Empa GEMS workshop 2014

1.1 Tutorial 1

Single system - Hydration of C_3A

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GEMS V.3.2 2482.930, CEMDATA14 (version April 17, 2014)

Hydration of C_3A

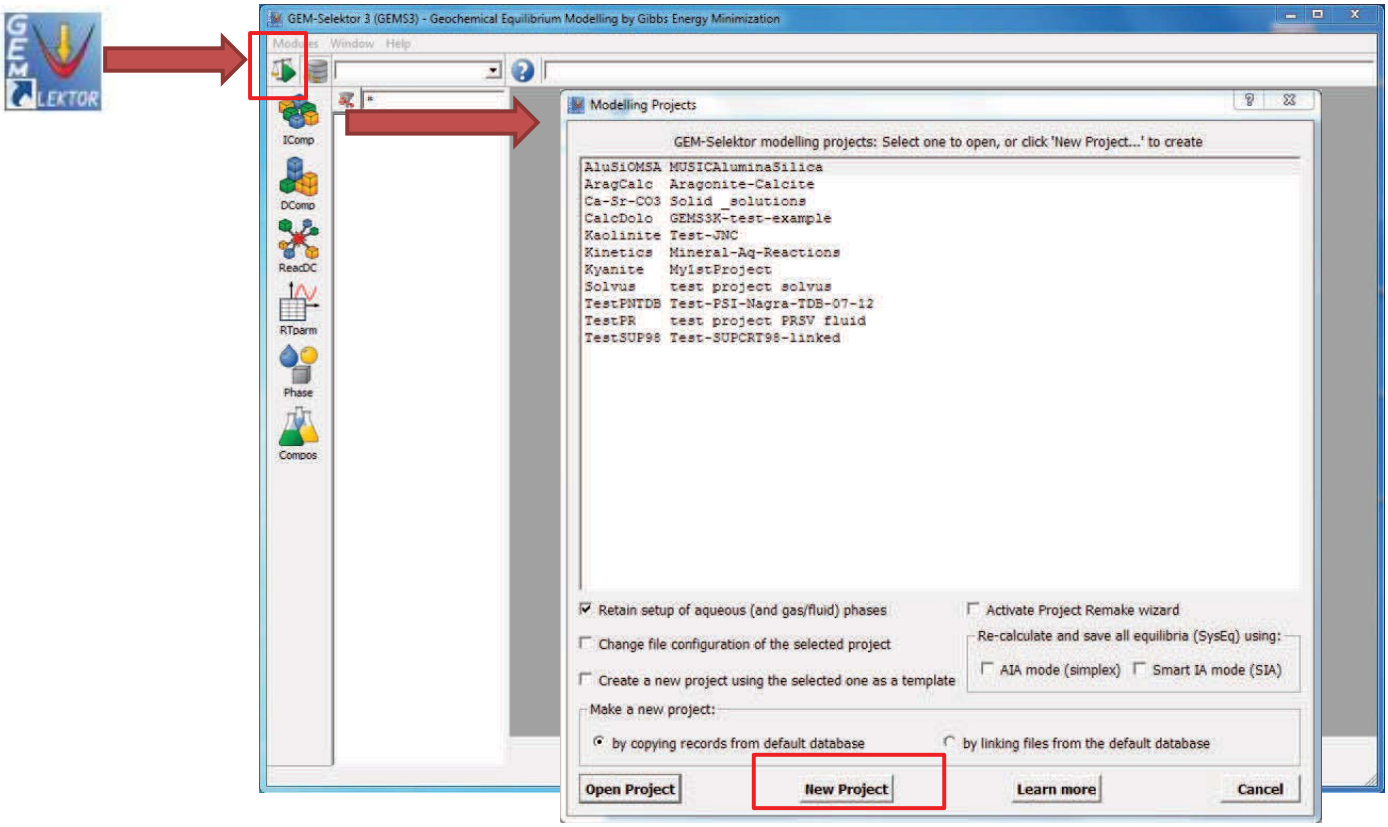
1) Simulation of reaction $C_3A + CaSO_4$

2) Simulation of reaction $C_3A + CaCO_3$

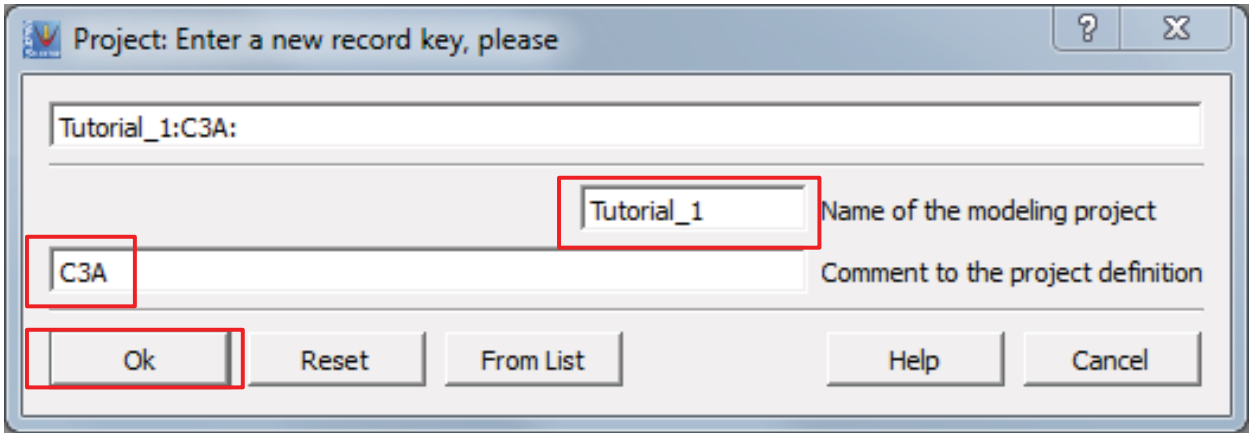
3) Simulation of reaction $C_3A + CaSO_4 + CaCO_3$

See Seligmann & Greening ICCC 1969 and various papers by Kuzel et al. (Kuzel & Pöllmann CCR 1991, Kuzel et. al CCR 1996) for experimental verification

Hydration of C_3A + $CaSO_4$ – project setup



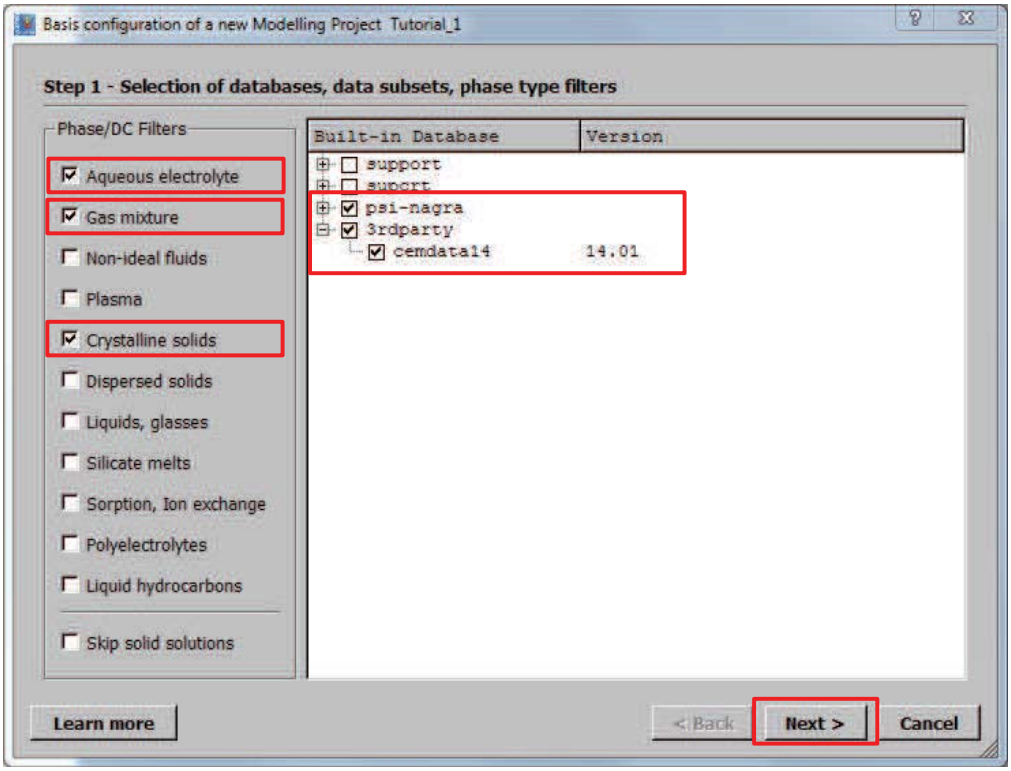
Hydration of C_3A + $CaSO_4$ – project setup



Hydration of C_3A + $CaSO_4$ – project setup

EMPA

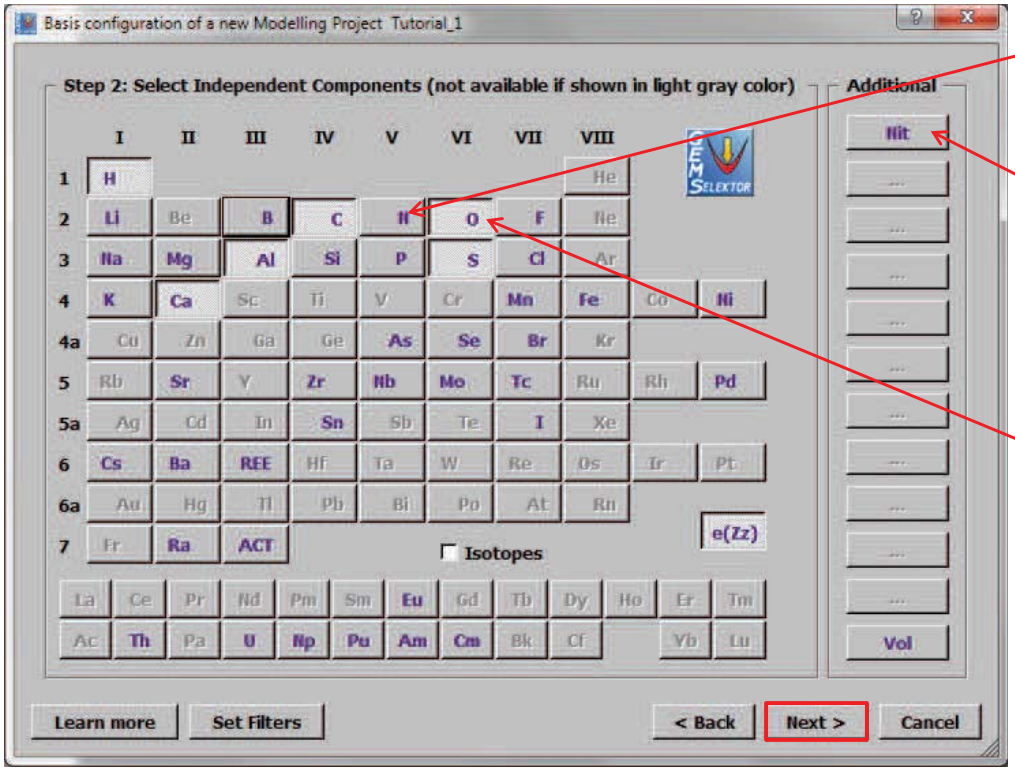
Select CEMDATA14 (3rd party data base)



Hydration of C_3A + $CaSO_4$ – project setup

EMPA

Select elements necessary to model C_3A hydration



„reactive N“ (don‘t use here)

Air: O_2, N_2, etc. (no reducing conditions, N_2 not reactive)

we can also use just oxygen (O_2)

Activity coefficients

Solubility product e. g. of gypsum

$K_{S0} = \{Ca^{2+}\}\cdot\{SO_4^{2-}\}\cdot\{H_2O\}^2/\{CaSO_4\cdot 2H_2O\}$

$K_{S0} = \{Ca^{2+}\}\cdot\{SO_4^{2-}\} = 10^{-4.58}$

{ } : activity; [ ]: concentration

$\{Ca^{2+}\} = [Ca^{2+}] \cdot \gamma_{Ca2+}$ ← Activity coefficicient

Correction of concentrations by activity coefficients, as the ions „feel" their neighbours (other ions, solvent).

Activity coefficients depend mainly on:

- ionic strength
- other ionic species
- temperature

Activity vs. ionic strength – selecting the right aqueous electrolyte model

Debye-Hückel $\log\gamma_{Ca^{2+}} = \frac{-AZ^2\sqrt{I}}{1+Ba\sqrt{I}}$ ionic strength I < 0.1 M

Extended Debye-Hückel $\log\gamma_{Ca^{2+}} = \frac{-AZ^2\sqrt{I}}{1+Ba\sqrt{I}} + bI$

common a, common b (Helgeson) I < 1-2 M

individual a, common b (Truesdell-Jones) I < 1 M

individual a, no b I < 0.3M

Davies $\log\gamma_{Ca^{2+}} = -AZ^2\left(\frac{\sqrt{I}}{1+\sqrt{I}} - 0.3I\right)$ 0.1 < I <0. 5 M

$$\log\gamma_{Ca^{2+}} = \frac{-AZ^2\sqrt{I}}{1+1.5\sqrt{I}} + \sum \varepsilon m_k$$ I < 3 M

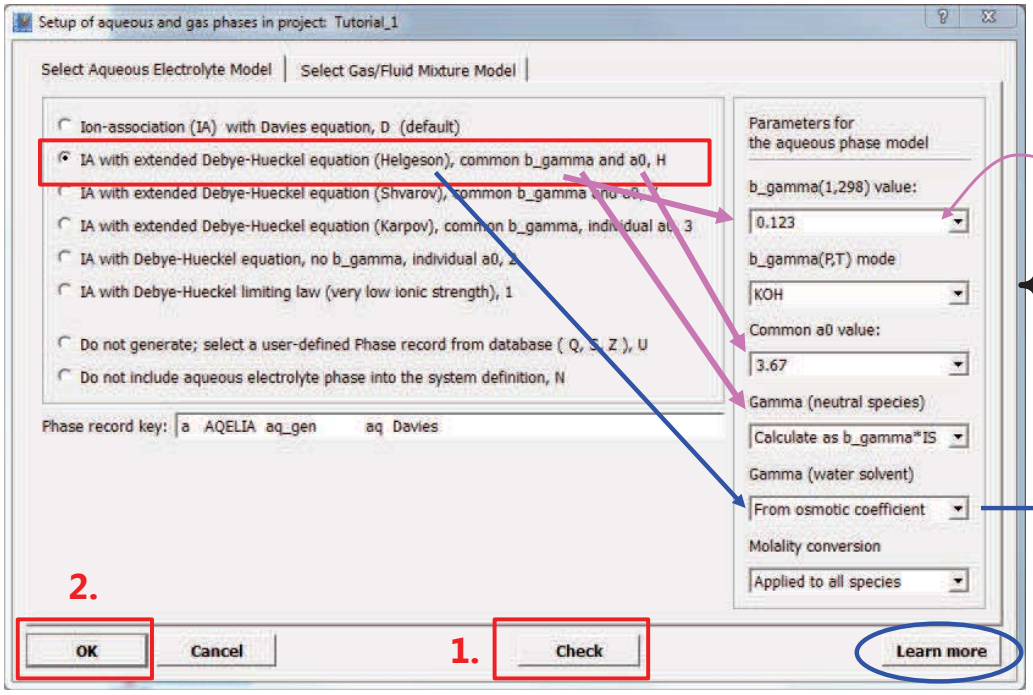
The calculation of activity coefficients is available as built-in function in the GEMS code.

For a detailed overview of different activity coefficients see :

C:\...\GEMS31\Gems3-app\Resources\doc\pdf and references therein

Hydration of C_3A + $CaSO_4$ – project setup

Select model for calculation of the aqueous phase

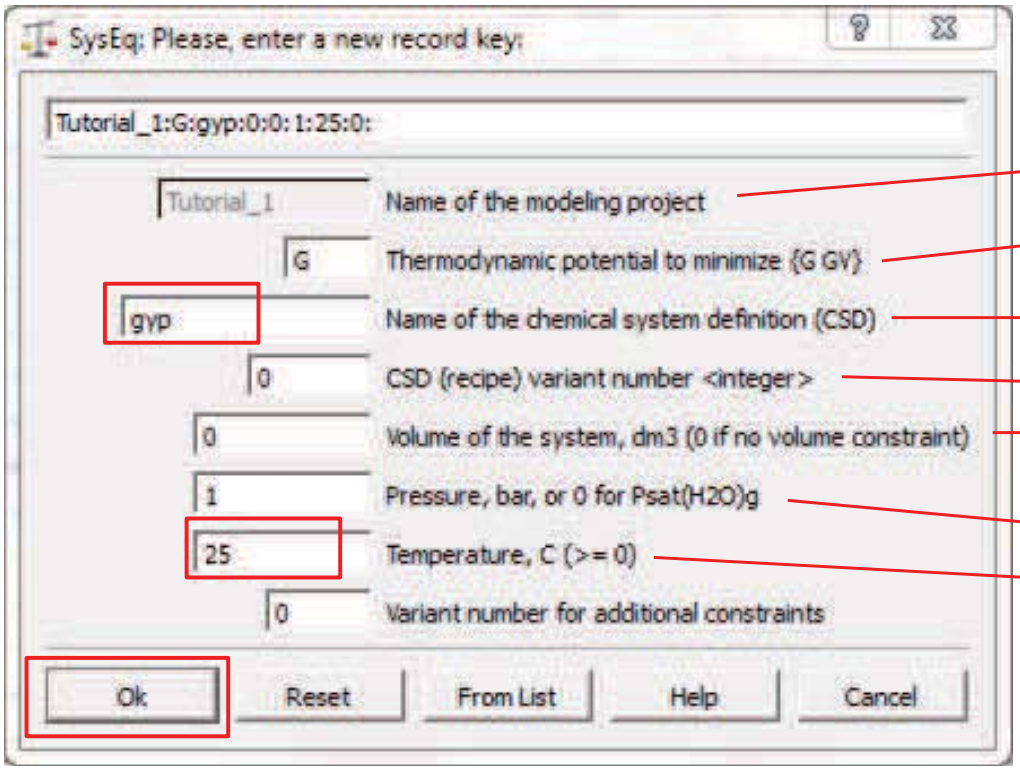


1) constant,
-> select at 298 K
2) f(pressure, temp)
-> electrolyte
a0=3.67 for KOH

Calculates activity of water

More details

Hydration of C_3A + $CaSO_4$ – project setup



Project name

Method (Gibbs free energy minimization)

System definition

Integer (default 0)

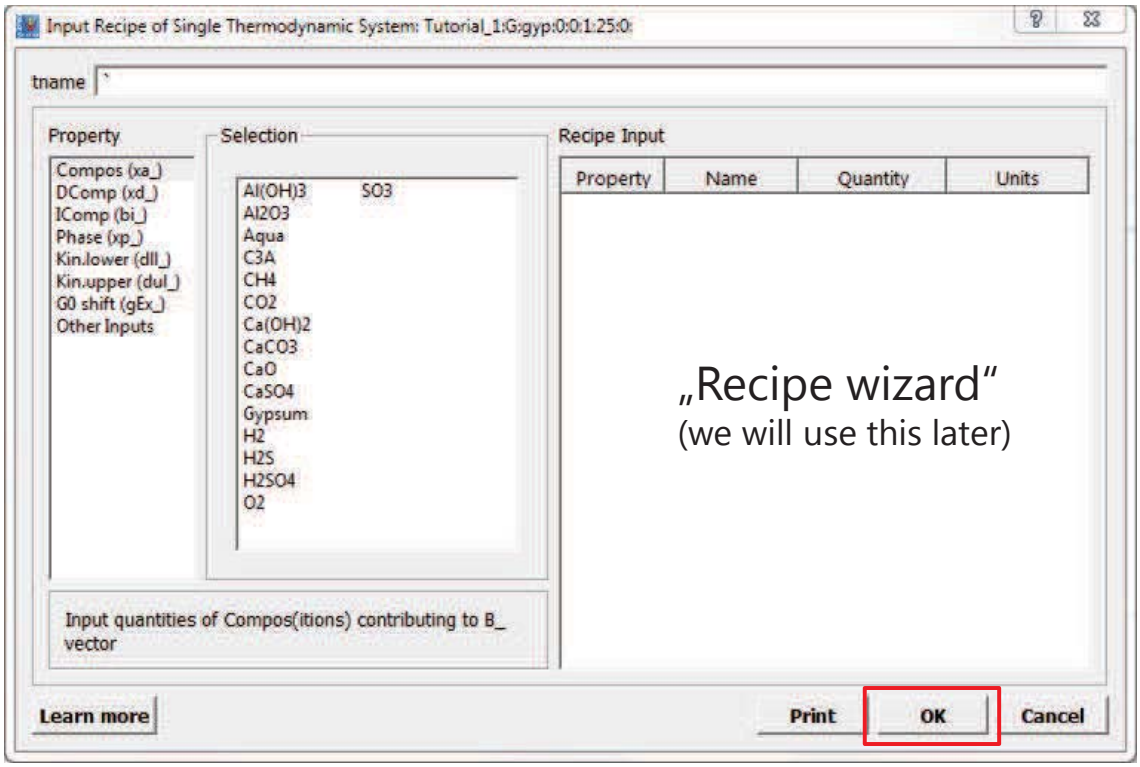
System volume unconstrained

Pressure (bar)

Temperature (°C)

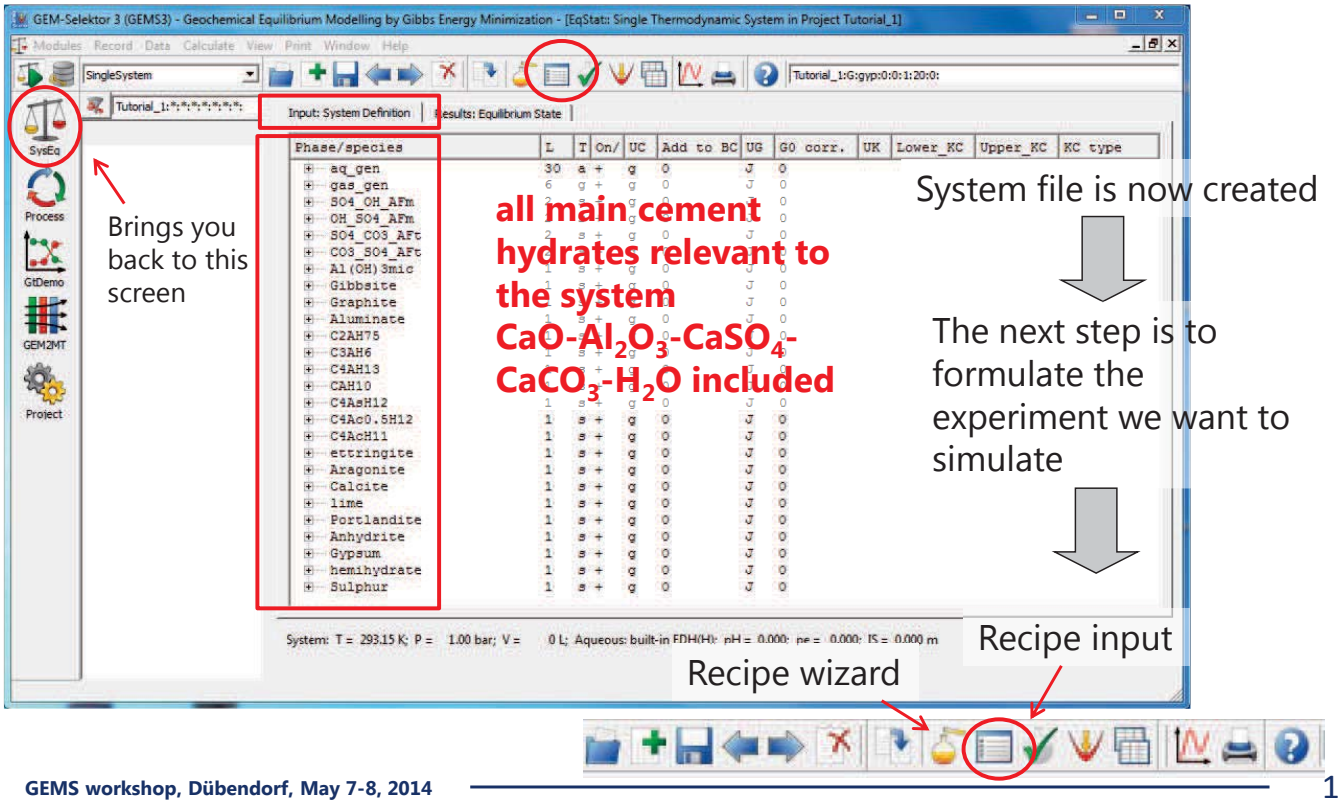
Hydration of C_3A + $CaSO_4$ – system creation (recipe)

It would be possible to create the recipe already now …

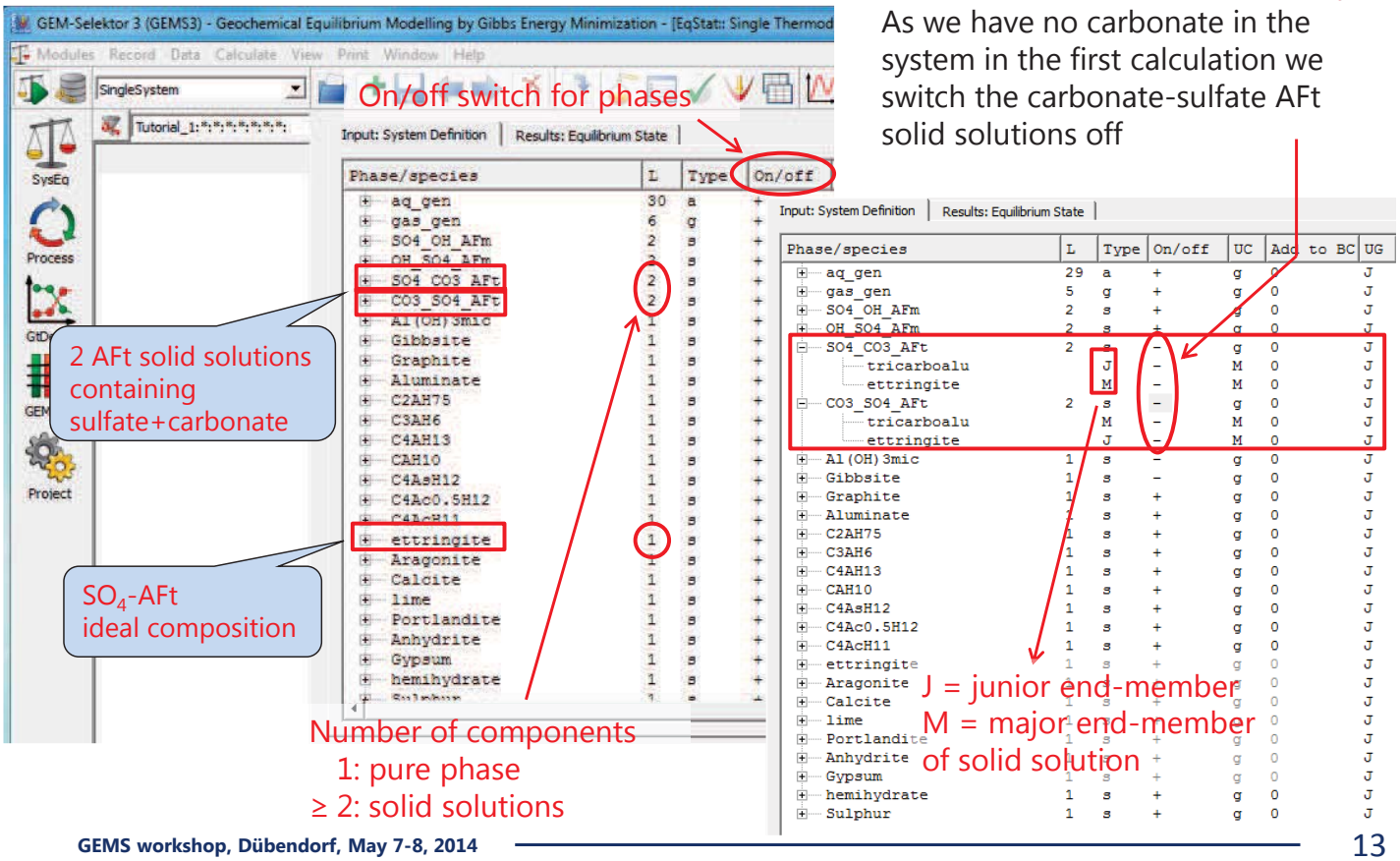


Hydration of C_3A + $CaSO_4$ – system creation (recipe)

… but we first look at the GEMS user interface more in detail.



Hydration of C_3A + $CaSO_4$ – system creation (recipe)



Hydration of C_3A + $CaSO_4$ – system creation (recipe)

Experimental problem part 1:

Reaction of C_3A with calcium sulfate

5 g C_3A + 2.52 g $CaSO_4$ + 2.5 g CaO + 50 g H_2O

+ 1 g O_2 (oxidizing conditions, CO_2-free = no carbonation)

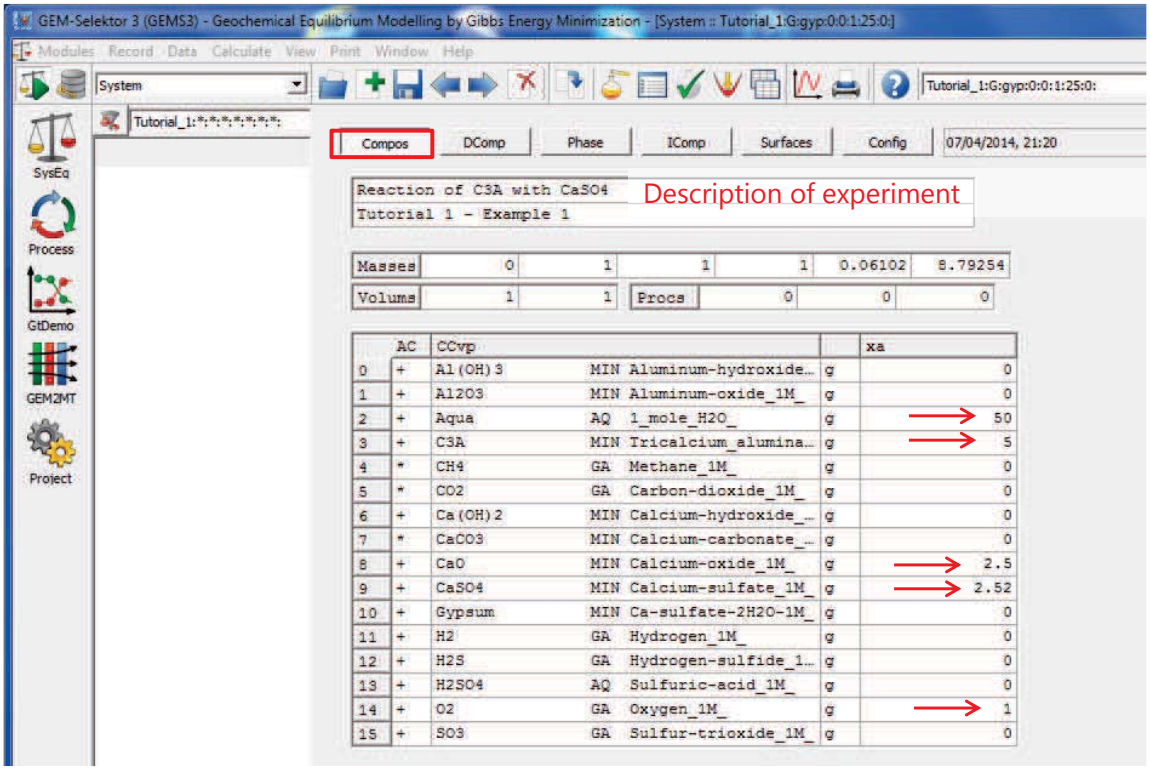
molar ratio SO_3/Al_2O_3 = 1, molar ratio CO_2/Al_2O_3 = 0

> Equilibrium speciation

recipe input

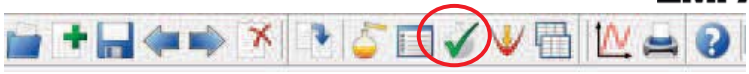
Hydration of C_3A + $CaSO_4$ – system creation (recipe)

Experimental conditions: React 5 g C_3A, 2.52 g $CaSO_4$ and 2.5 g CaO with 50 g water (add 1 g O_2 to simulate gas phase)



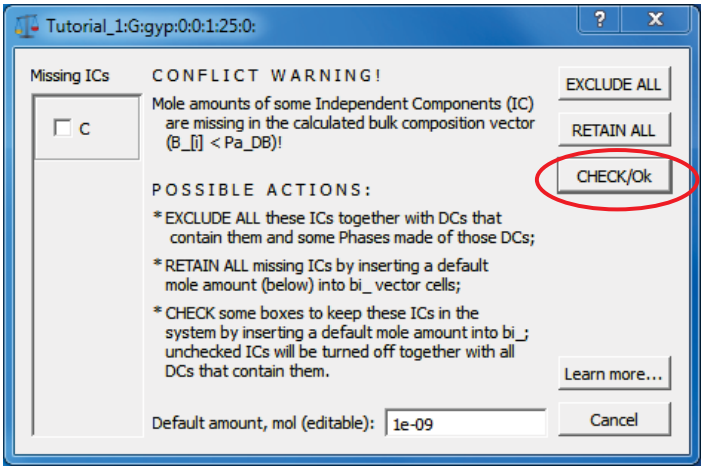
Hydration of C_3A + $CaSO_4$ – system creation (recipe)

Check system definition



we exclude carbonate in this example

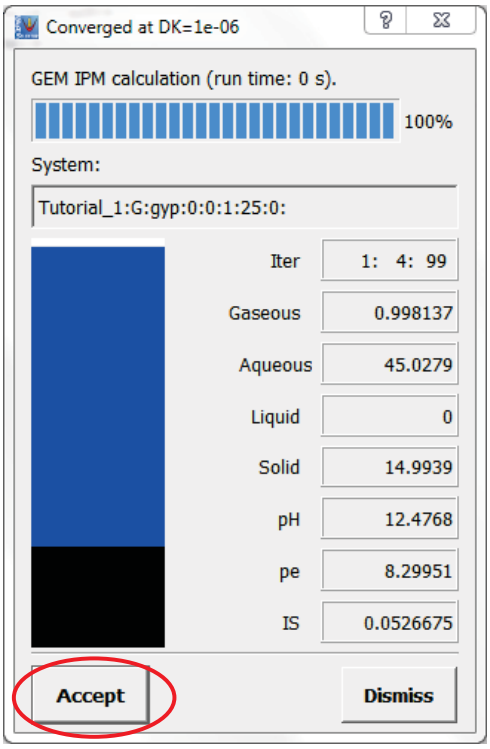
=> Switches off all phases containing C



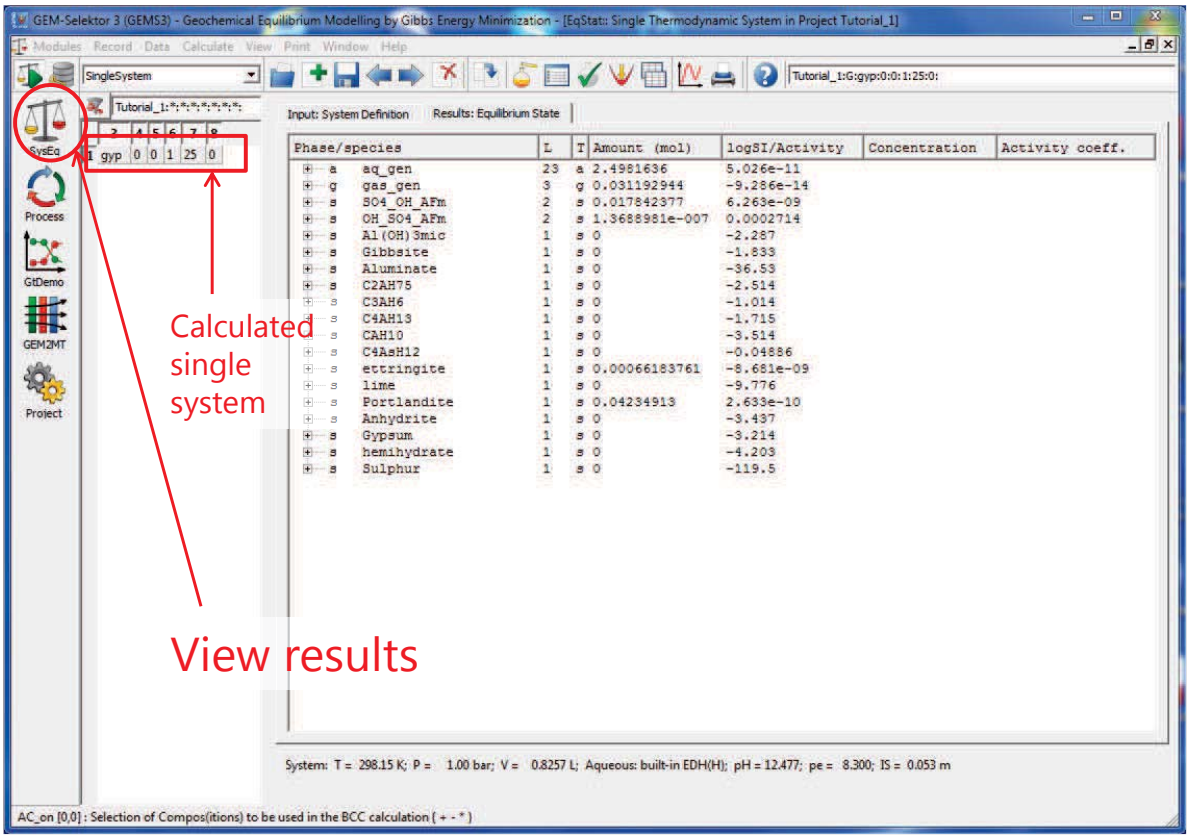
Hydration of C_3A + $CaSO_4$ – calculation of equilibrium

Experimental conditions: React 5 g C_3A, 2.52 g $CaSO_4$ and 2.5 g CaO with 50 g water (add 1 g O_2 to simulate gas phase)

Start calculation



Hydration of C_3A + $CaSO_4$ – results



Hydration of C_3A + $CaSO_4$ – results

2.498 mol aqueous phase (water + dissolved ions)

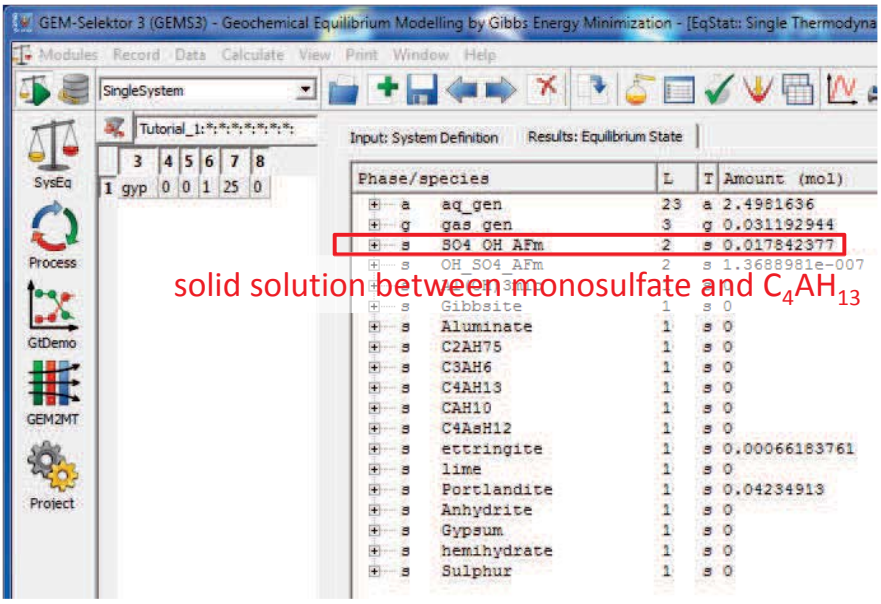
0.031 mol gaseous phase

Solid products:

0.0178 mol monosulfate

< 0.001 mol ettringite

0.0423 mol portlandite



solid solution between monosulfate and C_4AH_{13}

Hydration of C_3A + $CaSO_4$ – results

Consideration of solid solution formation

Input: System Definition | Results: Equilibrium State

Phase/species	L	Type	Amount (mol)	logSI/Activity	Concentration	Activity coeff.
a aq_gen	23	a	2.4981636	-3.107e-10		
g gas_gen	3	g	0.031192944	-9.342e-13		
s SO4_OH_AFm	2	s	0.017842377	3.588e-09		
C4AH13		M	0.00131839	0.0192869	0.073890942	0.26101866
monosulphate		J	0.016523987	0.893594	0.92610906	0.96489058
s OH_SO4_AFm	2	s	1.3710124e-007	0.0001159		
s Al(OH)3mic	1	s	0	-2.287		
s Gibbsite	1	s	0	-1.833		
s Aluminate	1	s	0	-36.53		
s C2AH75	1	s	0	-2.514		
s C3AH6	1	s	0	-1.014		
s C4AH13	1	s	0	-1.715		
s CAH10	1	s	0	-3.514		
s C4AsH12	1	s	0	-0.04886		
s ettringite	1	s	0.00066183746	5.906e-08		
s lime	1	s	0	-9.776		
s Portlandite	1	s	0.042349131	-1.816e-09		
s Anhydrite	1	s	0	-3.437		
s Gypsum	1	s	0	-3.214		
s hemihydrate	1	s	0	-4.203		
s Sulphur	1	s	0	-119.5		

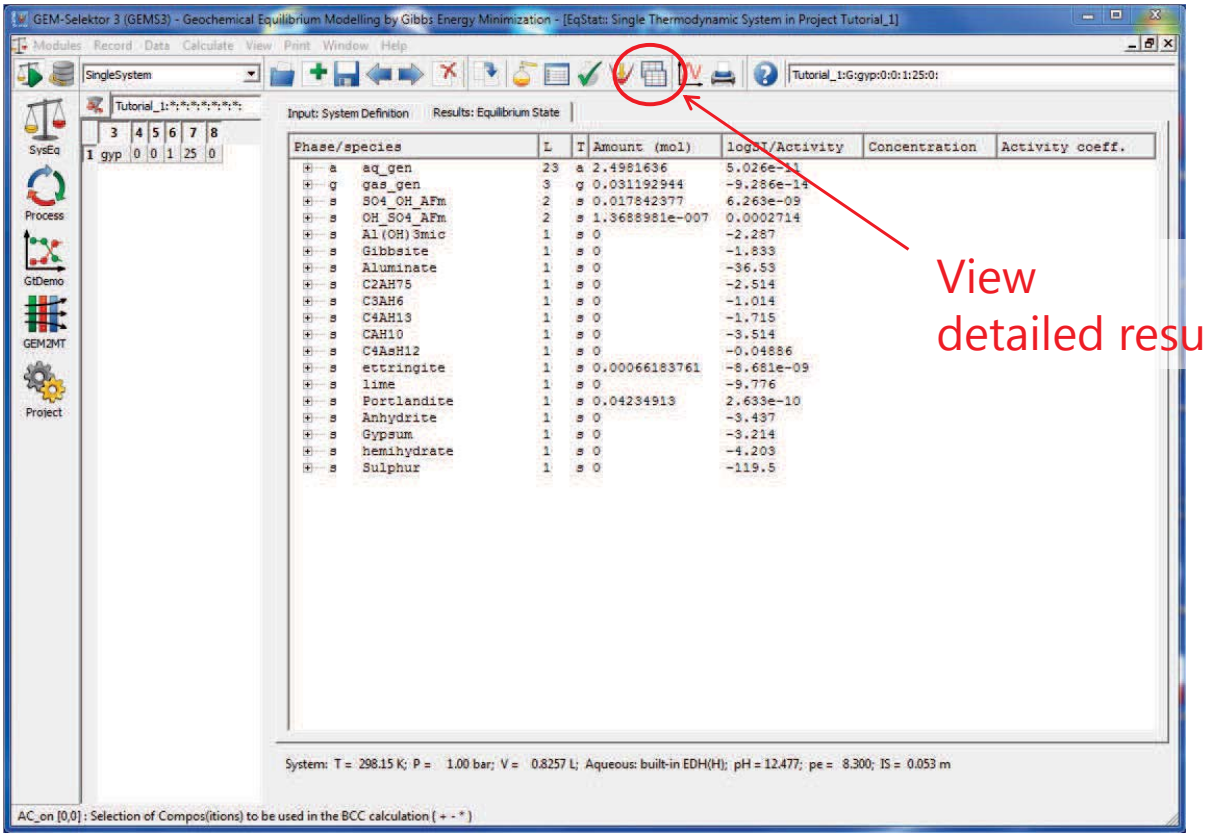
solid solution:

93 mol-% monosulfate

7 mol-% C_4AH_{13}

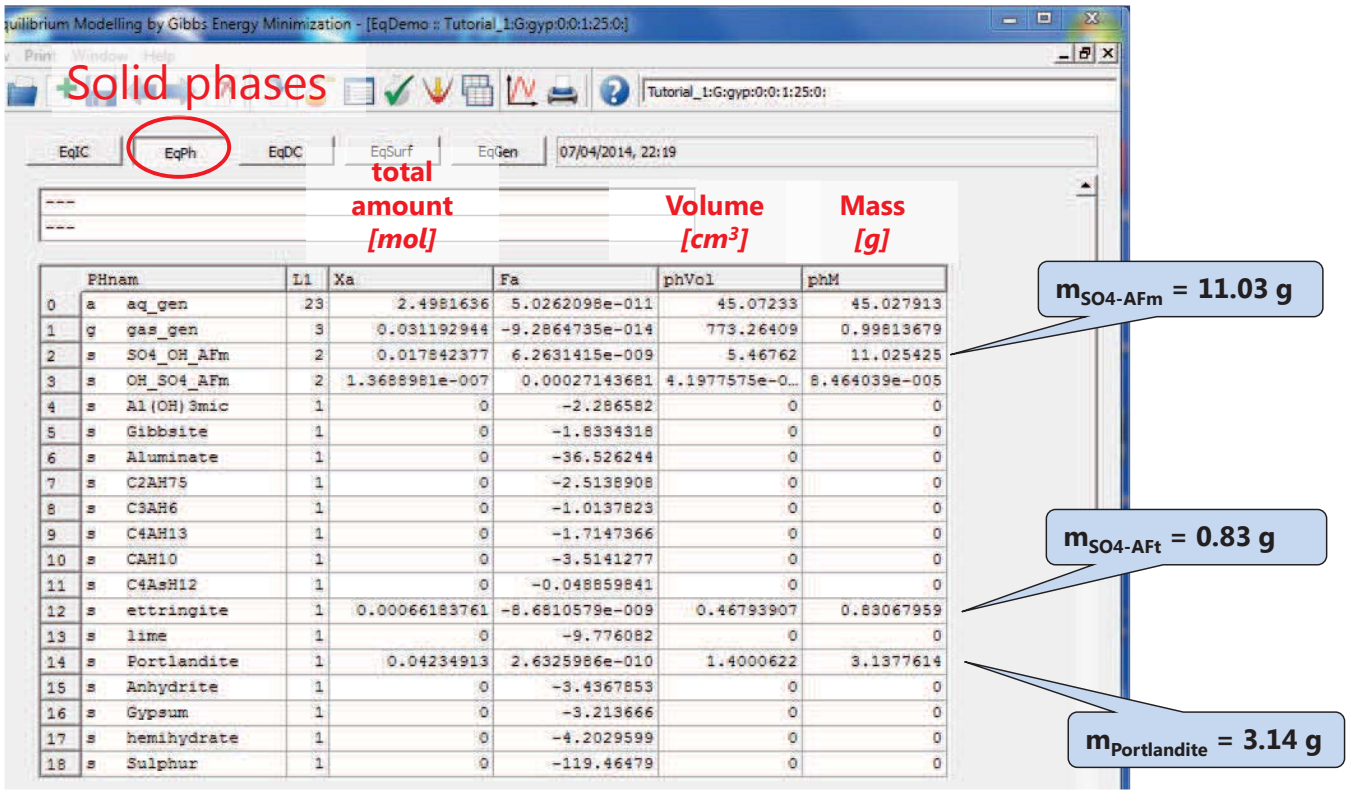
=> $Ca_4Al_2(OH)_{12.16}(SO_4)_{0.93}\cdot 6H_2O$

Hydration of C_3A + $CaSO_4$ – results



Hydration of C_3A + $CaSO_4$ – results

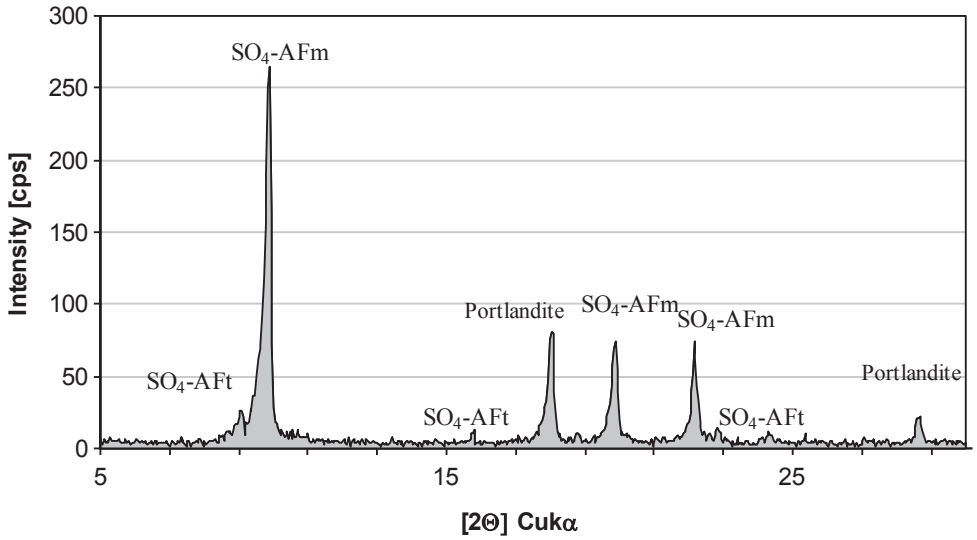
Detailed information about composition of aqueous, gaseous and solid phases



Hydration of C_3A + $CaSO_4$ – results

Comparison of modelling vs. experiments:

Hydration of C_3A at SO_3/Al_2O_3 = 1, 28 d at 25°C, solid phases by XRD



Qualitatively very good agreement between experimental and calculated results
Phase assemblage SO_4-AFm - SO_4-AFt - portlandite - aq. predicted and observed.
Quantification with help of GEMS possible.

Hydration of C_3A + $CaSO_4$ – results

Composition of aqueous phase

EqIC | EqPh | EqDC | EqSurf | EqGen | 07/04/2014, 22:19

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total molalities in aqueous phase

	ICnam	b	Cb	u	lgm t	m t	ICnam
0	Al	0.037010516	-4.3927555e-018	-325.00408	-4.394339	4.033304e-005	Al
1	Ca	0.11860702	-7.8093431e-018	-266.17062	-1.6905294	0.020392507	Ca
2	H	5.5508373	1.4056818e-016	-47.839143	-1.3901083	0.040727867	H
3	O	3.0675738	-3.436111e-016	-1.0692328e-013	-1.3621855	0.043432463	O
4	S	0.018510003	2.1963777e-018	-275.07784	-5.0753463	8.4072447e-006	S
5	Zz	0	-1.6683228e-019	19.11033	0	7.164635e-018	Zz

Hydration of C_3A + $CaCO_3$

Experimental problem part 2:

Reaction of C_3A with calcium carbonate

5 g C_3A + 1.86 g $CaCO_3$ + 2.5 g CaO + 50 g H_2O

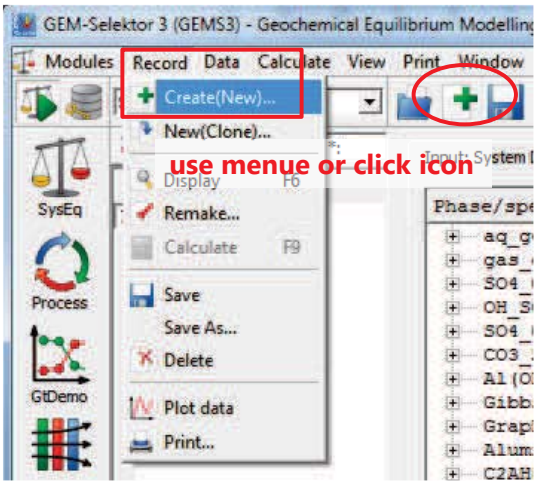
+ 1 g O_2 (oxidizing conditions, CO_2-free = no carbonation)

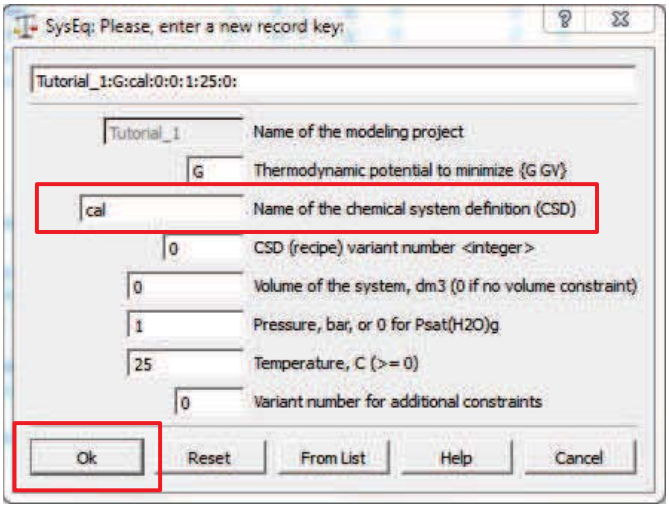
molar ratio SO_3/Al_2O_3 = 0, molar ratio CO_2/Al_2O_3 = 1

Hydration of C_3A + $CaCO_3$

Experimental conditions: **React 5 g C_3A, 1.86 g $CaCO_3$ and 2.5 g CaO with 50 g water (add 1 g O_2 to simulate gas phase)**

1) Create new system

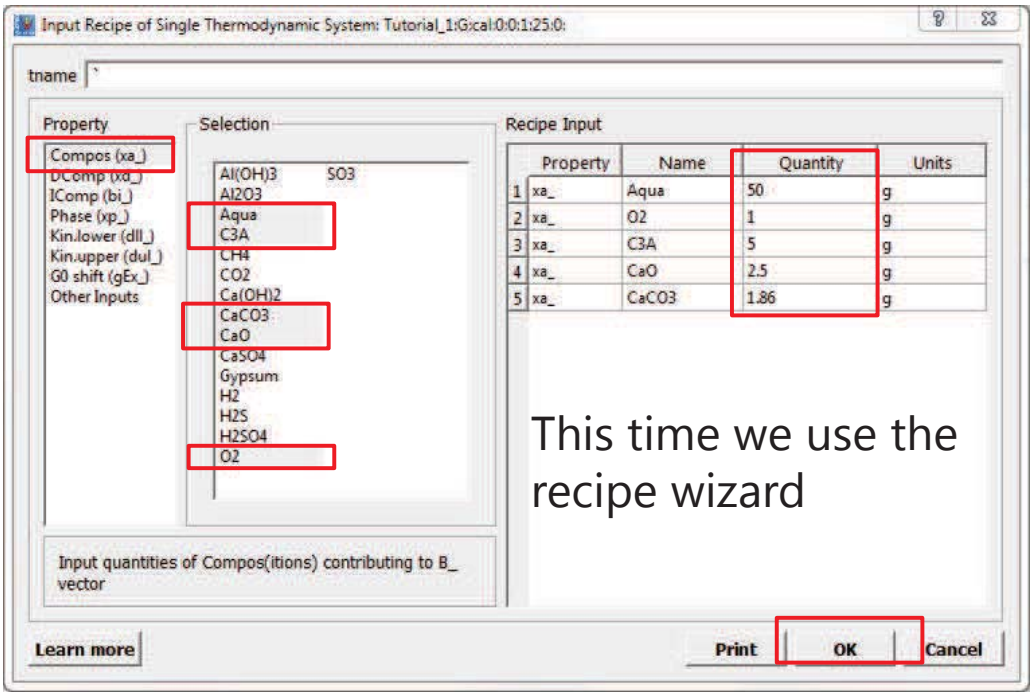




Hydration of C_3A + $CaCO_3$

Experimental conditions: **React 5 g C_3A, 1.86 g $CaCO_3$ and 2.5 g CaO with 50 g water (add 1 g O_2 to simulate gas phase)**

2) Enter initial system composition



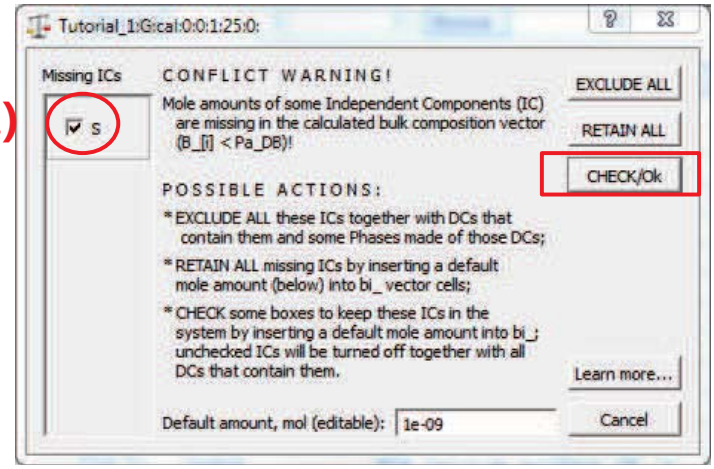
Hydration of C_3A + $CaCO_3$

Experimental conditions: **React 5 g C_3A, 1.86 g $CaCO_3$ and 2.5 g CaO with 50 g water (add 1 g O_2 to simulate gas phase)**

Check system definition

we leave the possibility of sulfate addition in the system

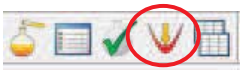
1.)

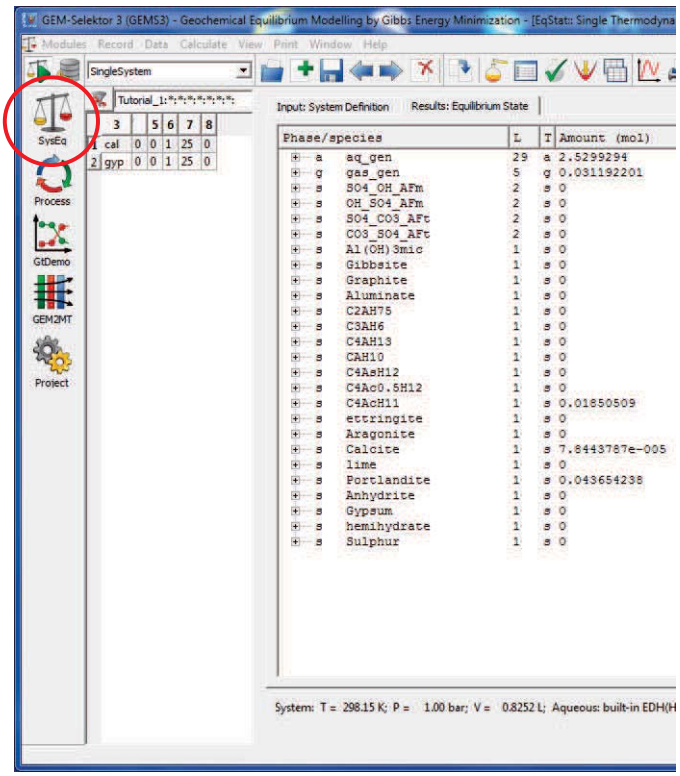


Hydration of C_3A + $CaCO_3$

Experimental conditions: **React 5 g C_3A, 1.86 g $CaCO_3$ and 2.5 g CaO with 50 g water (add 1 g O_2 to simulate gas phase)**

3) Calculate equilibrium





Formation of monocarboaluminate, small amounts of calcite and portlandite

Hydration of C_3A + $CaCO_3$

Detailed results

EqIC | EqPh | EqDC | EqSurf | EqGen | 08/04/2014, 14:11

Reaction of C3A with CaCO3
Tutorial 1 - Example 2

	PHnam		L1	Xa	Fa	phVol	phM
0	a	aq_gen	29	2.5299294	-7.6990275e-010	45.645478	45.60038
1	g	gas_gen	5	0.031192201	-1.5452046e-010	773.24568	0.99811302
2	s	SO4_OH_AFm	2	0	-1	0	0
3	s	OH_SO4_AFm	2	0	-1	0	0
4	s	SO4_CO3_AFt	2	0	-1	0	0
5	s	CO3_SO4_AFt	2	0	-1	0	0
6	s	Al(OH)3mic	1	0	-3.0243947	0	0
7	s	Gibbsite	1	0	-2.5712446	0	0
8	s	Graphite	1	0	-82.225518	0	0
9	s	Aluminate	1	0	-38.001871	0	0
10	s	C2AH75	1	0	-3.9895155	0	0
11	s	C3AH6	1	0	-2.4894077	0	0
12	s	C4AH13	1	0	-3.1903604	0	0
13	s	CAH10	1	0	-4.9897515	0	0
14	s	C4AsH12	1	0	-4.1075232	0	0
15	s	C4Ac0.5H12	1	0	-0.70017977	0	0
16	s	C4AcH11	1	0.01850509		5	10.519196
17	s	ettringite	1	0		0	0
18	s	Aragonite	1	0		0	0
19	s	Calcite	1	7.8443787e-005	-2.6182802e-010	0.0028972427	0.0078512033
20	s	lime	1	0	-9.7760823	0	0
21	s	Portlandite	1	0.043654238	1.4981742e-008	1.4432091	3.2344603
22	s	Anhydrite	1	0	-6.0198249		0
23	s	Gypsum	1	0	-5.7967051		0

$m_{CO3\text{-}AFm}$ = 10.52 g

$m_{Calcite}$ = 0.008 g

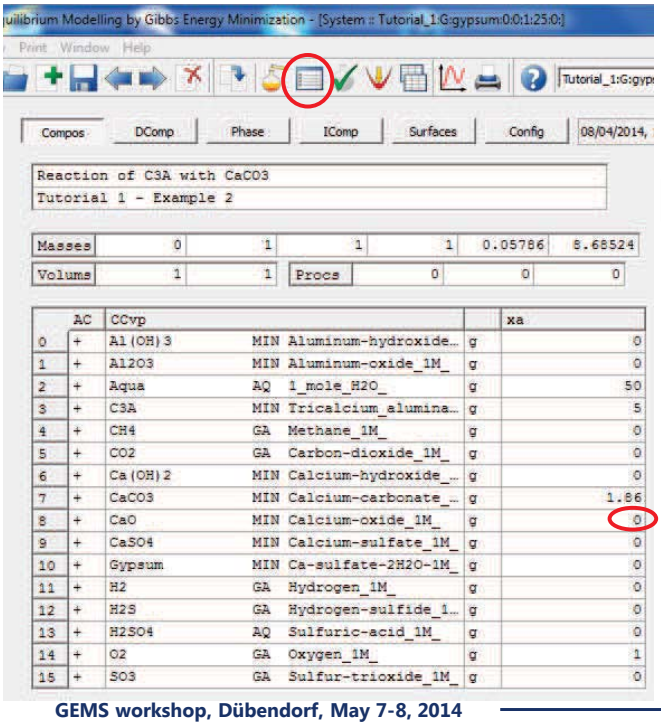
$m_{Portlandite}$ = 3.23 g

Formation of monocarboaluminate, small amounts of calcite and portlandite

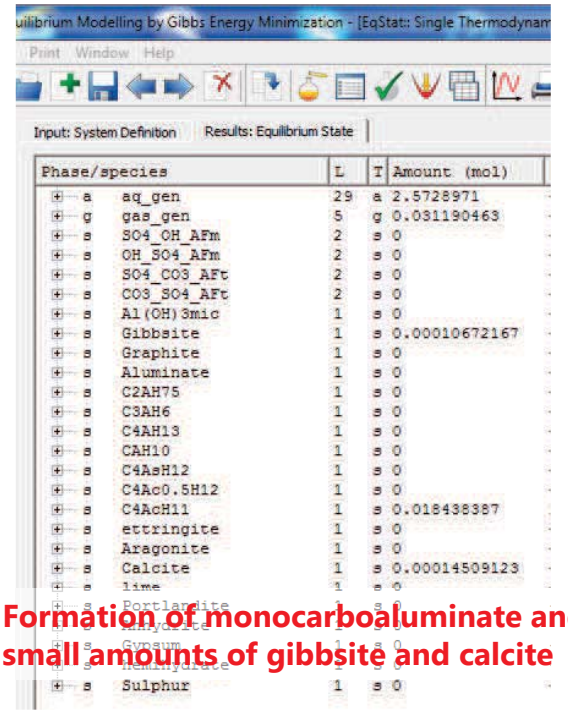
Hydration of C_3A + $CaCO_3$

Experimental conditions: **React 5 g C_3A and 1.86 g $CaCO_3$ with 50 g water (add 1 g O_2 to simulate gas phase)**

4) Repeat calculation without lime addition



	AC	CCvp			xa
0	+	Al(OH)3	MIN	Aluminum-hydroxide… g	0
1	+	Al2O3	MIN	Aluminum-oxide_1M_ g	0
2	+	Aqua	AQ	1_mole_H2O_ g	50
3	+	C3A	MIN	Tricalcium_alumina… g	5
4	+	CH4	GA	Methane_1M_ g	0
5	+	CO2	GA	Carbon-dioxide_1M_ g	0
6	+	Ca(OH)2	MIN	Calcium-hydroxide_… g	0
7	+	CaCO3	MIN	Calcium-carbonate_… g	1.86
8	+	CaO	MIN	Calcium-oxide_1M_ g	0
9	+	CaSO4	MIN	Calcium-sulfate_1M_ g	0
10	+	Gypsum	MIN	Ca-sulfate-2H2O-1M_ g	0
11	+	H2	GA	Hydrogen_1M_ g	0
12	+	H2S	GA	Hydrogen-sulfide_1… g	0
13	+	H2SO4	AQ	Sulfuric-acid_1M_ g	0
14	+	O2	GA	Oxygen_1M_ g	1
15	+	SO3	GA	Sulfur-trioxide_1M_ g	0



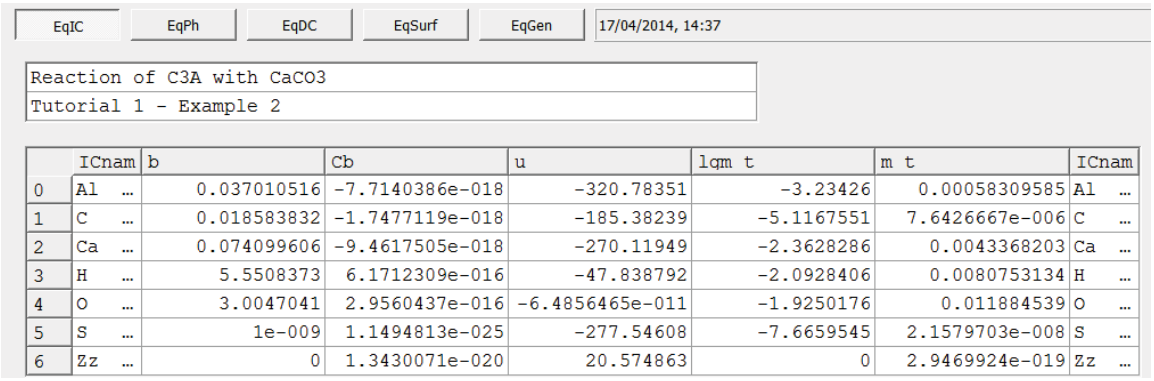
Phase/species		L	T	Amount (mol)
aq_gen		29	a	2.5728971
gas_gen		5	g	0.031190463
SO4_OH_AFm		2	s	0
OH_SO4_AFm		2	s	0
SO4_CO3_AFt		2	s	0
CO3_SO4_AFt		2	s	0
Al(OH)3mic		1	s	0
Gibbsite		1	s	0.00010672167
Graphite		1	s	0
Aluminate		1	s	0
C2AH75		1	s	0
C3AH6		1	s	0
C4AH13		1	s	0
CAH10		1	s	0
C4AsH12		1	s	0
C4Ac0.5H12		1	s	0
C4AcH11		1	s	0.018438387
ettringite		1	s	0
Aragonite		1	s	0
Calcite		1	s	0.000145091 23
lime		1	s	0
Portlandite		1	s	0
Gypsum		1	s	0
Sulphur		1	s	0

Formation of monocarboaluminate and small amounts of gibbsite and calcite

Hydration of C_3A + $CaCO_3$

Experimental conditions: **React 5 g C_3A and 1.86 g $CaCO_3$ with 50 g water (add 1 g O_2 to simulate gas phase)**

Without lime addition: check pore solution composition



	ICnam	b	Cb	u	lgm t	m t	ICnam
0	Al …	0.037010516	-7.7140386e-018	-320.78351	-3.23426	0.00058309585	Al …
1	C …	0.018583832	-1.7477119e-018	-185.38239	-5.1167551	7.6426667e-006	C …
2	Ca …	0.074099606	-9.4617505e-018	-270.11949	-2.3628286	0.0043368203	Ca …
3	H …	5.5508373	6.1712309e-016	-47.838792	-2.0928406	0.0080753134	H …
4	O …	3.0047041	2.9560437e-016	-6.4856465e-011	-1.9250176	0.011884539	O …
5	S …	1e-009	1.1494813e-025	-277.54608	-7.6659545	2.1579703e-008	S …
6	Zz …	0	1.3430071e-020	20.574863	0	2.9469924e-019	Zz …

measured *

2.32 mmol/l
< 0.1 mmol/l
3.19 mmol/l

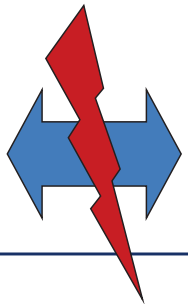
pHcalc = 11.84 pH = 11.59

* measured at 25°C, aged 56 d, undersaturation

Solid phase assemblage:

CO_3-AFm-calcite-aqueous phase

experiments modelling



Hydration of C_3A + $CaCO_3$

<u>Experimental conditions:</u> React 5 g C_3A and 1.86 g $CaCO_3$ with 50 g water (add 1 g O_2 to simulate gas phase)

Without lime addition: supress formation of gibbsite and microcrystalline $Al(OH)_3$ and repeat calculation

=>Introduction of metastability constraints

Input: System Definition | Results: Equilibrium State

Phase/species	L	T	On/	UC	Add to BC	UG	G0 corr.
aq_gen	29	a	+	g	0	J	0
gas_gen	5	g	+	g	0	J	0
SO4_OH_AFm	2	s	+	g	0	J	0
OH_SO4_AFm	2	s	+	g	0	J	0
SO4_CO3_AFt	2	s	+	g	0	J	0
CO3_SO4_AFt	2	s	+	g	0	J	0
Al(OH)3mic	1	s	-	g	0	J	0
AlOHmic		O	-	M	0	J	0
Gibbsite	1	s	-	g	0	J	0
Gbs		O	-	M	0	J	0
Graphite	1	s	+	g	0	J	0
Aluminate	1	s	+	g	0	J	0
C2AH75	1	s	+	g	0	J	0
C3AH6	1	s	+	g	0	J	0
C4AH13	1	s	+	g	0	J	0
CAH10	1	s	+	g	0	J	0
C4AsH12	1	s	+	g	0	J	0
C4Ac0.5H12	1	s	+	g	0	J	0
C4AcH11	1	s	+	g	0	J	0
ettringite	1	s	+	g	0	J	0
Aragonite	1	s	+	g	0	J	0
Calcite	1	s	+	g	0	J	0
lime	1	s	+	g	0	J	0
Portlandite	1	s	+	g	0	J	0
Anhydrite	1	s	+	g	0	J	0
Gypsum	1	s	+	g	0	J	0
hemihydrate	1	s	+	g	0	J	0
Sulphur	1	s	+	g	0	J	0

Hydration of C_3A + $CaCO_3$

<u>Experimental conditions:</u> React 5 g C_3A and 1.86 g $CaCO_3$ with 50 g water (add 1 g O_2 to simulate gas phase)

Without lime addition: supress formation of gibbsite and microcrystalline $Al(OH)_3$ and repeat calculation

Formation of monocarboaluminate and small amounts of calcite, as observed <u>in the experiment</u>

ibrium Modelling by Gibbs Energy Minimization - [EqStat: Single Thermodyna

Print Window Help

Input: System Definition | Results: Equilibrium State

Phase/species	L	T	Amount (mol)
aq_gen	29	a	2.5728615
gas_gen	5	g	0.031190419
SO4_OH_AFm	2	s	0
OH_SO4_AFm	2	s	0
SO4_CO3_AFt	2	s	0
CO3_SO4_AFt	2	s	0
Graphite	1	s	0
Aluminate	1	s	0
C2AH75	1	s	0
C3AH6	1	s	0
C4AH13	1	s	0
CAH10	1	s	0
C4AsH12	1	s	0
C4Ac0.5H12	1	s	0
C4AcH11	1	s	0.018452666
ettringite	1	s	0
Aragonite	1	s	0
Calcite	1	s	0.00013079679
lime	1	s	0
Portlandite	1	s	0
Anhydrite	1	s	0
Gypsum	1	s	0
hemihydrate	1	s	0
Sulphur	1	s	0

Hydration of C_3A + $CaCO_3$

Experimental conditions: **React 5 g C_3A and 1.86 g $CaCO_3$ with 50 g water (add 1 g O_2 to simulate gas phase)**

Without lime addition: supress formation of gibbsite and microcrystalline $Al(OH)_3$ and repeat calculation

Al = 2.27 mmol/kg

C ~ 0.008 mmol/kg

Ca = 3.41 mmol/kg

m t	ICnam
0.0022697558	Al ...
7.9685752e-006	C ...
0.0034126022	Ca ...
0.0045396865	H ...
0.011724956	O ...
2.157899e-008	S ...
8.9209963e-019	Zz ...

measured

2.32 mmol/l
< 0.1 mmol/l
3.19 mmol/l

pHcalc = 11.60

pH = 11.59

Phase assemblage:

CO_3-AFm-calcite-aqueous phase

Hydration of C_3A + $CaCO_3$ + $CaSO_4$

Experimental problem part 3:

Reaction of C_3A with calcium carbonate and calcium sulfate

5 g C_3A + + 1.86 g $CaCO_3$ + 2.52 g $CaSO_4$ + 2.5 g CaO + 50 g H_2O

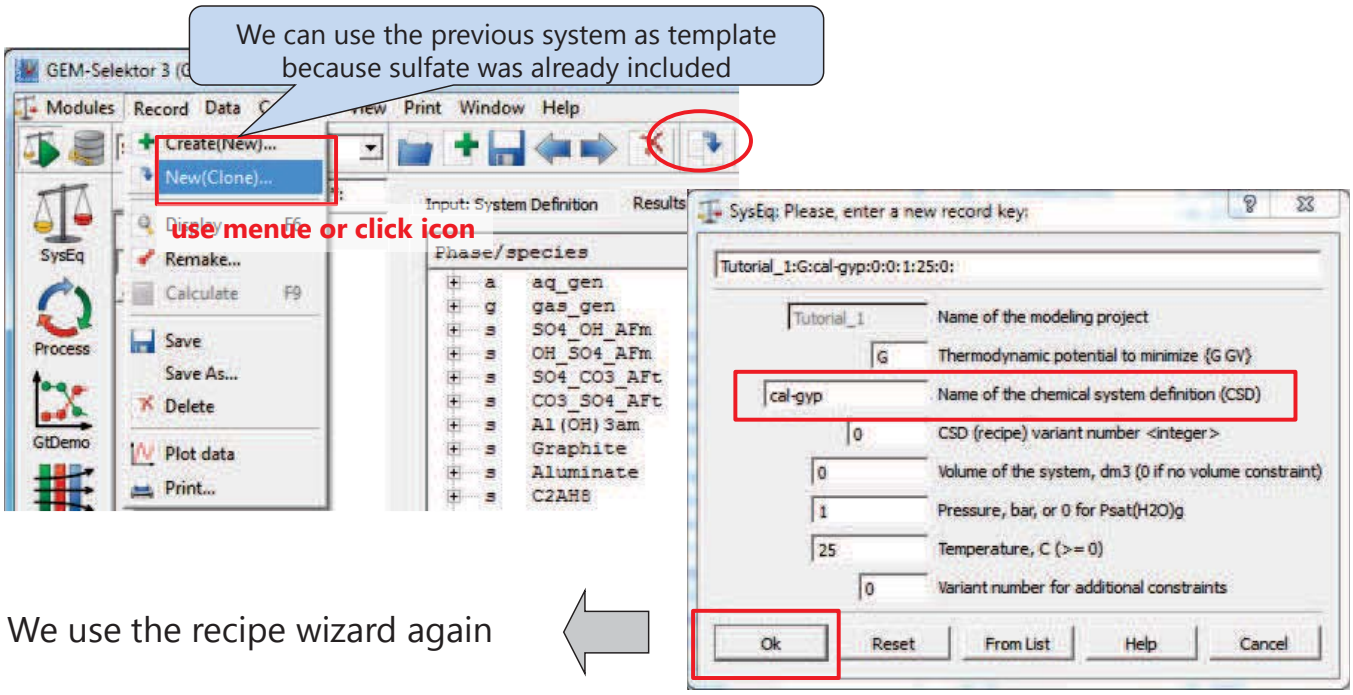
+ 1 g O_2 (oxidizing conditions, CO_2-free = no carbonation)

molar ratio SO_3/Al_2O_3 = 1, molar ratio CO_2/Al_2O_3 = 1

Hydration of C_3A + $CaCO_3$ + $CaSO_4$

Experimental conditions: **React 5 g C_3A, 1.86 g $CaCO_3$, 2.52 g $CaSO_4$ and 2.5 g CaO with 50 g water (add 1 g air CO_2-free to simulate gas phase)**

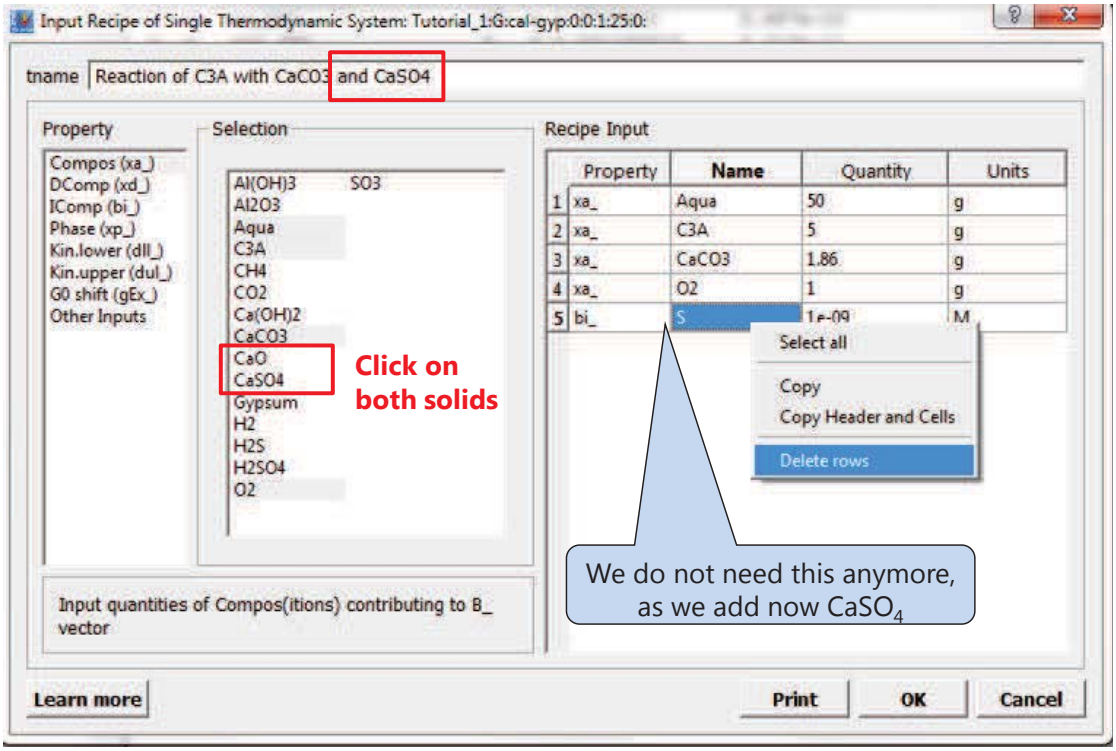
1) Create new system



We use the recipe wizard again

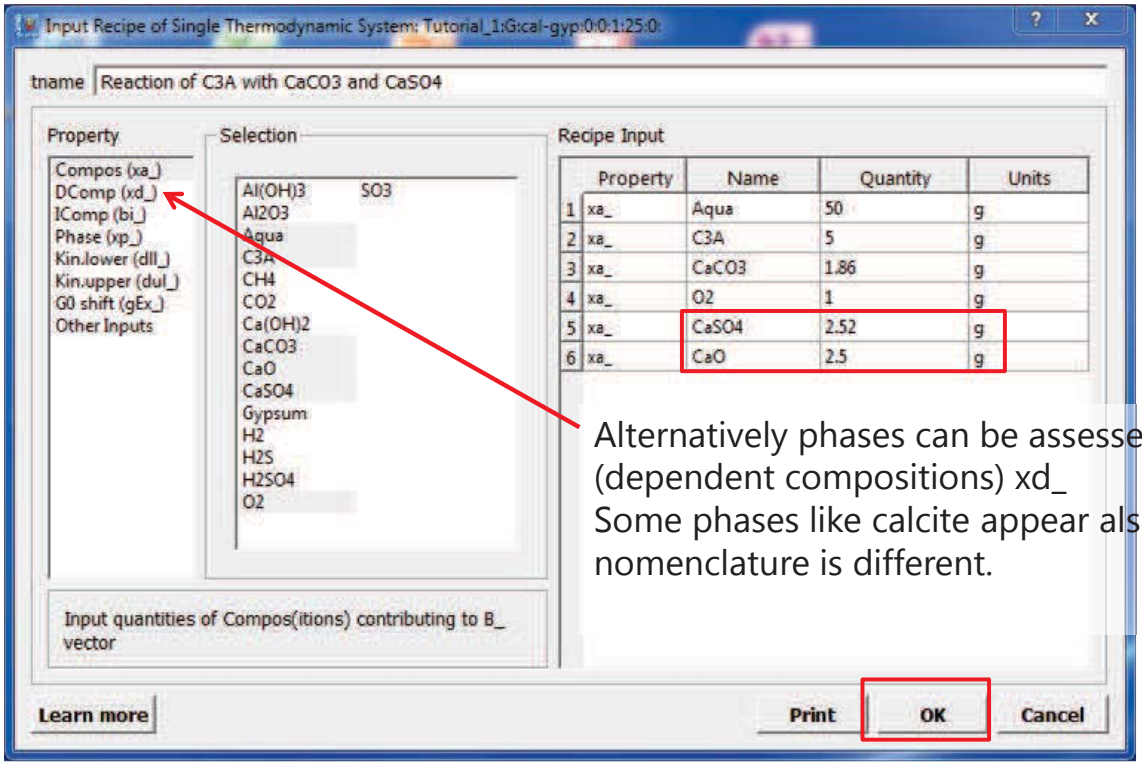
Hydration of C_3A + $CaCO_3$ + $CaSO_4$

Experimental conditions: **React 5 g C_3A, 1.86 g $CaCO_3$, 2.52 g $CaSO_4$ and 2.5 g CaO with 50 g water (add 1 g O_2 to simulate gas phase)**



Hydration of C_3A + $CaCO_3$ + $CaSO_4$

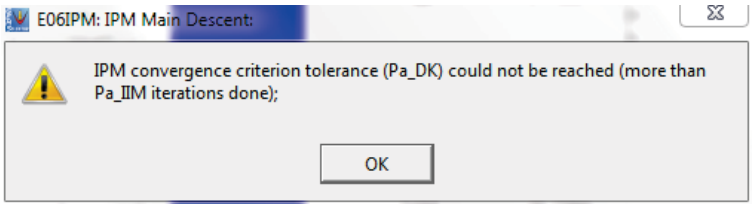
Experimental conditions: **React 5 g C_3A, 1.86 g $CaCO_3$, 2.52 g $CaSO_4$ and 2.5 g CaO with 50 g water (add 1 g O_2 to simulate gas phase)**



Alternatively phases can be assessed via Dcomp (dependent compositions) xd_
Some phases like calcite appear also there, nomenclature is different.

Hydration of C_3A + $CaCO_3$ + $CaSO_4$

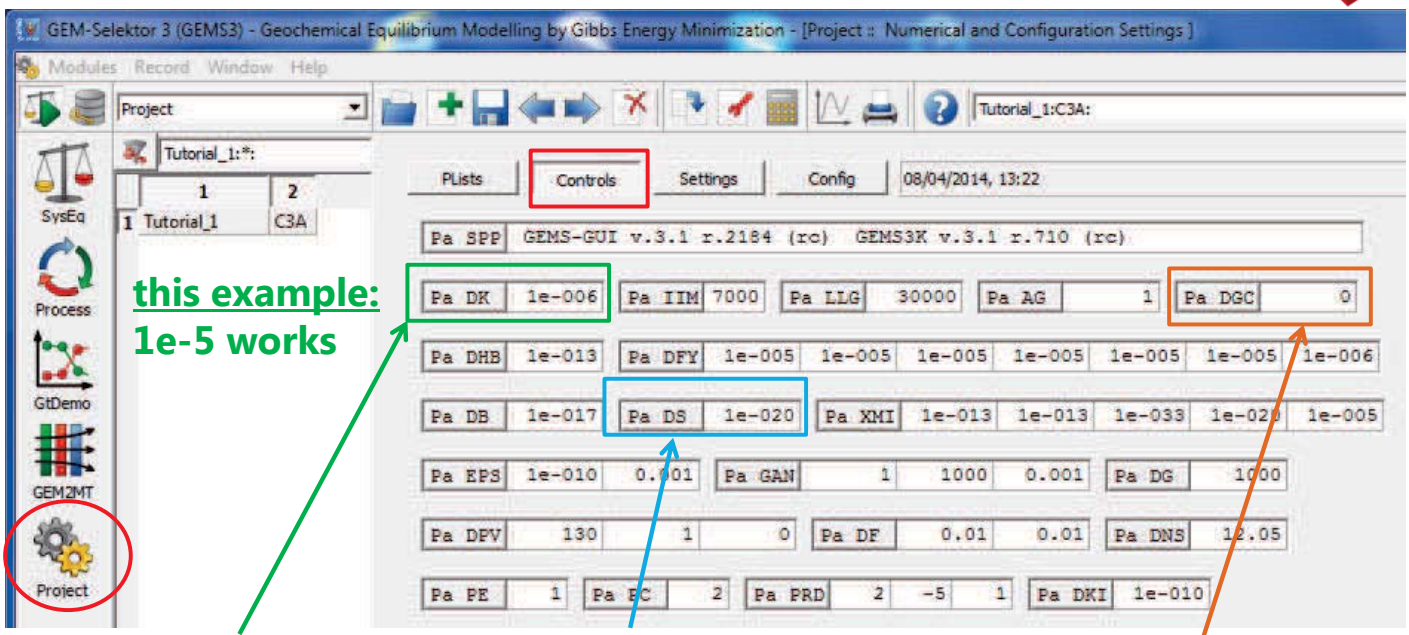
This error message might occur now:



The reason is the solid solution SO_4/CO_3-AFt.
We try to fix this in the near future. As a workaround there are two possible solutions:

1) Do not use this solid solution. Use the single phases instead.
2) Modify some of the settings of GEMS as shown on the next slide. In most cases this should work.

Convergence problem - workaround



this example: 1e-5 works

Covergence tolerance parameter:
use higher value, e.g. 1e-005,
maximum seems to be 5e-004

Minumum amount of stable phases:
use lower value, e.g. 1e-023

Smoothing parameter:
use low positive value, e.g. 0.01

Do not touch the other values !!!

Hydration of C_3A + $CaCO_3$ + $CaSO_4$

Experimental conditions: **React 5 g C_3A, 1.86 g $CaCO_3$, 2.52 g $CaSO_4$ and 2.5 g CaO with 50 g water (add 1 g O_2 to simulate gas phase)**

2) Calculate equilibrium

Formation of AFt, monocarboaluminate, calcite and portlandite

No formation of monosulfoaluminate despite SO_3/Al_2O_3 = 1

solid solution:

90.5 mol% SO_4-AFt

9.5 mol% CO_3-AFt

Input: System Definition | Results: Equilibrium State

Phase/species	L	T	Amount (mol)	logSI/Activity	Concentration
aq_gen	29	a	2.3865525	-3.114e-09	
gas_gen	5	g	0.031195546	-2.73e-10	
SO4_OH_AFm	2	s	0	-1	
OH_SO4_AFm	2	s	0	-1	
SO4_CO3_AFt	2	s	0.0068201901	6.873e-07	
tricarboalu		J	0.00065073471	0.01168	0.095412986
ettringite		M	0.0061694554	0.839471	0.90458701
CO3_SO4_AFt	2	s	1.9742038e-007	0.07018	
Graphite	1	s	0	-82.23	
Aluminate	1	s	0	-38	
C2AH75	1	s	0	-3.99	
C3AH6	1	s	0	-2.489	
C4AH13	1	s	0	-3.19	
CAH10	1	s	0	-4.99	
C4AsH12	1	s	0	-1.058	
C4Ac0.5H12	1	s	0	-0.7002	
C4AcH11	1	s	0.011684712	-3.061e-08	
ettringite	1	s	0	-0.07599	
Aragonite	1	s	0	-0.1438	
Calcite	1	s	0.0049466221	-1.445e-07	
lime	1	s	0	-9.776	
Portlandite	1	s	0.043706866	-6.743e-10	
Anhydrite	1	s	0	-2.97	
Gypsum	1	s	0	-2.747	
hemihydrate	1	s	0	-3.736	
Sulphur	1	s	0	-119	

Hydration of C_3A + $CaCO_3$ + $CaSO_4$

Experimental conditions: **React 5 g C_3A, 1.86 g $CaCO_3$, 2.52 g $CaSO_4$ and 2.5 g CaO with 50 g water (add 1 g O_2 to simulate gas phase)**

3) Assess Calculation

Formation of AFt, monocarboaluminate, calcite and portlandite

No formation of monosulfo-aluminate despite SO_3/Al_2O_3 = 1

EqIC | EqPh | EqDC | EqSurf | EqGen | 08/04/2014, 13:42

Reaction of C3A with CaCO3 and CaSO4
Tutorial 1 - Example 3

	PHnam		L1	Xa	Fa	phVol	phM
0	a	aq_gen	29	2.3865525	-3.1142163e-009	43.05862	43.016213
1	g	gas_gen	5	0.031195546		58	0.99822004
2	s	SO4_OH_AFm	2	0		0	0
3	s	OH_SO4_AFm	2	0	-1	0	0
4	s	SO4_CO3_AFt	2	0.0068201901	6.8728173e-007	4.7852281	8.489707
5	s	CO3_SO4_AFt	2	1.9742038e-007	0.070175618	0.00013934524	0.00024733198
6	s	Graphite	1	0	-82.225518	0	0
7	s	Aluminate	1	0	-38.001869	0	0
8	s	C2AH75	1	0	-3.9895148	0	0
9	s	C3AH6	1	0	-2.4894066	0	0
10	s	C4AH13	1	0	-3.2	0	0
11	s	CAH10	1	0	-4.8	0	0
12	s	C4AsH12	1	0	-1.057941	0	0
13	s	C4Ac0.5H12	1	0	-0.70017984	0	0
14	s	C4AcH11	1	0.0116847		9038	6.6421602
15	s	ettringite	1			0	0
16	s	Aragonite	1	0	-0.1438323	0	0
17	s	Calcite	1	0.0049466221	-1.4447295e-007	0.18269853	0.49509256
18	s	lime	1	0	-9.7760821	0	0
19	s	Portlandite	1	0.043706866	-6.742948e-010	1.444949	3.2383597
20	s	Anhydrite	1	0	-2.9702427	0	0
21	s	Gypsum	1	0		0	0
22	s	hemihydrate	1	0		0	0
23	s	Sulphur	1	0	-118.99824	0	0

$m_{AFt(ss)}$ = 8.49 g

$m_{CO3\text{-}AFm}$ = 6.64 g

$m_{Calcite}$ = 0.50 g

$m_{Portlandite}$ = 3.24 g

Hydration of C_3A + $CaCO_3$ + $CaSO_4$

Experimental conditions: **React 5 g C_3A, 1.86 g $CaCO_3$, 2.52 g $CaSO_4$ and 2.5 g CaO with 50 g water (add 1 g O_2 to simulate gas phase)**

3) Assess Calculation

Aqueous phase composition (speciation, acivities and activity coefficients) →

Aqueous phase composition (total molalities) ↓

EqIC | EqPh | EqDC | EqSurf | EqGen

m t	ICnam	
7.3772305e-006	Al	...
6.5547777e-006	C	...
0.020400467	Ca	...
0.04073122	H	...
0.043454407	O	...
2.4618063e-005	S	...
-1.2602745e-017	Zz	...

EqIC | EqPh | EqDC | EqSurf | EqGen | 08/04/2014, 13:42

Reaction of C3A with CaCO3 and CaSO4
Tutorial 1 - Example 3

total conc [mol] | lg (activity) | activity coeff. | molality (mol/kg)

	DCnam	x	lga	gamma	my
0	Al(SO4)+	1.5803402e-035	-33.519634	0.82143385	3.6795373e-034
1	Al(SO4)2-	0	-36.693995	0.82143385	0
2	Al+3	1.6153245e-033	-32.245398	0.15111242	3.7609919e-032
3	AlO+	6.7995432e-020	-17.885905	0.82143385	1.583151e-018
4	AlO2-	3.1684759e-007	-5.217534	0.82143385	7.3772249e-006
5	AlO2H@	2.3923556e-013	-11.24765	1.0150365	5.5701686e-012
6	AlOH+2	1.8543084e-026	-24.72593	0.4353569	4.3174227e-025
7	Ca(CO3)@	2.3481928e-007	-5.2557428	1.0150365	5.4673436e-006
8	Ca(HCO3)+	1.5710125e-011	-9.5222061	0.82143385	3.6578195e-010
9	Ca(SO4)@	3.9699481e-007	-5.0276907	1.0150365	9.2433085e-006
10	Ca+2	0.00069291553	-2.1534316	0.4353569	0.016133289
11	CaOH+	0.00018264103	-2.4567863	0.82143385	0.0042524672
12	CO2@	1.0653084e-016	-14.599001	1.0150365	2.4803786e-015
13	CO3-2	4.6513582e-008	-6.3265336	0.4353569	1.0829849e-006
14	HCO3-	1.7537942e-010	-8.4744073	0.82143385	4.0833937e-009
15	CH4@	0	-159.3121	1.0150365	0
16	H2@	0	-44.65852	1.0150365	0
17	O2@	5.5625946e-005	-2.8811982	1.0150365	0.0012951499
18	S2O3-2	0	-163.49781	0.4353569	0
19	HSO3-	0	-55.380556	0.82143385	0
20	SO3-2	0	-50.123735	0.4353569	0
21	HSO4-	1.1348816e-017	-15.663434	0.82143385	2.6423672e-016
22	SO4-2	6.603369e-007	-5.1743469	0.4353569	1.5374754e-005
23	H2S@	0	-155.6577	1.0150365	0
24	HS-	0	-150.17085	0.82143385	0

Hydration of C_3A – Summary of modelled results

1.) $C_3A+CaSO_4+CaO+H_2O \Rightarrow$ *monosulfoaluminate(ss) + AFt $_{traces}$ + CH*

2.) $C_3A+CaCO_3+CaO+H_2O \Rightarrow$ *monocarboaluminate + calcite$_{traces}$ + CH*

3.) $C_3A+CaCO_3+CaSO_4+CaO+H_2O \Rightarrow$ *monocarboaluminate + AFt(ss) + calcite + CH*

Phase diagram