GEMS workshop 2020

Lecture 02b

Single system - Hydration of C_3A (Pt. 2)

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Tutorial – single systems: hydration of C_3A

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Hydration of C_3A

1) Simulation of reaction $C_3A + CaO + CaSO_4$ Guided tutorial (Lecture 02)

2) Simulation of reaction $C_3A + CaO + CaCO_3$

3) Simulation of reaction $C_3A + CaCO_3$

4) Simulation of reaction $C_3A + CaO + CaSO_4 + CaCO_3$

} Individual work

Hydration of C_3A + CaO + $CaCO_3$

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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

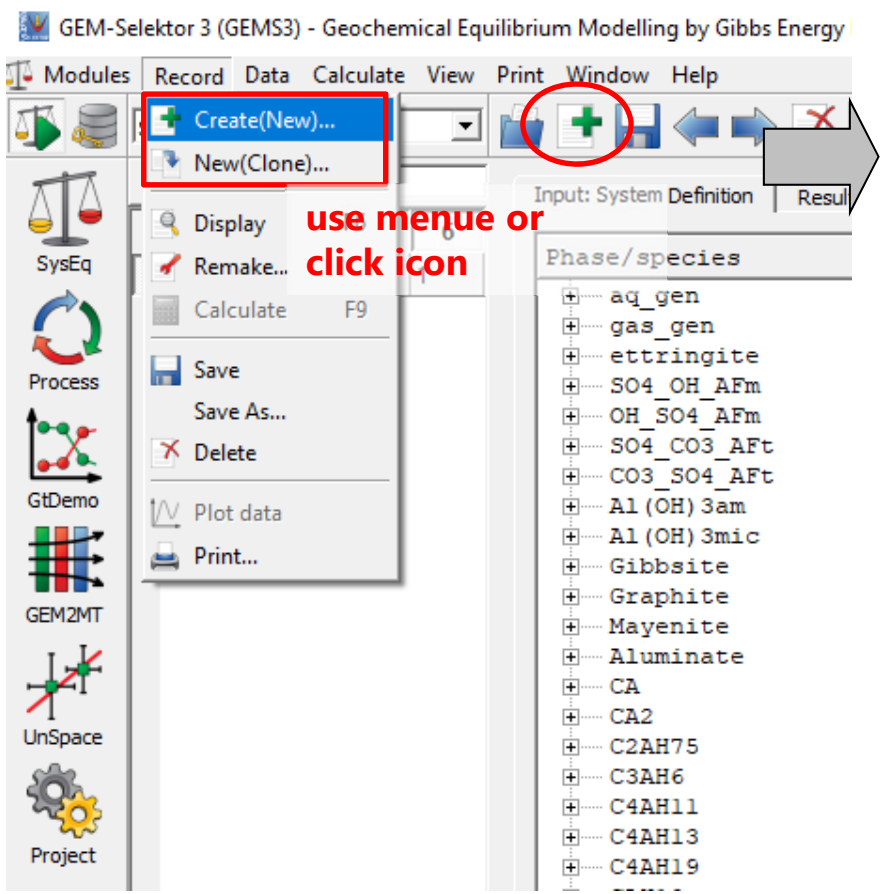
+ 0.1 g O_2 (oxidizing conditions, CO_2-free = no carbonation)

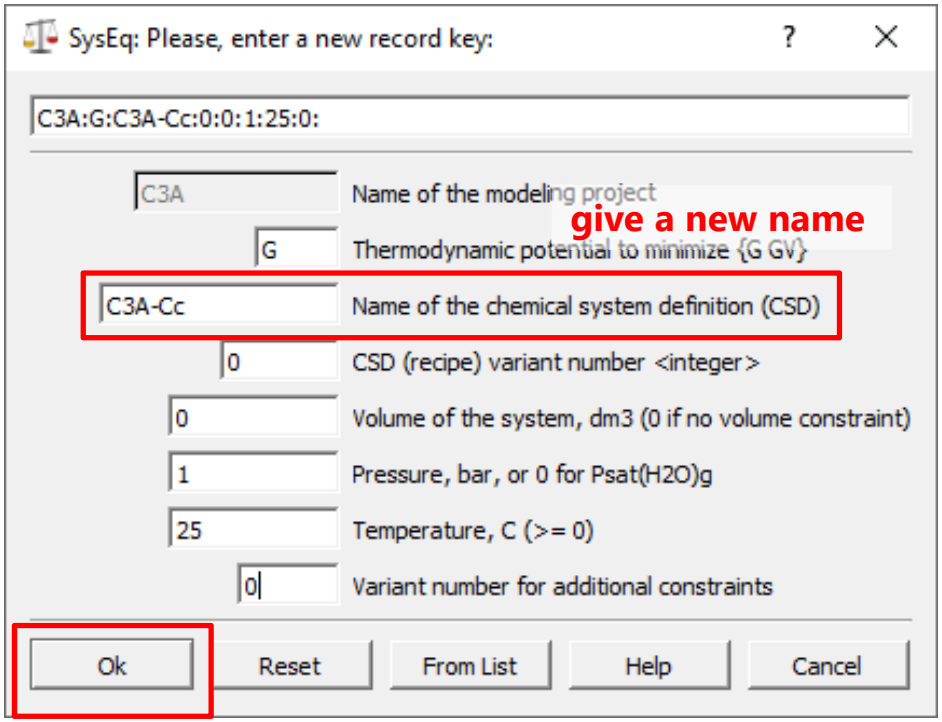
molar ratio SO_3/Al_2O_3 = 0, molar ratio CO_2/Al_2O_3 = 1

Hydration of C_3A + CaO + $CaCO_3$

Experimental conditions: **React 5 g C_3A, 1.86 g $CaCO_3$ and 2.5 g CaO with 50 g water (add 0.1 g O_2 to simulate gas phase)**

1) Create a new system within the same project



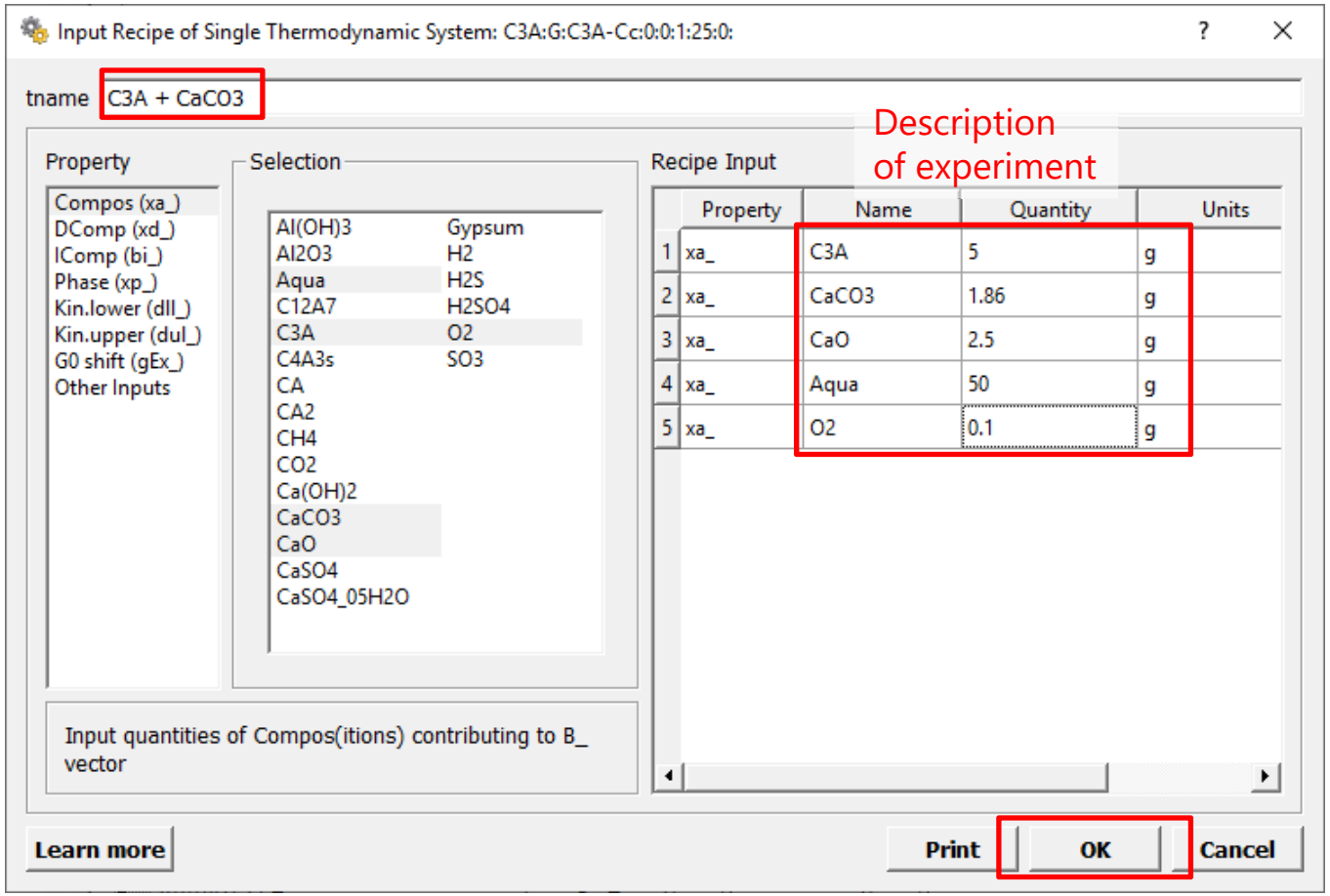


Hydration of C_3A + CaO + $CaCO_3$

<u>Experimental conditions:</u> React 5 g C_3A, 1.86 g $CaCO_3$ and 2.5 g CaO with 50 g water (add 0.1 g O_2 to simulate gas phase)

2) Enter initial system composition

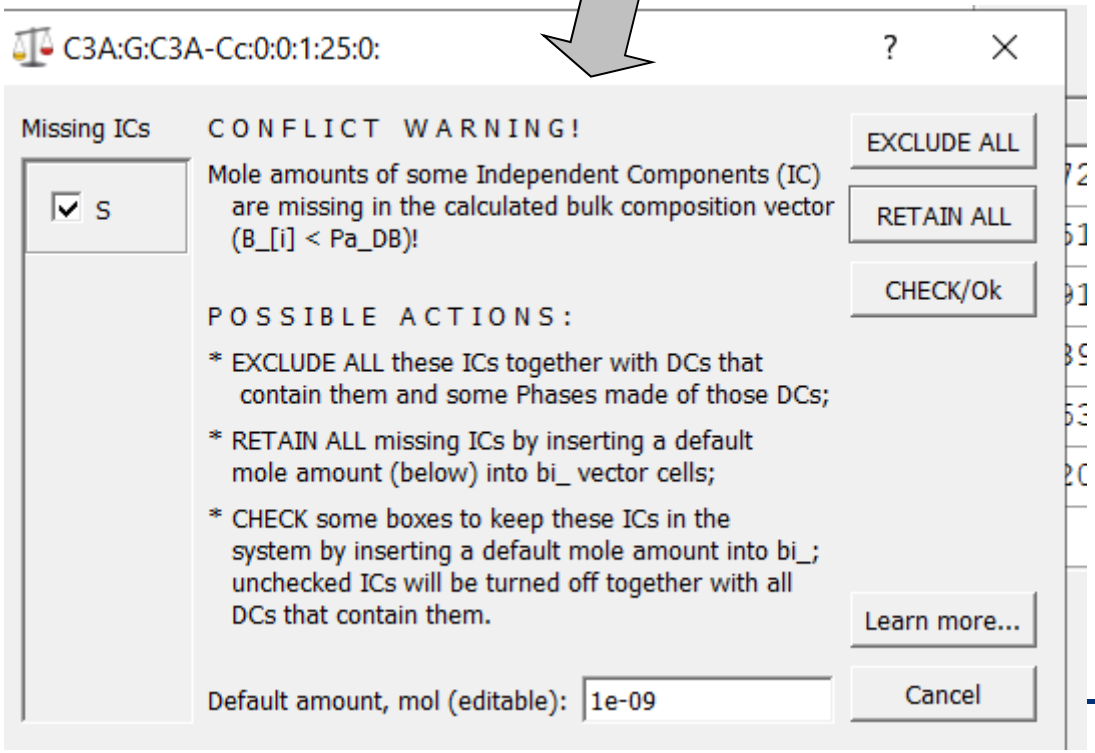
Recipe wizard

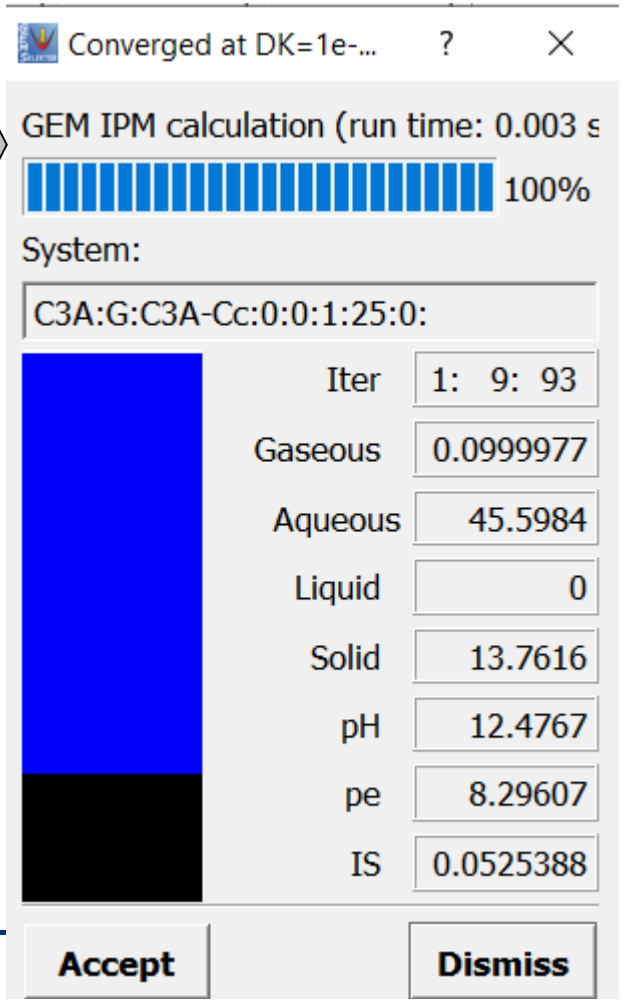


Hydration of C_3A + CaO + $CaCO_3$

<u>Experimental conditions:</u> React 5 g C_3A, 1.86 g $CaCO_3$ and 2.5 g CaO with 50 g water (add 0.1 g O_2 to simulate gas phase)

Start calculation

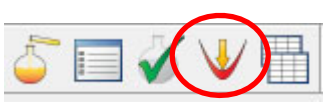


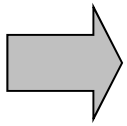


Hydration of C_3A + CaO + $CaCO_3$

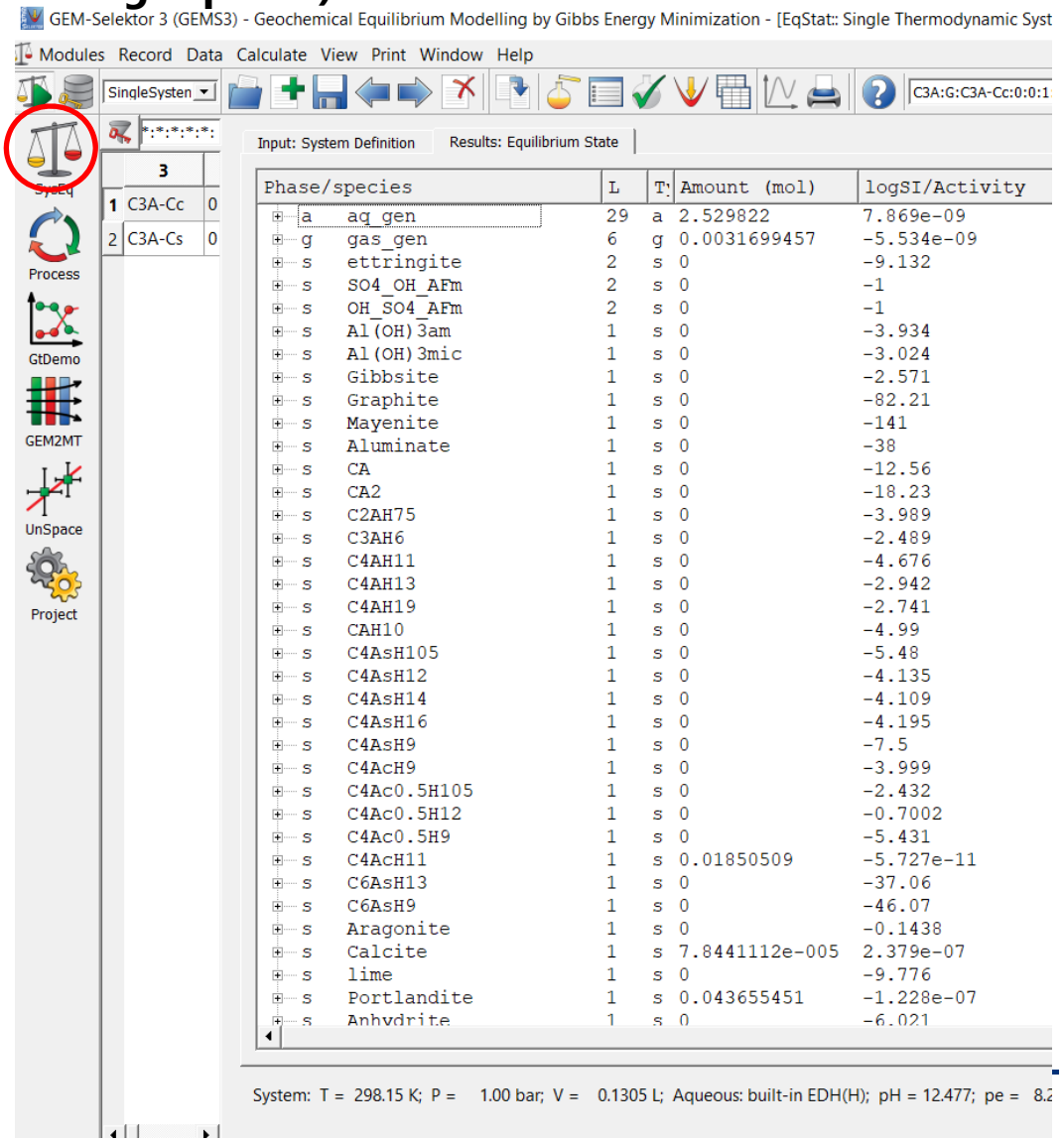
<u>Experimental conditions:</u> React 5 g C_3A, 1.86 g $CaCO_3$ and 2.5 g CaO with 50 g water (add 1 g O_2 to simulate gas phase)

3) Calculate equilibrium





Formation of monocarboaluminate, small amounts of calcite and portlandite



Hydration of C_3A + CaO + $CaCO_3$

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Detailed results

Formation of monocarboaluminate, small amounts of calcite and portlandite

EqIC | EqPh | EqDC | EqSurf | EqGen | 26/03/2020, 15:43

C3A + CaSO4

	PHnam		L1	Xa	Fa	phVol	phM
0	a	aq_gen	29	2.529822	6.4081814e-009	45.643622	45.598405
1	g	gas_gen	6	0.0031699457	-5.5338199e-009	78.58204	0.099997749
2	s	ettringite	2	0	-9.1324096	0	0
3	s	SO4_OH_AFm	2	0	-1	0	0
4	s	OH_SO4_AFm	2	0	-1		
5	s	Al(OH)3am	1	0	-3.934274		
26	s	C4Ac0.5H12	1	0	-0.70020345	0	0
27	s	C4Ac0.5H9	1	0	-5.4311886	0	0
28	s	C4AcH11	1	0.01850509	-5.7273337e-011	4.8475565	10.519196
29	s	C6AsH13	1	0		0	0
30	s	C6AsH9	1	0		0	0
31	s	Aragonite	1	0	-0.14383192	0	0
32	s	Calcite	1	7.8441112e-005	2.3794536e-007	0.002897144	0.0078509356
33	s	lime	1	0	-9.7760354	0	0
34	s	Portlandite	1	0.043655451	-1.2281381e-007	1.4432492	3.2345502
35	s	Anhydrite	1	0	-6.0210873	0	0
36	s	Gypsum	1	0	-5.7980614	0	0
37	s	hemihydrate	1	0	-6.7872852		0
38	s	Sulphur	1	0			0

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

$m_{Calcite}$ = 0.008 g

$m_{Portlandite}$ = 3.23 g

Hydration of C_3A + $CaCO_3$

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Experimental problem part 3:

Reaction of C_3A with calcium carbonate

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

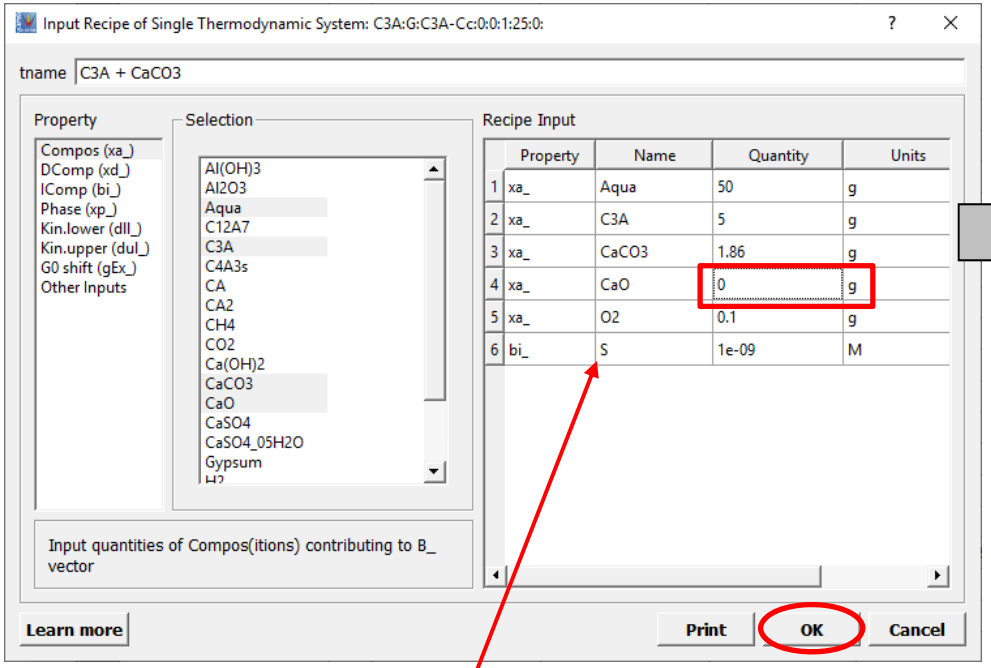
+ 0.1 g O_2 (oxidizing conditions, CO_2-free = no carbonation)

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 and 1.86 g $CaCO_3$ with 50 g water (add 0.1 g O_2 to simulate gas phase)**

Repeat calculation without lime addition



low amount of S added by GEMS as presence of S in the calculations was maintained

		PHnam	Ll	Xa	Fa	phVol	phM
6	s	CO3_SO4_AFt	2	0	-1	0	0
7	s	Al(OH)3am	1	0	-1.3631423	0	0
8	s	Al(OH)3mic	1	0	-0.45314547	0	0
9	s	Gibbsite	1	0.00010671355	4.6642162e-006	0.0034101384	0.0083240404
10	s	Graphite	1	0	-80.496214	0	0
11	s	Mayenite	1	0	-125.60593	0	0
12	s	Aluminate	1	0	-38.00523	0	0
	s	CA	1	0	-9.1357966	0	0
	s	CA2	1	0	-9.6643563	0	0
15	s	C2AH75	1	0	-2.2756047	0	0
16	s	C3AH6	1	0	-2.4909356	0	0
17	s	C4AH11	1	0	-6.3909619	0	0
18	s	C4AH13	1	0	-4.6562055	0	0
19	s	C4AH19	1	0	-4.4536514	0	0
20	s	CAH10	1	0	-1.5600969	0	0
21	s	C4AsH105	1	0	-5.6830641	0	0
22	s	C4AsH12	1	0	-4.3369726	0	0
23	s	C4AsH14	1	0	-4.310718	0	0
24	s	C4AsH16	1	0	-4.3955522	0	0
25	s	C4AsH9	1	0	-7.7028542	0	0
26	s	C4AcH9	1	0	-3.9997538	0	0
27	s	C4Ac0.5H105	1	0	-3.2895615	0	0
28	s	C4Ac0.5H12	1	0	-1.5573656	0	0
29	s	C4Ac0.5H9	1	0	-6.2894075	0	0
30	s	C4AcH11	1	0.018438391	-9.4062568e-009	4.8300841	10.481281
31	s	C6AsH13	1	0	-37.664961	0	0
32	s	C6AsH9	1	0	-46.674937	0	0
33	s	Aragonite	1	0	-0.14383064	0	0
34	s	Calcite	1	0.00014508719	1.5190626e-006	0.0053586501	0.014521341
35	s	lime	1	0	-11.491063	0	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 0.1 g O_2 to simulate gas phase)**

Without lime addition: check pore solution composition

EqIC | EqPh | EqDC | EqSurf | EqGen | 26/03/2020, 15:43

C3A + CaSO4

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molality

	ICnam	b	Cb	u	lgm t	m t	ICnam
0	Al …	0.037010516	-7.6640767e-018	-320.75864	-3.2343274	0.00058300544	Al …
1	C …	0.018583832	7.1850719e-019	-185.34933	-5.1157638	7.6601304e-006	C …
2	Ca …	0.074099606	4.5505455e-018	-270.10305	-2.3630329	0.0043347808	Ca …
3	H …	5.5508373	-6.1312614e-016	-47.830556	-2.0930571	0.0080712899	H …
4	O …	2.9484519	6.4210593e-016	-0.016487608	-1.9279604	0.011804282	O …
5	S …	1e-009	0	-277.49644	-7.6659371	2.1580567e-008	S …
6	Zz …	0	3.6244083e-020	20.566841	0	-7.4164313e-019	Zz …

measured *

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

pHcalc = 11.84

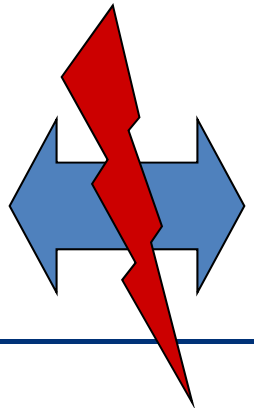
pH = 11.59

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

Solid phase assemblage:

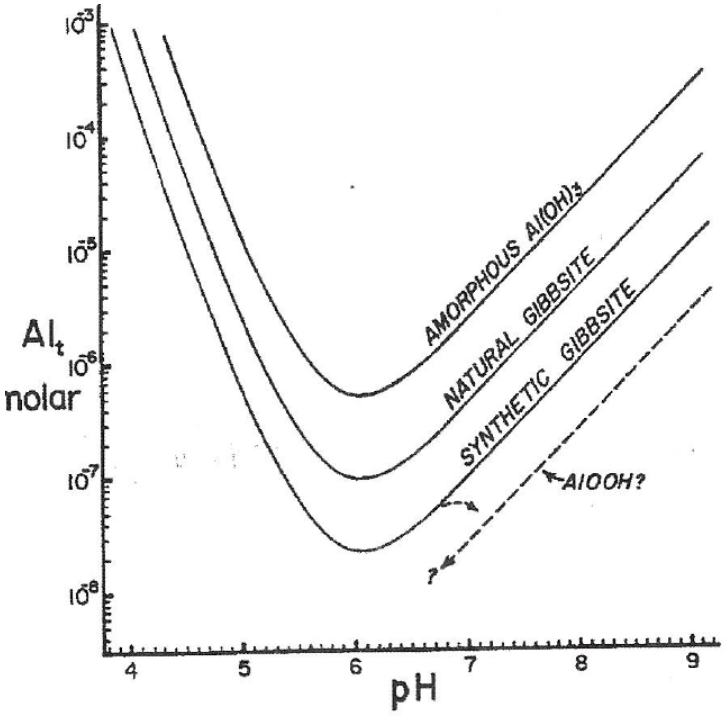
CO_3-AFm - calcite - aqueous phase

experiments



modelling

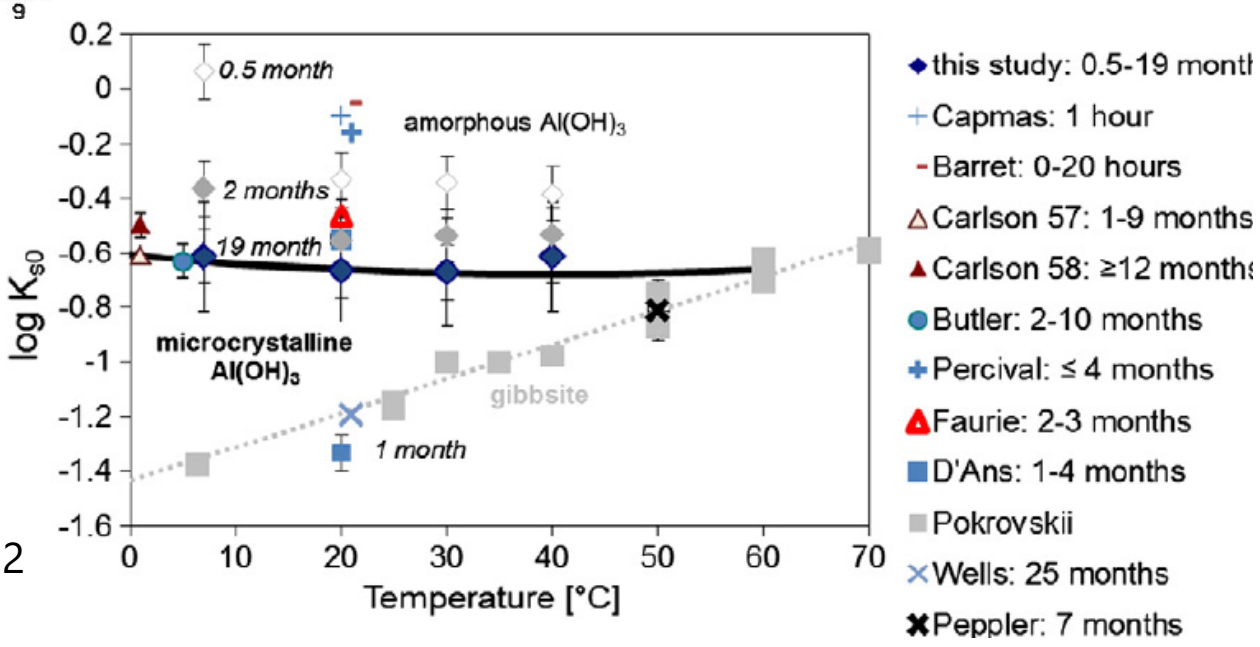
Solubility of Al-hydroxides



Mäder-Waber
Aqueous geochemistry

$Al(OH)_3$ solubility depends on crystallinity and time

In the database		log K_{S0}
$Al(OH)_3$(am)	→ $Al(OH)_4^-$ - OH^- - H_2O	**0.24**
$Al(OH)_3$(mic)	→ $Al(OH)_4^-$ - OH^- - H_2O	**-0.67**
$Al(OH)_3$(gibbsite)	→ *$Al(OH)_4^-$ - OH^- - H_2O*	***-1.12***



Lothenbach ea, CCR 2012

Hydration of C_3A + $CaCO_3$

=> supress formation of gibbsite and microcrystalline $Al(OH)_3$ and repeat calculation

=>***Introduction of metastability constraints,*** ***Option 1: deactivate compound***

Input: System Definition | Results: Equilibrium State

Phase/species	L	T	On/	UC	Add to BC	UG	G0 corr.	UK	Lower_KC	Upper_KC	KC ty
aq_gen	29	a	+	g	0	J	0				
gas_gen	6	g	+	g	0	J	0				
ettringite	2	s	+	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)3am	1	s	+	g	0	J	0				
AlOHam		O	+	M	0	J	0	M	0	1000000	B
Al(OH)3mic	1	s	-	g	0	J	0				
AlOHmic		O	-	M	0	J	0	M	0	0	B
Gibbsite	1	s	-	g	0	J	0				
Gbs		O	-	M	0	J	0	M	0	0	B
Graphite	1	s	+	g	0	J	0				

Phases disappear from results

Option 2: limit the amount formed to zero *=> phases still present in results, in 0 amount*

Phase/species	L	T	On/	UC	Add to BC	UG	G0 corr.	UK	Lower_KC	Upper_KC	KC ty
aq_gen	29	a	+	g	0	J	0				
gas_gen	6	g	+	g	0	J	0				
ettringite	2	s	+	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)3am	1	s	+	g	0	J	0				
AlOHam		O	+	M	0	J	0	M	0	1000000	B
Al(OH)3mic	1	s	+	g	0	J	0				
AlOHmic		O	+	M	0	J	0	M	0	0	B
Gibbsite	1	s	+	g	0	J	0				
Gbs		O	+	M	0	J	0	M	0	0	B
Graphite	1	s	+	g	0	J	0				

Upper restriction
dul_ = 0
Default 1000000

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 0.1 g O_2 to simulate gas phase)

supressed 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>

gibbsite and microcrystalline $Al(OH)_3$ are oversaturated (log SI > 0)
But none is allowed to form (amount = 0)

Phase/species	L	T	Amount (mol)	logSI/Activity
a aq_gen	29	a	2.5727565	1.056e-08
g gas_gen	6	g	0.0031689703	8.058e-08
s ettringite	2	s	0	-9.857
s SO4_OH_AFm	2	s	0	-1
s OH_SO4_AFm	2	s	0	-1
s Al(OH)3am	1	s	0	-0.5254
s Al(OH)3mic	1	s	0	0.3845
s Gibbsite	1	s	0	0.8377
s Graphite	1	s	0	-79.94
s Mayenite	1	s	0	-120.6
s Aluminate	1	s	0	-38.01
s CA	1	s	0	-8.019
s CA2	1	s	0	-6.872
s C2AH75	1	s	0	-1.717
s C3AH6	1	s	0	-2.491
s C4AH11	1	s	0	-6.949
s C4AH13	1	s	0	-5.215
s C4AH19	1	s	0	-5.012
s CAH10	1	s	0	-0.4431
s C4AsH105	1	s	0	-5.725
s C4AsH12	1	s	0	-4.379
s C4AsH14	1	s	0	-4.352
s C4AsH16	1	s	0	-4.437
s C4AsH9	1	s	0	-7.744
s C4AcH9	1	s	0	-4
s C4Ac0.5H105	1	s	0	-3.569
s C4Ac0.5H12	1	s	0	-1.837
s C4Ac0.5H9	1	s	0	-6.569
s C4AcH11	1	s	0.018452688	-8.039e-08
s C6AsH13	1	s	0	-37.79
s C6AsH9	1	s	0	-46.8
s Aragonite	1	s	0	-0.1438
s Calcite	1	s	0.00013077376	1.642e-05
s lime	1	s	0	-12.05

Hydration of C_3A + $CaCO_3$

Experimental conditions: **React 5 g C_3A and 1.86 g $CaCO_3$ with 50 g water (add 0.1 g O_2 to simulate gas phase)**

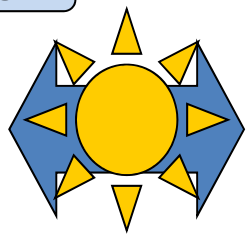
Without lime addition: supress formation of gibbsite and microcrystalline $Al(OH)_3$ and repeat calculation

Al = 2.27 mmol/kg

C ≈ 0.008 mmol/kg

Ca = 3.41 mmol/kg

m t	ICnam
0.0022688806	Al …
7.9829387e-006	C …
0.0034113038	Ca …
0.0045379362	H …
0.011643582	O …
2.1579854e-008	S …
1.1977761e-018	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 + CaO + $CaSO_4$ + $CaCO_3$

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Experimental problem part 4:

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

+ 0.1 g O_2 (oxidizing conditions, CO_2-free = no carbonation)

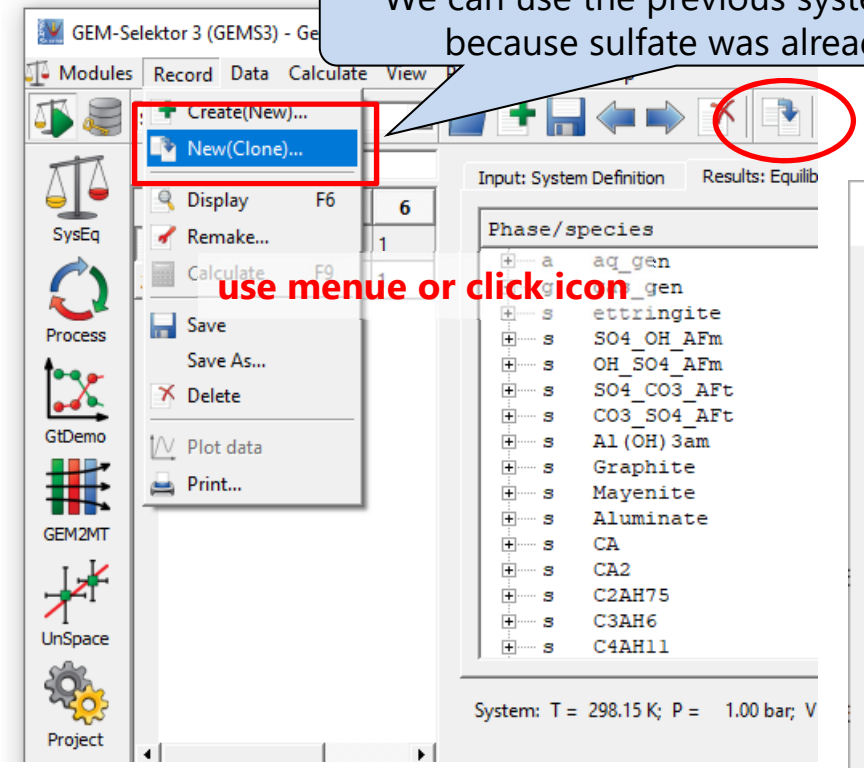
molar ratio SO_3/Al_2O_3 = 1, molar ratio CO_2/Al_2O_3 = 1

Hydration of C_3A + CaO + $CaSO_4$ + $CaCO_3$

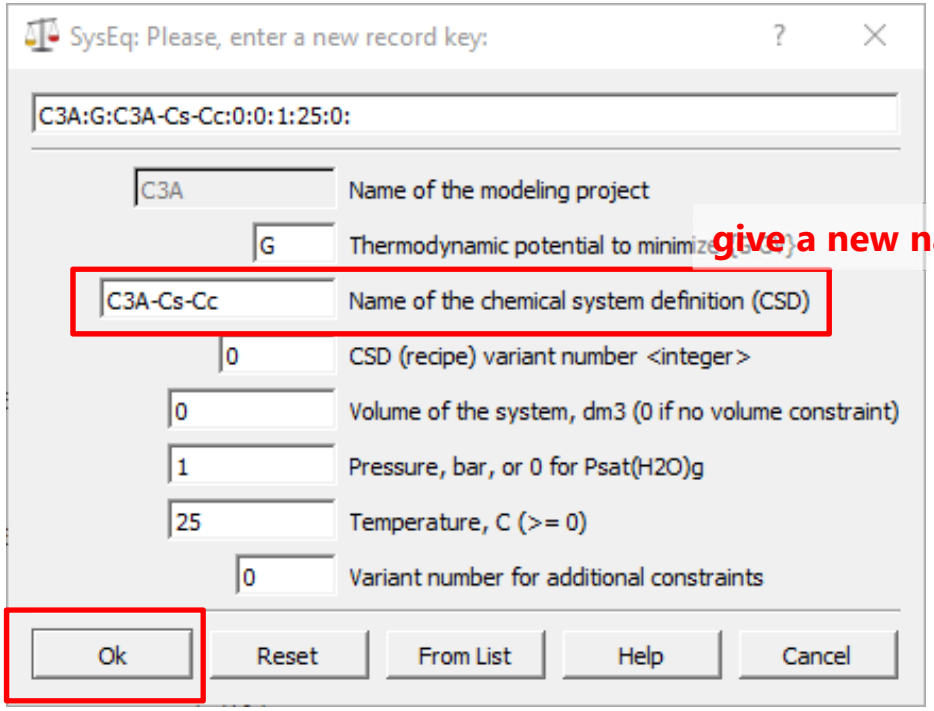
<u>Experimental conditions:</u> React 5 g C_3A, 1.86 g $CaCO_3$, 2.52 g $CaSO_4$ and 2.5 g CaO with 50 g water (add 0.1 g O_2 to simulate gas phase)

1) Create new system

We can use the previous system as template because sulfate was already included



use menue or click icon



give a new name

We use the recipe wizard again

Hydration of C_3A + CaO + $CaSO_4$ + $CaCO_3$

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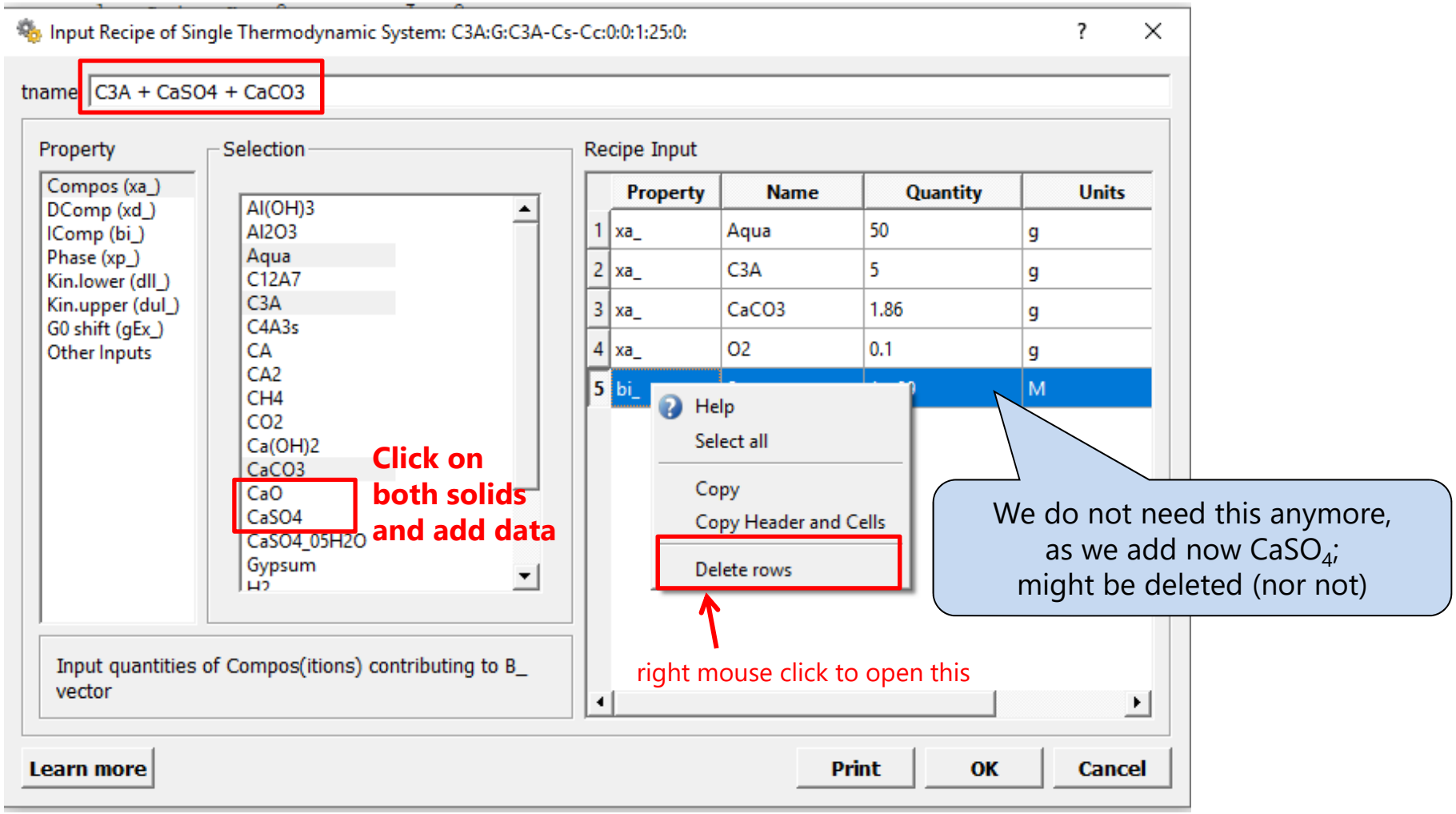
<u>Experimental conditions:</u> React 5 g C_3A, 1.86 g $CaCO_3$, 2.52 g $CaSO_4$ and 2.5 g CaO with 50 g water (add 0.1 g O_2 to simulate gas phase)



Hydration of C_3A + CaO + $CaSO_4$ + $CaCO_3$

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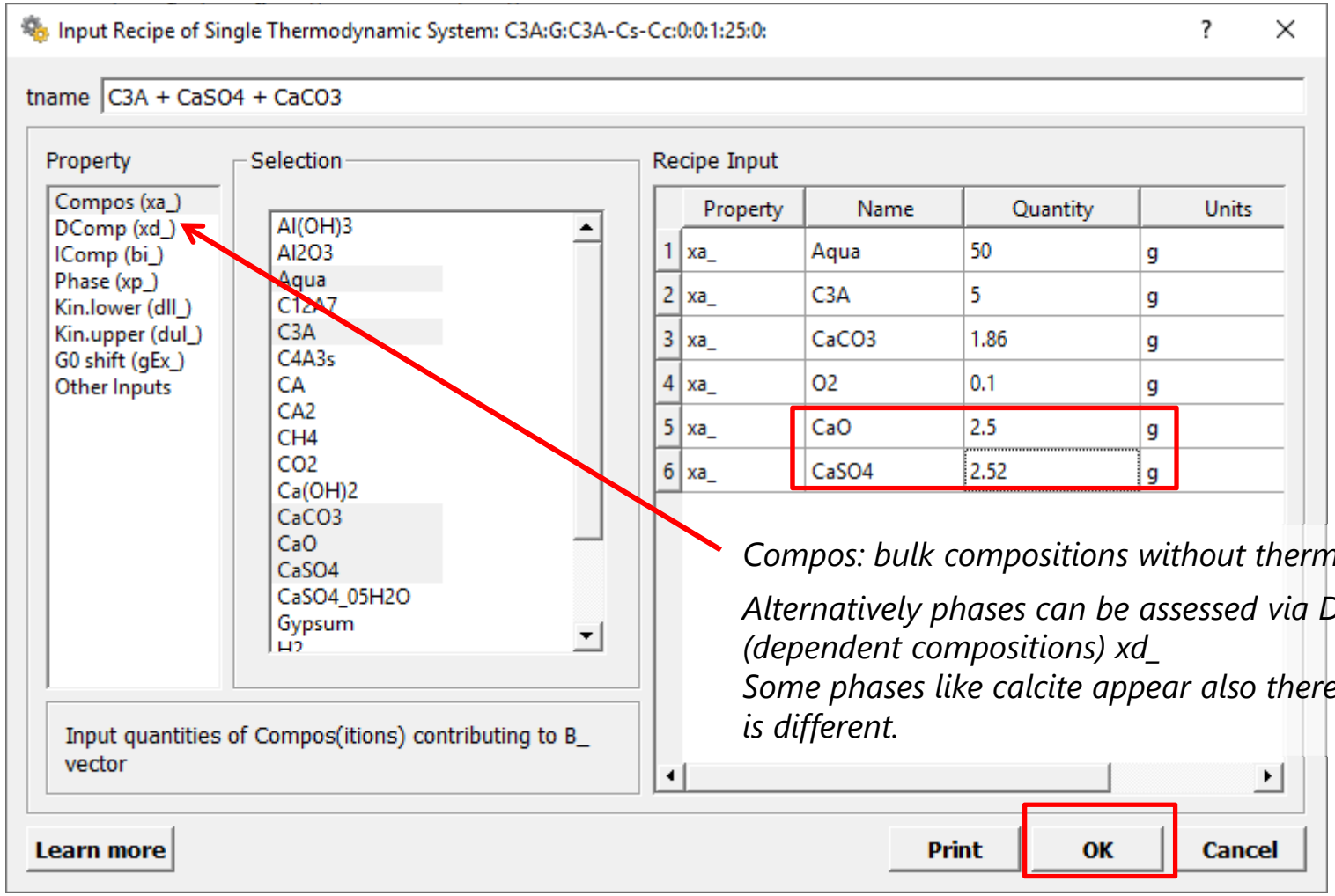
<u>Experimental conditions:</u> React 5 g C_3A, 1.86 g $CaCO_3$, 2.52 g $CaSO_4$ and 2.5 g CaO with 50 g water (add 0.1 g O_2 to simulate gas phase)



Compos: bulk compositions without thermodynamic data

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

Hydration of C_3A + CaO + $CaSO_4$ + $CaCO_3$

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<u>Experimental conditions:</u> 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 0.1 g O_2 to simulate gas phase)

2) Calculate equilibrium

(you may activate again SO4_CO3_AFt , CO3_SO4_AFt ,gibbsite and microcrystalline $Al(OH)_3$)

Formation of AFt, monocarboaluminate, calcite and portlandite

<u>No</u> formation of monosulfoaluminate despite SO_3/Al_2O_3 = 1

solid solution:

90.7 mol% SO_4-AFt

9.3 mol% CO_3-AFt

Input: System Definition | Results: Equilibrium State

Phase/species		L	T	Amount (mol)	logSI/Activity	Concentration
a	aq_gen	29	a	2.3867606	3.823e-10	
g	gas_gen	6	g	0.0031733326	1.096e-07	
s	ettringite	2	s	0	-0.04235	
s	SO4_OH_AFm	2	s	0	-1	
s	OH_SO4_AFm	2	s	0	-1	
s	SO4_CO3_AFt	2	s	0.02041597	4.874e-08	
	tricarboalu03		J	0.0019071421	0.226472	0.093414229
	ettringite03_ss		M	0.018508828	0.900165	0.90658577
s	CO3_SO4_AFt	2	s	1.8168586e-007	4.903e-08	
	tricarboalu03		M	1.6976312e-008	0.226472	0.093437717
	ettringite03_ss		J	1.6470955e-007	0.900165	0.90656228
s	Al(OH)3am	1	s	0	-3.934	
s	Al(OH)3mic	1	s	0	-3.024	
s	Gibbsite	1	s	0	-2.571	
s	Graphite	1	s	0	-82.21	
s	Mayenite	1	s	0	-141	
s	Aluminate	1	s	0	-38	
s	CA	1	s	0	-12.56	
s	CA2	1	s	0	-18.23	
s	C2AH75	1	s	0	-3.989	
s	C3AH6	1	s	0	-2.489	
s	C4AH11	1	s	0	-4.676	
s	C4AH13	1	s	0	-2.942	
s	C4AH19	1	s	0	-2.741	
s	CAH10	1	s	0	-4.99	
s	C4AsH105	1	s	0	-2.45	
s	C4AsH12	1	s	0	-1.105	
s	C4AsH14	1	s	0	-1.079	
s	C4AsH16	1	s	0	-1.165	
s	C4AsH9	1	s	0	-4.47	
s	C4AcH9	1	s	0	-3.999	
s	C4Ac0.5H105	1	s	0	-2.432	
s	C4Ac0.5H12	1	s	0	-0.7002	
s	C4Ac0.5H9	1	s	0	-5.431	
s	C4AcH11	1	s	0.011699715	-1.729e-08	
s	C6AsH13	1	s	0	-27.97	
s	C6AsH9	1	s	0	-36.98	

Hydration of C_3A + CaO + $CaSO_4$ + $CaCO_3$

<u>Experimental conditions:</u> 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 0.1 g O_2 to simulate gas phase)

3) Assess Calculation

Formation of AFt, monocarboaluminate, calcite and portlandite

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

EqIC | EqPh | EqDC | EqSurf | EqGen | 27/03/2020, 08:36

		PHnam	L1	Xa	Fa	phVol	phM
0	a	aq_gen	29	2.3867606	3.8233694e-010	43.062453	43.019923
1	g	gas_gen	6	0.0031733326	1.0959891e-007	78.665999	0.10010464
2	s	ettringite	2	0	-0.042351029	0	0
3	s	SO4_OH_AFm	2			0	0
4	s	OH_SO4_AFm	2			0	0
5	s	SO4_CO3_AFt	2	0.02041597	4.8737269e-008	4.7755733	8.4726721
6	s	CO3_SO4_AFt	2	1.8168586e-007	4.9026597e-008	4.2498715e-0…	7.5399875e-0…
7	s	Al(OH)3am	1	0	-3.9342733	0	0
29	s	C4Ac0.5H9	1	0	-5.4311878		0
30	s	C4AcH11	1	0.011699715	-1.7287463e-008	3.0648341	6.6506889
31	s	C6AsH13	1			0	0
32	s	C6AsH9	1	0	-36.9763	0	0
33	s	Aragonite	1	0	-0.14383223	0	0
34	s	Calcite	1	0.0049766728	-7.0941594e-008	0.18380843	0.49810025
35	s	lime	1	0	-9.7760351	0	0
36	s	Portlandite	1	0.043707887	-6.9026541e-008	1.4449827	3.2384353
37	s	Anhydrite	1	0	-2.9910661	0	0
38	s	Gypsum	1	0		0	0
39	s	hemihydrate	1	0		0	0

$m_{AFt(ss)}$ = 8.47 g

$m_{CO3\text{-}AFm}$ = 6.65 g

$m_{Calcite}$ = 0.50 g

$m_{Portlandite}$ = 3.24 g

Hydration of C_3A + CaO + $CaSO_4$ + $CaCO_3$

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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 0.1 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	
7.3706496e-006	Al	...
6.6329802e-006	C	...
0.020373895	Ca	...
0.040680088	H	...
0.043352788	O	...
2.3537278e-005	S	...
8.4386471e-019	Zz	...

EqIC | EqPh | EqDC | EqSurf | EqGen | 27/03/2020, 08:36

C3A + CaSO4

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

	DCnam	x	lga	gamma	my
0	Al(SO4)+	1.5068327e-035	-33.540047	0.82202255	3.508076e-034
1	Al(SO4)2-	0	-36.735817	0.82202255	0
2	Al+3	1.6083685e-033	-32.244404	0.15212732	3.7444628e-032
3	AlO+	6.8023658e-020	-17.885448	0.82202255	1.5836673e-018
4	AlO2-	3.1659312e-007	-5.2176143	0.82202255	7.3706439e-006
5	AlO2H@	2.4294309e-013	-11.247485	0.99999945	5.6559884e-012
6	AlOH+2	1.8521152e-026	-24.725228	0.43664655	4.3119326e-025
7	Ca(CO3)@	2.383873e-007	-5.2557427	0.99999945	5.5499245e-006
8	Ca(HCO3)+	1.5710576e-011	-9.521961	0.82202255	3.6575989e-010
9	Ca(SO4)@	3.8412382e-007	-5.0485142	0.99999945	8.9428346e-006
10	Ca+2	0.00069186196	-2.1528477	0.43664655	0.016107325
11	CaOH+	0.00018264054	-2.4564943	0.82202255	0.0042520773
12	CO2@	1.0814254e-016	-14.599048	0.99999945	2.5176801e-015
13	CO3-2	4.6329894e-008	-6.3271175	0.43664655	1.078612e-006
14	HCO3-	1.7515891e-010	-8.4747461	0.82202255	4.0778964e-009
15	CH4@	0	-159.28362	0.99999945	0
16	H2@	0	-44.651413	0.99999945	0
17	O2@	5.4634714e-005	-2.8955074	0.99999945	0.0012719576
18	S2O3-2	0	-163.51147	0.43664655	0
19	HSO3-	0	-55.394564	0.82202255	0
20	SO3-2	0	-50.137988	0.43664655	0
21	HSO4-	1.0803266e-017	-15.684597	0.82202255	2.5151219e-016

Hydration of C_3A – Summary of modelled results

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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

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

Phase diagramm