



1.2 Tutorial 2

Single system - Hydration of OPC

F. Winnefeld, T. Matschei, B. Lothenbach

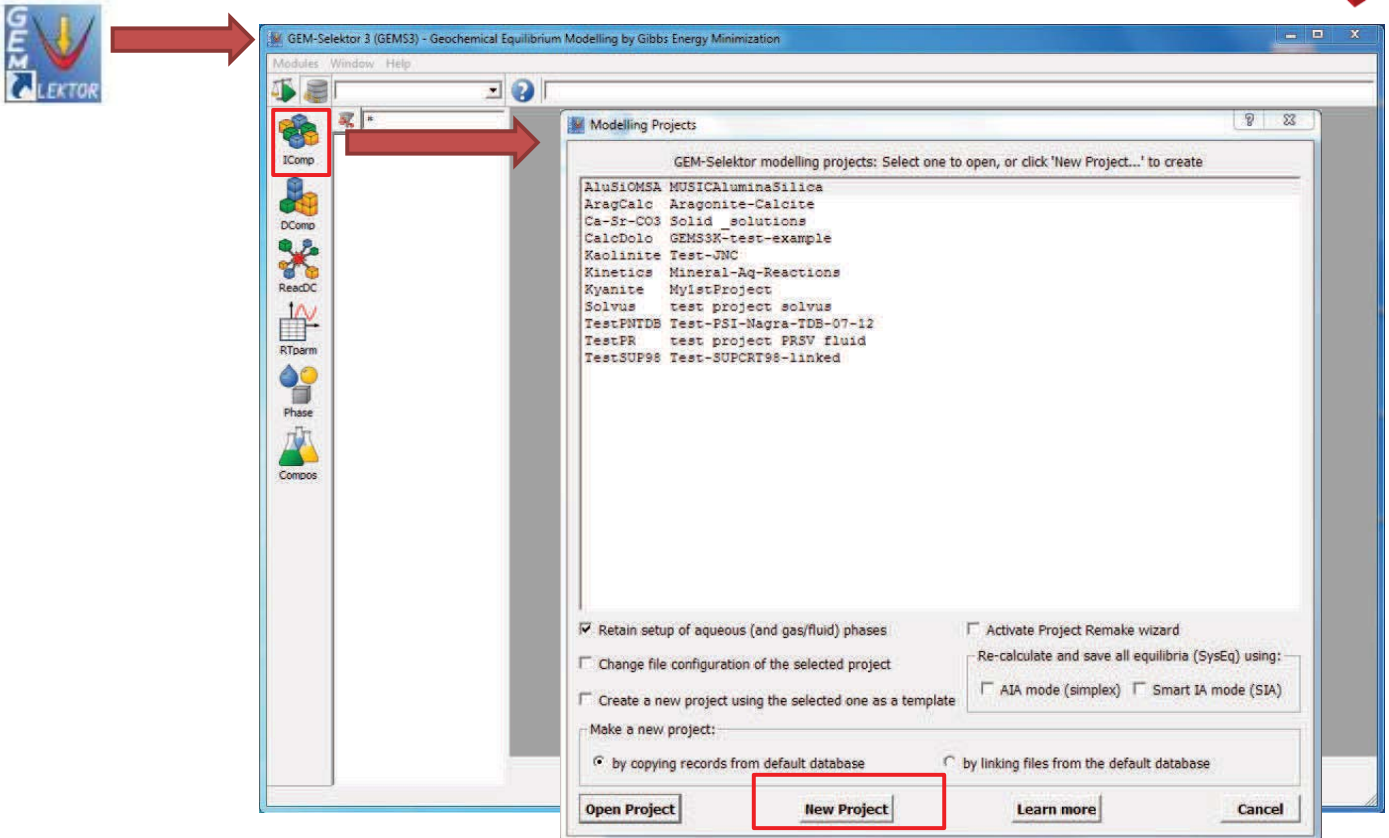
GEMS V.3.2 2482.930, CEMDATA14 (version April 14, 2014)

Tutorial 2 – OPC hydration

Hydration of a model cement composition

- The example will show the principle possibility to apply GEMS to simulate cement hydration.
- A simplified cement composition is used and 100% hydration assumed (other assumptions are possible).
- The impact of limestone on the predicted phase assemblage will be shown.

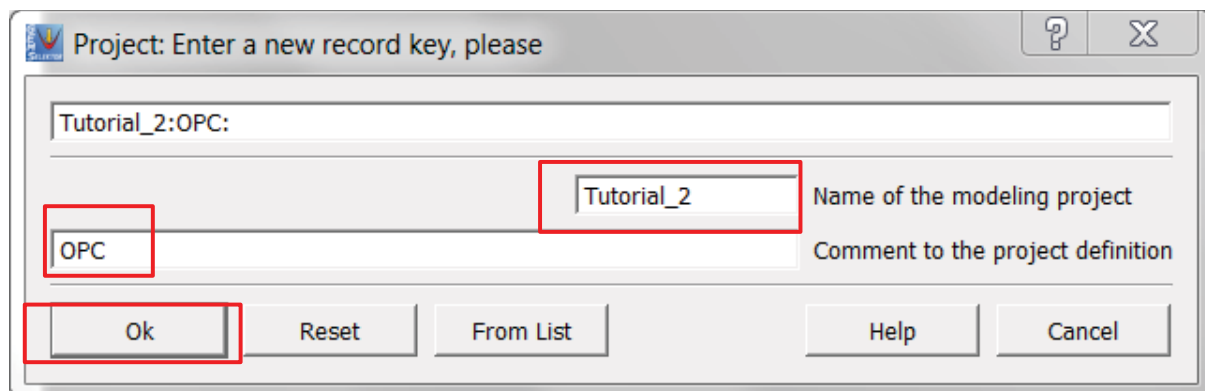
Hydration of OPC – project setup



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3

Hydration of OPC – project setup

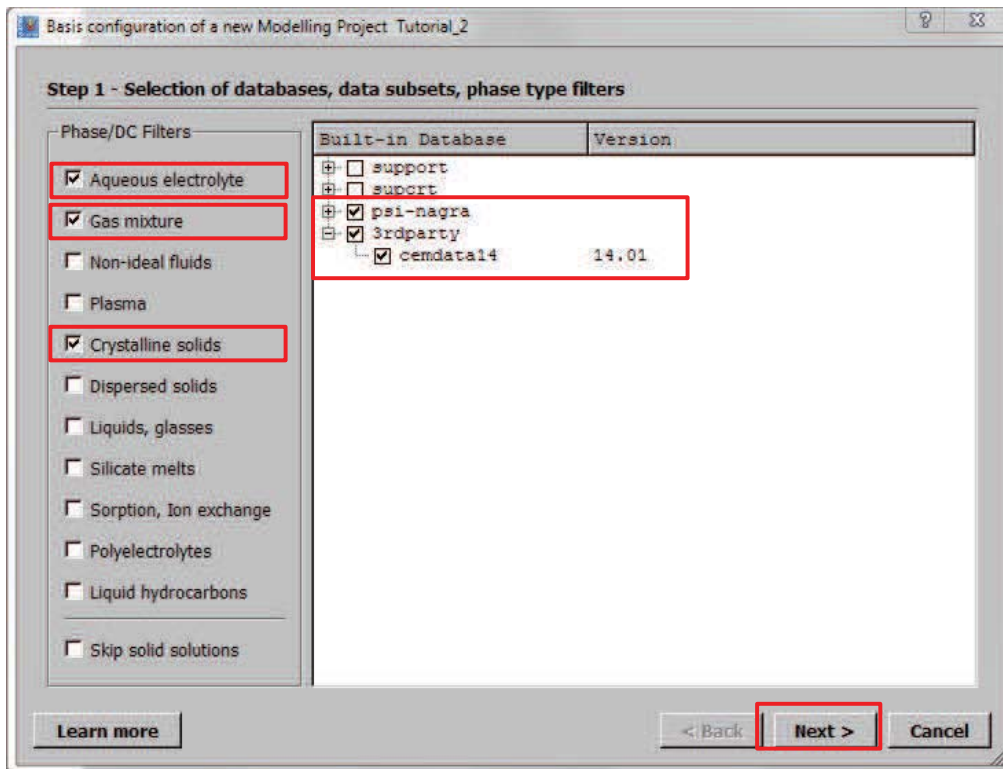


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4

Hydration of OPC – project setup

Select CEMDATA14 (3rd party data base)

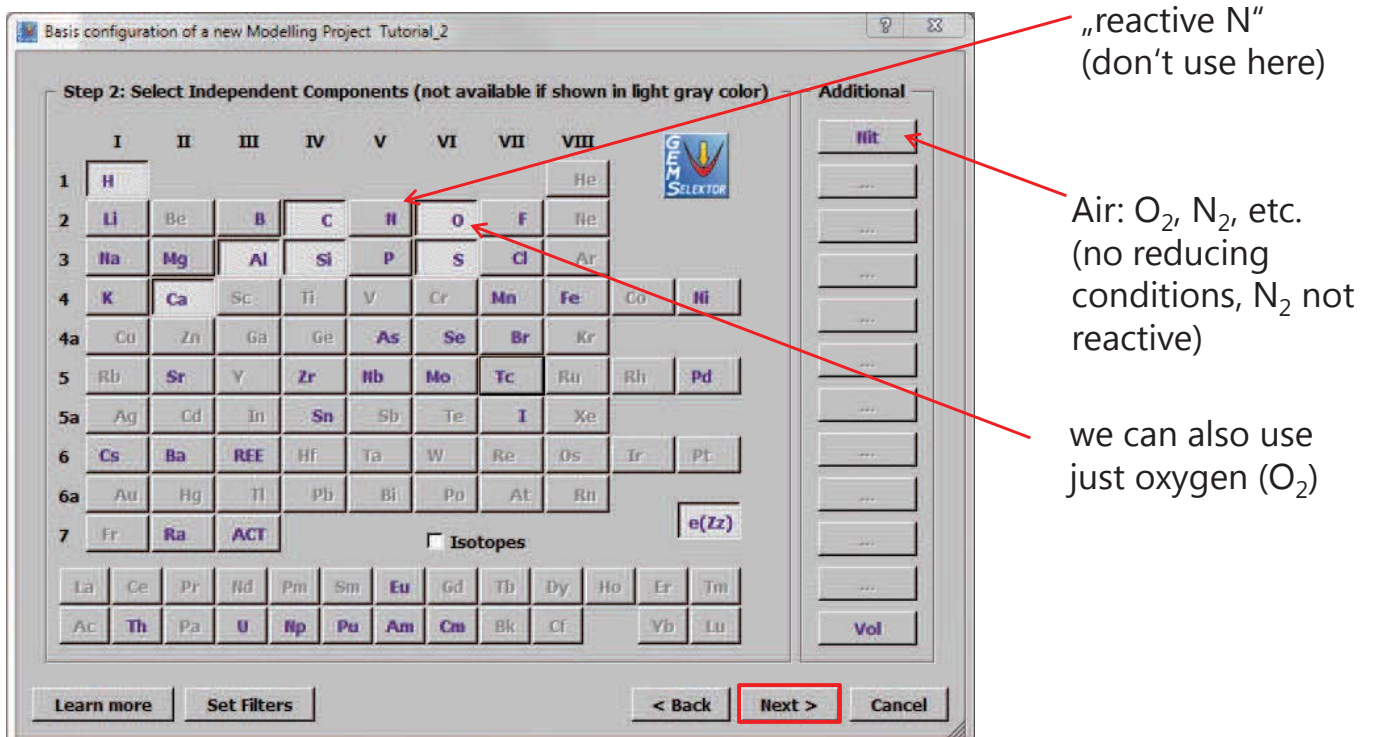


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5

Hydration of OPC – project setup

Modified project setup including elements necessary to model cement hydration
(as we use a model cement we neglect Na, K, Mg and Fe for the moment)



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6

Select model for calculation of the aqueous phase

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7

Hydration of OPC – project setup

We leave temperature at 25°C

Press OK again to leave the recipe wizard. We will use it later, but first some more explanations and definitions are needed.

Hydration of OPC – system creation

all main cement hydrates included in this project

System file is now created

The next step is to formulate the experiment we want to simulate

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

9

Hydration of OPC – system creation

On/off switch for phases

As we have no carbonate in the system in the first calculation we switch the carbonate-sulfate AFt solid solutions off

2 AFt solid solutions containing sulfate+carbonate

SO₄-Aft ideal composition

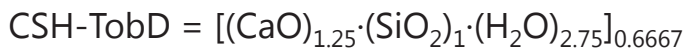
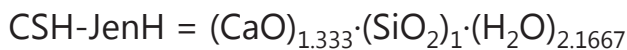
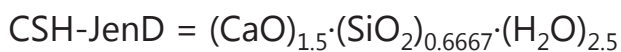
Number of components
1: pure phase
2: solid solutions

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

10

C-S-H is modeled as a solid solution of 4 different species:

Input: System Definition Results: Equilibrium State											
Phase/species	L	Type	On/off	UC	Add to BC	UG	G0 corr.	UK	Lower_KC	Upper_KC	KC
aq_gen	37	a	+	g	0	J	0				
gas_gen	5	g	+	g	0	J	0				
CSHQ	4	s	+	g	0	J	0				
CSH-JenD		I	+	M	0	J	0	M	0	1e+006	B
CSH-JenH		I	+	M	0	J	0	M	0	1e+006	B
CSH-TobD		I	+	M	0	J	0	M	0	1e+006	B
CSH-TobH		I	+	M	0	J	0	M	0	1e+006	B



For more detailed information see: Kulik D.A., Cem. Concr. Res. 41 (2011), 477.

Hydration of OPC – system creation

Experimental problem part 1:

Hydration of a model cement

CaO 70.6 wt.-%

SiO₂ 22.0 wt.-%

Al₂O₃ 4.5 wt.-%

SO₃ 2.9 wt.-%

w/c 0.50



Bogue calculation

C₃S 81.37 wt.-%

C₂S 1.70 wt.-%

C₃A 11.93 wt.-%

CaSO₄ 5.00 wt.-%

Assumption: 100% hydration

React 100 g of the model cement with 50 g water (add 1 g O₂)



> Recipe >



> Equilibrium speciation

Hydration of OPC – system creation

Experimental conditions: React 100 g OPC with 50 g water (add 1 g O₂)

Use recipe wizard



Enter phase composition

Property	Name	Quantity	Units
1 xa_	O2	1	g
2 xa_	Aqua	50	g
3 xa_	C3S	81.37	g
4 xa_	C2S	1.7	g
5 xa_	C3A	11.93	g
6 xa_	CaSO4	5	g

Alternatively you could enter the oxide composition

Hydration of OPC – system creation

Experimental conditions: React 100 g OPC with 50 g water (add 1 g O₂)

Check system definition



Missing ICs

CONFLICT WARNING!

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

POSSIBLE ACTIONS:

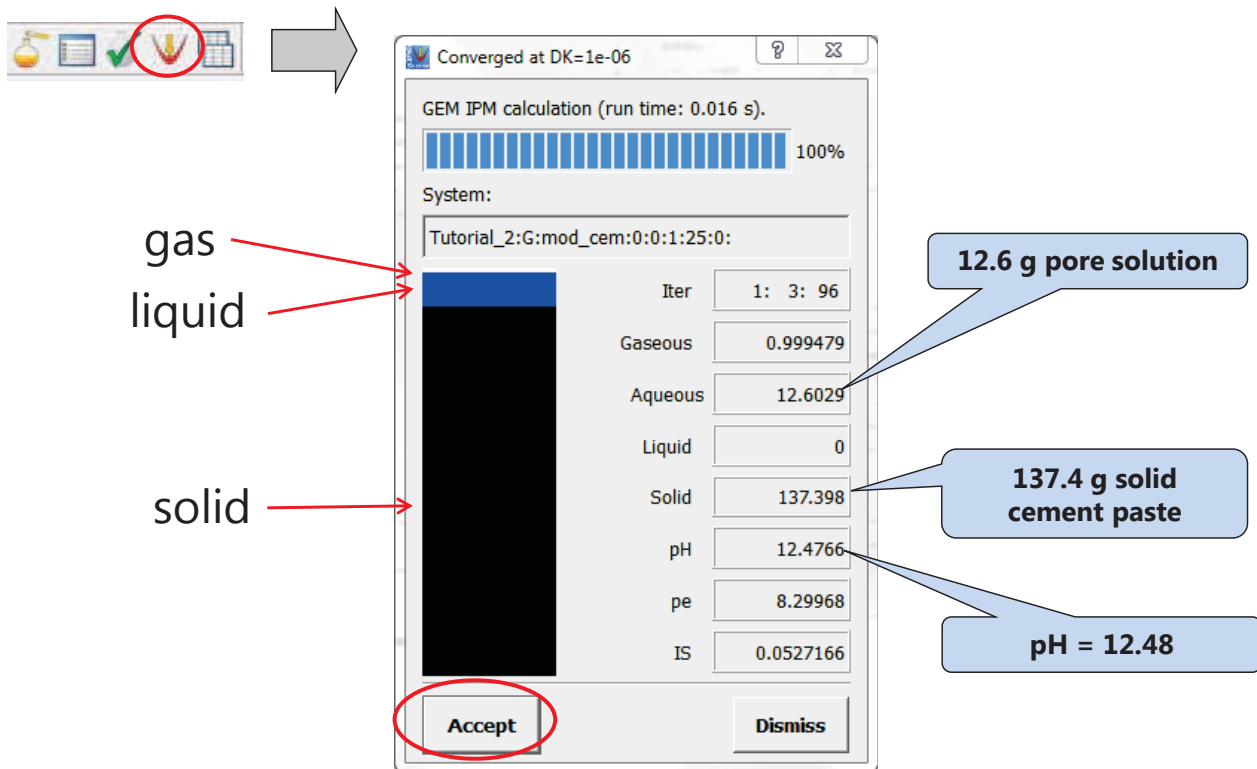
- * EXCLUDE ALL these ICs together with DCs that contain them and some Phases made of those DCs;
- * RETAIN ALL missing ICs by inserting a default mole amount (below) into bi_vector cells;
- * CHECK some boxes to keep these ICs in the system by inserting a default mole amount into bi_vector; unchecked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

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

We exclude carbonate in this example

Hydration of OPC – calculation of equilibrium

Experimental conditions: React 100 g OPC with 50 g water (add 1 g O₂)



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15

Hydration of OPC – results

Predicted stable phase assemblage

Input: System Definition		Results: Equilibrium State					
Phase/species	L	T	Amount (mol)	logSI/Activity	Concentration	Activity coeff.	
aq_gen	31	a	0.69920713	-7.238e-10			
gas_gen	3	g	0.031234875	4.938e-12			
CSHQ	4	s	0.48097803	1.812e-09			
CSH-JenD	I		0.19647065	0.408482	0.40848155	1	
CSH-JenH	I		0.13034662	0.271003	0.27100327	1	
CSH-TobD	I		0.14771528	0.307114	0.30711441	1	
CSH-TobH	I		0.0064454787	0.0134008	0.013400776	1	
SO4_OH_AfM	2	s	0.044152586	4.151e-09			
C4AH13	J		0.0074266998	0.109027	0.16820532	0.6481e002	
monosulphate	M		0.036725886	0.709781	0.83179468	0.85331218	
OH_SO4_AfM	2	s	3.563024e-007	4.151e-09			
Al(OH)3mic	1	s	0	-1.91			
Gibbsite	1	s	0	-1.457			
Kaolinite	1	s	0	-12.41			
Belite	1	s	0	-1.754			
Aluminate	1	s	0	-35.77			
Alite	1	s	0	-13.79			
C2AH7S	1	s	0	-1.762			
C3AH6	1	s	0	-0.2615			
C4AH13	1	s	0	-0.9625			
CAH10	1	s	0	-2.762			
C4AsH12	1	s	0	-0.1489			
C2ASH8	1	s	0	-0.4563			
ettringite	1	s	0	-1.805			
lime	1	s	0	-9.776			
Portlandite	1	s	0.48533506	-1.575e-09			
Anhydrite	1	s	0	-4.289			
Gypsum	1	s	0	-4.066			
hemihydrate	1	s	0	-5.055			
Sulphur	1	s	0	-120.3			
Quartz	1	s	0	-5.041			
Silica-amorph	1	s	0	-6.073			

CSH-JenD = (CaO)_{1.5}·(SiO₂)_{0.6667}·(H₂O)_{2.5}
 CSH-JenH = (CaO)_{1.333}·(SiO₂)₁·(H₂O)_{2.1667}
 CSH-TobD = [(CaO)_{1.25}·(SiO₂)₁·(H₂O)_{2.75}]_{0.6667}
 CSH-TobH = (CaO)_{0.6667}·(SiO₂)₁·(H₂O)_{1.5}

C-S-H solid solution
1.63 CaO · SiO₂ · 2.88 H₂O

SO₄-AFm solid solution
0.83 mol-% SO₄-AFm
0.17 mol-% OH-AFm

=> Ca₄Al₂(OH)_{12.34}(SO₄)_{0.83}·6H₂O

System: T = 298.15 K; P = 1.00 bar; V = 0.8495 L; Aqueous: built-in EDH(H); pH = 12.477; pe = 8.300; IS = 0.053 m

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16

Hydration of OPC – results

Assessment of calculations

Predicted phase assemblage (hydr. cement paste):

- C-S-H (solid solution)
- SO₄-AFm (solid solution)
- Portlandite

Total solid volume:
33.13+13.38+16.05
= 62.56 cm³

PHnam	Li	Xa	Fa	phVol	PM
0 a aq_gen	31			12.61208	12.602856
1 g gas_gen	3			774.3035	0.99947852
2 s CSHQ	4			33.130544	74.412635
3 s SO4_OH_AFm	3			13.384168	27.025028
4 s OH_SO4_AFm	3			0.00010800812	0.002180877
5 s SO4_CO3_AFm	1			0	0
6 s CO3_SO4_AFm	1			0	0
7 s Al(OH)3mic	1			0	0
8 s Gibbsite	1			0	0
9 s Kaolinite	1			0	0
10 s Belite	1			0	0
11 s Aluminite	1			0	0
12 s Alite	1			0	0
13 s C2AH75	1			0	0
14 s C3AH6	1			0	0
15 s C4AH13	1			0	0
16 s CAH10	1			0	0
17 s C4AsH12	1			0	0
18 s C2ASH8	1			0	0
19 s ettringite	1			0	0
20 s lime	1			0	0
21 s Portlandite	1			16.045177	35.959785
22 s Anhydrite	1			0	0
23 s Gypsum	1			0	0

Hydration of OPC – results

Assessment of calculations

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

Aqueous phase composition (total molalities)

DCnam	x	lga	gamma	my
0 Al(SO4)+	0	-33.724304	0.82138317	0
1 Al(SO4)2-	0	-38.217918	0.82138317	0
2 Al+3	6.1654384e-033	-31.130816	0.15101216	4.8997336e-031
3 AlO+	2.5912107e-019	-16.771743	0.82138317	2.0592602e-017
4 AlO2-	1.2062931e-006	-4.1037929	0.82138317	9.5865278e-005
5 AlO2H0	9.1118271e-013	-10.133699	1.0150502	7.2412572e-011
6 AlOH+2	7.0715173e-026	-23.611558	0.43523178	5.6198032e-024
7 AlHSiO3+2	4.0727468e-032	-29.851184	0.43523178	3.2366513e-030
8 AlSiO5-3	2.3618467e-012	-10.547528	0.15101216	1.8769825e-010
9 Ca(SO4)0	5.5818969e-009	-6.3465221	1.0150502	4.4359875e-007
10 Ca+2	0.00020326399	-2.1530105	0.43523178	0.016153586
11 CaOH+	5.353897e-005	-2.4565757	0.82138317	0.0042547938
12 Ca(HSiO3)+	1.2939784e-009	-7.0733187	0.82138317	1.0283372e-007
13 CaSiO30	3.6858892e-007	-4.5267617	1.0150502	2.9292118e-005
14 HSiO3-	1.161123e-008	-6.1203675	0.82138317	9.227557e-007
15 Si4O10-4	1.0549231e-022	-21.541151	0.034309925	8.3835758e-021
16 SiO20	2.0252543e-011	-8.7868244	1.0150502	1.6094892e-009
17 SiO3-2	3.0712829e-009	-6.9737511	0.43523178	2.4407783e-007
18 H20	0	-44.658521	1.0150502	0
19 O20	1.629693e-005	-2.8811982	1.0150502	0.0012951328
20 SiO3-2	0	-166.13589	0.43523178	0
21 HSO3-	0	-56.699599	0.82138317	0
22 SO3-2	0	-51.442988	0.43523178	0
23 HSO4-	1.5950289e-019	-16.982477	0.82138317	1.2675849e-017
24 SO4-2	9.2783654e-009	-6.4935994	0.43523178	7.3736068e-007

Hydration of a model cement composition – summary

- possibility to apply GEMS to simulate cement hydration with metastability constraints (e.g. siliceous hydrogarnet suppressed – see appendix)
- additional iron and alkalis present in real “OPC”.
Thus to improve accuracy of the calculation one has to consider:
 - Additional iron containing phases
(Moeschner et al. Geoch. Cosm. Acta 2007, Dilnesa et al. CCR 2014a+b included in the cement database)
 - Sorption of alkalis on C-S-H
(experimental data: Hong and Glasser CCR 1999)
 - Sorption of sulfate on C-S-H
(experimental data: Divet et al. CCR 1998, Barbarulo et al. 2002, Skapa in progress 2008)
 - Substitution of alumina (Richardson CCR 1994, Chen et al. ICCS 2007, Pardal et al. CCR 2009 & Inorg. Chem. 2012)
- kinetics can be taken into account as function of clinker reactivity over time
(e.g. Lothenbach et al. CCR 2006 & 2008)

Hydration of OPC with limestone – system creation

Experimental problem part 2:

Blending of the model cement with 5% limestone

C_3S	81.37 wt.-%	$\xrightarrow{+ 5\% CaCO_3}$	C_3S	77.30 wt.-%
C_2S	1.70 wt.-%		C_2S	1.62 wt.-%
C_3A	11.93 wt.-%		C_3A	11.33 wt.-%
$CaSO_4$	5.00 wt.-%		$CaSO_4$	4.75 wt.-%
			$CaCO_3$	5.00 wt.-%
w/c	0.50			

Assumption: 100% hydration



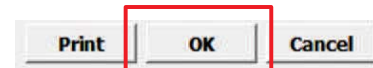
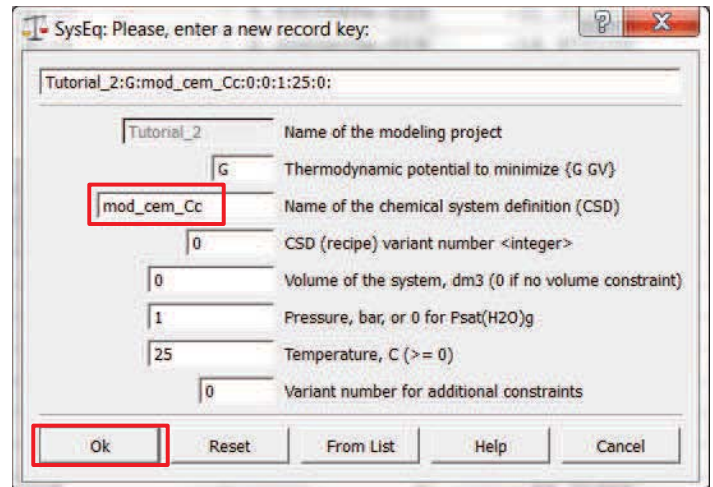
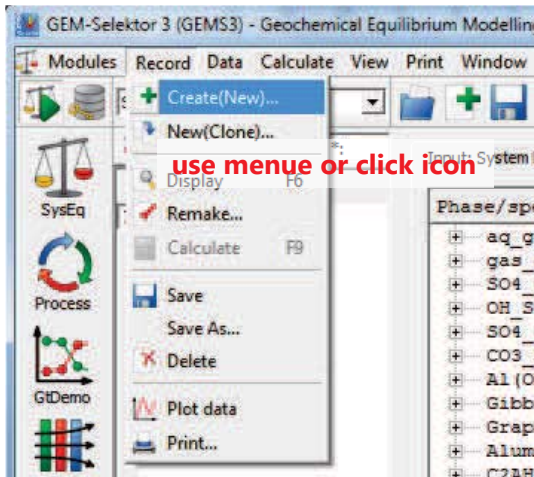
Hydration of OPC with limestone – system creation



Limestone addition:

repeat calculations with 95% OPC blended with 5% CaCO_3

Create new system



Press OK again to leave the recipe wizard

Hydration of OPC with limestone – system creation



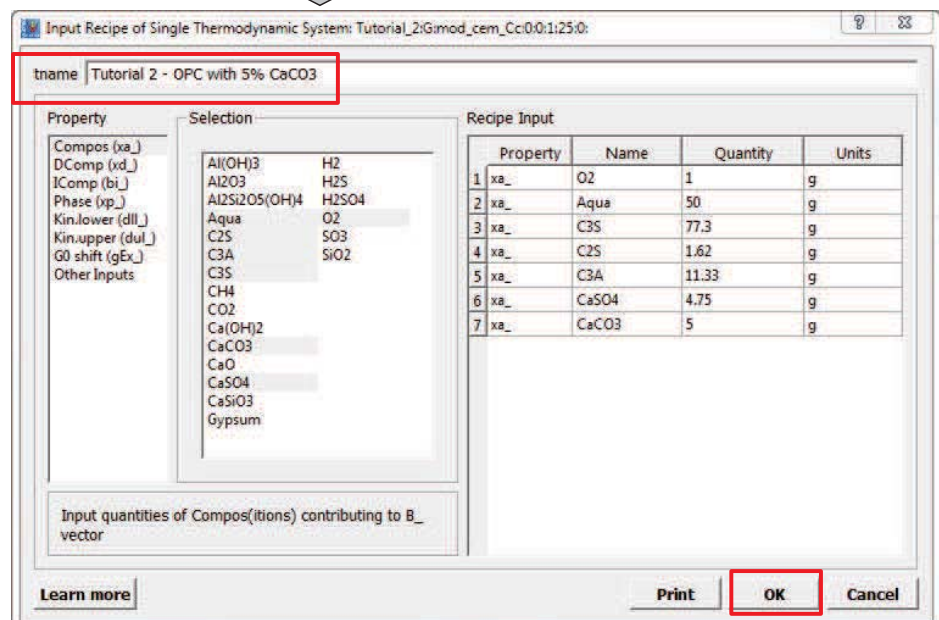
Experimental conditions: React 100 g OPC blended with 5% CaCO_3 with 50 g water

(add 1 g O_2)

Use recipe wizard



Enter phase composition



Hydration of OPC with limestone - results

Experimental conditions: React 100 g OPC blended with 5% CaCO₃ with 50 g water

(add 1 g O₂)

Input: System Definition		Results: Equilibrium State			
Phase/species	L	T	Amount (mol)	logSI/Activity	Concentration
a aq_gen	37	a	0.57495244	1.582e-10	
g gas_gen	5	g	0.031237771	1.058e-11	
s CSHQ	4	s	0.45695871	1.132e-09	
CSH-JenD		I	0.18665924	0.408482	0.40848163
CSH-JenH		I	0.12383725	0.271003	0.27100314
CSH-TobD		I	0.14033863	0.307114	0.30711446
CSH-TobH		I	0.0061235984	0.0134008	0.01340077
s SO4_OH_AfM	2	s	0	-1	
s OH_SO4_AfM	2	s	0	-1	
s SO4_CO3_AfT	2	s	0.0064282692	-3.818e-11	
tricarboalu		J	0.00061333041	0.0116799	0.095411439
ettringite		M	0.0058149388	0.83947	0.90458856
s CO3_SO4_AfT	2	s	0.0064282692	-3.818e-11	
tricarboalu		M	0.00061333041	0.0116799	0.095411439
ettringite		J	0.0058149388	0.83947	0.90458856
s Al(OH)3mic	1	s	0	-3.024	
s Gibbsite	1	s	0	-2.571	
s Belite	1	s	0	-1.754	
s Aluminate	1	s	0	-38	
s Alite	1	s	0	-13.79	
s C2AH75	1	s	0	-3.99	
s C3AH6	1	s	0	-2.489	
s C4AH13	1	s	0	-3.19	
s C4AH19	1	s	0	-2.741	
s CAH10	1	s	0	-4.99	
s C4AsH12	1	s	0	-1.058	
s C2ASH8	1	s	0	-2.684	
s C4Ac0.5H12	1	s	0	-0.7002	
s C4AcH11	1	s	0.029076338	2.494e-10	
s ettringite	1	s	0	-0.07599	
s Aragonite	1	s	0	-0.1438	
s Calcite	1	s	0.01720015	8.41e-10	
s lime	1	s	0	-9.776	
s Portlandite	1	s	0	-2.97	
s Anhydrite	1	s	0	-2.747	

CSH-JenD = (CaO)_{1.5}·(SiO₂)_{0.6667}·(H₂O)_{2.5}
 CSH-JenH = (CaO)_{1.333}·(SiO₂)₁·(H₂O)_{2.1667}
 CSH-TobD = [(CaO)_{1.25}·(SiO₂)₁·(H₂O)_{2.75}]_{0.6667}
 CSH-TobH = (CaO)_{0.6667}·(SiO₂)₁·(H₂O)_{1.5}

C-S-H solid solution
1.63 CaO · SiO₂ · 2.88 H₂O

Aft solid solution:
0.905 mol SO₄-ettringite
0.095 mol CO₃-ettringite
=> Ca₆Al₂(OH)₁₂(SO₄)_{2.715}(CO₃)_{0.285} · 26H₂O

Monocarboaluminate
(CO₃-AFm)

=> Significant mineralogical changes due to limestone addition

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23

Hydration of OPC with limestone - results

Experimental conditions: React 100 g OPC blended with 5% CaCO₃ with 50 g water

(add 1 g O₂)

Predicted phase assemblage (hydrated cement paste):

- C-S-H (solid solution)
- SO₄-Aft (solid solution)
- CO₃-AFm
- Calcite
- Portlandite

Tutorial 2 - OPC with 5% CaCO3							
PHnam	L1	Xa	Fa	hVol	phM		
0 a aq_gen	37	0.57495244	1.5816157e-010	10.373392	10.363212		
1 g gas_gen				0.22e-011	774.37532	0.99957118	
2 s CSHQ				31.476055	70.696579		
3 s SO4_OH_AfM	2		0	-1	0		
4 s OH_SO4_AfM	2		0	-1	0		
5 s SO4_CO3_AfT	2		0	0.11	4.5102464	8.0018486	
6 s CO3_SO4_AfT	2	0.0064282692	-3.8178544e-011	0.11	4.5102464	8.0018486	
7 s Al(OH)3mic	1		0	-3.0243936	0	0	
8 s Gibbsite	1		0	-2.5712435	0	0	
9 s Belite	1		0	-1.7543913	0	0	
10 s Aluminate	1		0	-38.001866	0	0	
11 M calcite							
13 s C3A	1		0	-2.4894033	0	0	
14 s C4AH13	1		0	-3.1903608	0	0	
15 s C4AH19	1		0	-2.7411143	0	0	
16 s CAH10	1		0	-4.9897519	0	0	
17 s C4AsH12	1		0	-1.0579398	0	0	
18 s C2ASH8	1		0	0	0	0	
19 s C4Ac0.5H12	1		0	0	0	0	
20 s C4AcH11	1	0.029076338	2.4943526e-010	7.6167795	15.520400		
21 s ettringite			0.7599459	0	0	0	
22 s Aragonite			0.2216	0	0	0	
23 s Calcite	1	0.01720015	8.4095527e-010	0.63527032	1.7215114		
24 s lime	1		0	-9.7760819	0	0	
25 s Portlandite	1	0.46815706	-3.3746833e-011	15.477272	34.68702		

V_{pore sol.} = 10.37 cm³

m_{pore sol.} = 10.36 g

V_{C-S-H} = 31.48 cm³

V_{Aft(ss)} = 9.02 cm³

m_{C-S-H} = 70.70 g

m_{Aft(ss)} = 16.00 g

M_{calcite} = 1.72 g => 5.00-1.72 = **3.28 g** calcite had reacted

m_{CO3-AfM} = 16.53 g

V_{CO3-AfM} = 7.62 cm³

V_{calcite} = 0.64 cm³

m_{calcite} = 1.72 g

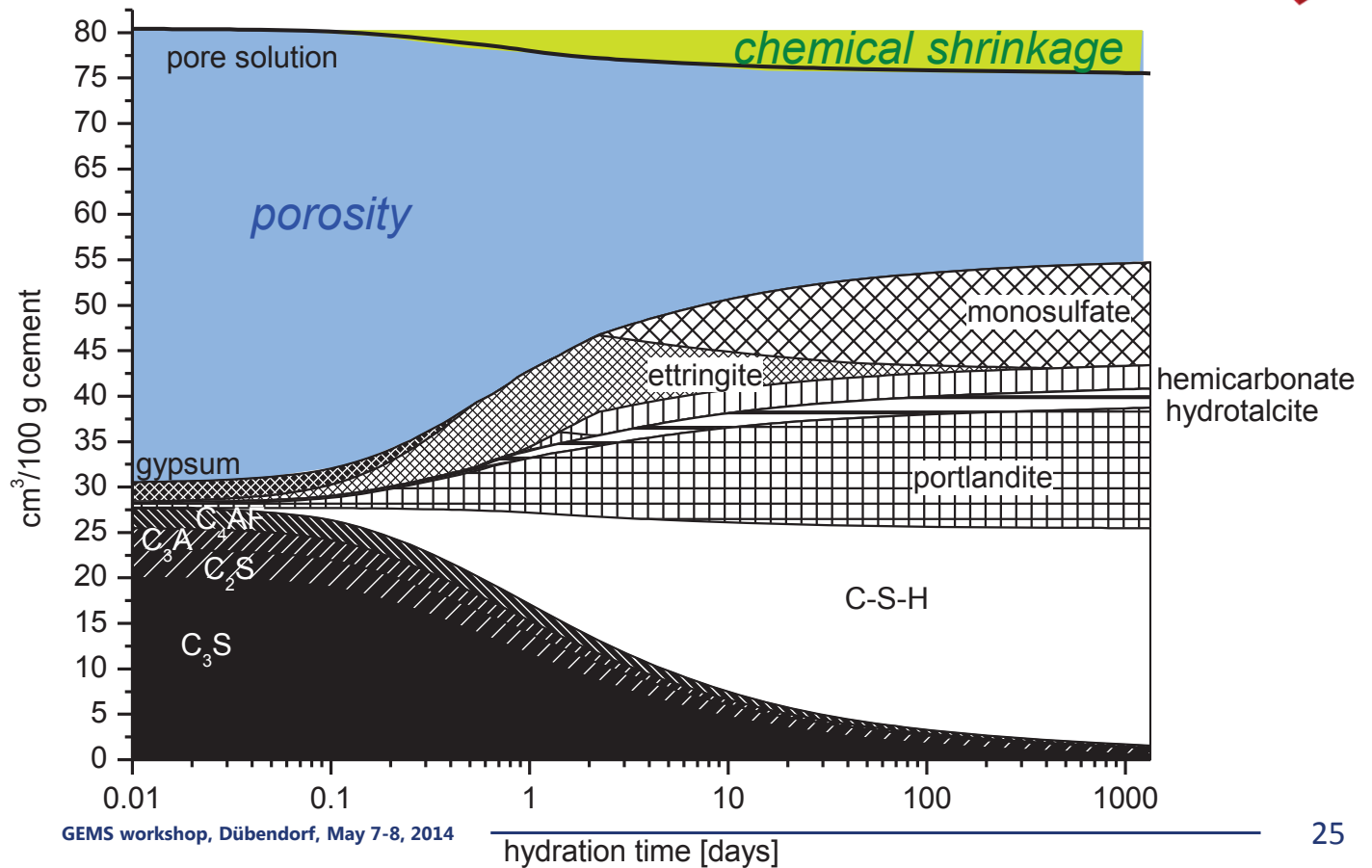
V_{Portlandite} = 15.48 cm³

m_{portlandite} = 34.69 g

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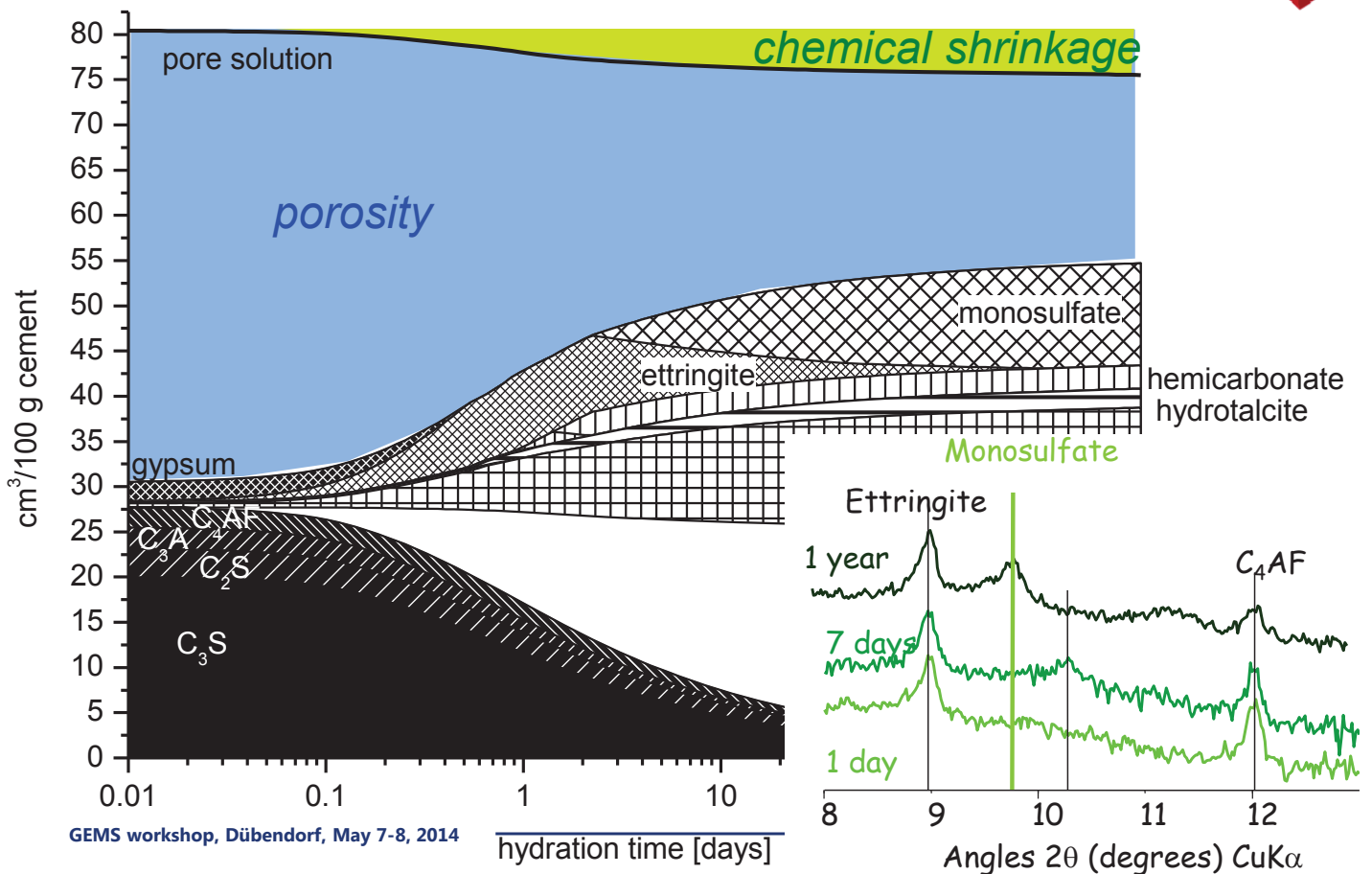
24

Comparison experimental data and modelling: Hydration of OPC without limestone

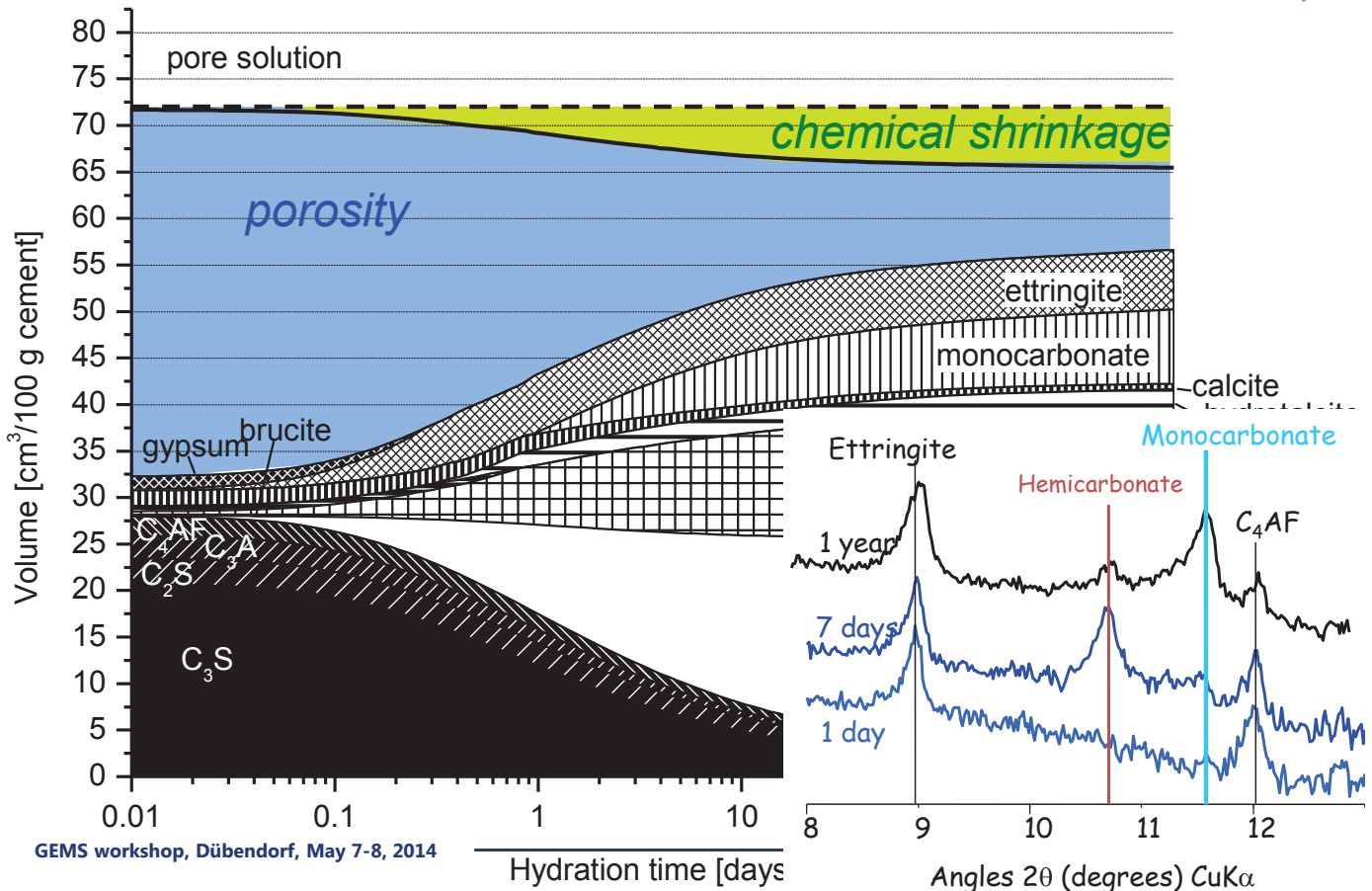


25

Comparison experimental data and modelling: Hydration of OPC without limestone



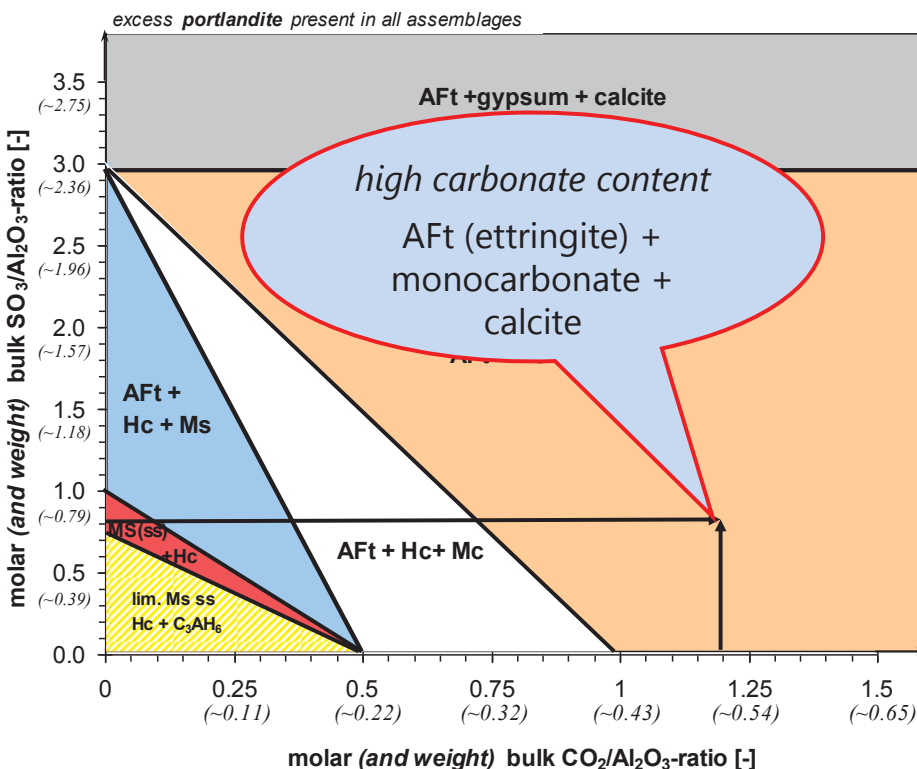
Comparison experimental data and modelling: Hydration of OPC with limestone



Hydration of OPC with limestone – phase diagram



Estimation of phase assemblages



Our cement:

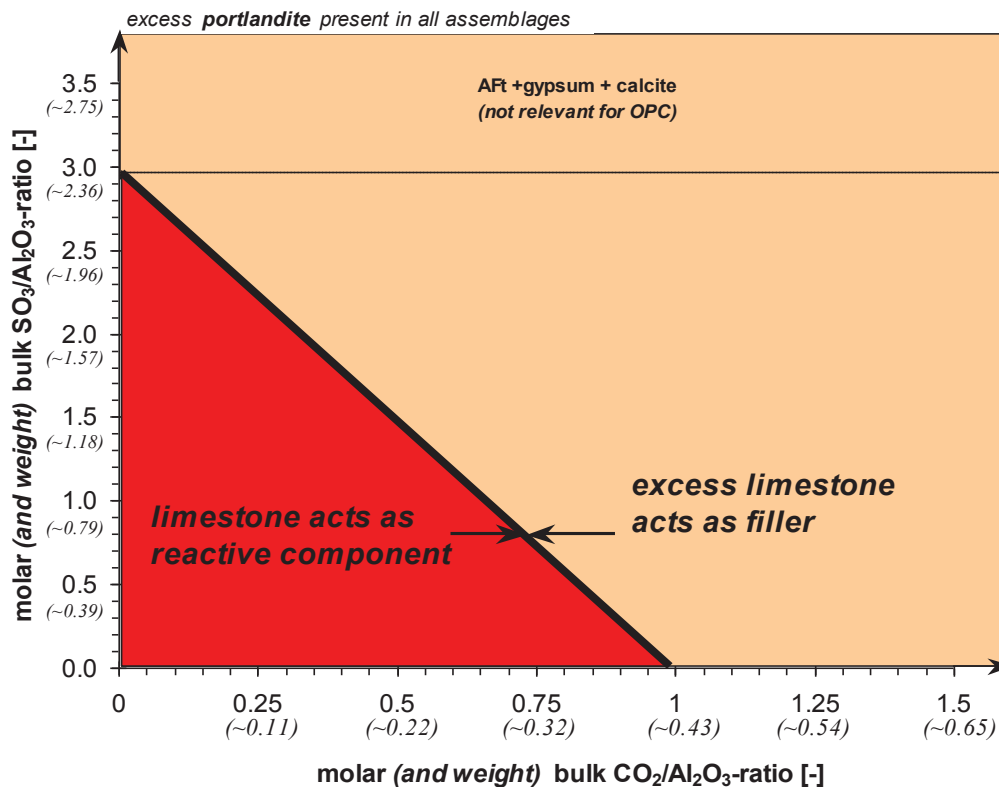
molar SO₃/Al₂O₃=0.82
weight SO₃/Al₂O₃=0.64

molar CO₂/Al₂O₃= 1.19
weight CO₂/Al₂O₃= 0.52

=> **Formation of monocarboaluminate, Aft and calcite expected**

Hydration of OPC with limestone – phase diagram

Distinction between limestone as reactive admixture and as filler



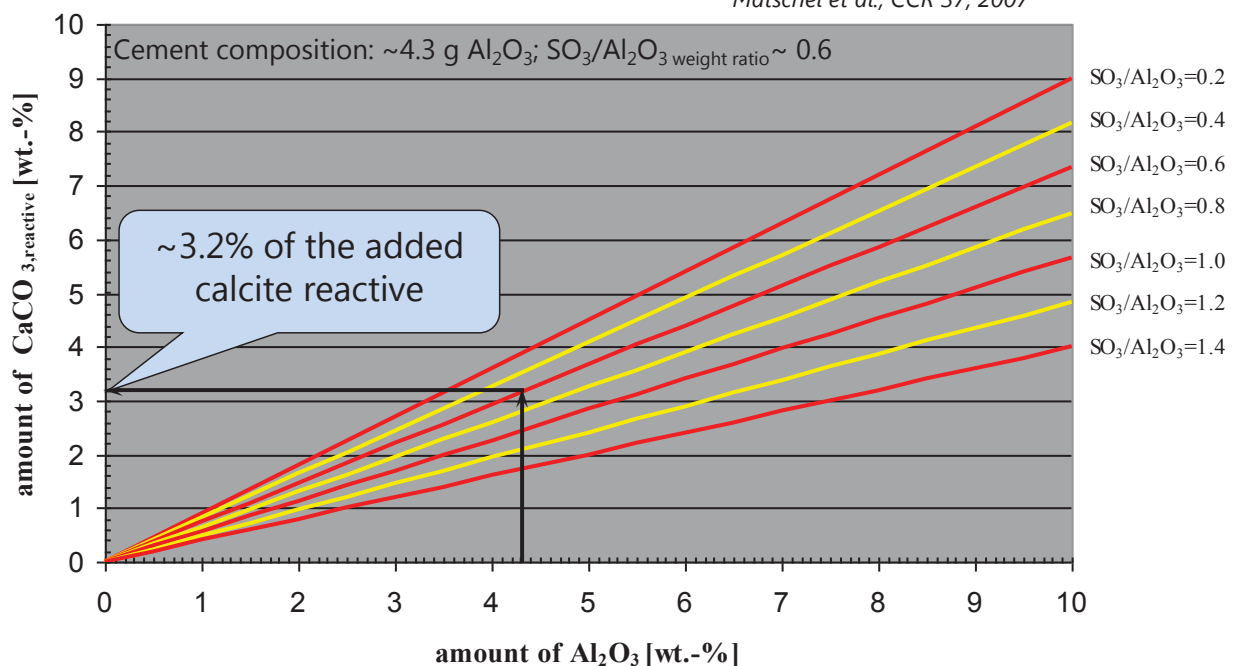
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29

Hydration of OPC with limestone – phase diagram

Previous calculations $M_{\text{calcite}} = 1.81 \text{ g} \Rightarrow 5 - 1.71 = 3.19 \text{ g}$ calcite have reacted

Matschei et al., CCR 37, 2007



=> Determination of reactive calcite content by using diagrams based on thermodynamic phase predictions

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30

Predicted stable phase assemblage

Possibility of formation of siliceous hydrogarnet in the system
 $\text{CaO-SiO}_2\text{-Al}_2\text{O}_3\text{-CaSO}_4\text{-CaCO}_3\text{-H}_2\text{O}$ at 25°C

- according to the literature the formation of siliceous hydrogarnet is likely in heat treated concretes
- AFm phases are abundant and generally observed in cement paste cured at 25°C
- knowledge on thermodynamic properties of solid solutions between different hydrogarnets containing Fe, Ca, Si has improved recently (Dilnesa et. al. CCR 2014a+b)
- formation of siliceous hydrogarnet apparently kinetically restraint

To reproduce reality, the formation of siliceous hydrogarnet is by default suppressed in GEMS. The data however is included in the cement database (DComp) and can be introduced (Phase) if desired.

Appendix – siliceous hydrogarnet

Import of siliceous Al-hydrogarnets (Dcomp -> Phase)

1. Selecting 'DComp' from the menu.

2. Selecting 'DComp' from the component list.

3. Selecting 'CaASiOH' from the list of components.

The main window displays thermochemical data for dependent components, including the following table:

Component	Formula	SiO2 (mol)	H2O (mol)
C3AS0.41H5.18	Ca3Al2O6(SiO2)0.41(H2O)5.18	0.41	5.18
C3AS0.84H4.32	Ca3Al2O6(SiO2)0.84(H2O)4.32	0.84	4.32

Appendix – siliceous hydrogarnet

Import of siliceous Al-hydrogarnets (Dcomp -> Phase)

1. **Record -> Create new**

2. **Record -> Create new**

3. **CaAlSiOH**

4. **Reset**

GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization

Phase: Please, set a new record key

s:CaAlSiOH:C3AS0.41H5.15:c:cem_

s Code of phase state { a g f p l m h s d x }

CaAlSiOH Group identifier for such phases (letters, digits)

C3AS0.41H5.15 Name of this phase definition (letters, digits)

c Phase class { c d l gm ss ssd ls aq xsa xc }

cem_ Comment to phase definition

Ok Reset From List Help Cancel

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33

Appendix – siliceous hydrogarnet

Import of siliceous Al-hydrogarnets (Dcomp -> Phase)

GEM-Selektor Phase Setup: s:CaAlSiOH:C3AS0.41H5.15:c:cem_

Step 1 - Defining the Phase and the Model of Mixing

Selection of the codes below will configure the Phase record and tell the program what kind of phase and which model of (non-ideal) mixing should be used, and how it should be calculated.

Phase aggregate state code:
s Condensed solid phase, also multi-component solid solution

Select a model of mixing for this phase:
I Ideal mixture or pure phase (default)

Select a mode of calculation of activity coefficients of end members:
I Activity coefficients will be set to 1 (pure phase, simple ideal mixing), default

Select a mode of execution of DcEq user-defined script for end-members:
N No DcEq script will be provided in this Phase definition (default)

Select a mode of execution of PhEq user-defined script for the whole phase:
N No PhEq script will be provided in this Phase definition (default)

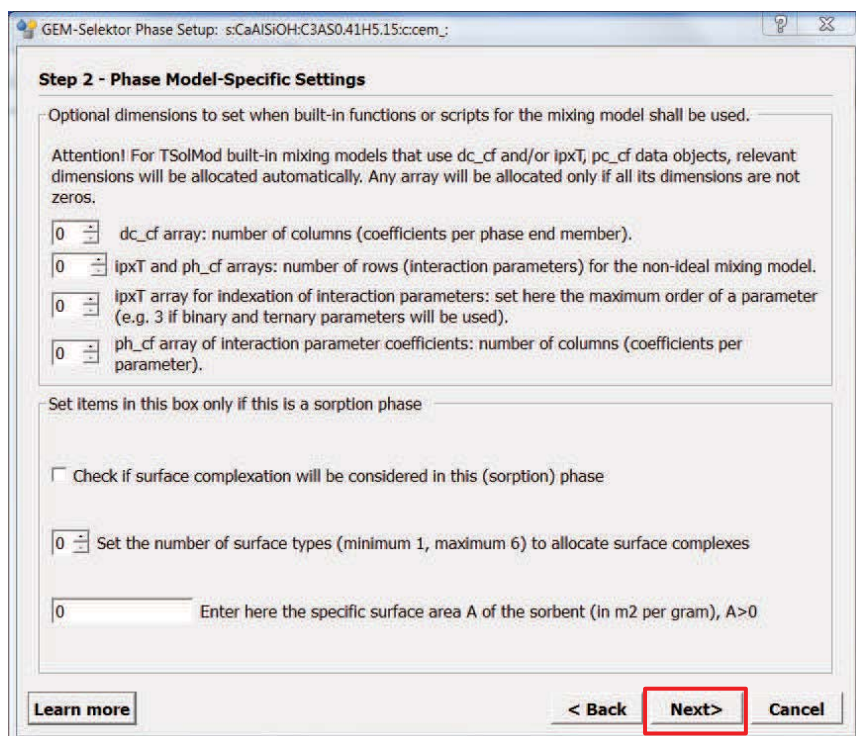
Select a mode of a linking user-defined DcEq script to phase end members:
N No DcEq script will be provided (pure phase, built-in or ideal model), default

Select specific mixing rules (temperature corrections) for EoS and activity models:
N Default mixing rule or form of interaction parameter coefficients

Learn more < Back Next> Cancel

34

Import of siliceous Al-hydrogarnets (Dcomp -> Phase)



GEM-Selektor Phase Setup: s:\CaAlSiOH:C3AS0.41H5.15\ccem_

Step 2 - Phase Model-Specific Settings

Optional dimensions to set when built-in functions or scripts for the mixing model shall be used.

Attention! For TSolMod built-in mixing models that use dc_cf and/or lpxT, pc_cf data objects, relevant dimensions will be allocated automatically. Any array will be allocated only if all its dimensions are not zeros.

0 dc_cf array: number of columns (coefficients per phase end member).

0 lpxT and ph_cf arrays: number of rows (interaction parameters) for the non-ideal mixing model.

0 lpxT array for indexation of interaction parameters: set here the maximum order of a parameter (e.g. 3 if binary and ternary parameters will be used).

0 ph_cf array of interaction parameter coefficients: number of columns (coefficients per parameter).

Set items in this box only if this is a sorption phase

☐ Check if surface complexation will be considered in this (sorption) phase

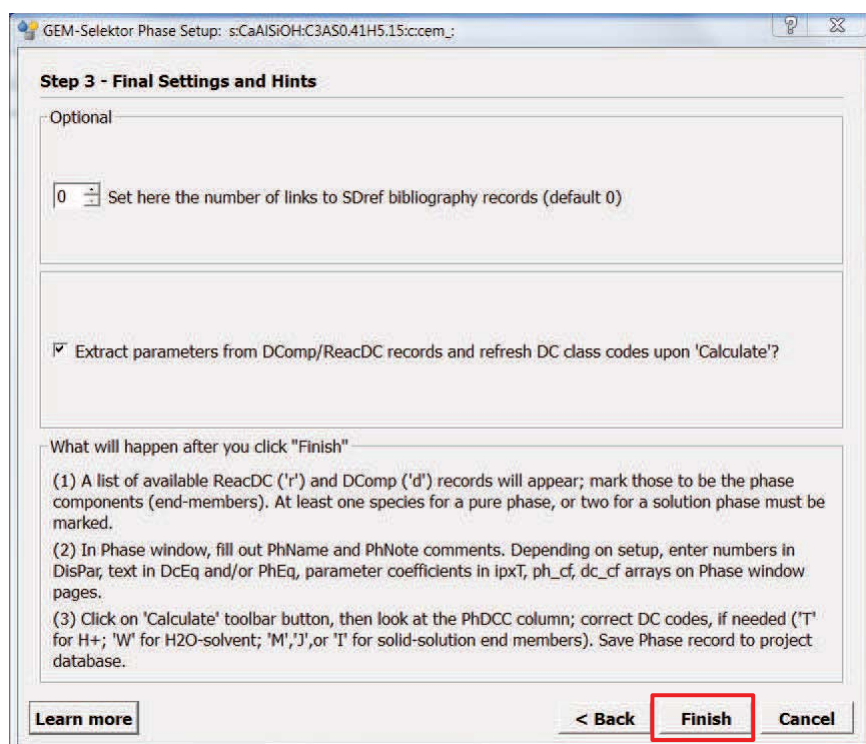
0 Set the number of surface types (minimum 1, maximum 6) to allocate surface complexes

0 Enter here the specific surface area A of the sorbent (in m² per gram), A>0

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Appendix – siliceous hydrogarnet

Import of siliceous Al-hydrogarnets (Dcomp -> Phase)



GEM-Selektor Phase Setup: s:\CaAlSiOH:C3AS0.41H5.15\ccem_

Step 3 - Final Settings and Hints

Optional

0 Set here the number of links to SDref bibliography records (default 0)

☒ Extract parameters from DComp/ReacDC records and refresh DC class codes upon 'Calculate'?

What will happen after you click "Finish"

(1) A list of available ReacDC ('r') and DComp ('d') records will appear; mark those to be the phase components (end-members). At least one species for a pure phase, or two for a solution phase must be marked.

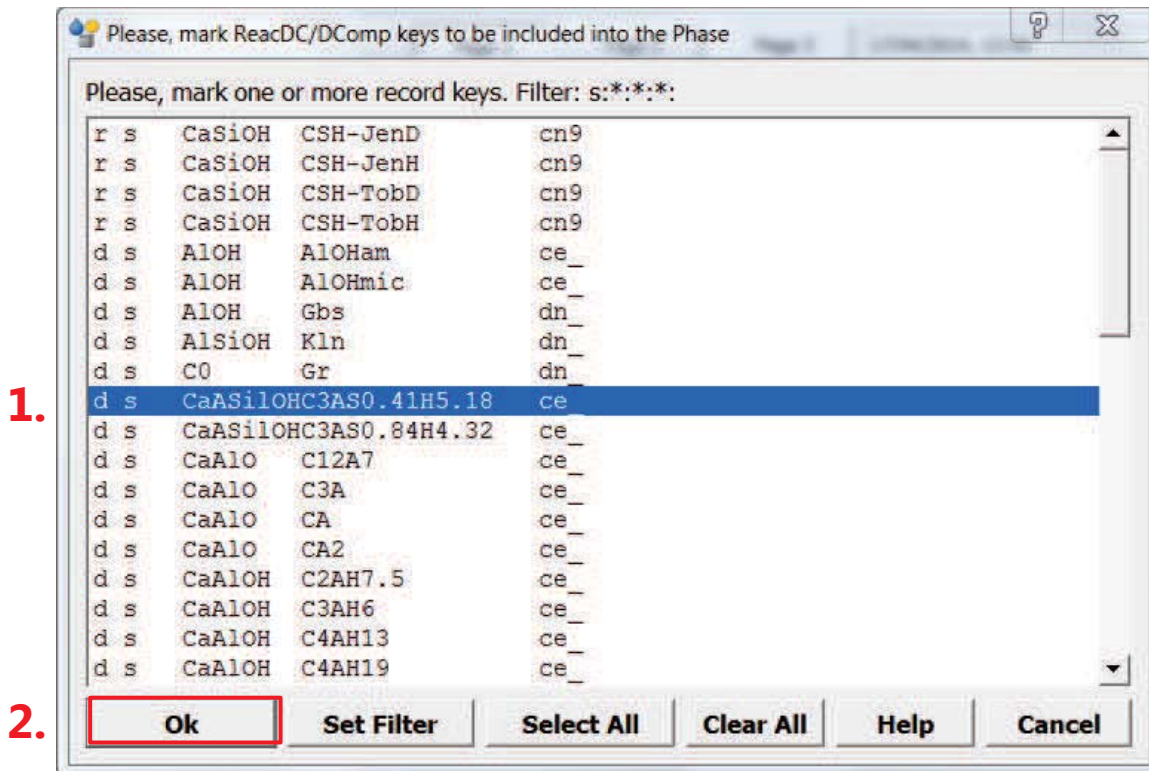
(2) In Phase window, fill out PhName and PhNote comments. Depending on setup, enter numbers in DisPar, text in DcEq and/or PhEq, parameter coefficients in lpxT, ph_cf, dc_cf arrays on Phase window pages.

(3) Click on 'Calculate' toolbar button, then look at the PhDCC column; correct DC codes, if needed ('T' for H+; 'W' for H₂O-solvent; 'M', 'J', or 'I' for solid-solution end members). Save Phase record to project database.

[Learn more](#) [< Back](#) [Finish](#) [Cancel](#)

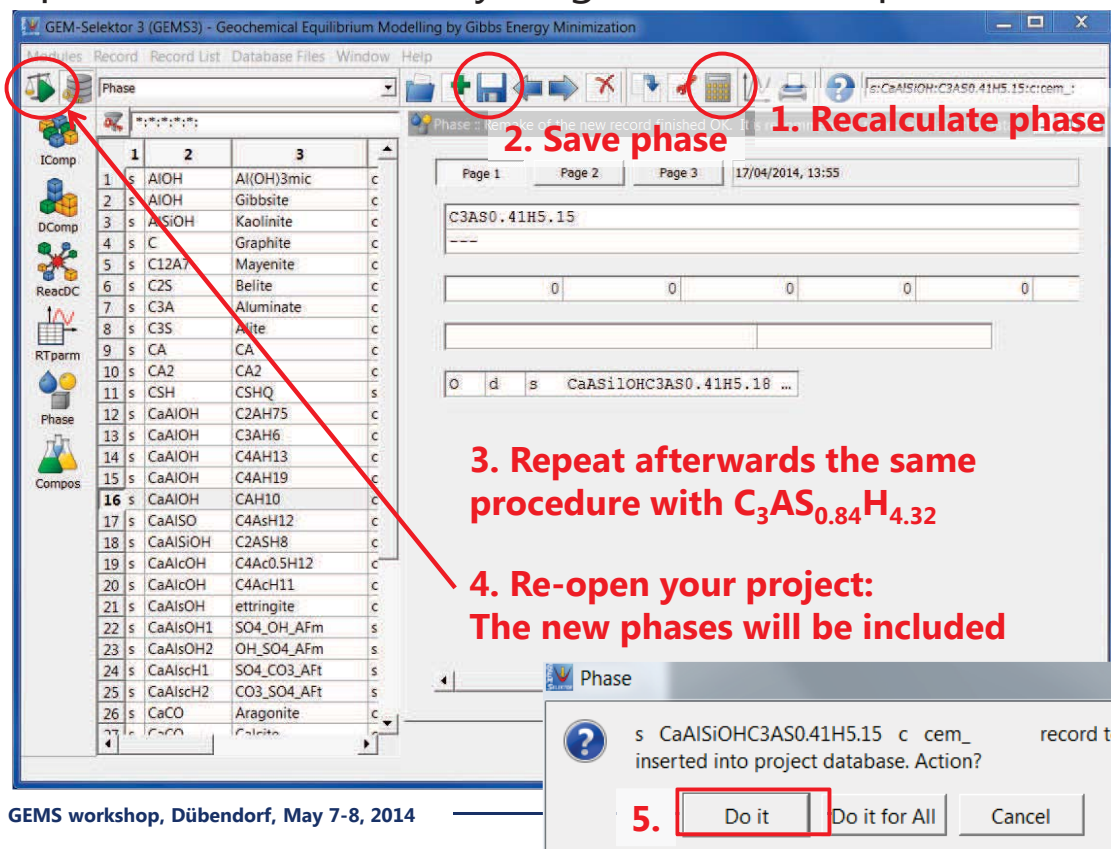
Appendix – siliceous hydrogarnet

Import of siliceous Al-hydrogarnets (Dcomp -> Phase)



Appendix – siliceous hydrogarnet

Import of siliceous Al-hydrogarnets (Dcomp -> Phase)

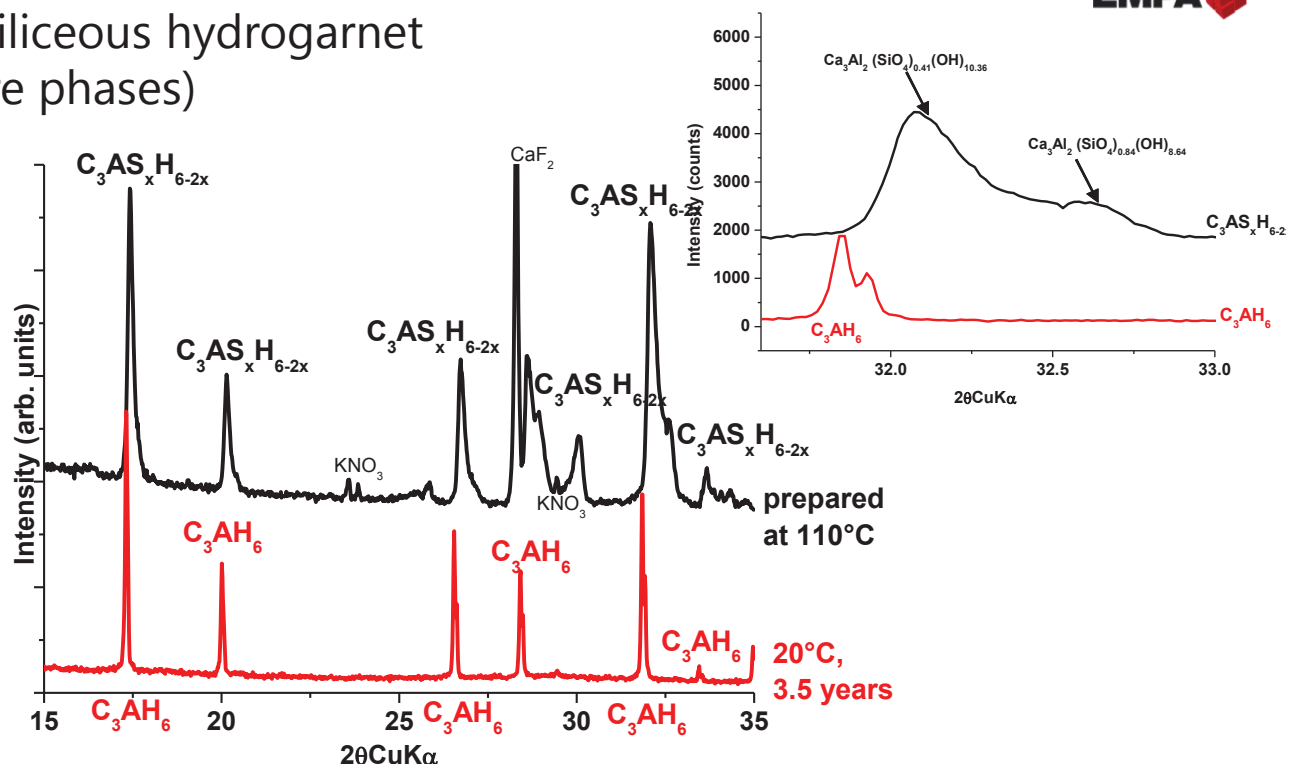


Predicted stable phase assemblage in presence of Si-Hg
(for OPC+calcite)

Input: System Definition		Results: Equilibrium State	
Phase/species	L	T	Amount (mol)
+ a	aq_gen	37	a 0.77375998
+ g	gas_gen	5	g 0.031233137
+ s	CSHQ	4	s 0.44101851
+ s	SO4_OH_AfM	2	s 0
+ s	OH_SO4_AfM	2	s 0
+ s	SO4_CO3_AfT	2	s 0.0061637368
+ s	CO3_SO4_AfT	2	s 0.0061637368
+ s	Al(OH)3mic	1	s 0
+ s	Gibbsite	1	s 0
+ s	Belite	1	s 0
+ s	Aluminate	1	s 0
+ s	Alite	1	s 0
+ s	C2AH75	1	s 0
+ s	C3AH6	1	s 0
+ s	C4AH13	1	s 0
+ s	C4AH19	1	s 0
+ s	CAH10	1	s 0
+ s	C4AsH12	1	s 0
+ s	C2ASH8	1	s 0
+ s	C3AS0.41H5.15	1	s 0.029605411
+ s	C3AS0.84H4.32	1	s 0
+ s	C4Ac0.5H12	1	s 0
+ s	C4AcH11	1	s 0
+ s	ettringite	1	s 0
+ s	Aragonite	1	s 0
+ s	Calcite	1	s 0.047863404
+ s	lime	1	s 0
+ s	Portlandite	1	s 0.48783282
+ s	Anhydrite	1	s 0
+ s	Gypsum	1	s 0

Appendix – siliceous hydrogarnet

Al-siliceous hydrogarnet (pure phases)



Room temperature: only C_3AH_6 forms;
 $C_3AS_2H_{6-2x}$ forms at 110 °C, but also stable at 20 °C

Al-siliceous hydrogarnet (OPC blended with fly ash)

Deschner, CCR 2013

