

## Lecture 02

### Single system – hydration of $C_3A$

- 1) Simulation of reaction  $C_3A + CaO + CaSO_4$
- 2) Simulation of reaction  $C_3A + CaO + CaCO_3$
- 3) Simulation of reaction  $C_3A + CaCO_3$
- 4) Simulation of reaction  $C_3A + C + CaSO_4 + CaCO_3$



Ellina Bernard

Version GEMS 3.9.6 (June 2023)

Software development/fitting  
tools/kinetic:

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### First Tutorial – single systems: hydration of $C_3A$

Hydration of  $C_3A$  ( $Ca_3Al_2O_6$ )\*

1) Simulation of reaction  $C_3A + CaO + CaSO_4$  **Guided tutorial**

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

3) Simulation of reaction  $C_3A + CaCO_3$

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

Individual  
work

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

\* cement notation

C => CaO

S =>  $SiO_2$

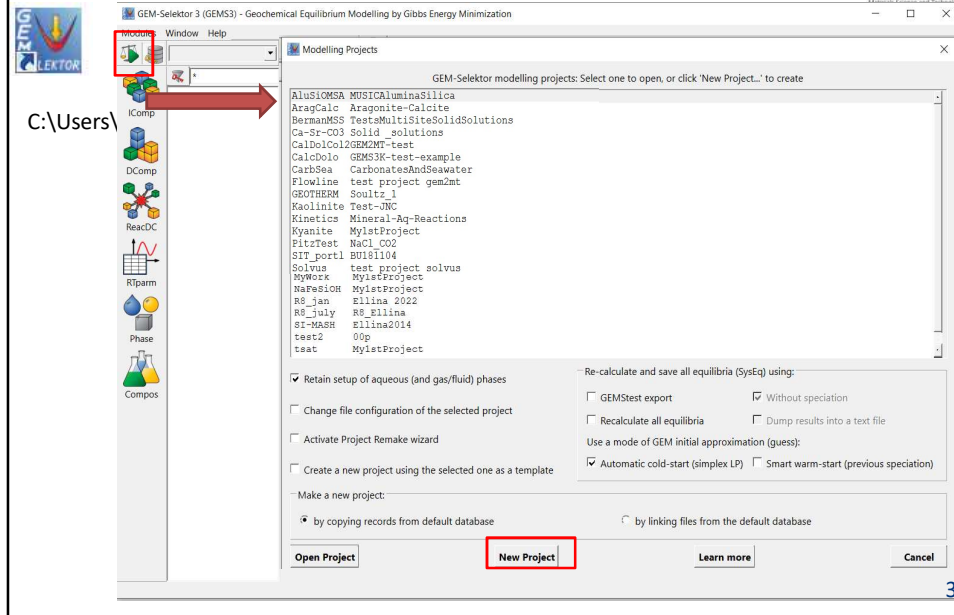
s =>  $SO_3$

A =>  $Al_2O_3$

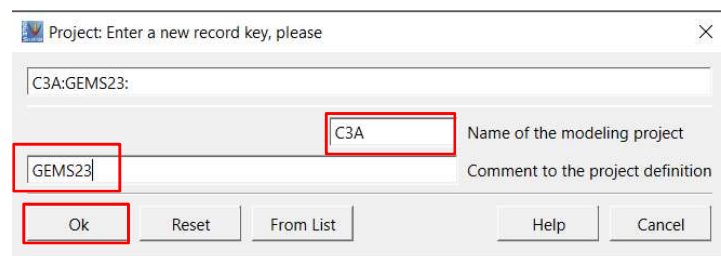
H =>  $H_2O$

c=>  $CO_2$

## Hydration of $C_3A$ + $CaO$ + $CaSO_4$ – project setup

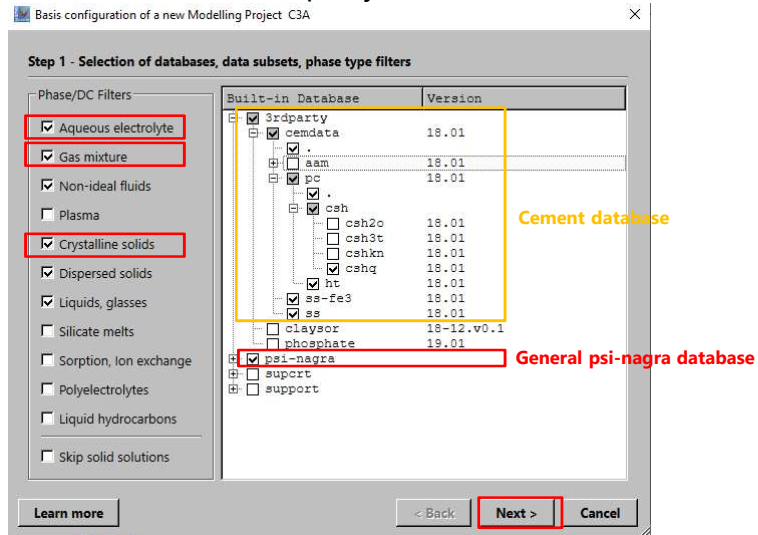


## Hydration of $C_3A$ + $CaO$ + $CaSO_4$ – project setup



## Hydration of $C_3A + CaO + CaSO_4$ – project setup

### Select CEMDATA18 (3<sup>rd</sup> party data base)

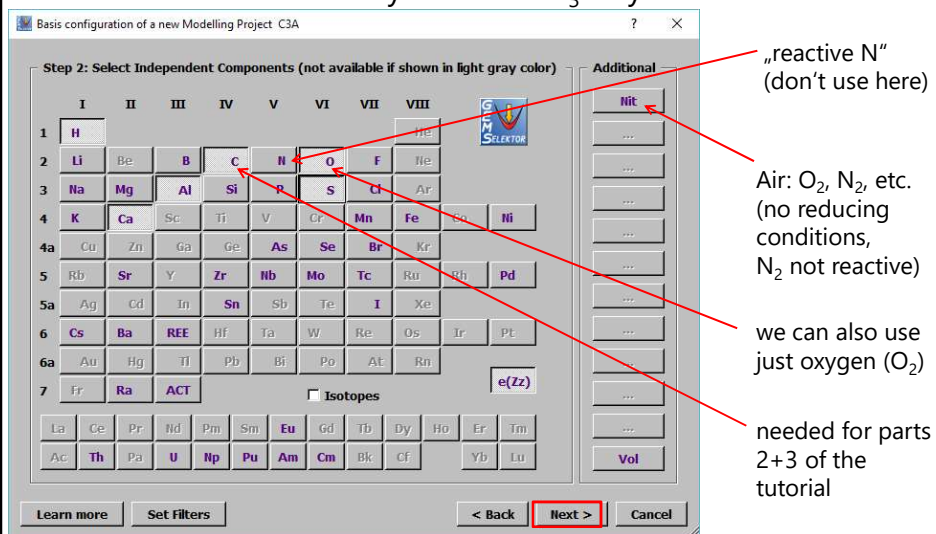


Recommended selection for PC and blended cements

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## Hydration of $C_3A + CaO + CaSO_4$ – project setup

### Select elements necessary to model $C_3A$ hydration



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## Hydration of $C_3A + CaO + CaSO_4$ – project setup

### Select model for calculation of the aqueous phase

Setup of aqueous and gas phases in project: C3A

Select Aqueous Electrolyte Model | Select Gas/Fluid Mixture Model

☐ Ion-association (IA) with Davies equation, D (default)

☒ IA with extended Debye-Hueckel equation (Helgeson), common  $b_{\gamma}$  and  $a_0$ , H

☐ IA with extended Debye-Hueckel equation (Sivakov), common  $b_{\gamma}$  and  $a_0$ , H

☐ IA with extended Debye-Hueckel equation (Karpov), common  $b_{\gamma}$  and individual  $a_0$ , 3

☐ IA with Debye-Hueckel equation, no  $b_{\gamma}$ , individual  $a_0$ , 2

☐ IA with Debye-Hueckel limiting law (very low ionic strength), 1

☐ Do not generate; select a user-defined Phase record from database ( Q, S, Z ), U

☐ Do not include aqueous electrolyte phase into the system definition, N

Phase record key: | a AQELIA aq\_gen aq EDH\_H

Parameters for the aqueous phase model

$b_{\gamma}(1,298)$  value: 0.123

$b_{\gamma}(P,T)$  mode: KOH

Common  $a_0$  value: 3.67

Gamma (neutral species): Calculate as  $b_{\gamma} \cdot IS$

Gamma (water solvent): From osmotic coefficient

Molality conversion: Applied to all species

OK Cancel Check Learn more

2. KOH good for cements

2) f(pressure, temp) -> electrolyte

$a_0=3.67$  for KOH  
 $b_0= 0.123$

Calculates activity of water

More details

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## 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

$$\{Ca^{2+}\} = [Ca^{2+}] \cdot \gamma_{Ca^{2+}} \leftarrow \text{Activity coefficient}$$

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

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## 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 $I < 0.1 \text{ M}$
Extended Debye-Hückel	$\log \gamma_{Ca^{2+}} = \frac{-AZ^2\sqrt{I}}{1+Ba\sqrt{I}} + bI$	
common a, common b (Helgeson)		$I < 1-2 \text{ M}$
individual a, common b (Truesdell-Jones)		$I < 1 \text{ M}$
individual a, no b		$I < 0.3 \text{ M}$
Davies	$\log \gamma_{Ca^{2+}} = -AZ^2\left(\frac{\sqrt{I}}{1+\sqrt{I}} - 0.3I\right)$	$0.1 < I < 0.5 \text{ M}$
SIT	$\log \gamma_{Ca^{2+}} = \frac{-AZ^2\sqrt{I}}{1+1.5\sqrt{I}} + \sum \varepsilon m_k$	$I < 3 \text{ M}$

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:\GEMS36\Gems3-app\Resources\doc\pdf\Activity-Coeffs.pdf and references therein

## Hydration of $C_3A$ + $CaO$ + $CaSO_4$ – project setup



SysEq: Please, enter a new record key:

C3A:G:C3A-Cs:0:0:1:25:0:

C3A	Name of the modeling project	Project name
G	Thermodynamic potential to minimize {G GV}	Method (Gibbs free energy minimization)
C3A-Cs	Name of the chemical system definition (CSD)	System definition
0	CSD (recipe) variant number <integer>	Integer (default 0)
0	Volume of the system, dm3 (0 if no volume constraint)	System volume unconstrained
1	Pressure, bar, or 0 for Psat(H2O)g	Pressure (bar)
25	Temperature, C (>= 0)	Temperature (°C)
0	Variant number for additional constraints	

Ok Reset From List Help Cancel

Avoid special signs such as \$ & % ä ö ü æ å ø 好 ...

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

We need a recipe

Input Recipe of Single Thermodynamic System: C3A:G:C3A-Cs:0:0:1:25:0:

Title: C3A + CaSO4 comments

Comment:

Property Selection

Compos (xa\_) Al(OH)3  
DComp (xd\_) Al2O3  
IComp (bi\_) Aqua  
Phase (xp\_) CT2A7  
Kin.lower (dll\_) C3A  
Kin.upper (du\_) C4A3s  
G0 shift (gEx\_) CA  
Other inputs CA2  
CH4

Recipe Input

Property	Name	Quantity	Units
----------	------	----------	-------

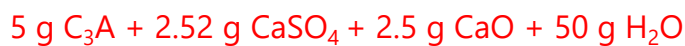
Input quantities of Compos(itions) contributing to B\_vector

Learn more Print OK Cancel

More comments if you like

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

1 Reaction of  $C_3A$  with calcium sulfate



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

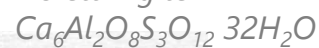
molar ratio  $SO_3/Al_2O_3 = 1$ , molar ratio  $CO_2/Al_2O_3 = 0$

Reaction products?

*Expectation: monosulfate*



*No ettringite*



> Recipe >



> Equilibrium speciation

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

Input Recipe of Single Thermodynamic System: C3A:G:C3A-Cs:0:0:1:25:0:

Title: **C3A + CaSO4**

Comment: ---

Property	Selection	Recipe Input
Compos (xa_)	Al(OH)3 CaCO3	1 xa_ Aqua 50 g
DComp (xd_)	Al2O3 CaO	2 xa_ C3A 5 g
IComp (bi_)	Aqua CaSO4	3 xa_ CaO 2.5 g
Phase (xp_)	C12A7 CaSO4_05H2O	4 xa_ CaSO4 2.52 g
Kin.lower (dll_)	C3A Gypsum	5 xa_ O2 0.1 g
Kin.upper (dul_)	C4A3s H2	
G0 shift (gEx_)	CA H2S	
Other Inputs	CA2 H2SO4	
	CH4 O2	
	CO2 SO3	
	Ca(OH)2	

Input quantities of Compos(itions) contributing to B\_ vector

**A bit of O<sub>2</sub> to guarantee oxidizing conditions**

Learn more Print **OK** Cancel

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

Check system definition



we keep carbonate in this example

=> adds a very small amount of C ( $10^{-9}$  M), has a negligible effect

C3A:G:C3A-Cs:0:0:1:25:0:

Missing ICs: **CONFLICT WARNING!**

☒ C

Mole amounts of some Independent Components (IC) are missing in the calculated bulk composition vector ( $B_{[i]} < Pa_{DB}$ ):

POSSIBLE ACTIONS:

- \* EXCLUDE ALL these ICs together with DCs that contain them and some Phases made of those DCs;
- \* RETAIN ALL missing ICs by inserting a default mole amount (below) into bi\_ vector cells;
- \* CHECK some boxes to keep these ICs in the system by inserting a default mole amount into bi\_ ; unchecked ICs will be turned off together with all DCs that contain them.

Default amount, mol (editable): **1e-09**

EXCLUDE ALL RETAIN ALL CHECK/OK

Learn more... Cancel

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## GEMS interface

2 equivalent input options    Recipe wizard (previous page)    Detailed input recipe

Empa  
Materials Science and Technology

Brings you always back to this screen

all main cement hydrates relevant to the system  
 $\text{CaO}$ - $\text{Al}_2\text{O}_3$ - $\text{CaSO}_4$ - $\text{CaCO}_3$ - $\text{H}_2\text{O}$  included

System: T = 298.15 K; P = 1.00 bar; V = 0 L; Aqueous: built-in EDH(H); pH = 0.000; pe = 0.000; IS = 0.000 m

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## Hydration of $\text{C}_3\text{A} + \text{CaO} + \text{CaSO}_4$ – system creation (input)

Empa  
Materials Science and Technology

On/off switch for phases

I = ideal solid solution

Number of components  
 1: pure phase  
 $\geq 2$ : solid solutions

J = junior end-member  
 M = major end-member of solid solution

SO<sub>4</sub>-Aft solid solution 30-32 H<sub>2</sub>O

2 Aft solid solutions containing sulfate+carbonate

SO<sub>4</sub>-Aft with less water (metaettringite; for low water content)

Monosulfate with different water content (relevant for low w/c)

System: T = 298.15 K; P = 1.00 bar; V = 0 L; Aqueous: built-in Davies; pH = 0.000; pe = 0.000; IS = 0.000 m

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## Hydration of $C_3A$ + $CaO$ + $CaSO_4$ – 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)

Compos DComp Phase IComp Surfaces Config 30/01/2018, 15:19

C3A + CaSO4  
Description of experiment

Masses	0	1	1	1	0	0
Volumes	1	1	Procs	0	0	0
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	+	C12A7	MIN Mayenite_1M	g		0
4	+	C3A	MIN Tricalcium_alumina...	g		5
5	+	C4A3s	MIN Yeelimite_1M	g		0
6	+	CA	MIN Calcium_aluminate...	g		0
7	+	CA2	MIN Calcium_dialuminat...	g		0
8	+	CH4	GA Methane_1M	g		0
9	+	CO2	GA Carbon-dioxide_1M	g		0
10	+	Ca (OH)2	MIN Calcium-hydroxide...	g		0
11	+	CaCO3	MIN Calcium-carbonate...	g		0
12	+	CaO	MIN Calcium-oxide_1M	g		2.5
13	+	CaSO4	MIN Calcium-sulfate_1M	g		2.52
14	+	CaSO4_05H2O	MIN hemihydrate_1M	g		0
15	+	Gypsum	MIN Ca-sulfate-2H2O-1M	g		0
16	+	H2	GA Hydrogen_1M	g		0
17	+	H2S	GA Hydrogen-sulfide_1...	g		0

Detailed input recipe

Input generated before  
by the input wizard  
=> 2 equivalent options  
to input data

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## Hydration of $C_3A$ + $CaO$ + $CaSO_4$ – 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)

Compos DComp Phase IComp Surfaces Config 24/04/2019, 16:

Summary of input in mol

IC	ICvp	B	bi
0	+	Al e Aluminum_	0.037010516 M
1	+	C e Carbon_	1e-009 M
2	+	Ca e Calcium_	0.11860702 M
3	+	H h Hydrogen_	5.5508373 M
4	+	O o Oxygen_	3.0113217 M
5	+	S e Sulfur_	0.018510003 M
6	+	Zz z Electric_cha...	0 M

Al/SO<sub>3</sub> = 2  
A/S = Al<sub>2</sub>O<sub>3</sub>/SO<sub>3</sub> = 1

Calculated during check

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## Hydration of $C_3A + CaO + CaSO_4$ – 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

Convergence problem can occur

- 1) Can be solved in «projects» by setting smoothing parameter to 0.01
- 2) Remove solid solution with only 1 solid

### Convergence problem - workaround

Tolerances and controls: GEMSGUI v.3.7.0 and GEMS3K v.3.7.0											
Pa_SPP	Pa_DK	1e-005	Pa_IIM	7000	Pa_ILG	30000	Pa_AG	1	Pa_DGC	0.01	
Pa_DHB	1e-013	Pa_DFY	1e-005	1e-005	1e-005	1e-005	1e-005	1e-005	1e-005	1e-006	
Pa_DB	1e-017	Pa_DS	1e-020	Pa_XMI	1e-013	1e-013	1e-033	1e-020	1e-005		
Pa_EPS	1e-010	0.001	Pa_GAN	1	1000	0.001	Pa_DG	1000			
Pa_DPV	130	1	0	Pa_DF	0.01	0.01	Pa_DNS	12.05			
Pa_PE	1	Pa_PC	2	Pa_PRD	2	-5	1	Pa_DKI	1e-010		

2. Coverage tolerance parameter:  
use higher value, e.g. 1e-004,  
maximum seems to be 5e-003

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

1. Smoothing parameter:  
use low positive value, e.g. 0.01  
=> 0.01 works

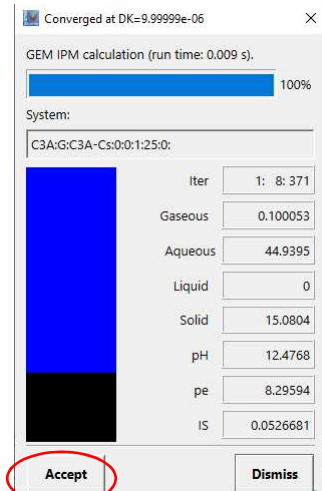
**Do not touch the other values !!!**

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## Hydration of $C_3A$ + $CaO$ + $CaSO_4$ – 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 $C_3A$ + $CaO$ + $CaSO_4$ – results

GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [EqStat: Single Thermodynamic System ...]

Modules Record Data Calculate View Print Window Help

SingleSystem

C3A:G:C3A-Cs:0:0:1:25:0

Input: System Definition Results: Equilibrium State

Phase/species	L	T	Amount (mol)	logSI/Activity	Concentration
aq_gen	29	a	2.4932653	-8.615e-09	
gas_gen	6	g	0.0031708121	-1.23e-09	
ettringite	2	s	0.00091958053	1.187e-06	
SO4_OH_Afm	2	s	0.008792363	-6.154e-08	
OH_SO4_Afm	2	s	0.008792363	-6.154e-08	
SO4_CO3_Aft	2	s	0	-0.03101	
CO3_SO4_Aft	2	s	0	-0.03101	
Al(OH)3am	1	s	0	-3.174	
Al(OH)3mic	1	s	0	-2.264	
Gibbsite	1	s	0	-1.811	
Graphite	1	s	0	-84.68	
Mayenite	1	s	0	-130.4	
Aluminate	1	s	0	-36.48	
CA	1	s	0	-11.04	
CA2	1	s	0	-15.19	
C2AH75	1	s	0	-2.469	
C3AH6	1	s	0	-0.9693	
C4AH11	1	s	0	-3.156	
C4AH13	1	s	0	-1.422	
C4AH19	1	s	0	-1.222	
CAH10	1	s	0	-3.47	
C4AsH105	1	s	0	-1.423	
C4AsH12	1	s	0	-0.07732	
C4AsH14	1	s	0	-0.05177	

System: T = 298.15 K; P = 1.00 bar; V = 0.131 L; Aqueous: built-in EDH(H); pH = 12.477; pe = 8.296; IS = 0.053 m

Calculated single system

Calculations

## Hydration of C<sub>3</sub>A + CaO + CaSO<sub>4</sub> – results

GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [EqStat: Single Thermody]

Name of single system

2.5 mol aqueous phase (water + dissolved ions)

0.0032 mol gaseous phase

Solid products:

0.0009 mol ettringite

0.0176 mol monosulfate

0.0418 mol portlandite

solid solution between monosulfate (C<sub>4</sub>AsH<sub>12</sub>) and C<sub>4</sub>AH<sub>13</sub>

System: T = 298.15 K; P = 1.00 bar; V = 0.131 L; Aqueous: built-in EDH(H); pH

## Hydration of C<sub>3</sub>A + CaO + CaSO<sub>4</sub> – results

### Solid solutions



Phase/species	L	T	Amount (mol)	logSI/Activity	Concentration	Activity coeff.
aq_gen	29	a	2.49326	-3.448e-09		
gas_gen	6	g	0.003171698	-1.957e-09		
ettringite	2	s	0.0009199661	4.729e-07		
ettringite	I	I	0.0007356808	0.799683	0.7996826	1
ettringite30	I	I	0.0001842852	0.200318	0.2003174	1
SO4 OH AFm	2	s	0.00879217	-2.421e-08		
C4AH13	J	J	0.0009172862	0.037881	0.1043299	0.3630883
monosulphate12	M	M	0.007874883	0.836829	0.8956701	0.9343053
OH SO4 AFm	2	s	0.00879217	-2.421e-08		
C4AH13	M	M	0.0009172862	0.037881	0.1043299	0.3630883
monosulphate12	J	J	0.007874883	0.836829	0.8956701	0.9343053
SO4 CO3 AFt	2	s	0	-0.031		
tricarboalu03	J	J	0	0.00247516	0	1
ettringite03_ss	M	M	0	0.92992	0	1
CO3 SO4 AFt	2	s	0	-0.031		
tricarboalu03	M	M	0	0.00247516	0	1
ettringite03_ss	J	J	0	0.92992	0	1
Al(OH)3am	1	s	0	-3.174		
Al(OH)3mic	1	s	0	-2.264		
Gibbsite	1	s	0	-1.811		

ideal solid solution:

80 mol-% ettringite-32H<sub>2</sub>O

20 mol-% ettringite-30 H<sub>2</sub>O

Non ideal solid solution:

10 mol-% C<sub>4</sub>AH<sub>13</sub>

90 mol-% C<sub>4</sub>AsH<sub>12</sub>

Incomplete solid solution (hardly any CO<sub>3</sub> endmember;  
normally not stable, can be deactivated:

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

Input: System Definition													
Results: Equilibrium State													
Phase/species	L	T	On/UC	Add to BC	UG	G0 corr.	UK	Lower_KC	Upper_KC	KC type			
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						
tricarboalu03		J	-	M	0	J	0	M	0	1000000	B		
ettringite03_ss		M	-	M	0	J	0	M	0	1000000	B		
CO3_SO4_AfT	2	s	+	g	0	J	0						
tricarboalu03		M	-	M	0	J	0	M	0	1000000	B		
ettringite03_ss		M	-	M	0	J	0	M	0	1000000	B		
Al(OH)3am	1	s	+	g	0	J	0						
Al(OH)3mic	1	s	+	g	0	J	0						
Gibbsite	1	s	+	g	0	J	0						
Graphite	1	s	+	g	0	J	0						

As we have very little carbonate in the system in the first calculation we may switch off the carbonate-sulfate AfT solid solutions (In the input page)

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## Hydration of $C_3A$ + $CaO$ + $CaSO_4$ – results

EM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [EqStat]: Single Thermodynamic System in Project C3A ...

SingleSystem

Input: System Definition Results: Equilibrium State

Phase/species	L	T	Amount (mol)	logSI/Activity	Concentration	Acti
aq_gen	29	a	2.49326	-3.488e-09		
gas_gen	6	g	0.003171698	-1.93e-09		
ettringite	2	s	0.0009199661	4.729e-07		
SO4_OH_AfM	2	s	0.00879217	-2.421e-08		
OH_SO4_AfM	2	s	0.00879217	-2.421e-08		
SO4_CO3_AfT	2	s	0	-0.031		
CO3_SO4_AfT	2	s	0	-0.031		
Al(OH)3am	1	s	0	-3.174		
Al(OH)3mic	1	s	0	-2.264		
Gibbsite	1	s	0	-1.811		
Graphite	1	s	0	-84.68		
Mayenite	1	s	0	-92.94		
Aluminate	1	s	0	-36.48		
CA	1	s	0	-11.04		
CA2	1	s	0	-15.19		
C2AH75	1	s	0	-2.469		
C3AH6	1	s	0	-0.9692		
C4AH11	1	s	0	-3.156		
C4AH13	1	s	0	-1.422		
C4AH19	1	s	0	-1.221		

Title: C3A +CaSO4

Comment: Please, enter here a comment about the purpose of this system definition

System: T = 298.15 K; P = 1.00 bar; V = 0.131 L; Aqueous: built-in EDH(H); pH = 12.477; pe = 8.296; IS = 0.053 m

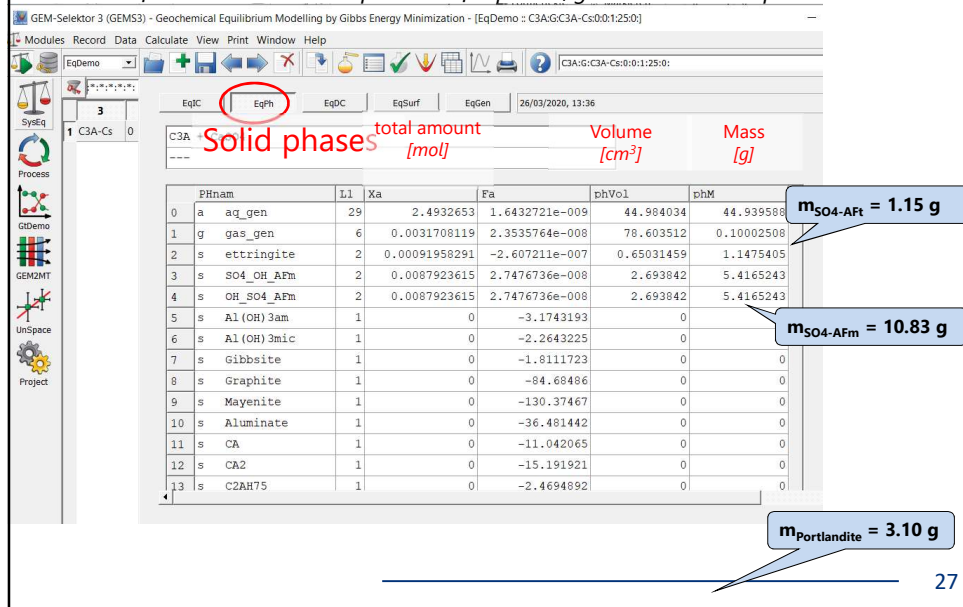
View detailed results

General information: pH, ionic strength, redox, ...

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## Hydration of $C_3A + CaO + CaSO_4$ – results

Detailed information about composition of aqueous, gaseous and solid phases

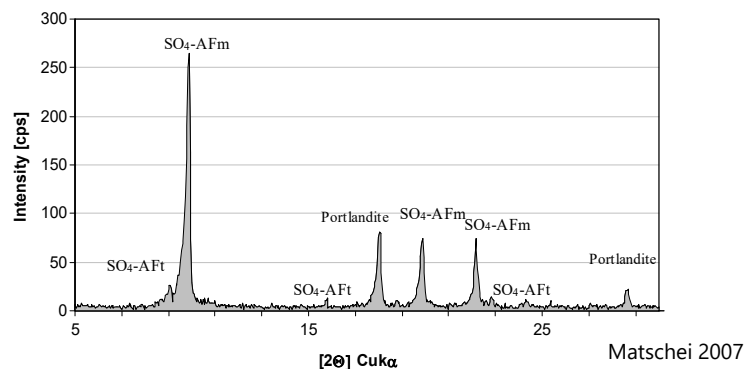


## Hydration of $C_3A + CaO + CaSO_4$ – results



Comparison to experiments:

Hydration of  $C_3A$  at  $SO_3/Al_2O_3 = 1$ , cured 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.

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## Hydration of $C_3A + CaO + CaSO_4$ – results

### Composition of aqueous phase

EqIC EqPh EqDC EqSurf EqGen 09/06/2023, 16:21

C3A +CaSO4  
Please, enter here a comment about the purpose of this system de...

	ICnam	b	Cb	u	lgm t	m t	ICnam
0	Al e	0.03701052	1.387779e-17	-324.928	-4.372027	4.245927e-05	Al e
1	C e	1e-09	3.797537e-26	-194.9822	-7.651954	2.22867e-08	C e
2	Ca e	0.118607	-2.081668e-17	-266.1541	-1.690528	0.02039259	Ca e
3	H h	5.550837	-2.872702e-15	-47.8309	-1.390111	0.0407276	H h
4	O o	3.011322	1.249001e-16	-0.01647609	-1.36302	0.04334909	O o
5	S e	0.01851	6.938894e-18	-275.1372	-5.122594	7.540599e-06	S e
6	Zz z	0	-4.012578e-19	19.1021	0	-2.480751e-18	Zz z

Output: total  
molalities in aqueous  
phase  
(mol/kg  $H_2O$ )

total mol in  
system (input)

$\log_{10}$  of total  
molalities

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## Tutorial – single systems: hydration of $C_3A$

### Hydration of $C_3A$

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

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

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