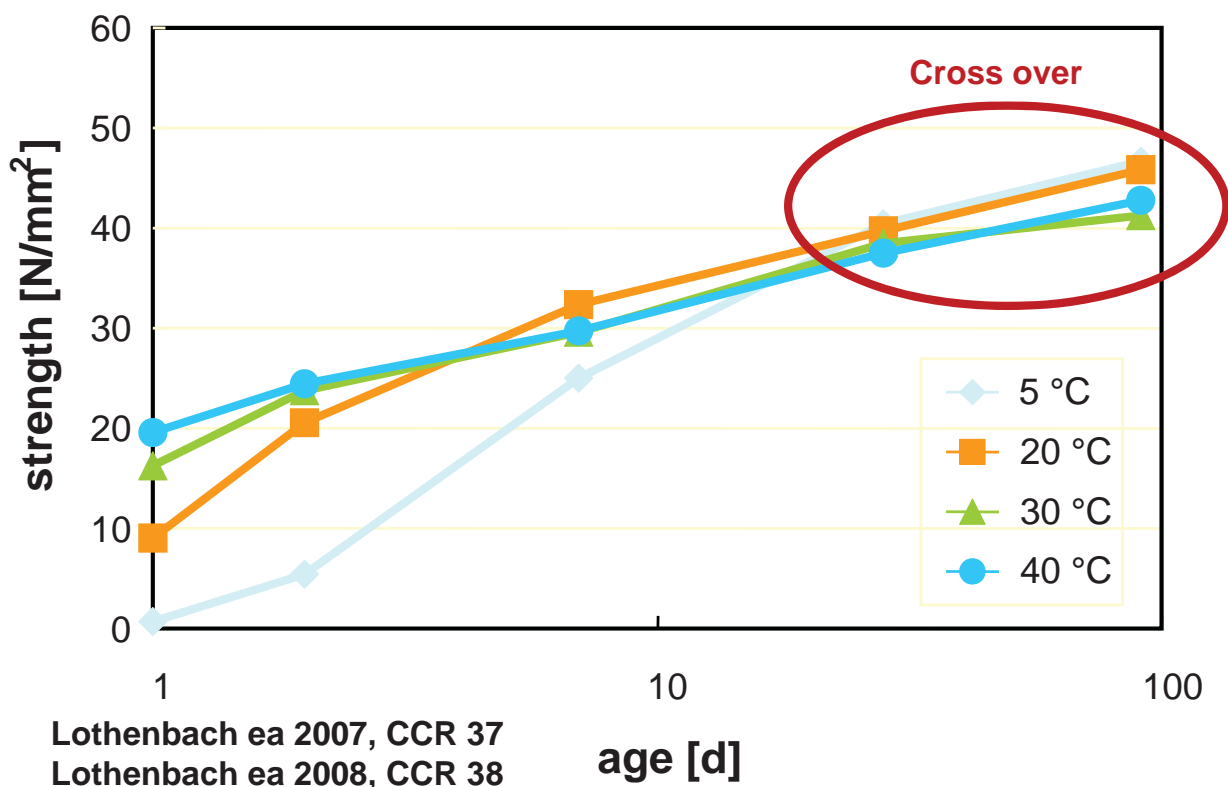




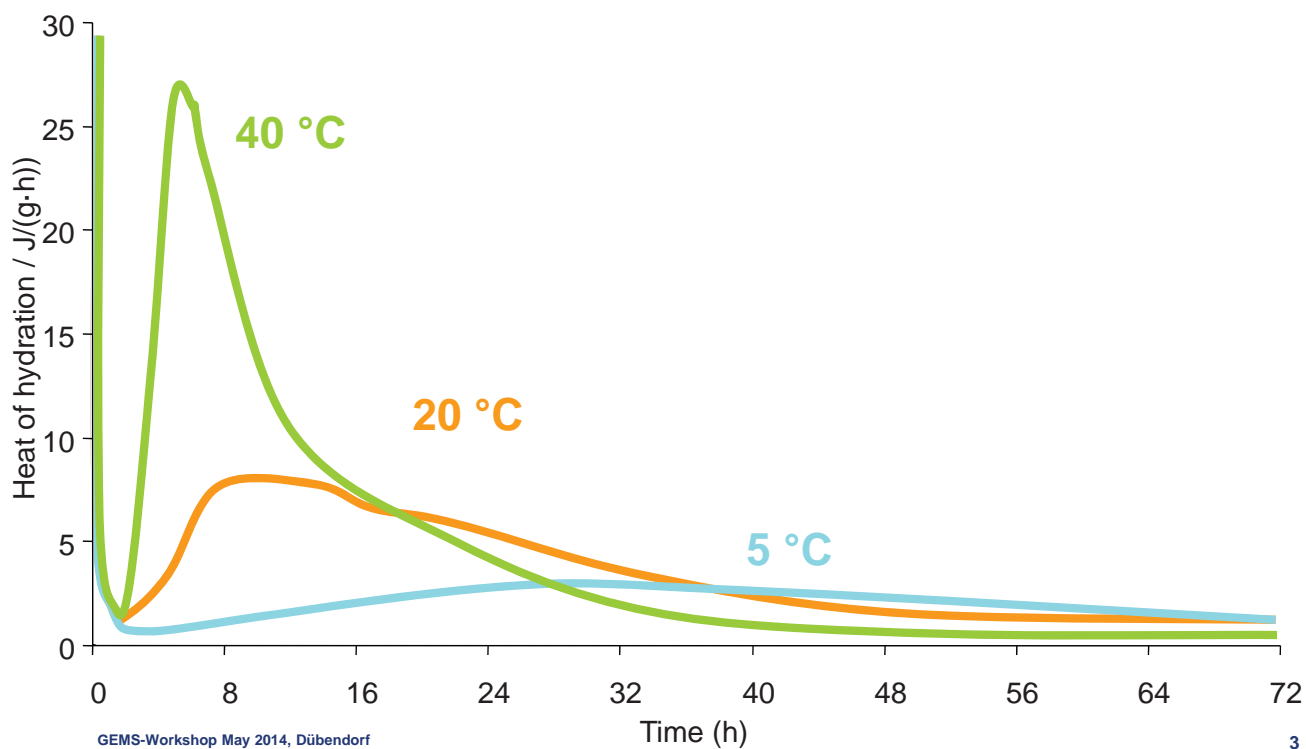
## 2) Influence of temperature

- a. Experimental evidence
- b. Temperature extrapolation
- c. Blended systems

### Influence of temperature: Compressive strength

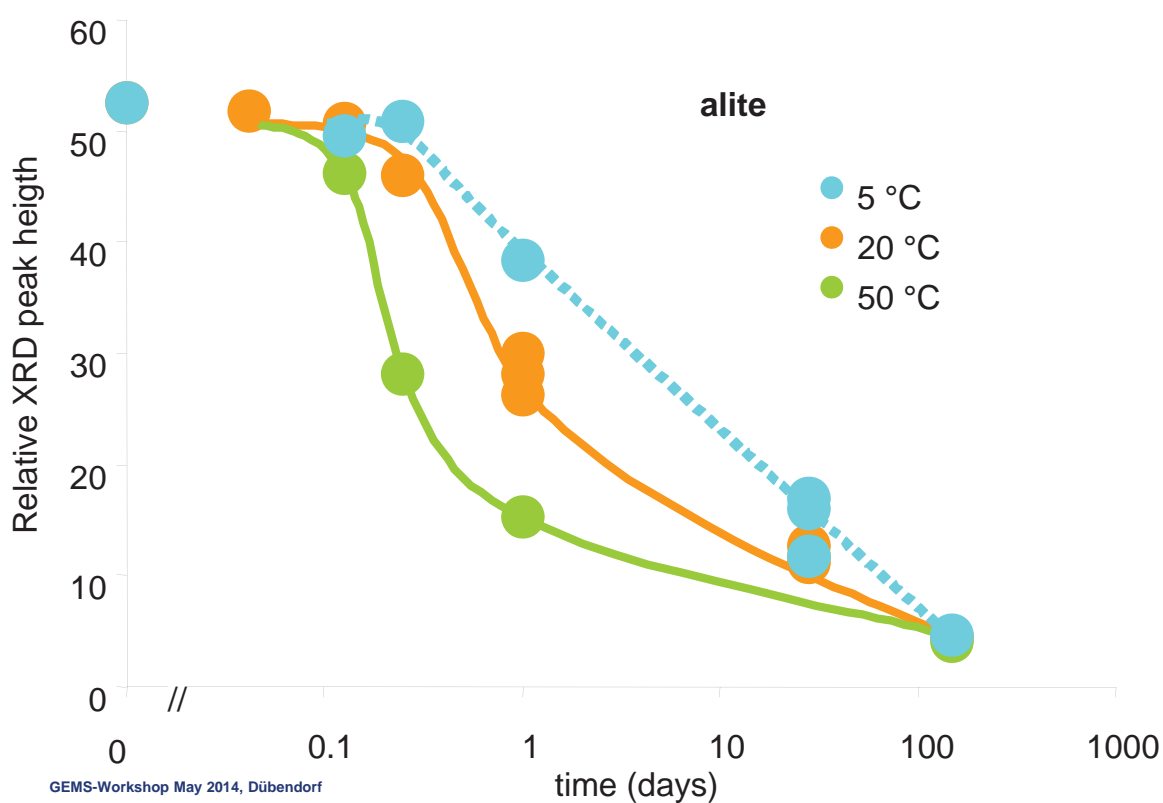


# Calorimetry



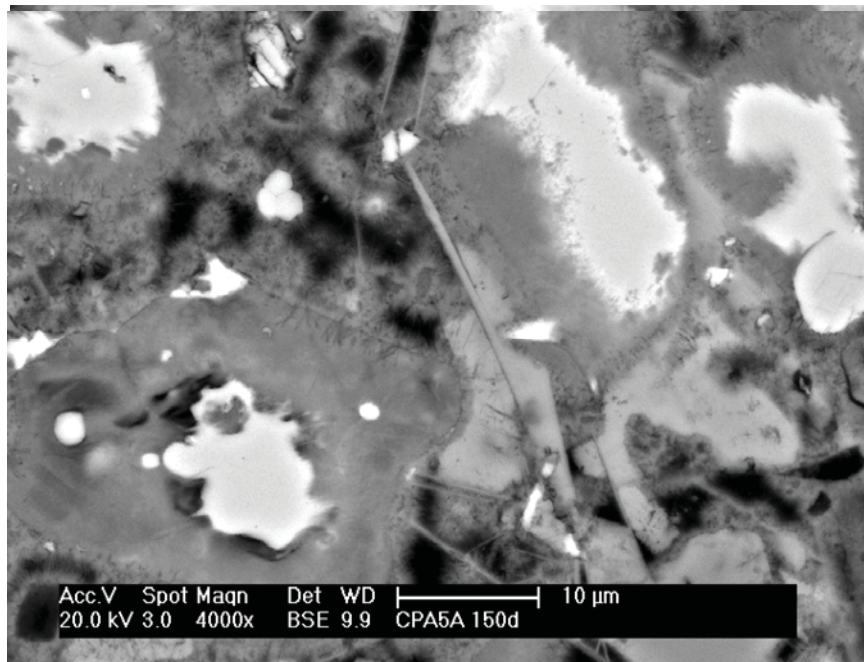
3

# Progress of hydration

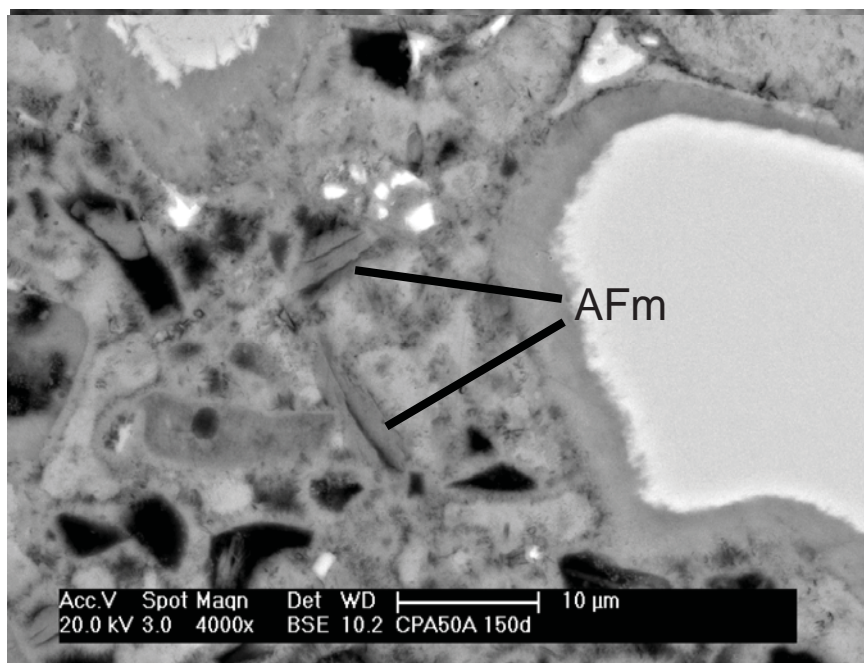


4

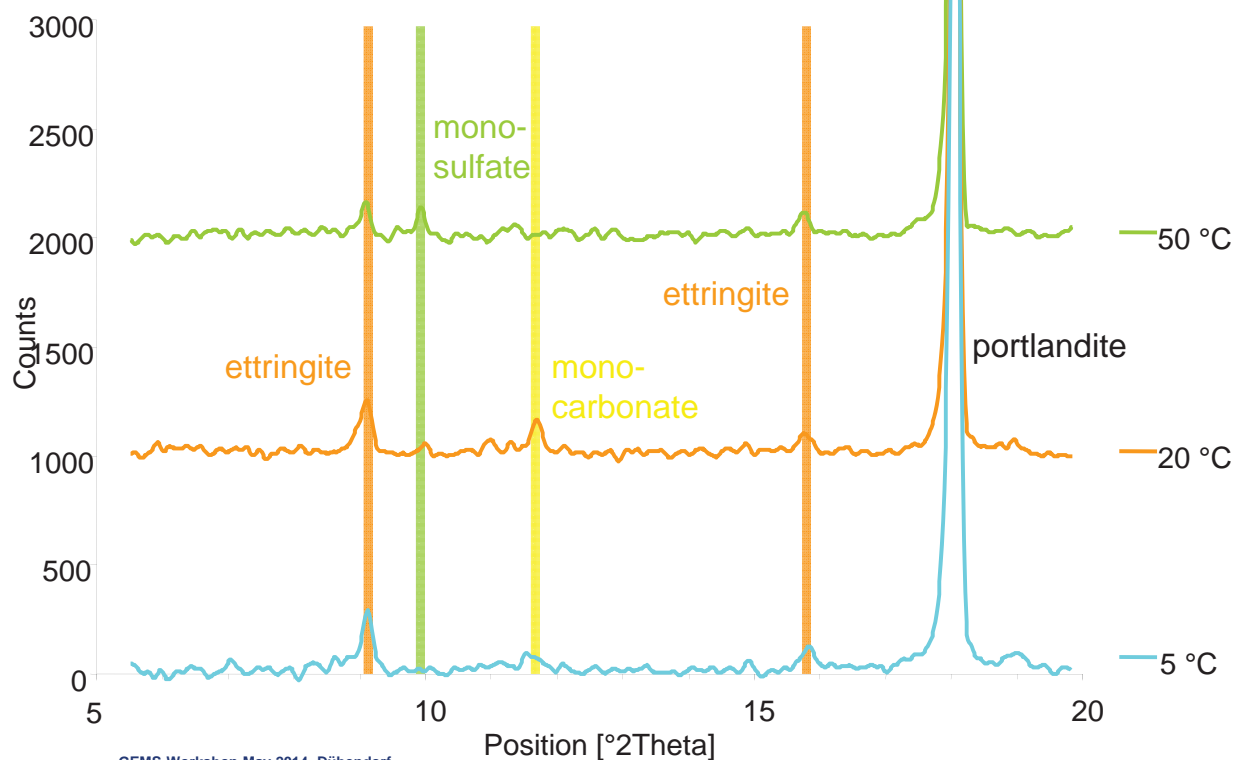
5 °C, 150 days



50 °C, 150 days

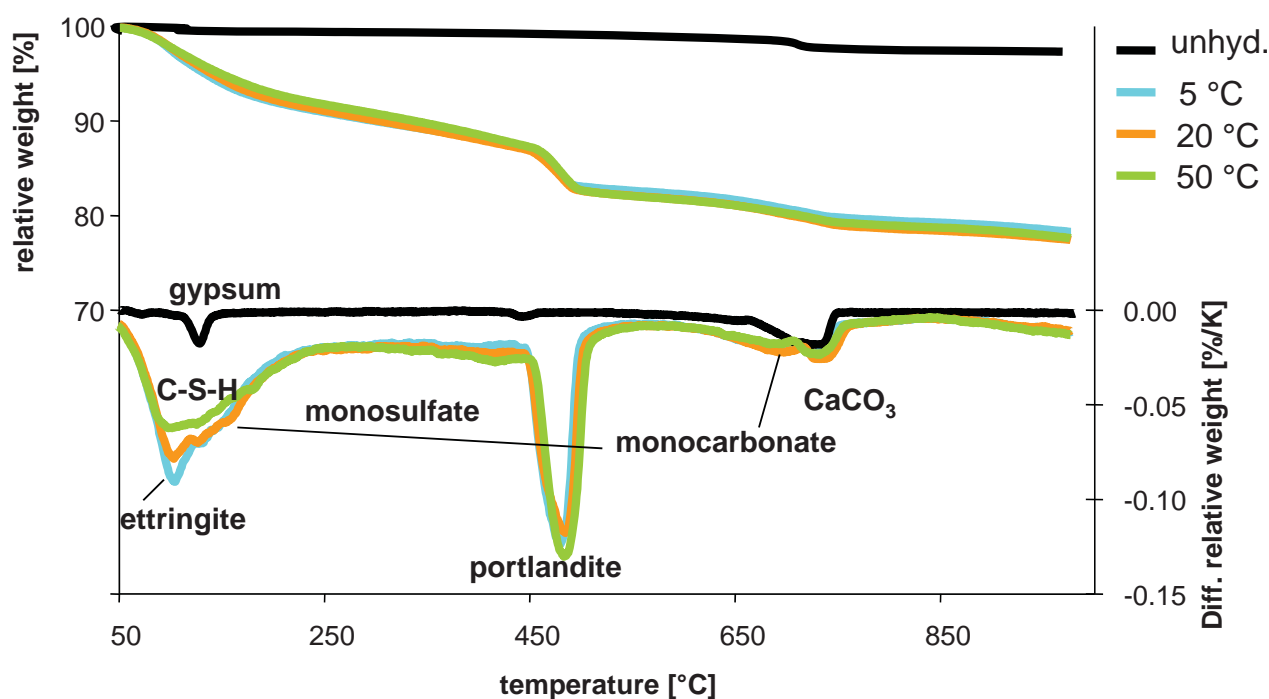


# XRD, 150 days



7

# 150 days



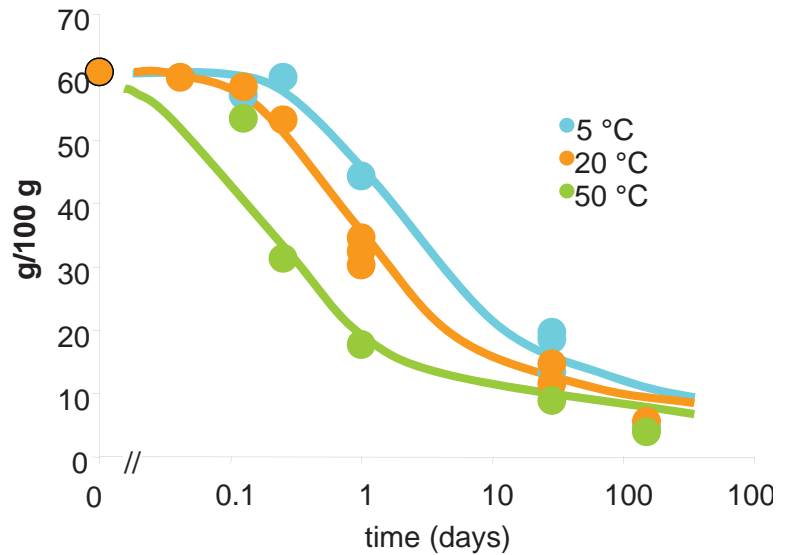
8

# Modeling: Temperature

## Arrhenius equation

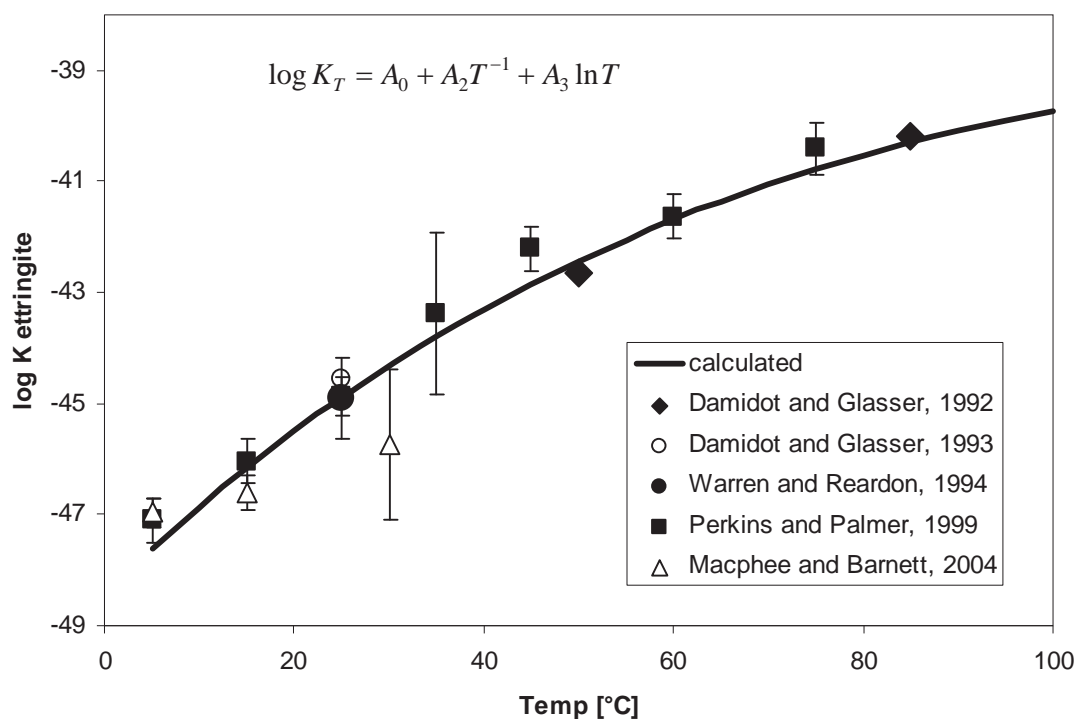
$$R_T = A e^{-\frac{E_a}{RT}}$$

$E_a$ : activation energy

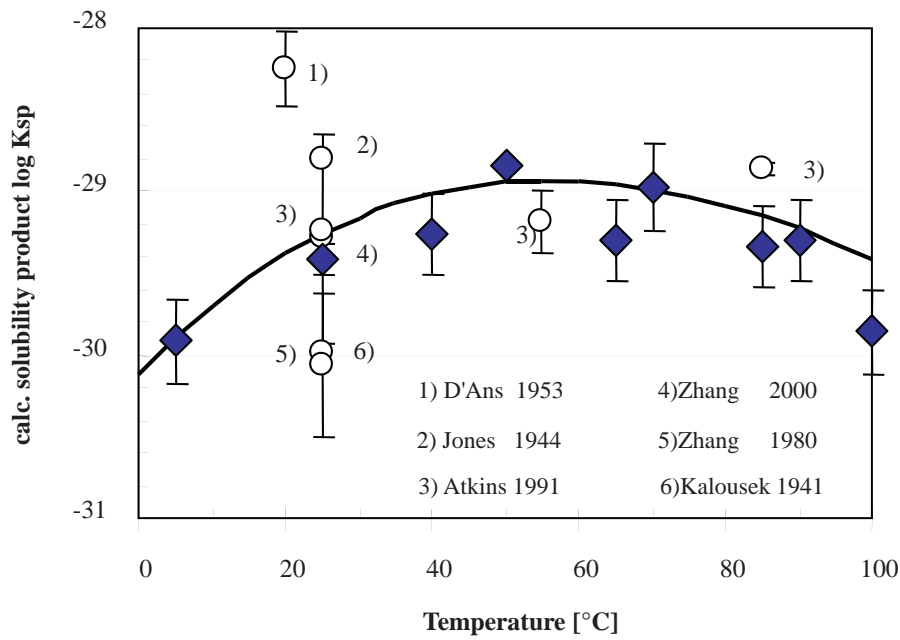


**Chemical reactions accelerate with increasing temperature**

## Solubility of ettringite as f(T)



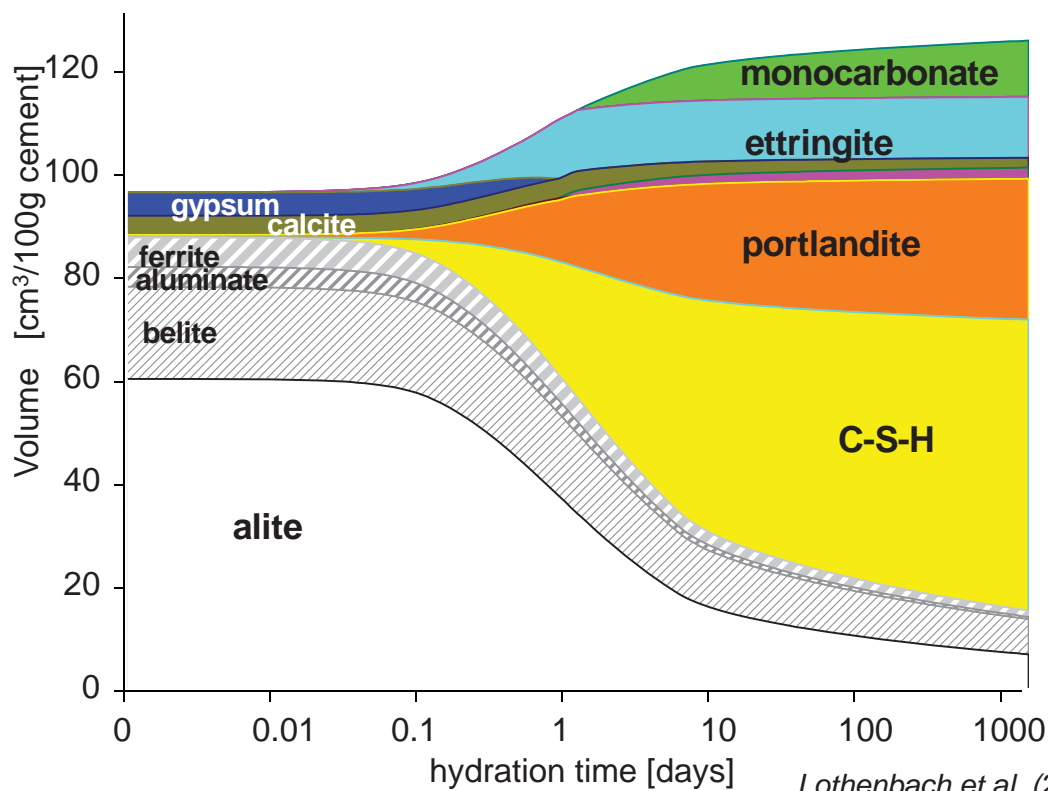
# Solubility of monosulfate



Matschei et al. (2007), CCR 37, 1379-1410

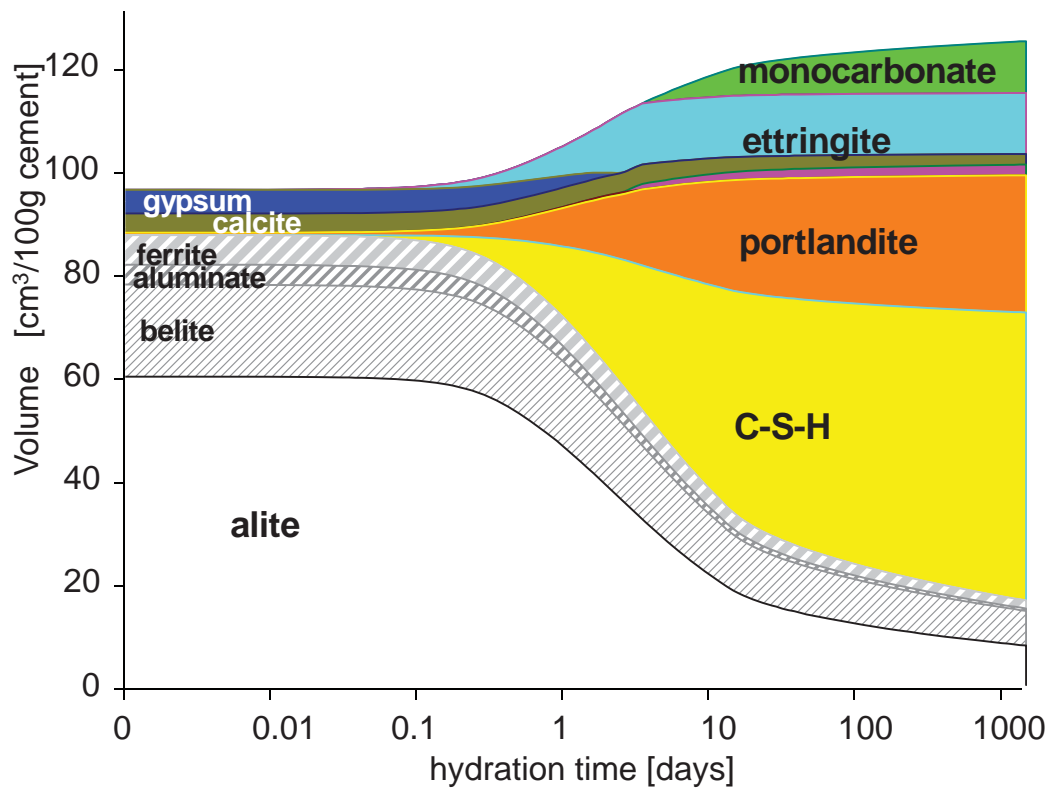


## Hydration: 20 °C

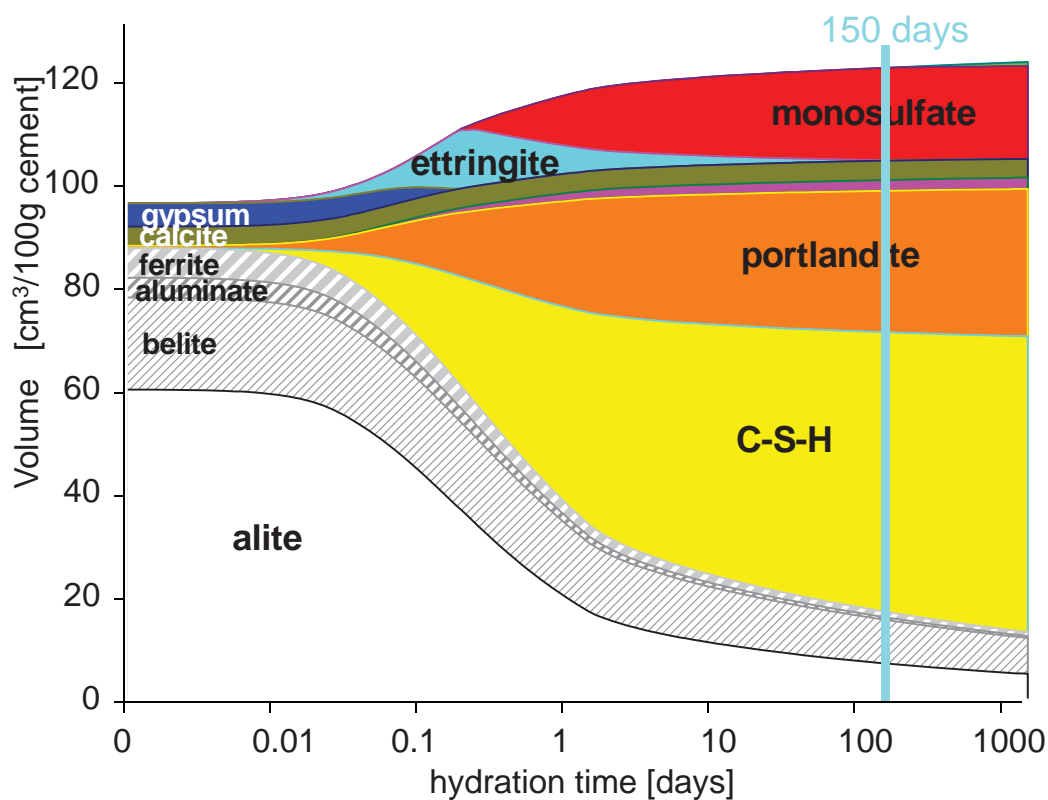


Lothenbach et al. (2008), CCR 38,

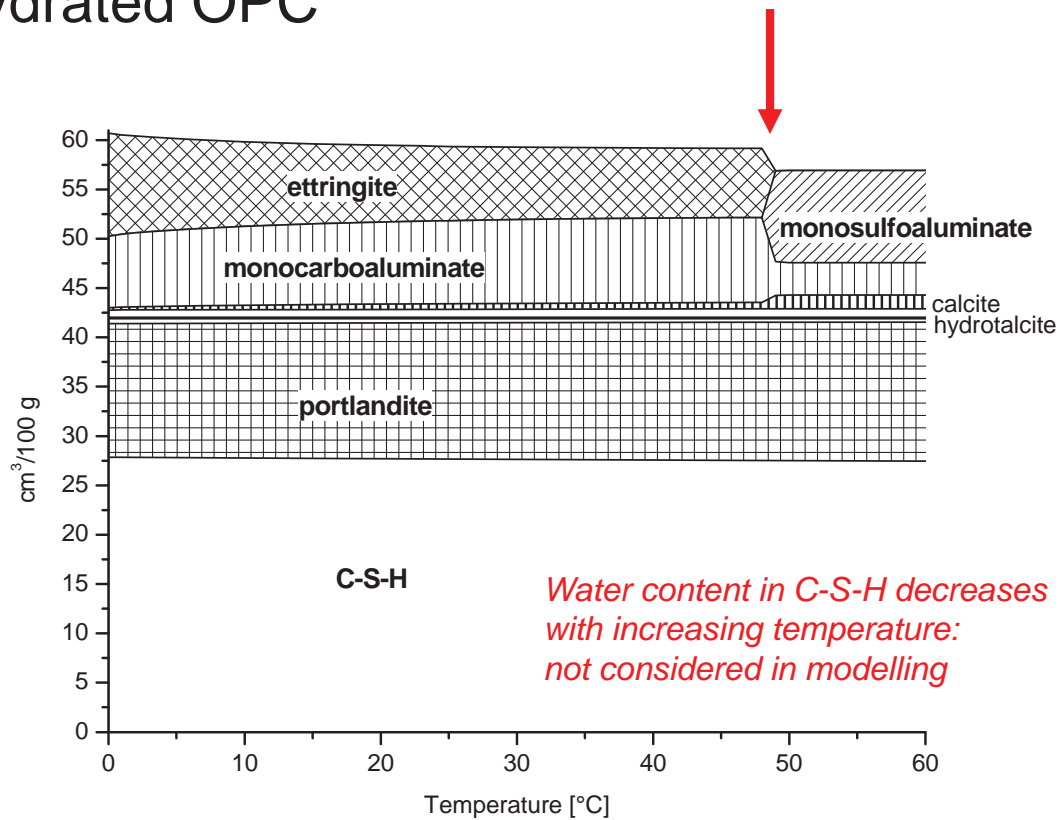
## hydration: 5 °C



## hydration: 50 °C

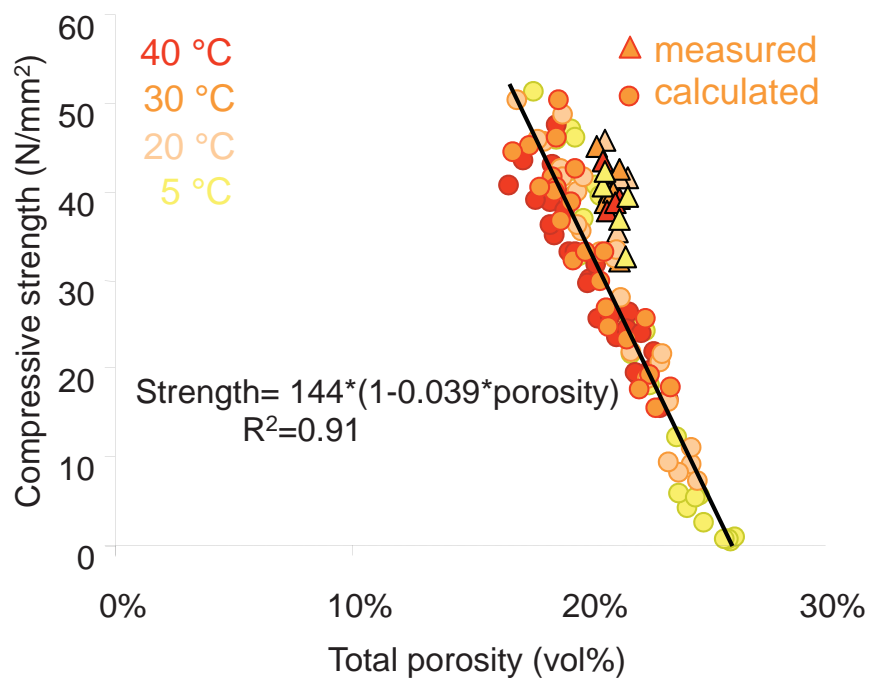


# Hydrated OPC



Lothenbach et al. (2010), *Advances Cem Res* 22, 211-223

## Strength-porosity



# Influence of temperature

Higher temperature:

- kinetic of hydration
- morphology (inhomogenous), denser C-S-H
- coarser porosity
- pore solution ( $\text{SO}_4$ , Al)
- hydrates (ettringite, monocarb. → monosulfate)
  - volume decrease
  - decrease in strength

Solubility of ettringite increases with temperature  
 -> less stable

## Influence of temperature: tutorial

### ■ Cement: «OPC» in project «Temp»

Input Recipe of Single Thermodynamic System: Temp:G:OPC:0:0:1:20:0:

tname OPC-all reacted 5% of calcite (2.8 g CaO, 2.2 g CO<sub>2</sub>)

Property	Name	Quantity	Units
1 xa_	Al <sub>2</sub> O <sub>3</sub>	5	g
2 xa_	Aqua	50	g
3 xa_	CO <sub>2</sub>	2.2	g
4 xa_	CaO	67	g
5 xa_	Fe <sub>2</sub> O <sub>3</sub>	1	g
6 xa_	K <sub>2</sub> O	0.1	g
7 xa_	MgO	1	g
8 xa_	Na <sub>2</sub> O	0.1	g
9 xa_	O <sub>2</sub>	0.1	g
10 xa_	SO <sub>3</sub>	4	g
11 xa_	SiO <sub>2</sub>	21.8	g

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

Learn more | Print | OK | Cancel

Cement composition in g/100 g:  
 => All reacts!

w/b = 0.5

Some O<sub>2</sub> to ensure oxic conditions

Input: System Definition   Results: Equilibrium State							
Phase/species	L	T	On/	UC	Add to BC	UG	G0
aq_gen	69	a	+	g	0	J	0
gas_gen	5	g	+	g	0	J	0
C3(AF)S0.84H	2	s	-	g	0	J	0
CSHQ	4	s	+	g	0	J	0
CSH-JenD		I	+	M	0	J	0
CSH-JenH		I	+	M	0	J	0
CSH-TobD		I	+	M	0	J	0
CSH-TobH		I	+	M	0	J	0
ettringite-Al	2	s	-	g	0	J	0
ettringite-Fe	2	s	-	g	0	J	0
monosulphate-Al	2	s	-	g	0	J	0
monosulphate-Fe	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
hydrocalc-pyro	2	s	+	g	0	J	0
Al(OH)3mic	1	s	+	g	0	J	0
Gibbsite	1	s	+	g	0	J	0
Kaolinite	1	s	+	g	0	J	0
Graphite	1	s	+	g	0	J	0
Mayenite	1	s	+	g	0	J	0
Belite	1	s	+	g	0	J	0
Aluminate	1	s	+	g	0	J	0
Alite	1	s	+	g	0	J	0
Ferrite	1	s	+	g	0	J	0
CA	1	s	+	g	0	J	0
CA2	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
C4AH10	1	s	+	g	0	J	0
C4AsH12	1	s	-	g	0	J	0
C2ASH6	1	s	+	g	0	J	0
C4AcO.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

No siliceous hydrogarnet (C3(AF)S0.84H) dolomite, quartz, ... formation at room temperature and short time frames

Quarternary solid solution model for C-S-H (Kulik 2010); Ca/Si varies from 0.67 to  $\approx 1.5$  (in the presence of portlandite)

Al-Fe monosulphate and Al-Fe-ettringite excluded for this example (duplicates can cause mathematical problems; iron more stable in hydroandradite:  $C_3FS_{0.84}H_{4.32}$ )

Single solids (ettringite/monosulphate) deactivated as already considered as solid solutions

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Input: System Definition   Results: Equilibrium State							
Phase/species	L	T	On/	UC	Add to BC	UG	G0 cor
C2ASH8	1	s	+	g	0	J	0
C4AcO.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
C3FH6	1	s	+	g	0	J	0
C4FH13	1	s	+	g	0	J	0
C3FS0.84H4.32	1	s	+	g	0	J	0
C3FS1.34H3.32	1	s	+	g	0	J	0
C4FcO5H10	1	s	+	g	0	J	0
C4FcH12	1	s	+	g	0	J	0
Dolomite-dis	1	s	-	g	0	J	0
Dolomite-ord	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
thaumasite	1	s	-	g	0	J	0
Iron	1	s	+	g	0	J	0
Fe-carbonate	1	s	+	g	0	J	0
Siderite	1	s	+	g	0	J	0
Hematite	1	s	-	g	0	J	0
Magnetite	1	s	+	g	0	J	0
Ferrihydrite-am	1	s	+	g	0	J	0
Ferrihydrite-mo	1	s	+	g	0	J	0
Goethite	1	s	-	g	0	J	0
Pyrite	1	s	+	g	0	J	0
Troilite	1	s	+	g	0	J	0
Melanterite	1	s	+	g	0	J	0
syngenite	1	s	+	g	0	J	0
OH-hydrocalcite	1	s	+	g	0	J	0
Magnesite	1	s	+	g	0	J	0
Brucite	1	s	+	g	0	J	0
Sulphur	1	s	+	g	0	J	0
Quartz	1	s	+	g	0	J	0
Silica-amorph	1	s	+	g	0	J	0

Single solids deactivated as already considered as solid solutions

No thaumasite, hematite, dolomite, goethite, quartz, ... formation at room temperature and short time frames

Amorphous SiO<sub>2</sub>

C\_on [33]: Selection of Phases to be included into GEM task { + - }

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Input: System Definition    Results: Equilibrium State

Phase/species	L	T	Amount (mol)	logSI/Activity	Concentration
a aq_gen	69	a	0.43500338	2.192e-09	
g gas_gen	5	g	0.0031158762	-2.094e-11	
s CSHQ	4	s	0.46917649	1.379e-09	
s SO4 OH AFm	2	s	0	-1	
s OH SO4 AFm	2	s	0	-1	
s SO4 CO3 AFt	2	s	0.018717018	-3.32e-09	
s CO3 SO4 AFt	2	s	2.9848203e-007	0.0001596	
s hydrotalc-pyro	2	s	0	-8.646	
s Al(OH)3mic	1	s	0	-3.192	
s Gibbsite	1	s	0	-2.669	
s Kaolinite	1	s	0	-15.11	
s Graphite	1	s	0	-83.76	
s Mayenite	1	s	0	-145.1	
s Belite	1	s	0	-1.856	
s Aluminate	1	s	0	-38.91	
s Alite	1	s	0	-14.11	
s Ferrite	1	s	0	-36.62	
s CA	1	s	0	-13	
s CA2	1	s	0	-18.96	
s C2AH75	1	s	0	-4.162	
s C3AH6	1	s	0	-2.668	
s C4AH13	1	s	0	-3.239	
s CAH10	1	s	0	-5.212	
s C2ASH8	1	s	0	-2.895	
s C4Ac0.5H12	1	s	0	-0.7397	
s C4AcH11	1	s	0.024117778	2.299e-09	
s Aragonite	1	s	0	-0.1441	
s Calcite	1	s	0.01959412	5.851e-09	
s C3FH6	1	s	0	-2.316	
s C4FH13	1	s	0	-2.476	
s C3FS0.84H4.32	1	s	0.0062622026	0	
s C3FS1.34H3.32	1	s	0	-0.6439	
s C4Fc05H10	1	s	0	-4.76	
s C4FcH12	1	s	0	-2.433	
s lime	1	s	0	-9.956	
s Portlandite	1	s	0.36532113	-3.761e-10	
s Anhydrite	1	s	0	-3.092	
s Gypsum	1	s	0	-2.838	

Solution  
C-S-H  
CH  
Ettringite  
Monocarbonate  
Calcite  
Hydroandradite ( $C_3FS_{0.84}H_{4.32}$ )  
Hydrotalcite

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## Influence of temperature: tutorial

### ■ New process file to calculate variation of temperature

GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [Process :: Definition of a Process Simulator (batch calculation)]

Modules Record Window Help

Process

Temp:\*\*\*\*

Create a new record from scratch

Controls Sampling Results Config 10/04/2014, 16:26

Process: Please, set a new record key

Temp:G:OPC:0:0:1:20:0:PC:P:

Temp Name of the modeling project

G Thermodynamic potential to minimize {G}

OPC Name of the parent chemical system definition (CSD)

0 CSD (recipe) variant number <integer>

0 Volume of the system, dm3

1 Pressure, bar, or 0 for Psat(H2O)g

20 Temperature, C

0 Variant number for additional constraints

PC Name of this process simulation task

P Process simulation mode code {P, S, L, G, T, R}

Ok Reset From List Help Cancel

iTau ipXi iNu

0 0 0

0 0 0

0 0 0

0 0 0

name  
Temperature and pressure variation

# Influence of temperature: tutorial

GEM-Selektor Process Setup: blended:G:OPC:0:0:1:25:000:Temp:P:

## Step 1 - Process Simulator Configuration

This is a tool for 'batch' calculation of multiple equilibrium states, sampling and plotting of results. In this way, irreversible geochemical processes (e.g. mixing, dissolution, hydration, titration, corrosion, weathering) can be simulated.

The Process record can be configured in several modes to perform specific simulation scenarios by execution of process control script 'P\_expr' and simulation output script 'pgExpr'. Simple scripts can be easily produced using this wizard.

Any process simulator belongs to one of three types:

1. 'Sequential': only input GEM parameters are modified (modes P, S, L);
2. 'Reciprocal': next step depends on GEM output parameters (e.g. pH) from previous step (mode R);
3. 'Inverse': GEM input adjusted to obtain prescribed values of GEM output (e.g. pH; modes G, T).

Please, choose a process simulation mode:

☒ P Sequential temperature and/or pressure change at fixed bulk composition

☐ S Direct sequential change of bulk composition and/or constraints (default)

☐ G Batch inverse titration sequence for incremented pH values etc.

☐ T One arbitrary inverse titration calculation as defined in Process control script

☐ R Sequential reactor scheme, uses equilibrium bulk compositions of phases

☐ L Lippmann diagram (transposed) for a binary solid solution

[Learn more](#) < Back Next> Cancel

Temperature and pressure variation

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# Influence of temperature: tutorial

GEM-Selektor Process Setup: Temp:G:OPC:0:0:1:20:0:PC:P:

## Step 2 - Process Simulation Controls (click 'Next' to retain the old script)

	iTm	iP	iTC	iNu	iTau	ipXi	iNu	ipH	ipe
From	1000	0	1	4	0	0	0	0	0
Until	1200	0	1	96	0	0	0	0	0
Step	1	0	2	0	0	0	0	0	0

☒ No script ☐ User-defined script ☐ PT phase diagram

Please, check iP and iT iterator contents, and set Step to 0 in all other iterators.

For PT phase diagram: select phases to plot, then skip the next wizard page.

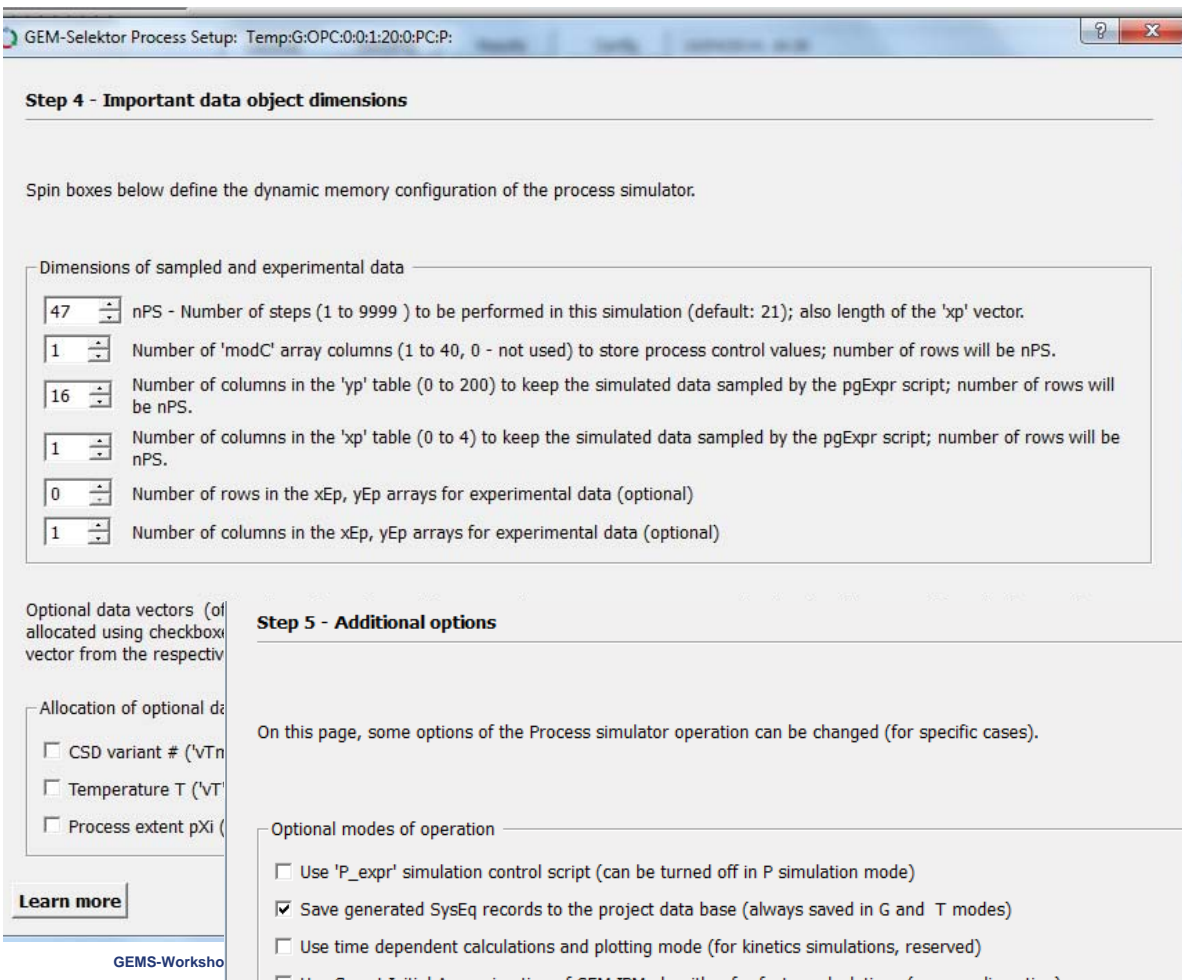
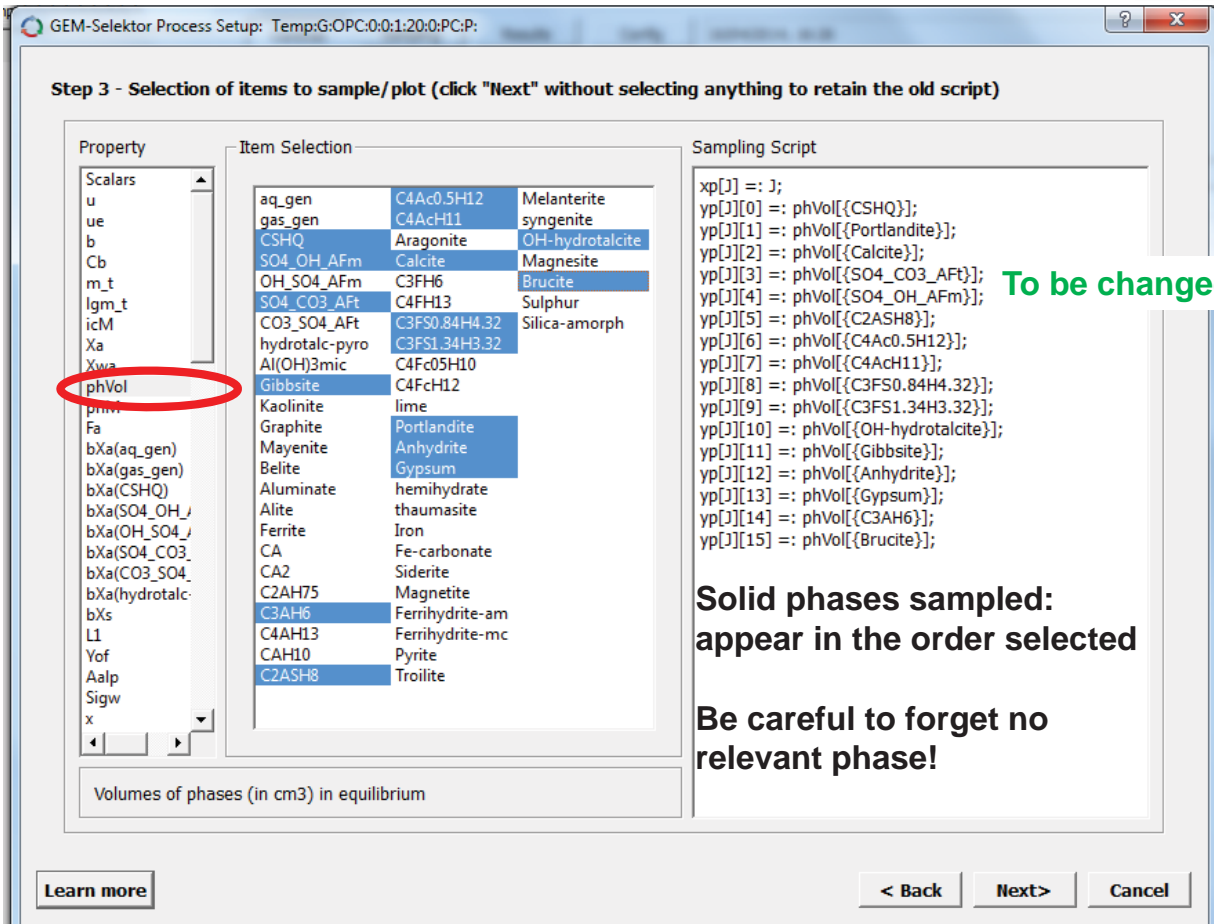
Phases

aq_gen	C3AH6	Iron
gas_gen	C4AH13	Fe-carbonate
CSH0	C4AH10	Siderite

Numbering of the single calculations

Start temperature  
Stop temperature  
Step size

No script needed



Temp:G:OPC:0:0:1:20:0:PC:P:

Controls | Sampling | Results | Config | 10/04/2014, 16:26

NeIt 9999 0 Next 1 I 0 J 0 Jp 0

pSTkey cTm 1000 cNV 0

cTau 0 cpXi 0 cXi 1 cNu 0

cpH 0 cpe 0 cEh 0 cT 277.15

**cTC: Temperature in °C**

**Ettringite and monosulphate: both parts of the solid solution needed**

```

xp[J] =: cTC;
yp[J][0] =: phVol[{CSHQ}];
yp[J][1] =: phVol[{Portlandite}];
yp[J][2] =: phVol[{Calcite}];
yp[J][3] =: phVol[{SO4_CO3_Aft}]+phVol[{CO3_SO4_Aft}];
yp[J][4] =: phVol[{SO4_OH_Afm}]+phVol[{OH_SO4_Afm}];
yp[J][5] =: phVol[{C2ASH8}];
yp[J][6] =: phVol[{C4Ac0.5H12}];
yp[J][7] =: phVol[{C4AcH11}];
yp[J][8] =: phVol[{C3FS0.84H4.32}];
yp[J][9] =: phVol[{C3FS1.34H3.32}];
yp[J][10] =: phVol[{OH-hydratalcite}];
yp[J][11] =: phVol[{Gibbsite}];
yp[J][12] =: phVol[{Anhydrite}];
yp[J][13] =: phVol[{Gypsum}];
yp[J][14] =: phVol[{C3AH6}];
yp[J][15] =: phVol[{Brucite}];

```

cT  
temperature  
in K

## Influence of temperature: tutorial

Modelling by Gibbs Energy Minimization - [Process :: Remake of the new record finished OK. It is recommended to re-calculate data]

Temp:G:OPC:0:0:1:20:0:PC:P:

Controls | Sampling | Results | Config | 10/04/2014, 16:26

--- pY Nam phVol

pX Nam	Temp C	CSHQ	Portlandite	Calcite	Ettringite	monosulfate	C2ASH8
0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0
9	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0
11	0	0	0	0	0	0	0
12	0	0	0	0	0	0	0
13	0	0	0	0	0	0	0
14	0	0	0	0	0	0	0
15	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0
17	0	0	0	0	0	0	0
18	0	0	0	0	0	0	0
19	0	0	0	0	0	0	0
20	0	0	0	0	0	0	0

yp [2,4] : Data table of c



## OPC without calcite



**EMPA** 

- Cement: «OPC\_noCc» in project «Temp»





# Influence of temperature: 5% Cc

Controls	Sampling	Results	Config	17/04/2014, 11:19
NeIt	9999	47	Next	0
I	0	J	46	Jp
Jp	46			
pSTkey	Temp:G:OPC:0:0:1:20:0:			cTm
cTm	1000	cNV	0	
cTau	0	cpXi	0	cXi
cXi	1	cNu	0	
cpH	0	cpe	0	cEh
cEh	0	cT	369.15	

```

xp[J] =: cTC;
yp[J][0] =: pH;
$ plotting Ca/Si in CSH
yp[J][1] =: bXa[{CSHQ}][{Ca}]/bXa[{CSHQ}][{Si}];
$ plotting H/Si in CSH: H/2 = H2O
yp[J][2] =: bXa[{CSHQ}][{H}]/2/bXa[{CSHQ}][{Si}];
$ log OH- conc
yp[J][3] =: 14+lg(my[{OH-}]);
    
```

## Plotting of changes in pH, OH- and C-S-H

$bXa[{CSHQ}][{Ca}]/bXa[{CSHQ}][{Si}]$ :

**molar Ca/Si in C-S-H solid solution**

$bXa[{CSHQ}][{H}]/2/bXa[{CSHQ}][{Si}]$ :

**molar H/Si in C-S-H solid solution (H/2 = H<sub>2</sub>O)**

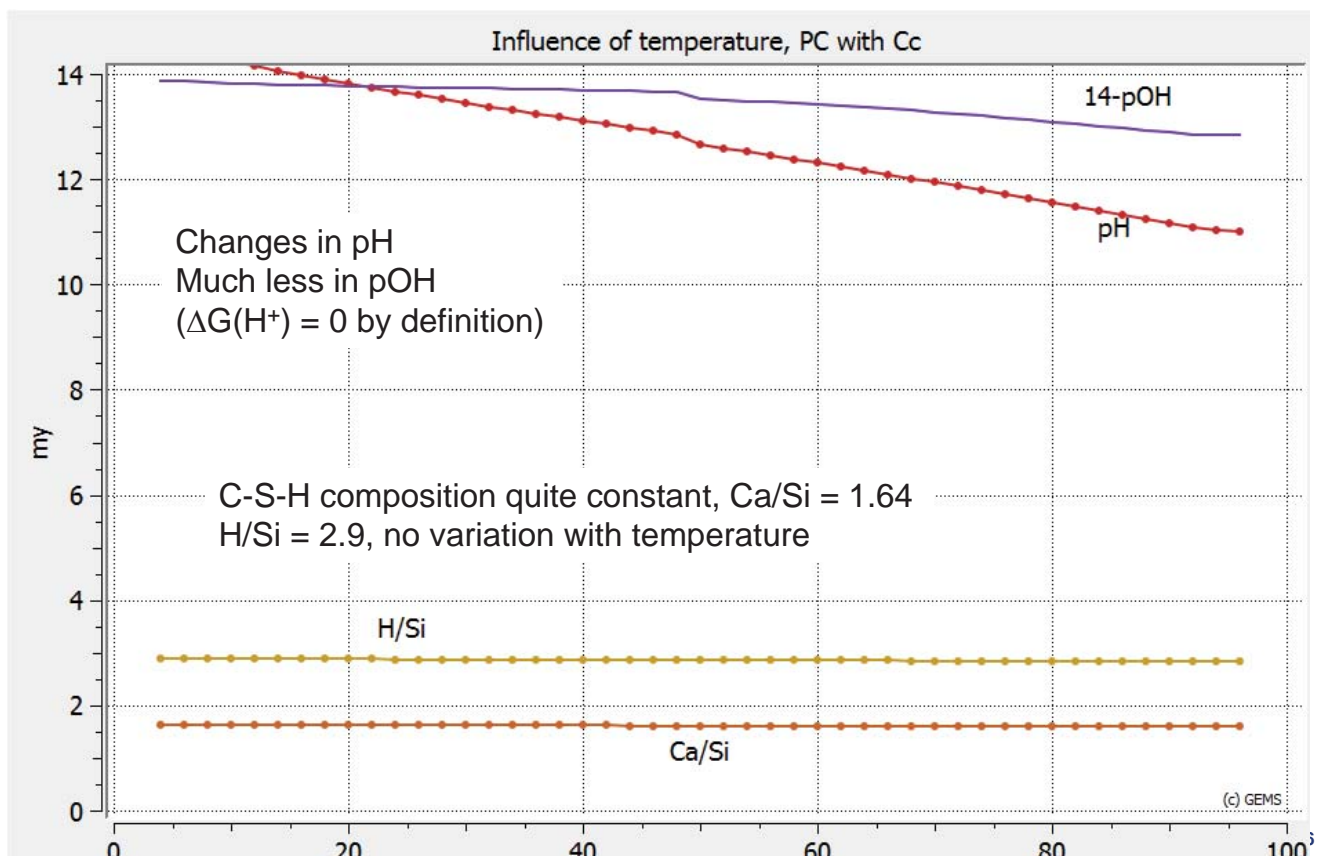
**14+lg(my[{OH-}]) equals pH at 25 °C**

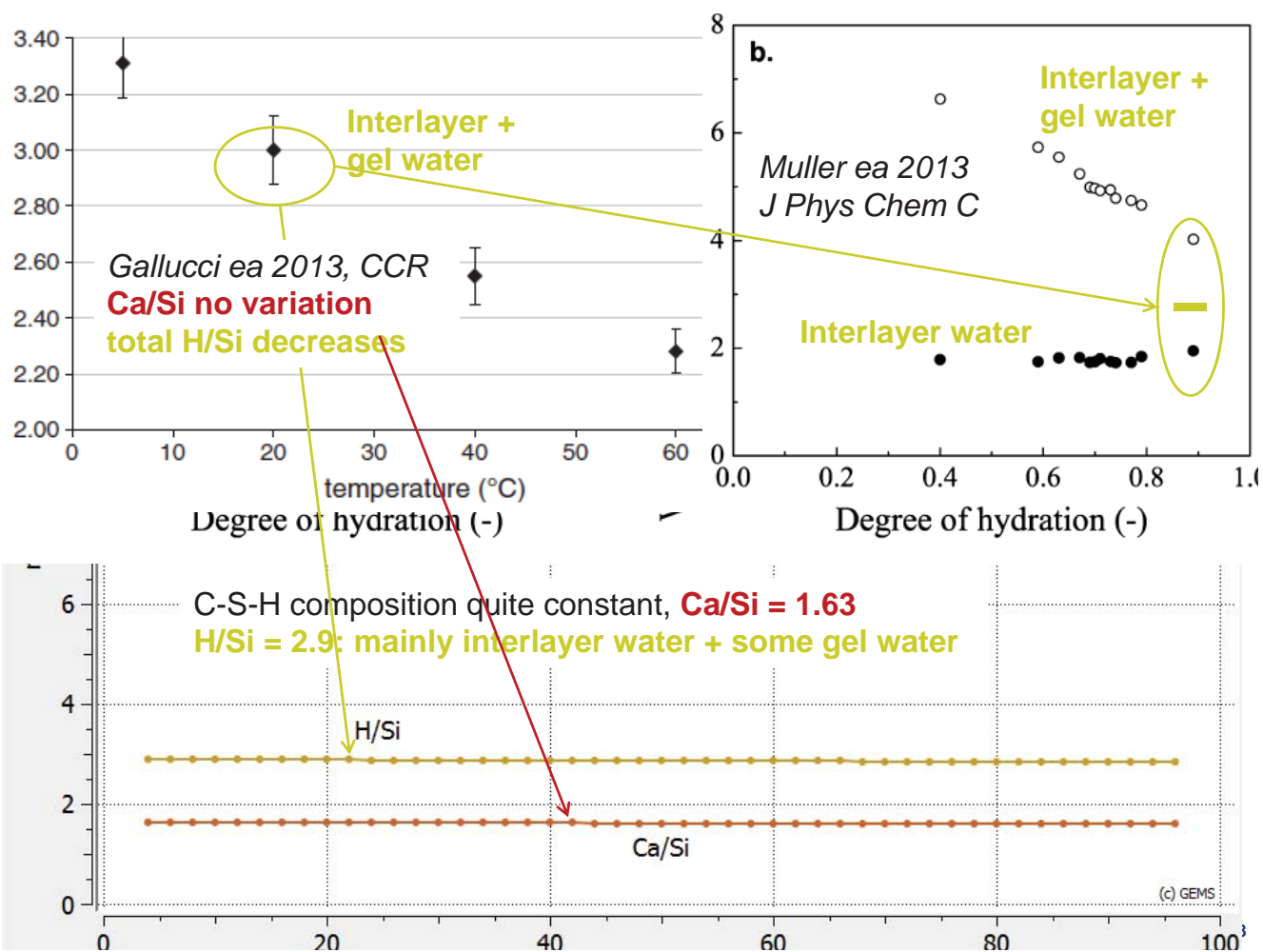
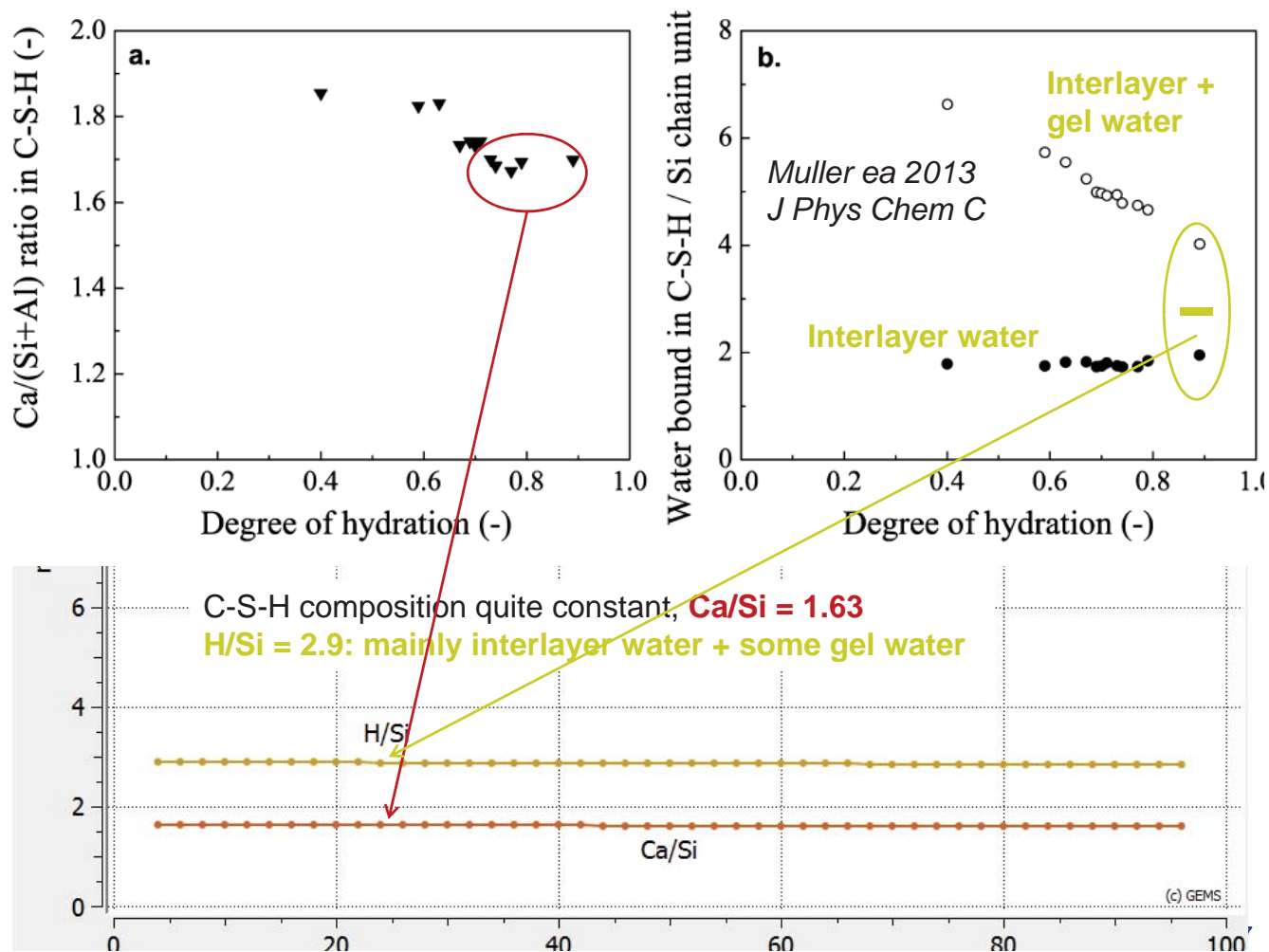
**=> to illustrate temperature effect on pH:**

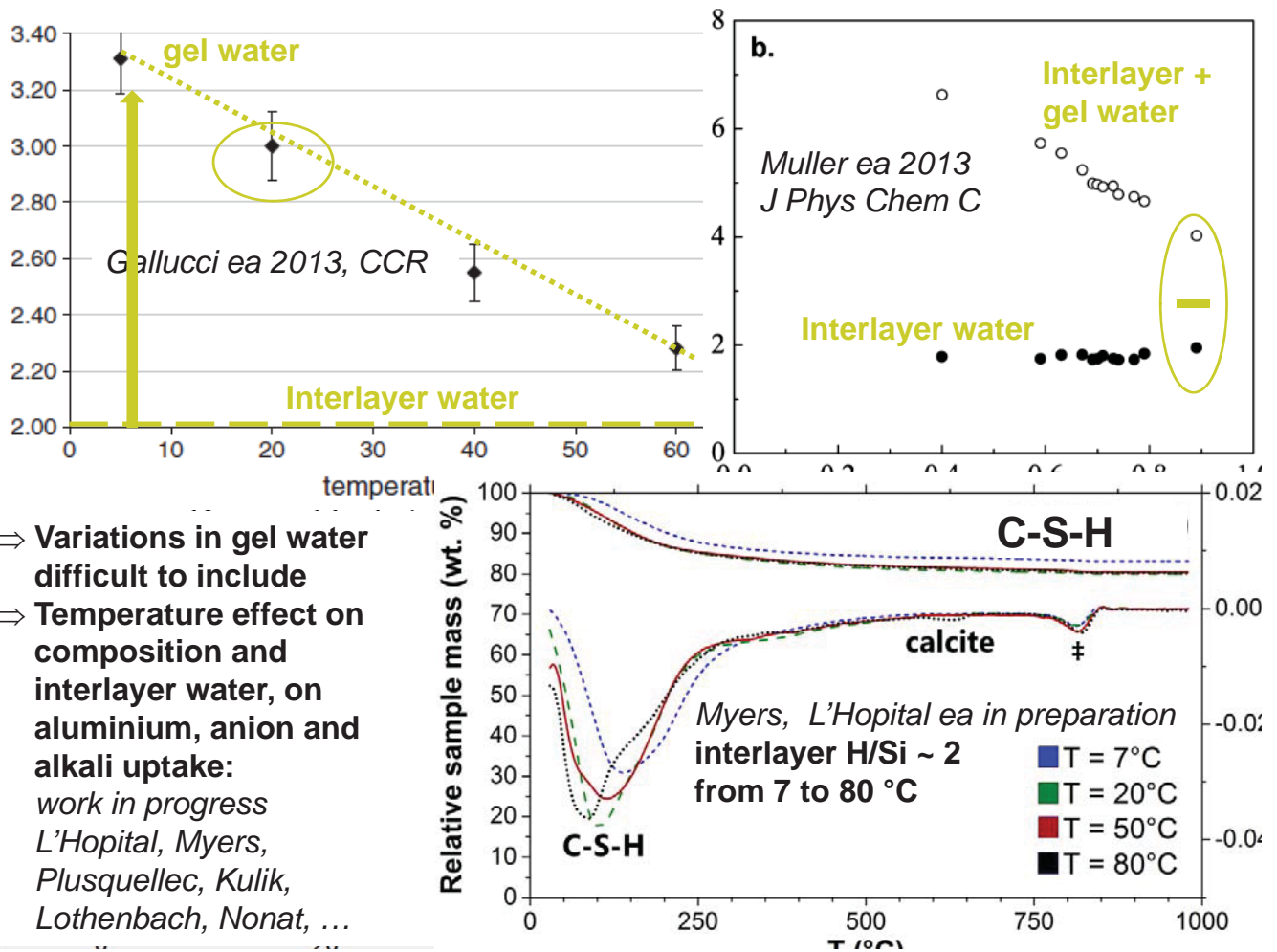
GEMS-Workshop May 2014, Dübendorf

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# Influence of temperature: 5% Cc

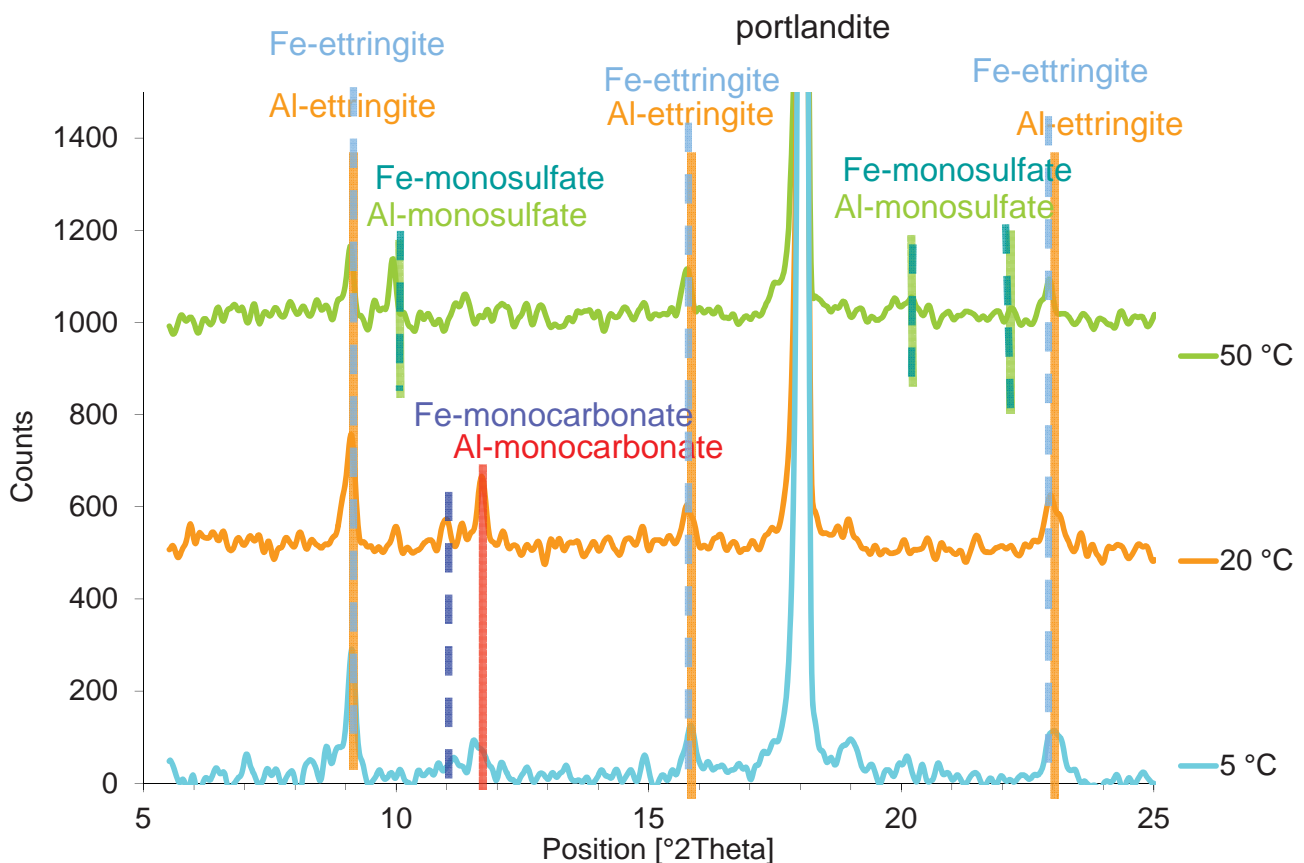






⇒ Variations in gel water difficult to include  
 ⇒ Temperature effect on composition and interlayer water, on aluminium, anion and alkali uptake:  
 work in progress  
 L'Hopital, Myers, Plusquellec, Kulik, Lothenbach, Nonat, ...

## What happens with the iron?



Lothenbach et al 2007, CCR 37

## Stability of Fe and Al-hydrates at 25 °C

(Solubility products refer to  $\text{Ca}^{2+}$ ,  $\text{OH}^-$ ,  $\text{Fe,Al}(\text{OH})_4^-$ ,  $\text{HSiO}_3^-$ ,  $\text{SO}_4^{2-}$ ,  $\text{CO}_3^{2-}$ )

Fe-hydrates		Al-hydrates		$\Delta$ Al-Fe
FH	-11.2	-1.3	$\text{AH}_3$	<b>-10</b>
$\text{C}_6\text{FsH}_{32}$	-44.0	-45.0	$\text{C}_6\text{AsH}_{32}$	1
$\text{C}_4\text{FsH}_{12}$	-31.6	-29.3	$\text{C}_4\text{AsH}_{12}$	-2
$\text{C}_4\text{FcH}_{12}$	-34.6	-31.5	$\text{C}_4\text{AcH}_{11}$	-3
$\text{C}_4\text{Fc}_{0.5}\text{H}_{10}$	-30.8	-29.1	$\text{C}_4\text{Ac}_{0.5}\text{H}_{10}$	-2
$\text{C}_3\text{FH}_6$	-26.3	-20.5	$\text{C}_3\text{AH}_6$	-6
$\text{C}_3\text{FS}_{0.84}\text{H}_{4.32}$	-34.2	-26.7	$\text{C}_3\text{AS}_{0.84}\text{H}_{4.32}$	<b>-8</b>

➡ Lower solubility product => higher stability

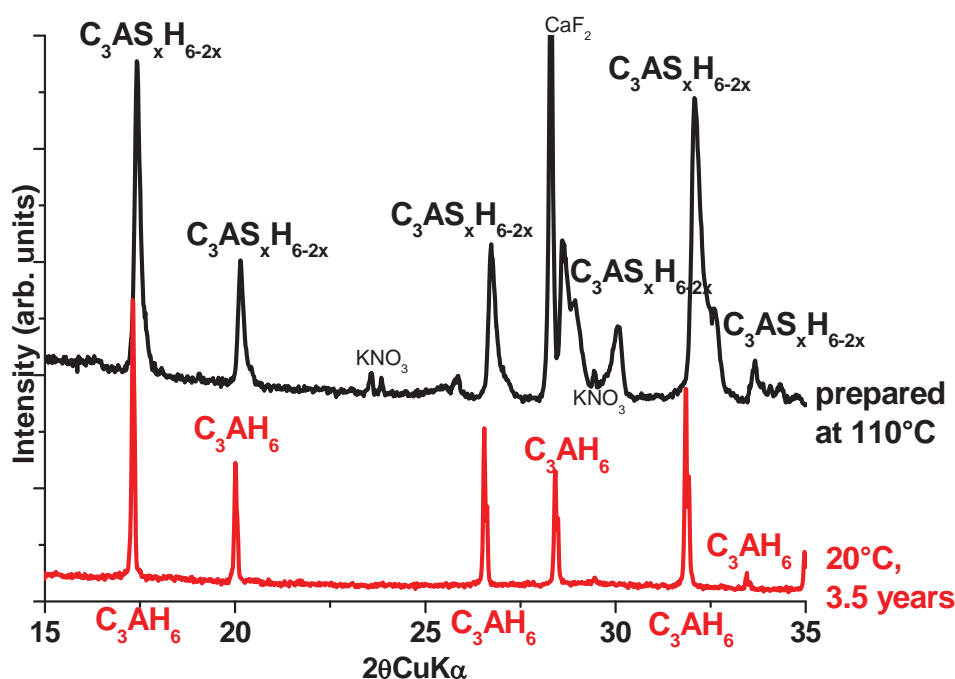
➡ **Stability Fe-ettringite < Fe-AFm <  $\text{FH}_3$ /Fe-siliceous hydrogarnet**

➡ **Formation of Al-containing siliceous hydrogarnet kinetically hindered at room temperature**

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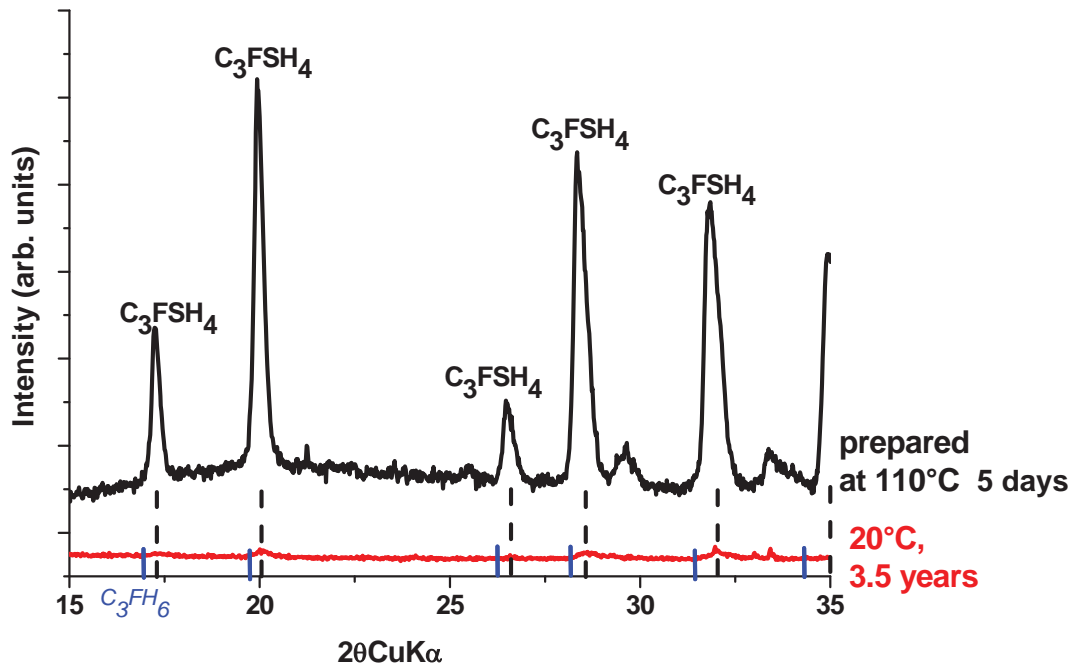
## Al siliceous hydrogarnet



Room temperature: only  $\text{C}_3\text{AH}_6$  + C-S-H forms;  
 $\text{C}_3\text{AS}_x\text{H}_{6-2x}$  forms at 110 °C, but remains stable at 20 °C

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# Fe siliceous hydrogarnet



**Low temperature Fe-siliceous hydrogarnet poorly crystalline  
=> difficult to detect by XRD**

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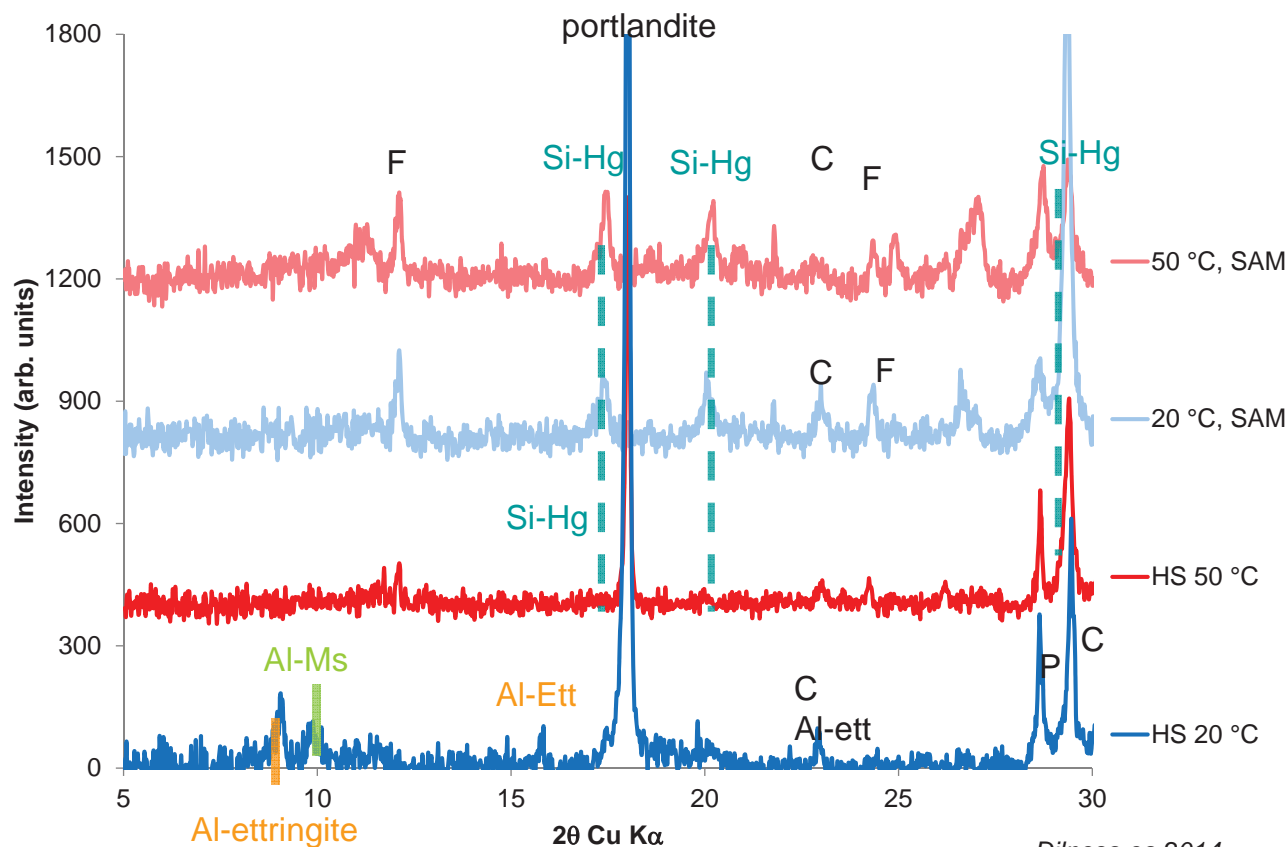
## Selective Dissolution using SAM

Salicylic Acid/Methanol Extraction (SAM)

Better identification of minor phases

- Dissolves
  - alite, belite, lime
  - CH, C-S-H, AFt and AFm phases
- Not affected:
  - $C_2(A,F)$ , periclase, calcite,
  - $C_3(A,F)SH_4$ , hydrotalcite, ...

# XRD OPC, 150 days: Siliceous hydrogarnet observed



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## EXAFS: Fe in siliceous hydrogarnet in the hydrated cement

At 20 °C								
Age	C <sub>2</sub> (A,F)	Fe(OH) <sub>3</sub>	C <sub>3</sub> FSH <sub>4</sub>	C <sub>3</sub> (A,F)SH <sub>4</sub>	Fe-Ht	C <sub>4</sub> FcH <sub>12</sub>	C <sub>6</sub> FS <sub>3</sub> H <sub>32</sub>	R-factor
Unhyd	1.00*	-	-	-	-	-	-	0.12
4 hrs	0.78(3)	0.20(3)	First hours			-	-	0.08
16 hrs	0.56(3)	0.44(3)	-	-	-	-	-	0.09
1 day	0.62(2)	-	-	0.38(2)	-	-	-	0.18
28 days	0.57(2)	-	-	0.43(2)	At ≥ 1 days			0.09
150 days	0.56(2)	-	-	0.44(2)	-	-	-	0.09
1 year	0.56(2)	-	-	0.44(2)	-	-	-	0.07
At 50 °C								
Age	C <sub>4</sub> AF	Fe(OH) <sub>3</sub>	C <sub>3</sub> FSH <sub>4</sub>	C <sub>3</sub> (A,F)SH <sub>4</sub>	Fe-Ht	C <sub>4</sub> FcH <sub>12</sub>	C <sub>6</sub> FS <sub>3</sub> H <sub>32</sub>	R-factor
Unhyd	1.00*	-	-	-	-	-	-	0.12
1 hrs	0.70(4)	0.30(4)	First hours			-	-	0.14
4 hrs	0.65(2)	0.35(2)	-	-	-	-	-	0.09
16 hrs	0.64(2)	-	-	0.36(2)	-	-	-	0.18
150 days	0.59(1)	-	-	0.41(1)	At ≥ 16 hours			0.09
1 year	0.58(2)	-	-	0.42(2)	-	-	-	0.07

20 °C

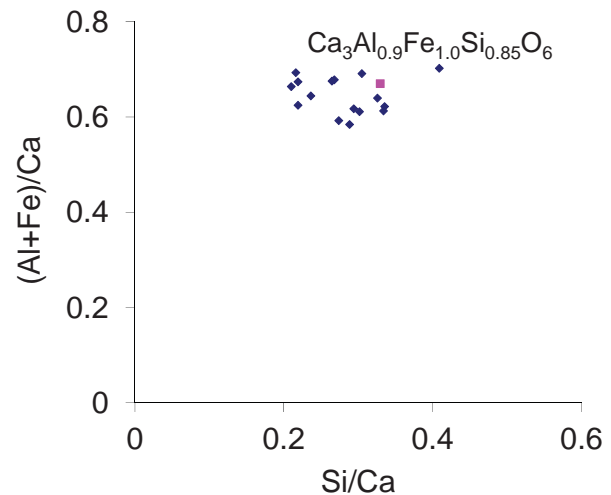
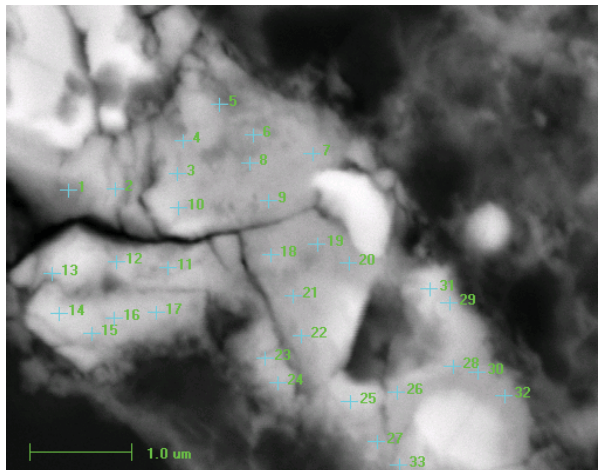
50 °C

>1 day:

iron present only in Fe siliceous hydrogarnet C<sub>3</sub>(A,F)S<sub>x</sub>H<sub>6-2x</sub>

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- Siliceous hydrogarnet observed in all samples
- Mixed siliceous hydrogarnet  $(C_3(A,F)S_{0.9}H_{4.2})$

## Conclusion: Fate of iron oxides

### Thermodynamic modelling:

$C_3FSH_4$  stable from 1 to 60 °C

$C_3ASH_4$  stable but formation kinetically hindered (suppressed in calculations)

### Experimental evidence:

XAFS spectroscopy => Fe associated with  $C_3(A,F)S_xH_{6-2x}$

Similar amount of siliceous hydrogarnet at 20 and 50 °C

XRD, TGA,  $C_3(A,F)SH_4$  present in hydrated cements  
but difficult to detect; more crystalline at 50°C

SEM: Mixed Al/Fe siliceous hydrogarnet

Phase/species	L	T	Amount (mol)	logSI/Activity	Concentration	A
a aq_gen	69	a	0.47421475	8.907e-10		
g gas_gen	5	g	0.0031148901	1.938e-10		
s C3(A,F)S0.84H	2	s	0.011454257	-3.416e-09		
C3AS0.84H4.32	I	I	0.005192054	0.453286	0.45328598	1
C3FS0.84H4.32	I	I	0.0062622028	0.546714	0.54671402	1
s CSHQ	4	s	0.46350181	2.004e-09		
s SO4 OH AFm	2	s	0	-1		
s OH SO4 AFm	2	s	0	-1		
s SO4 CO3 AFt	2	s	0.018760835	-1.991e-09		
s CO3 SO4 AFt	2	s	3.9158123e-009	0.004993		
s hydrotalc-pyro	2	s	0	-8.645		
s Al(OH)3mic	1	s	0	-3.194		
s Gibbsite	1	s	0	-2.671		
s Kaolinite	1	s	0	-15.12		
s Graphite	1	s	0	-83.75		
s Mayenite	1	s	0	-145.1		
s Belite	1	s	0	-1.859		
s Aluminat	1	s	0	-38.92		
s Alite	1	s	0	-14.12		
s Ferrite	1	s	0	-36.89		
s CA	1	s	0	-13		
s CA2	1	s	0	-18.97		
s C2AH75	1	s	0	-4.164		
s C3AH6	1	s	0	-2.672		
s C4AH13	1	s	0	-3.238		
s C4AH19	1	s	0	-2.835		
s CAH10	1	s	0	-5.211		
s C2ASH8	1	s	0	-2.898		
s C4Ac0.5H12	1	s	0	-0.7393		
s C4AcH11	1	s	0.0188822	5.777e-09		
s Aragonite	1	s	0	-0.1441		
s Calcite	1	s	0.0247094	3.357e-09		
s C3FH6	1	s	0	-2.576		
s C4FH13	1	s	0	-2.731		
s C3FS0.84H4.32	1	s	0	-0.2622		
s C3FS1.34H3.32	1	s	0	-0.9075		
s C4Fc05H10	1	s	0	-5.017		
s C4FcH12	1	s	0	-2.688		
s lime	1	s	0	-9.957		

**Solution**  
**Hydrogarnet/hydroandradite**  
**(C3(A,F)S0.84H4.32)**  
**C-S-H**  
**CH**  
**Ettringite**  
**Monocarbonate**  
**hydrotalcite**

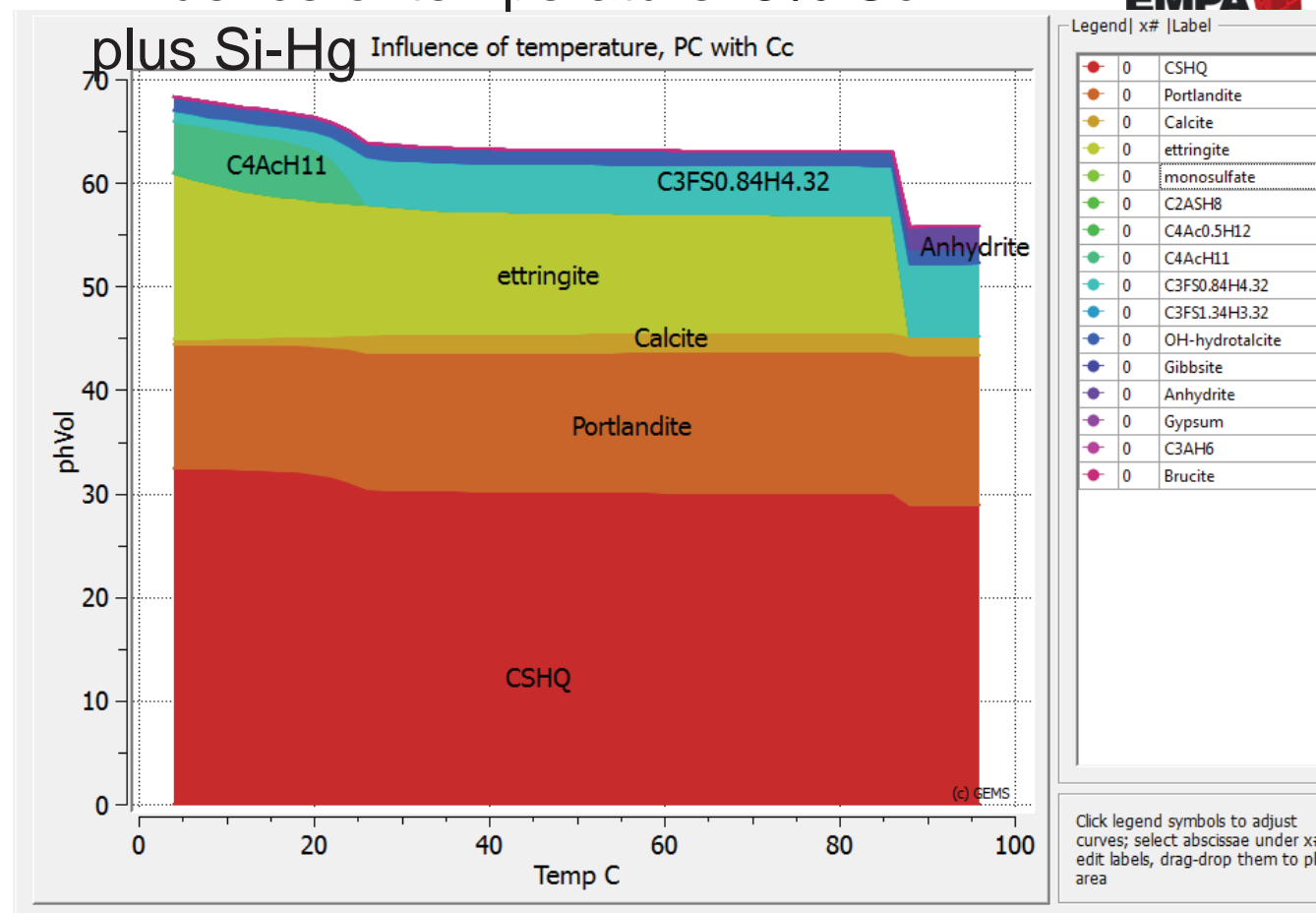
**Note  $C_3AS_{0.42}H_{5.16}$ :**  
**not activated in database**  
**=> suppressed during all**  
**calculations as its formation not**  
**observed at ambient conditions**  
**(to include create an additional**  
**Phase refering to**  
**Dcomp:  $C_3AS_{0.42}H_{5.16}$ )**

ystem: T = 293.15 K; P = 1.00 bar; V = 0.1506 L; Aqueous: built-in EDH(H); pH = 13.785; pe = 7.365; IS = 0.568 m

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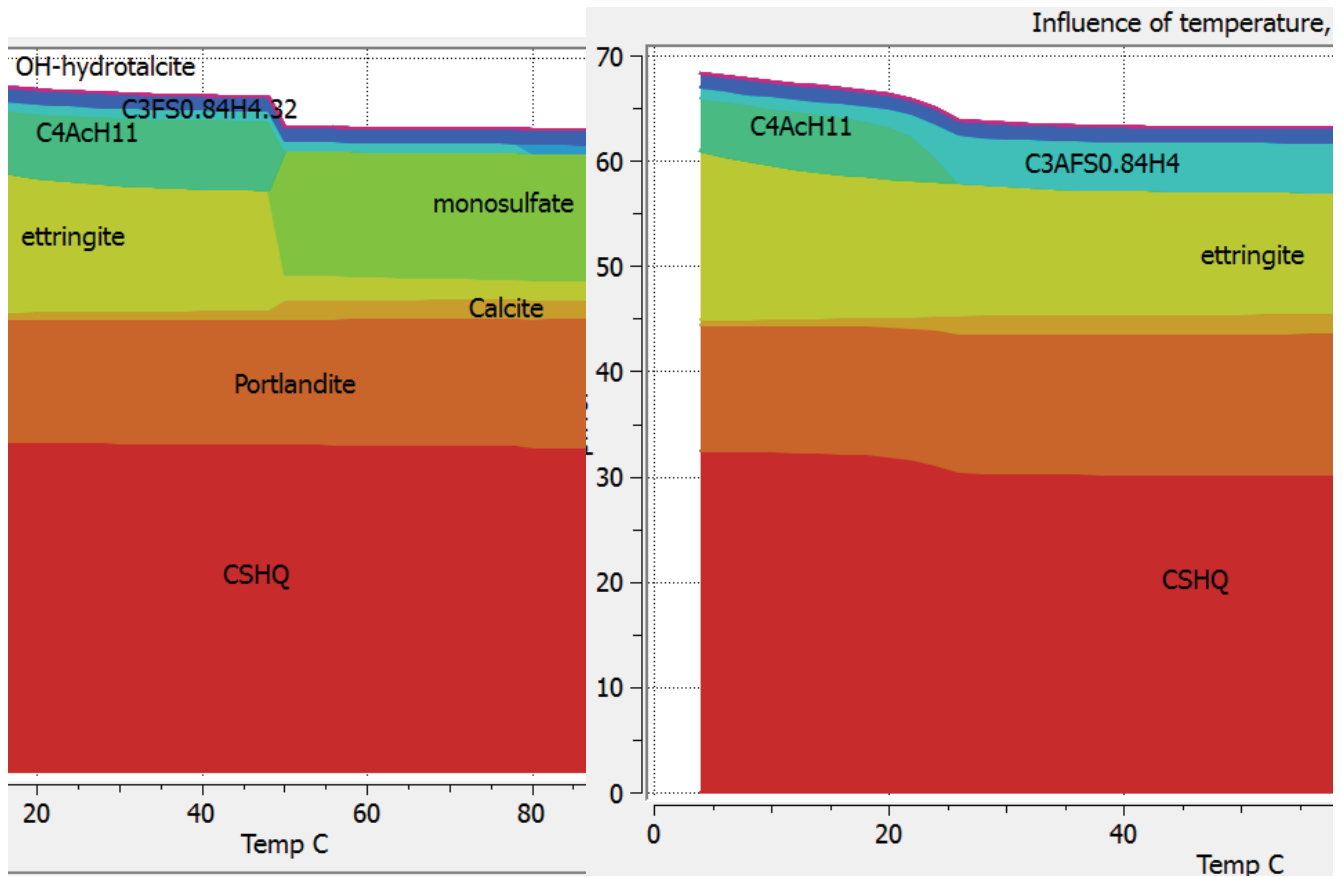
## Influence of temperature: 5% Cc

plus Si-Hg Influence of temperature, PC with Cc



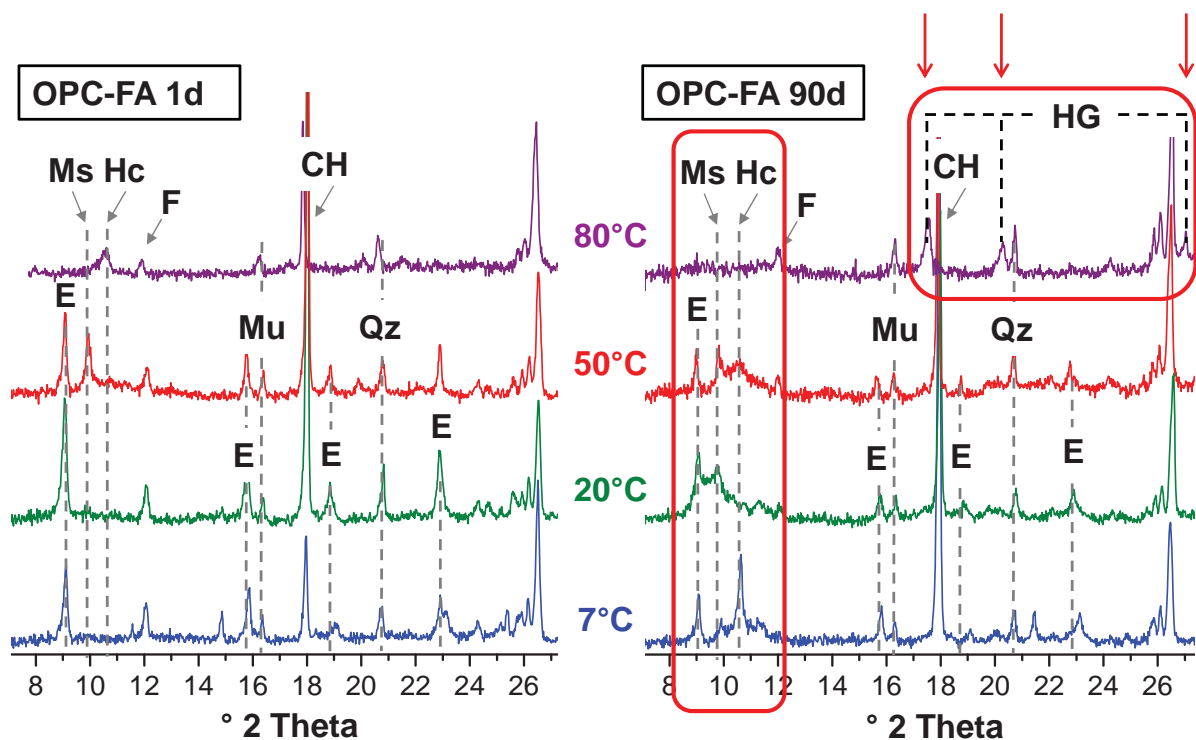
No  $C_3AS_{0.84}H_{4.32}$

With  $C_3AS_{0.84}H_{4.32}$

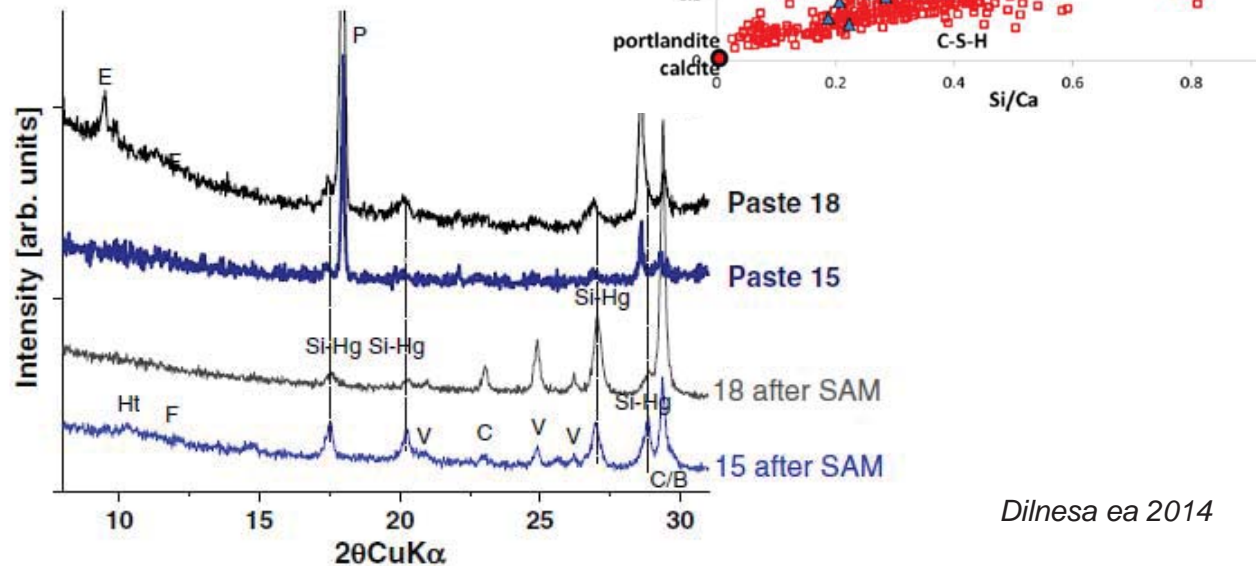


## siliceous hydrogarnet

siliceous hydrogarnet in OPC blended with fly ash)



**Si-hydrogarnet / no AFm  
observed in very old cements  
hydrated 50 years at 20 °C**



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## Influence of temperature



Higher temperature:

→ faster kinetic of PC hydration and  $SiO_2$  reaction:

### OPC

→ **47 °C**: ettringite, monocarb. → monosulfate

→ volume decrease => decrease in strength

### longterm

→ Hydrogarnet-hydrogrossular instead of AFm

**In addition changes in CSH volume (water content);**

**Not captured in present CSH model (no gel water present)!**