->|Amount destroyed (moles) | 0.00000E+00| (modr(n)) |
	|Reactant |CSH(0.8) | (ureac(n)) | |->|Type |Pure mineral | (urcjco(jcode(n))) | |->|Status |Reacting | (urcjre(jreac(n))) |

Number	Excerpt of input file

	`|->|Amount remaining (moles) | 5.00000E+00| (morr(n)) |`
	`|----------|`
	`|->|Amount destroyed (moles) | 0.00000E+00| (modr(n)) |`

9	Metastable assemblage of Kerolite and SiO2(am)

Excerpts of EQ3-input file	`|Mg++ | 1.00000E-20|Molality |`
	`|Si(OH)4(aq) | 1.00000E-20|Molality |`
	`|Al(OH)4- | 1.00000E-20|Molality |`
	`|H+ | 1.00000E-07|Molality |`

	`|Alter/Suppress Options | (nxmod) |`
	`|----------|`
	`|Species |Option |Alter value |`
	`| (uxmod(n)) |(ukxm(kxmod(n)))| (xlkmod(n))|`
	`|----------|`
	`|SiO2_alpha_Qtz(cr) |Suppress | |`
	`|Sepiolite |Suppress | |`

Excerpts of EQ6-input file	`|Reactant |SiO2(am) | (ureac(n)) |`
	`|----------|`
	`|->|Type |Pure mineral | (urcjco(jcode(n))) |`
	`|----------|`
	`|->|Status |Reacting | (urcjre(jreac(n))) |`
	`|----------|`
	`|->|Amount remaining (moles) | 5.00000E+00| (morr(n)) |`
	`|----------|`
	`|->|Amount destroyed (moles) | 0.00000E+00| (modr(n)) |`

	`|Reactant |Kerolite | (ureac(n)) |`
	`|----------|`
	`|->|Type |Pure mineral | (urcjco(jcode(n))) |`
	`|----------|`
	`|->|Status |Reacting | (urcjre(jreac(n))) |`
	`|----------|`
	`|->|Amount remaining (moles) | 5.00000E+00| (morr(n)) |`
	`|----------|`
	`|->|Amount destroyed (moles) | 0.00000E+00| (modr(n)) |`

10a	Solubility of SiO2(am) in 0.1 molal MgCl2 solution

Excerpts of EQ3-input file	`|Mg++ | 0.10000E+00|Molality |`
	`|Si(OH)4(aq) | 1.00000E-20|Molality |`
	`|Cl- | 0.20000E+00|Molality |`
	`|H+ | 7.00000E+00|pH |`

	`|Alter/Suppress Options | (nxmod) |`
	`|----------|`
	`|Species |Option |Alter value |`
	`| (uxmod(n)) |(ukxm(kxmod(n)))| (xlkmod(n))|`
	`|----------|`
	`|SiO2_alpha_Qtz(cr) |Suppress | |`

Excerpt of EQ6-input file	`|Reactant |SiO2(am) | (ureac(n)) |`
	`|----------|`
	`|->|Type |Pure mineral | (urcjco(jcode(n))) |`
	`|----------|`
	`|->|Status |Reacting | (urcjre(jreac(n))) |`
	`|----------|`
	`|->|Amount remaining (moles) | 5.00000E+00| (morr(n)) |`
	`|----------|`
	`|->|Amount destroyed (moles) | 0.00000E+00| (modr(n)) |`

10b	Solubility of SiO2(am) in 3 molal MgCl2 solution

Excerpts of EQ3-input file	`|Mg++ | 3.00000E+00|Molality |`
	`|Si(OH)4(aq) | 1.00000E-20|Molality |`
	`|Cl- | 6.00000E+00|Molality |`
	`|H+ | 7.00000E+00|pH |`

	`|Alter/Suppress Options | (nxmod) |`
	`|----------|`
	`|Species |Option |Alter value |`
	`| (uxmod(n)) |(ukxm(kxmod(n)))| (xlkmod(n))|`
	`|----------|`
	`|SiO2_alpha_Qtz(cr) |Suppress | |`

Excerpt of EQ6-input file	`|Reactant |SiO2(am) | (ureac(n)) |`
	`|----------|`
	`|->|Type |Pure mineral | (urcjco(jcode(n))) |`
	`|----------|`

Number	Excerpt of input file
	|->|Status |Reacting | (urcjre(jreac(n))) | |----------| |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) | |----------| |->|Amount destroyed (moles) | 0.00000E+00| (modr(n)) |
10c	Solubility of SiO2(am) in 5 molal MgCl2 solution
Excerpts of EQ3-input file	|Mg++ | 5.00000E+00|Molality | |Si(OH)4(aq) | 1.00000E-20|Molality | |Cl- | 1.00000E+01|Molality | |H+ | 7.00000E+00|pH |
	|Alter/Suppress Options | (nxmod) | |----------| |Species |Option |Alter value | | (uxmod(n)) |(ukxm(kxmod(n)))| (xlkmod(n))| |----------| |SiO2_alpha_Qtz(cr) |Suppress | |
Excerpt of EQ6-input file	|Reactant |SiO2(am) | (ureac(n)) | |----------| |->|Type |Pure mineral | (urcjco(jcode(n))) | |----------| |->|Status |Reacting | (urcjre(jreac(n))) | |----------| |->|Amount remaining (moles) | 5.00000E+00| (morr(n)) | |----------| |->|Amount destroyed (moles) | 0.00000E+00| (modr(n)) |

5.3 Remarks

Note that in calculation No. 4, where carbonate is present, and in calculations No. 10 a-c, the initial composition needed to be charge balanced with H<+>. Otherwise the iterator did not find any solution.

6 Numerical Results

Table 6-1: Result for calculations 1a – c and 2

Calculation	Ca^{2+}	$Al(OH)_4^-$	pH
	[mol/kg H_2O]		
PHREEQC			
1a	2.034E-02	6.987E-05	12.498
1b	7.877E-03	1.062E-03	12.095
1c	6.570E-03	2.248E-03	11.971
2	1.154E-02	2.080E-03	12.237
CHEMAPP			
1a	2.033E-02	6.976E-05	12.498
1b	7.871E-03	1.062E-03	12.095
1c	6.566E-03	2.247E-03	11.971
2	1.153E-02	2.079E-03	12.236
GWB			
1a	2.034E-02	6.983E-05	12.499
1b	7.874E-03	1.062E-03	12.095
1c	6.568E-03	2.248E-03	11.971
2	1.154E-02	2.080E-03	12.237
EQ3/6			
1a	2.032E-02	6.977E-05	12.498
1b	7.870E-03	1.062E-03	12.095
1c	6.565E-03	2.247E-03	11.971
2	1.153E-02	2.078E-03	12.236

Table 6-2: Differences in results (in %) for calculations 1a – c and 2

Calculation	Ca^{2+}	$Al(OH)_4^-$	pH
	[mol/kg H_2O]		
PHREEQC-CHEMAPP			
1a	-0.0688	-0.1517	0.0000
1b	-0.0787	-0.0471	0.0000
1c	-0.0685	-0.0267	0.0000
2	-0.0867	-0.0721	-0.0082
PHREEQC-GWB			
1a	0	-0.0572	0.0080
1b	-0.0381	0.0000	0.0000
1c	-0.0304	0.0000	0.0000
2	0.0000	0.0000	0.0000
PHREEQC-EQ3/6			
1a	-0.0934	-0.1503	0.0000
1b	-0.0927	-0.0471	0.0000
1c	-0.0807	-0.0311	0.0000
2	-0.1040	-0.0769	-0.0082

Note that for species with very small concentration the percental error may become very high. This shall not be understood as an indicator for poor quality.

Table 6-3: Result for calculations 3, 4 and 6

Calculation	Ca^{2+}	$CaSO_4$	$CaCO_3$	Cl^-	CO_3^{2-}	HCO_3^-	SO_4^{2-}	$Al(OH)_4^-$	pH
				[mol/kg H_2O]					
PHREEQC									
3	2.092E-03	1.203E-07					1.046E-03	3.649E-04	11.196
4	3.287E-03		5.715E-06	0.000E+00	2.677E-06	1.017E-07		2.190E-03	11.593
6	1.416E-01			7.079E-02				9.757E-08	13.072
CHEMAPP									
3	2.091E-03	1.205E-07					1.045E-03	3.648E-04	11.196
4	3.286E-03		5.712E-06		2.672E-06	1.016E-07		2.189E-03	11.594
6	1.412E-01			7.062E-02				9.741E-08	13.072
GWB									
3	2.092E-03	1.204E-07					1.046E-03	3.649E-04	11.196
4	3.287E-03		5.712E-06		2.675E-06	1.016E-07		2.190E-03	11.594
6	1.415E-01			7.077E-02				9.756E-08	13.072
EQ3/6									
3	2.091E-03	1.205E-07					1.045E-03	3.648E-04	11.196
4	3.286E-03		5.712E-06		2.671E-06	1.016E-07		2.189E-03	11.594
6	1.412E-01			7.059E-02				9.740E-08	13.072

Table 6-4: Differences in results (in %) for calculations 3, 4 and 6

Calculation	Ca^{2+}	$CaSO_4$	$CaCO_3$	Cl^-	CO_3^{2-}	HCO_3^-	SO_4^{2-}	$Al(OH)_4^-$	pH
				[mol/kg H_2O]					
PHREEQC-CHEMAPP									
3	-0.0669	0.1330					-0.0669	-0.0274	0.0000
4	-0.0274		-0.0490		-0.2017	-0.0983		-0.0502	0.0086
6	-0.2613			-0.2472				-0.1650	0.0000
PHREEQC-GWB									
3	0.0000	0.0831					0.0000	0.0000	0.0000
4	0.0000		-0.0525		-0.0747	-0.0983		0.0000	0.0000
6	-0.0706			-0.0283				-0.0102	0.0000
PHREEQC-EQ3/6									
3	-0.0717	0.1247					-0.0765	-0.0301	0.0000
4	-0.0365		-0.0490		-0.2167	-0.1377		-0.0594	0.0086
6	-0.2966			-0.2825				-0.1794	0.0000

Note that for species with very small concentration the percental error may become very high. This shall not be understood as an indicator for poor quality.

Table 6-5: Result for calculations 5, 7 and 9

Calculation	Ca^{2+}	Mg^{2+}	$Mg(OH)^{+}$	$Al(OH)_4^{-}$	$Si(OH)_4$	$SiO(OH)_3^{-}$	$SiO2(OH)_2^{2-}$	pH
				[mol/kg H_2O]				
PHREEQC								
5		1.533E-04	8.855E-06	1.789E-10				10.489
7	8.155E-04			9.920E-05	1.009E-05	2.059E-04	1.518E-06	11.097
9		3.711E-05	1.714E-08		1.932E-03	7.183E-05	8.294E-10	8.375
CHEMAPP								
5		1.532E-04	8.848E-06	1.791E-10				10.489
7	8.152E-04			9.920E-05	1.009E-05	2.058E-04	1.517E-06	11.097
9		3.711E-05	1.713E-08		1.934E-03	7.185E-05	8.290E-10	8.375
GWB								
5	0.000E+00	1.532E-04	8.848E-06	1.791E-10	0.000E+00	0.000E+00	0.000E+00	10.489
7	8.152E-04	0.000E+00	0.000E+00	9.917E-05	1.012E-05	2.065E-04	1.522E-06	11.097
9	0.000E+00	3.779E-05	1.728E-08	2.000E-06	1.934E-03	7.123E-05	8.148E-10	8.371
EQ3/6								
5		1.532E-04	8.849E-06	1.791E-10				10.489
7	8.151E-04			9.920E-05	1.009E-05	2.058E-04	1.517E-06	11.097
9		3.715E-05	1.713E-08		1.934E-03	7.182E-05	8.281E-10	8.375

Table 6-6: Differences in results (in %) for calculations 5, 7 and 9

Calculation	Ca^{2+}	Mg^{2+}	$Mg(OH)^{+}$	$Al(OH)_4^{-}$	$Si(OH)_4$	$SiO(OH)_3^{-}$	$SiO2(OH)_2^{2-}$	pH
				[mol/kg H_2O]				
PHREEQC-CHEMAPP								
5		-0.0718	-0.0768	0.1230				0.0000
7	-0.0392			-0.0010	-0.0396	-0.0583	-0.0659	0.0000
9		0.0081	-0.0700		0.0932	0.0306	-0.0543	0.0000
PHREEQC-GWB								
5		-0.0652	-0.0791	0.1118				0.0000
7	-0.0368			-0.0302	0.2973	0.2914	0.2635	0.0000
9		1.8324	0.8168		0.1035	-0.8353	-1.7603	-0.0478
PHREEQC-EQ3/6								
5		-0.0522	-0.0678	0.1062				0.0000
7	-0.0441			-0.0030	-0.0396	-0.0631	-0.0791	0.0000
9		0.0970	-0.0350		0.1035	-0.0139	-0.1592	0.0000

Note that for species with very small concentration the percental error may become very high. This shall not be understood as an indicator for poor quality.

Table 6-7: Result for calculations 8 a - d

Calculation	Ca^{2+}	$Si(OH)_4$	$SiO(OH)_3^-$	$SiO2(OH)_2^{2-}$	pH
			[mol/kg H_2O]		
PHREEQC					
8a	2.032E-02	1.448E-09	8.353E-07	3.854E-07	12.499
8b	1.032E-02	2.787E-08	8.483E-06	1.619E-06	12.233
8c	2.109E-03	3.087E-06	1.900E-04	4.842E-06	11.565
8d	1.315E-03	1.931E-03	2.541E-03	1.285E-06	9.901
CHEMAPP					
8a	2.030E-02	1.446E-09	8.338E-07	3.842E-07	12.499
8b	1.031E-02	2.787E-08	8.479E-06	1.617E-06	12.233
8c	2.108E-03	3.087E-06	1.899E-04	4.839E-06	11.565
8d	1.315E-03	1.933E-03	2.542E-03	1.284E-06	9.901
GWB					
8a	2.031E-02	1.446E-09	8.345E-07	3.854E-07	12.499
8b	1.032E-02	2.787E-08	8.484E-06	1.620E-06	12.233
8c	2.109E-03	3.087E-06	1.900E-04	4.842E-06	11.563
8d	1.316E-03	1.933E-03	2.541E-03	1.284E-06	9.901
EQ3/6					
8a	2.030E-02	1.446E-09	8.338E-07	3.841E-07	12.499
8b	1.031E-02	2.787E-08	8.478E-06	1.616E-06	12.233
8c	2.108E-03	3.087E-06	1.899E-04	4.838E-06	11.565
8d	1.315E-03	1.933E-03	2.541E-03	1.283E-06	9.901

Table 6-8: Differences in results (in %) for calculations 8 a - d

Calculation	Ca^{2+}	$Si(OH)_4$	$SiO(OH)_3^-$	$SiO2(OH)_2^{2-}$	pH
			[mol/kg H_2O]		
PHREEQC-CHEMAPP					
8a	-0.1033	-0.1519	-0.1784	-0.3088	0.0000
8b	-0.0872	-0.0108	-0.0448	-0.1544	0.0000
8c	-0.0474	0.0097	-0.0316	-0.0640	0.0000
8d	-0.0152	0.0880	0.0197	-0.1167	0.0000
PHREEQC-GWB					
8a	-0.0492	-0.1381	-0.0958	0.0000	0.0000
8b	0.0000	0.0000	0.0118	0.0618	0.0000
8c	0.0000	0.0000	0.0000	0.0000	-0.0173
8d	0.0760	0.1036	0.0000	-0.0778	0.0000
PHREEQC-EQ3/6					
8a	-0.1230	-0.1381	-0.1772	-0.3425	0.0000
8b	-0.0969	-0.0144	-0.0542	-0.1915	0.0000
8c	-0.0569	0.0065	-0.0368	-0.0847	0.0000
8d	-0.0152	0.0984	0.0157	-0.1401	0.0000

Note that for species with very small concentration the percental error may become very high. This shall not be understood as an indicator for poor quality.

Table 6-9: Result for calculations 10 a - c

Calculation	Mg^{2+}	$Mg(OH)^{+}$	Cl^{-}	$Si(OH)_4$	$SiO(OH)_3^{-}$	$SiO2(OH)_2^{2-}$	pH
			[mol/kg H_2O]				
PHREEQC							
10a	1.000E-01	1.100E-07	2.000E-01	1.849E-03	6.653E-07	3.057E-13	6.259
10b	3.000E+00	2.154E-06	6.000E+00	3.574E-04	3.598E-09	3.835E-15	5.208
10c	5.000E+00	4.190E-06	1.000E+01	6.550E-05	3.129E-11	1.486E-17	4.348
CHEMAPP							
10a	1.000E-01	1.101E-07	2.000E-01	1.851E-03	6.652E-07	3.049E-13	6.258
10b	3.000E+00	2.157E-06	6.000E+00	3.577E-04	3.583E-09	3.785E-15	5.206
10c	5.000E+00	4.195E-06	1.000E+01	6.554E-05	3.115E-11	1.463E-17	4.347
GWB							
10a	1.000E-01	1.100E-07	2.000E-01	1.851E-03	6.657E-07	3.058E-13	6.258
10b	3.000E+00	2.149E-06	6.000E+00	3.578E-04	3.602E-09	3.822E-15	5.208
10c	5.000E+00	4.178E-06	1.000E+01	6.557E-05	3.133E-11	1.480E-17	4.348
EQ3/6							
10a	1.000E-01	1.102E-07	2.000E-01	1.851E-03	6.651E-07	3.048E-13	6.258
10b	3.000E+00	2.157E-06	6.000E+00	3.577E-04	3.581E-09	3.777E-15	5.206
10c	5.000E+00	4.196E-06	1.000E+01	6.554E-05	3.112E-11	1.460E-17	4.347

Table 6-10: Differences in results (in %) for calculations 10 a - c

Calculation	Mg^{2+}	$Mg(OH)^{+}$	Cl^{-}	$Si(OH)_4$	$SiO(OH)_3^{-}$	$SiO2(OH)_2^{2-}$	pH
			[mol/kg H_2O]				
PHREEQC-CHEMAPP							
10a	0.0000	0.0909	0.0000	0.1082	-0.0150	-0.2617	-0.0160
10b	0.0000	0.1393	0.0000	0.0839	-0.4169	-1.3038	-0.0384
10c	0.0000	0.1193	0.0000	0.0611	-0.4474	-1.5478	-0.0230
PHREEQC-GWB							
10a	0.0000	0.0000	0.0000	0.1082	0.0601	0.0327	-0.0160
10b	0.0000	-0.2321	0.0000	0.1119	0.1112	-0.3390	0.0000
10c	0.0000	-0.2864	0.0000	0.1069	0.1278	-0.4038	0.0000
PHREEQC-EQ3/6							
10a	0.0100	0.1455	0.0050	0.1028	-0.0286	-0.3075	-0.0160
10b	0.0000	0.1346	0.0017	0.0811	-0.4808	-1.5072	-0.0384
10c	0.0000	0.1313	0.0000	0.0672	-0.5465	-1.7497	-0.0230

Note that for species with very small concentration the percental error may become very high. This shall not be understood as an indicator for poor quality.

7 References

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