Lecture 05
Hydration

a) **Reaction of cement clinker**
b) **Hydration modelling with GEMS**

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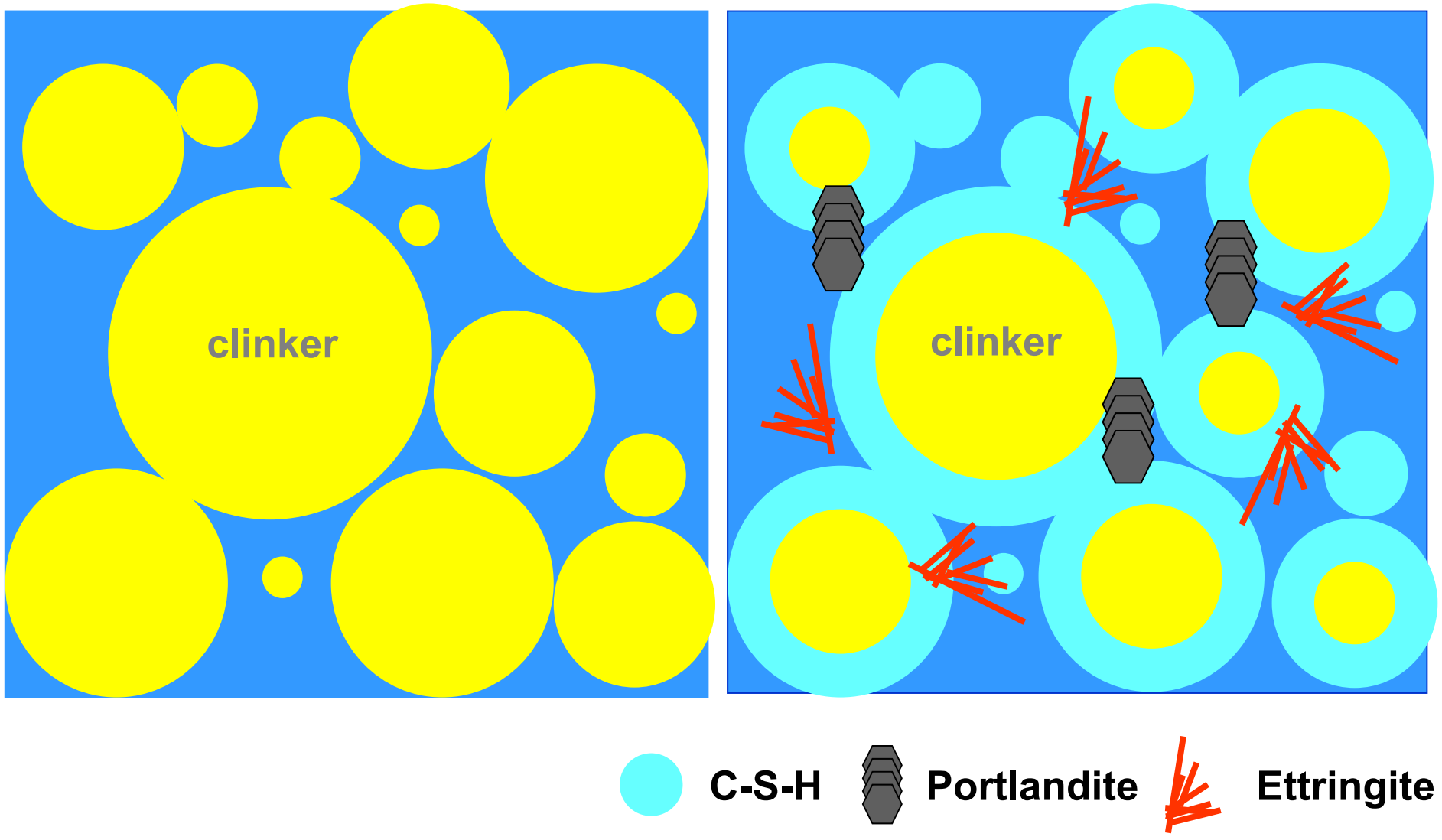
Hydration



Modeling: Dissolution

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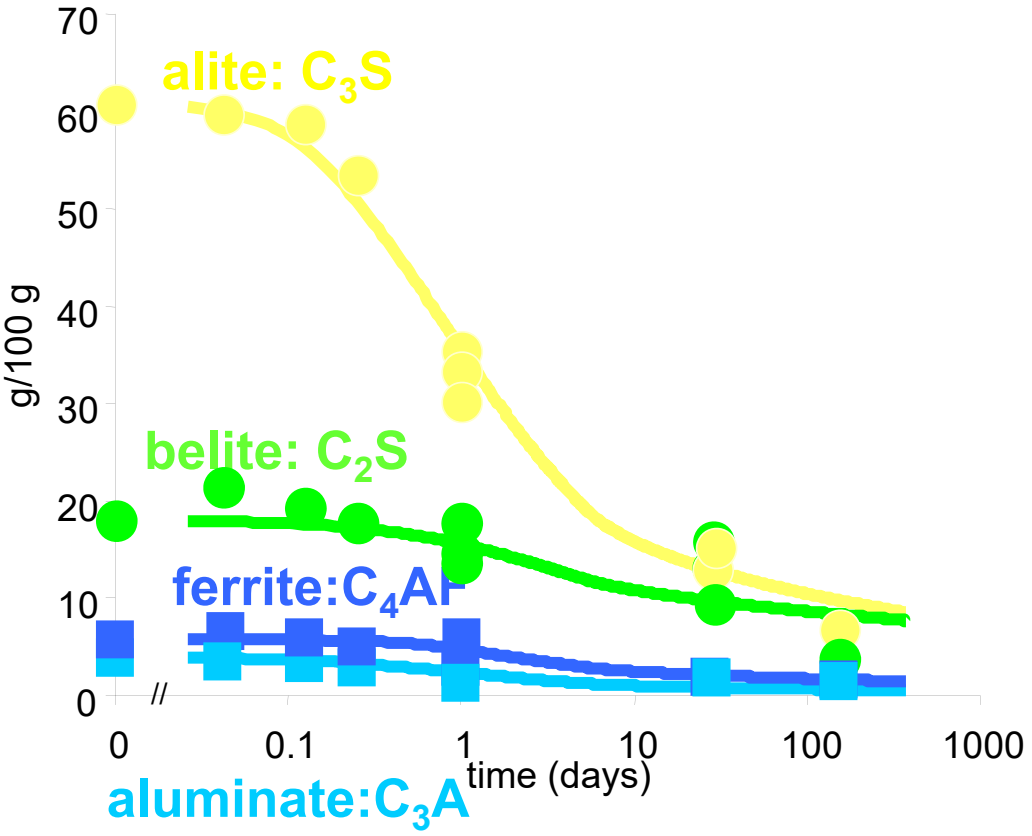
Empirical Approach: Parrot and Killoh (1984)

$$R_t = \frac{K_1}{N_1}(1-\alpha_t)(-\ln(1-\alpha_t))^{(1-N_1)}$$

$$R_t = \frac{K_2 \times (1-\alpha_t)^{2/3}}{1-(1-\alpha_t)^{1/3}}$$

$$R_t = K_3 \times (1-\alpha_t)^{N_3}$$

All parameters (K_i, N_i) from Parrot and Killoh (1984)



Cement specific input: surface area, w/c, composition

Modeling: Dissolution

Empirical Approach: Parrot and Killoh (1984)

nucleation

$$R_t = \frac{K_1}{N_1}(1-\alpha_t)(-\ln(1-\alpha_t))^{(1-N_1)}$$

diffusion

$$R_t = \frac{K_2 \times (1-\alpha_t)^{2/3}}{1-(1-\alpha_t)^{1/3}}$$

shell

$$R_t = K_3 \times (1-\alpha_t)^{N_3}$$

degree of hydration

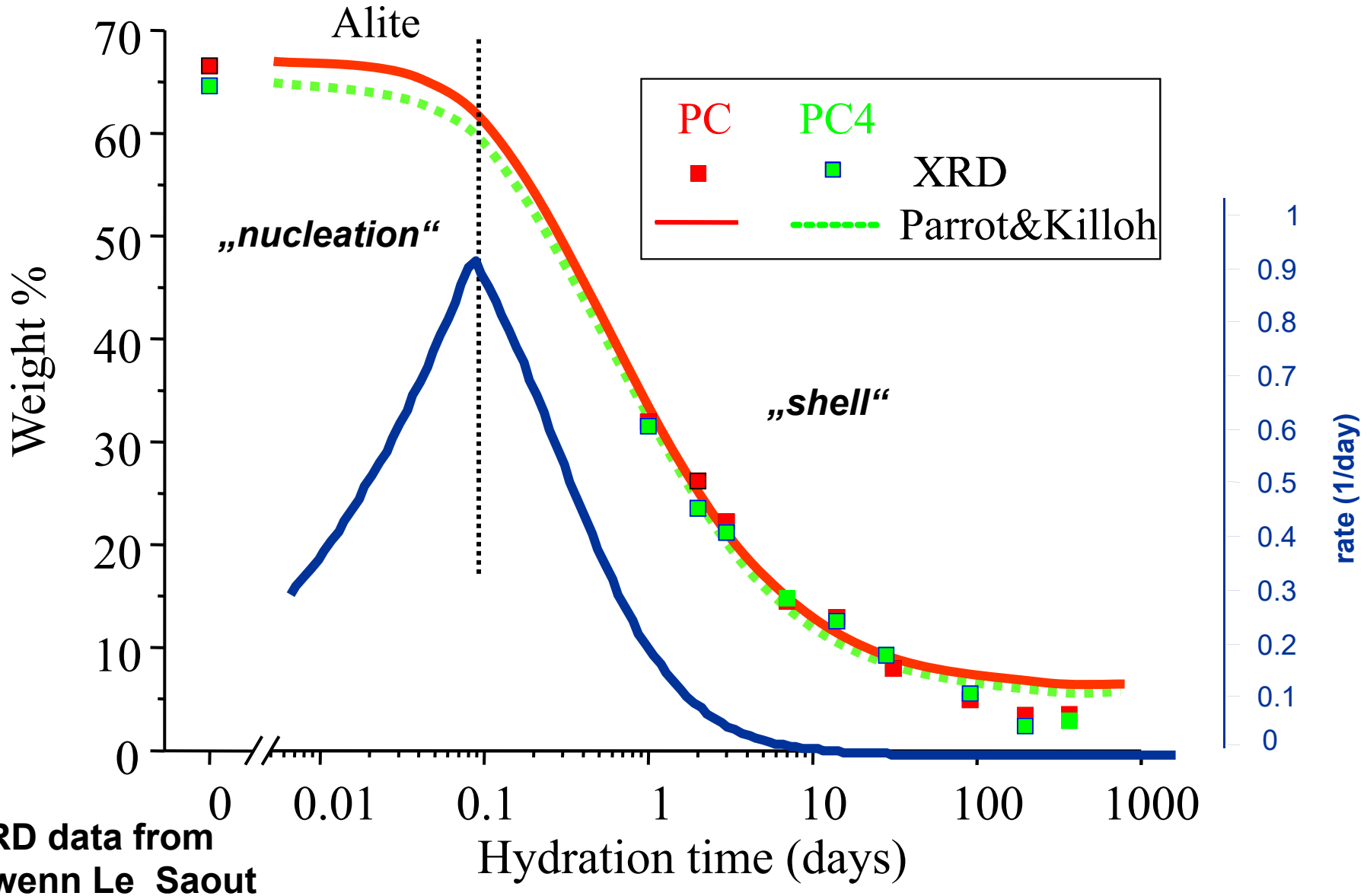
$$\alpha_t = \alpha_{t-1} + \Delta t \cdot R_{t-1} \cdot (1+3.333 \cdot (H \cdot {}^{w}/_{c} - \alpha_t))^4$$

for $\alpha_t > H \cdot {}^{w}/_{c}$.

	alite	belite	alum.	ferrite
K_1	1.5	0.5	1.0	0.37
N_1	0.7	1.0	0.85	0.7
K_2	0.05	0.006	0.04	0.015
K_3	1.1	0.2	1.0	0.4
N_3	3.3	5.0	3.2	3.7
H	1.33	1.33	1.33	1.33

Cement specific input: surface area, w/c

Modeling: Dissolution



XRD data from Gwenn Le Saout

Modeling: Dissolution

Empirical Approach: Parrot and Killoh adapted

Lothenbach et al. (2008) 38, 848-860

nucleation

$$R_t = \frac{K_1}{N_1}(1-\alpha_t)(-\ln(1-\alpha_t))^{(1-N_1)}$$

$$R_t = \frac{K_2 \times (1-\alpha_t)^{2/3}}{1-(1-\alpha_t)^{1/3}}$$ *diffusion*

$$R_t = K_3 \times (1-\alpha_t)^{N_3}$$ *shell*

degree of hydration

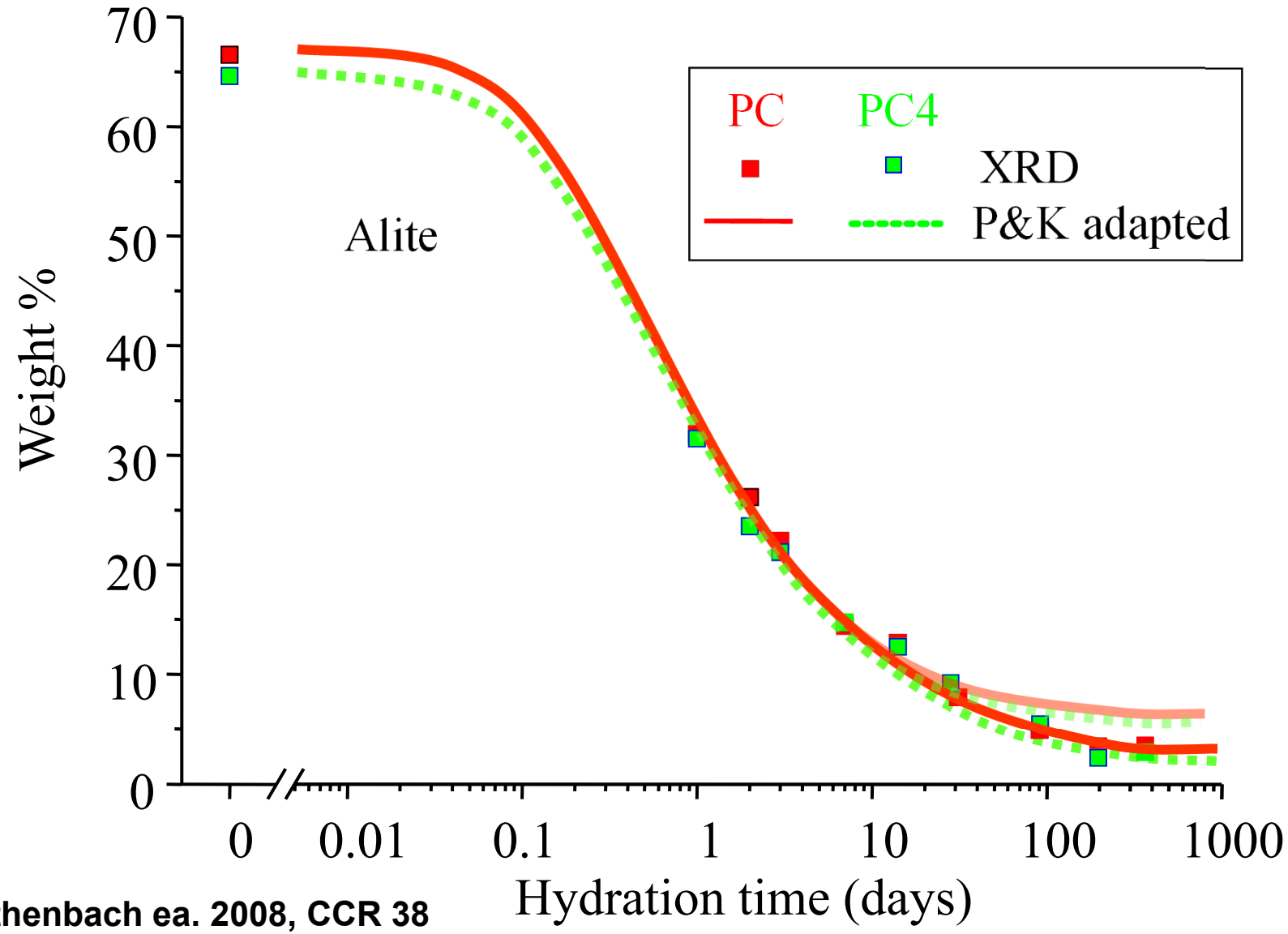
$$\alpha_t = \alpha_{t-1} + \Delta t \cdot R_{t-1} \cdot (1+3.333 \cdot (H \cdot {}^{w}/_{c} - \alpha_t))^4$$

for $\alpha_t > H \cdot {}^{w}/_{c}$.

	alite	belite	alum.	ferrite
K_1	1.5	0.5	1.0	0.37
N_1	0.7	1.0	0.85	0.7
K_2	0.05	**0.02**	0.04	0.015
K_3	1.1	**0.7**	1.0	0.4
N_3	3.3	5.0	3.2	3.7
H	**2.0**	**1.55**	**1.8**	**1.65**

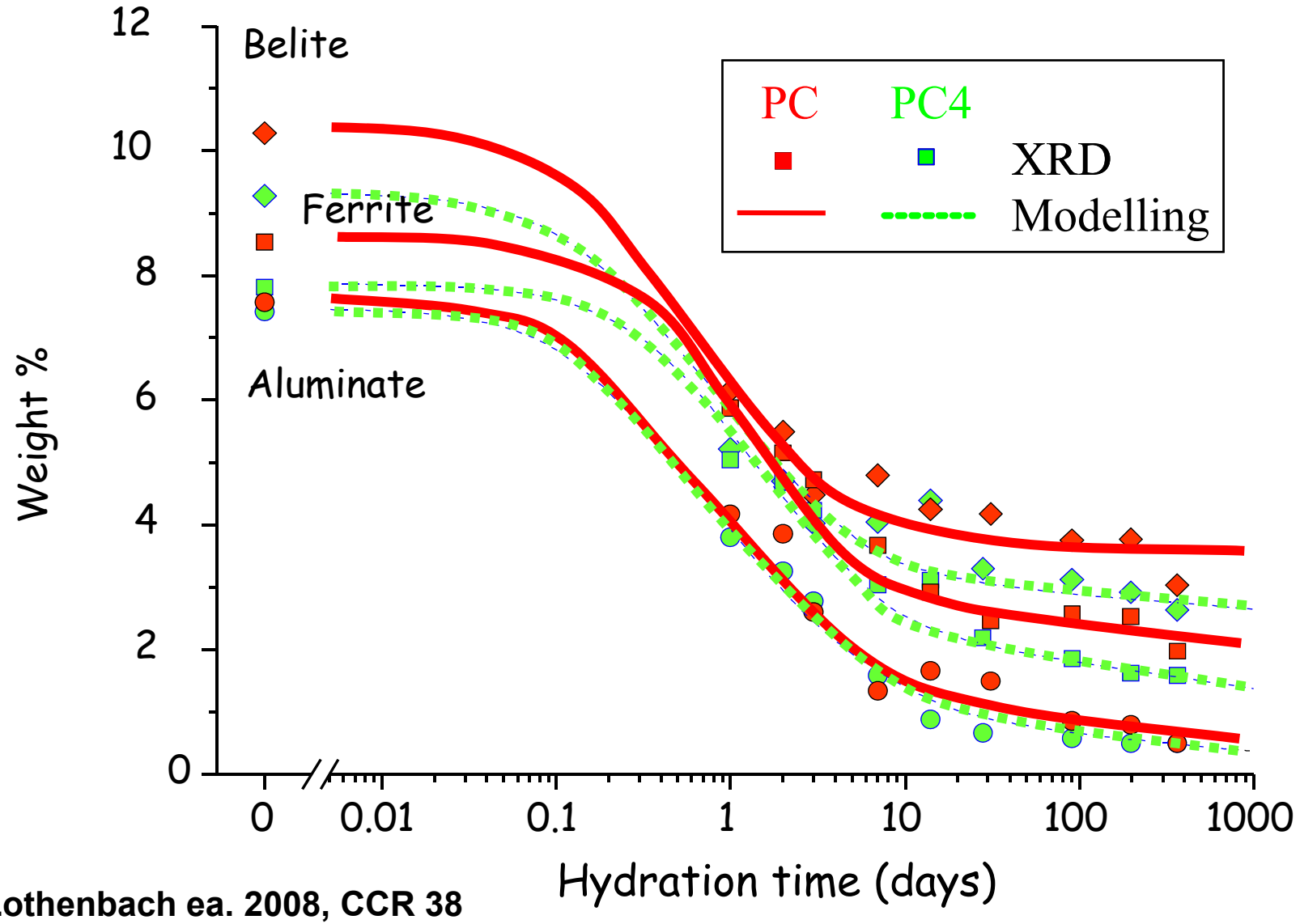
Cement specific input: surface area, w/c

Modeling: Dissolution



Lothenbach ea. 2008, CCR 38

Modeling: Dissolution



Lothenbach ea. 2008, CCR 38

Thermodyn. calculations

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Multi-component input

I Slowly soluble clinkers

C_3S C_2S
C_3A C_4AF

K_2O
Na_2O
MgO

II Soluble solids

K_2SO_4
Na_2SO_4
Hemihydrate
CaO

Gypsum
Anhydrite
Calcite

III Water

H_2O

Thermodynamic modeling
GEMS-PSI

Ca^{2+}
$CaOH^+$
$CaSO_4^0$
Speciation in solution

Portlandite

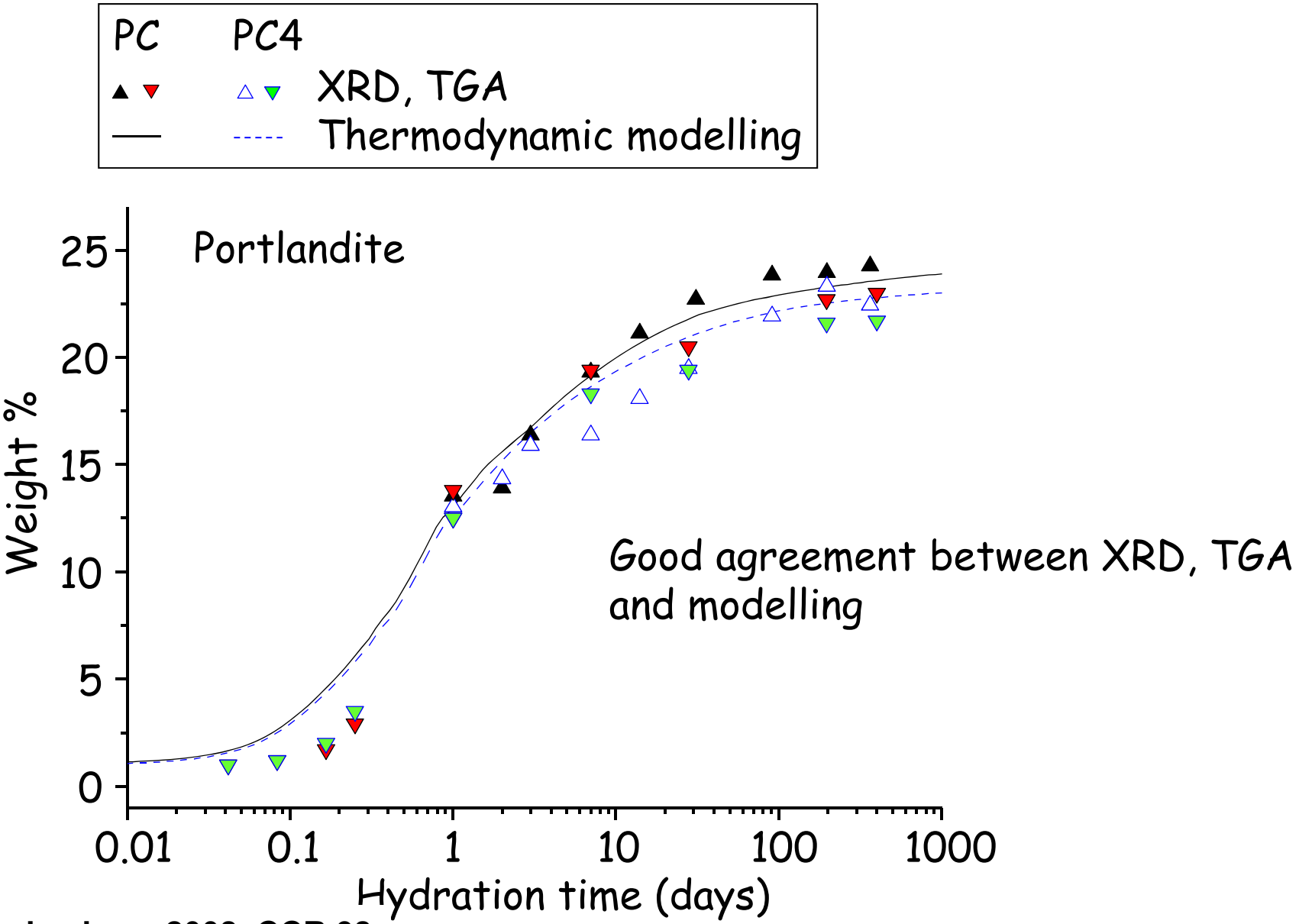
C-S-H

Ettringite

AFm

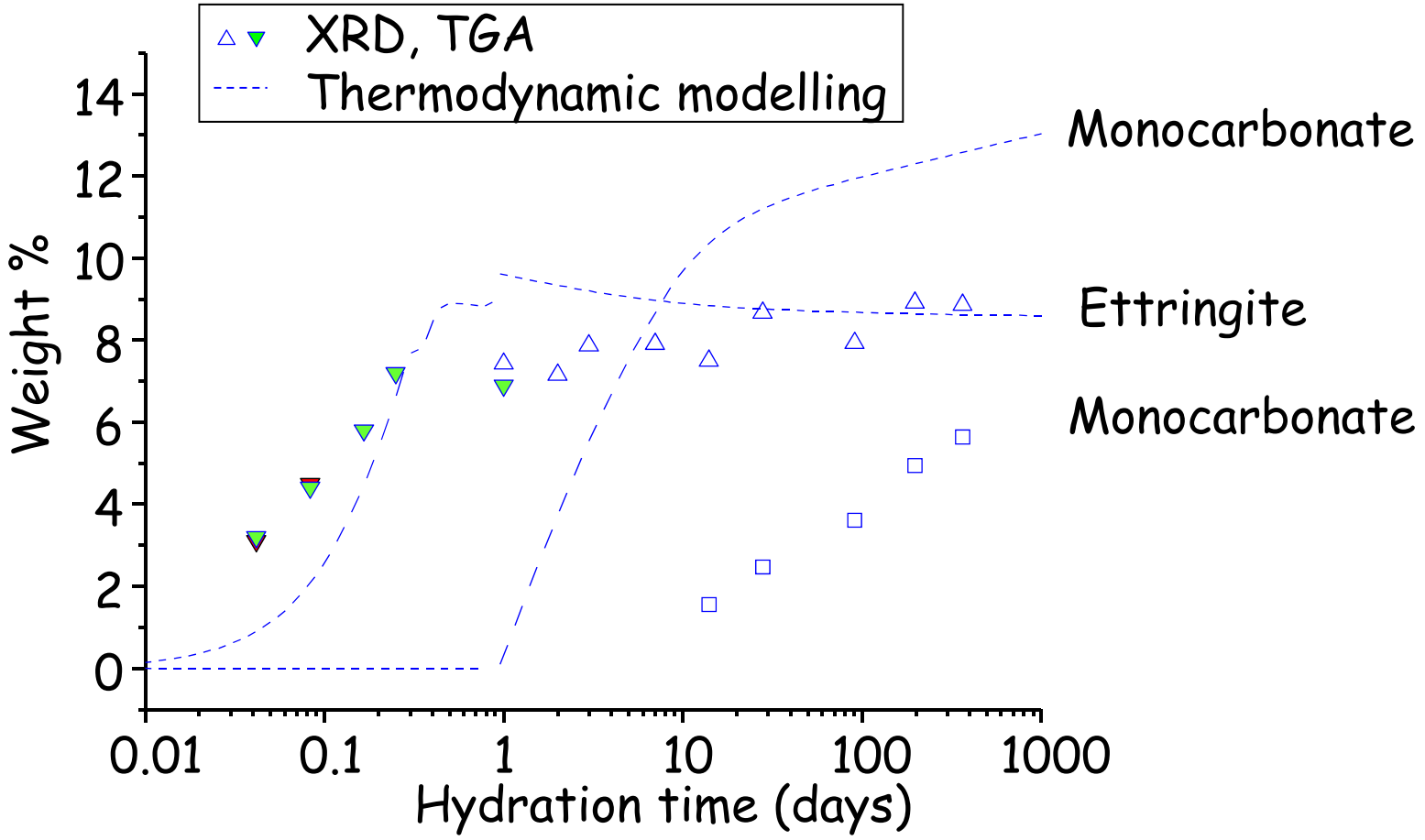
Hydrotalcites, ...

Output data, Portlandite



Lothenbach ea. 2008, CCR 38

Output data, AFt, AFm phases



- Overestimation of monocarbonate (<= hemicarbonate, Al in C-S-H)
- Correct amount of ettringite in the PC sample

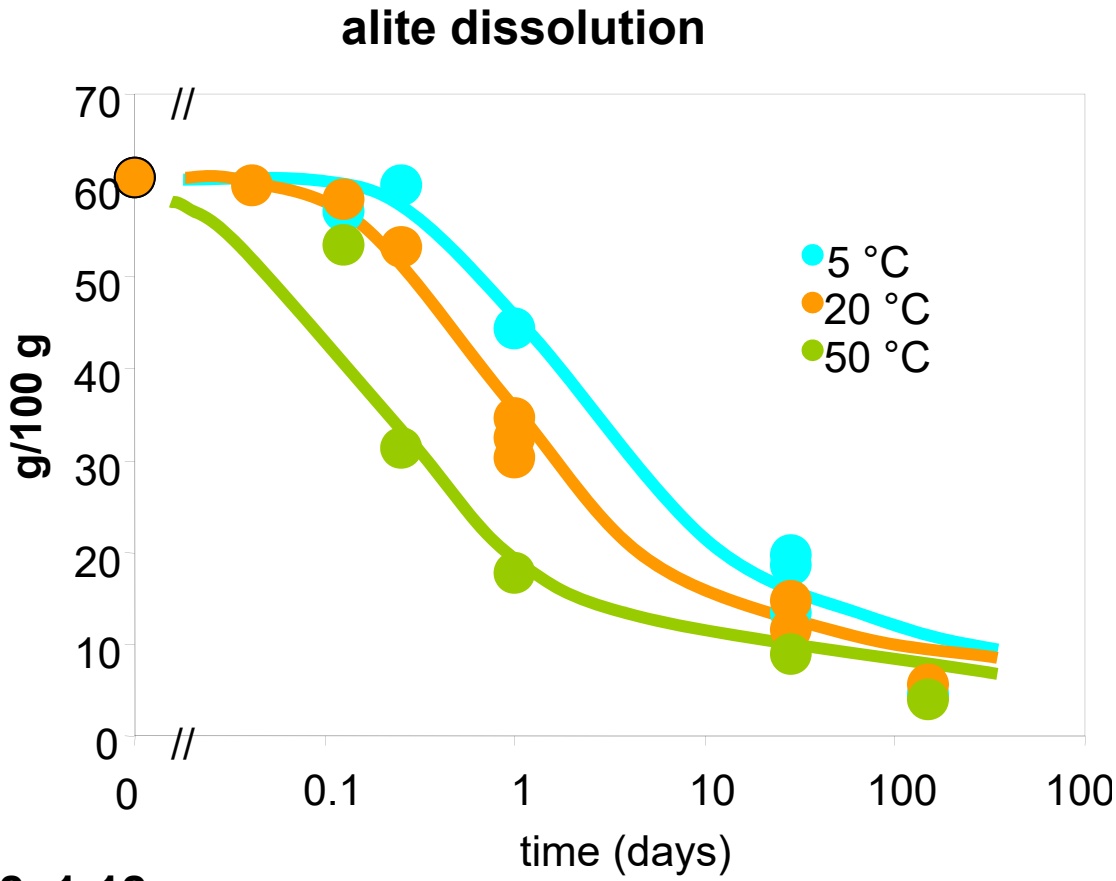
Lothenbach ea. 2008, CCR 38

Modeling: Temperature

Arrhenius equation

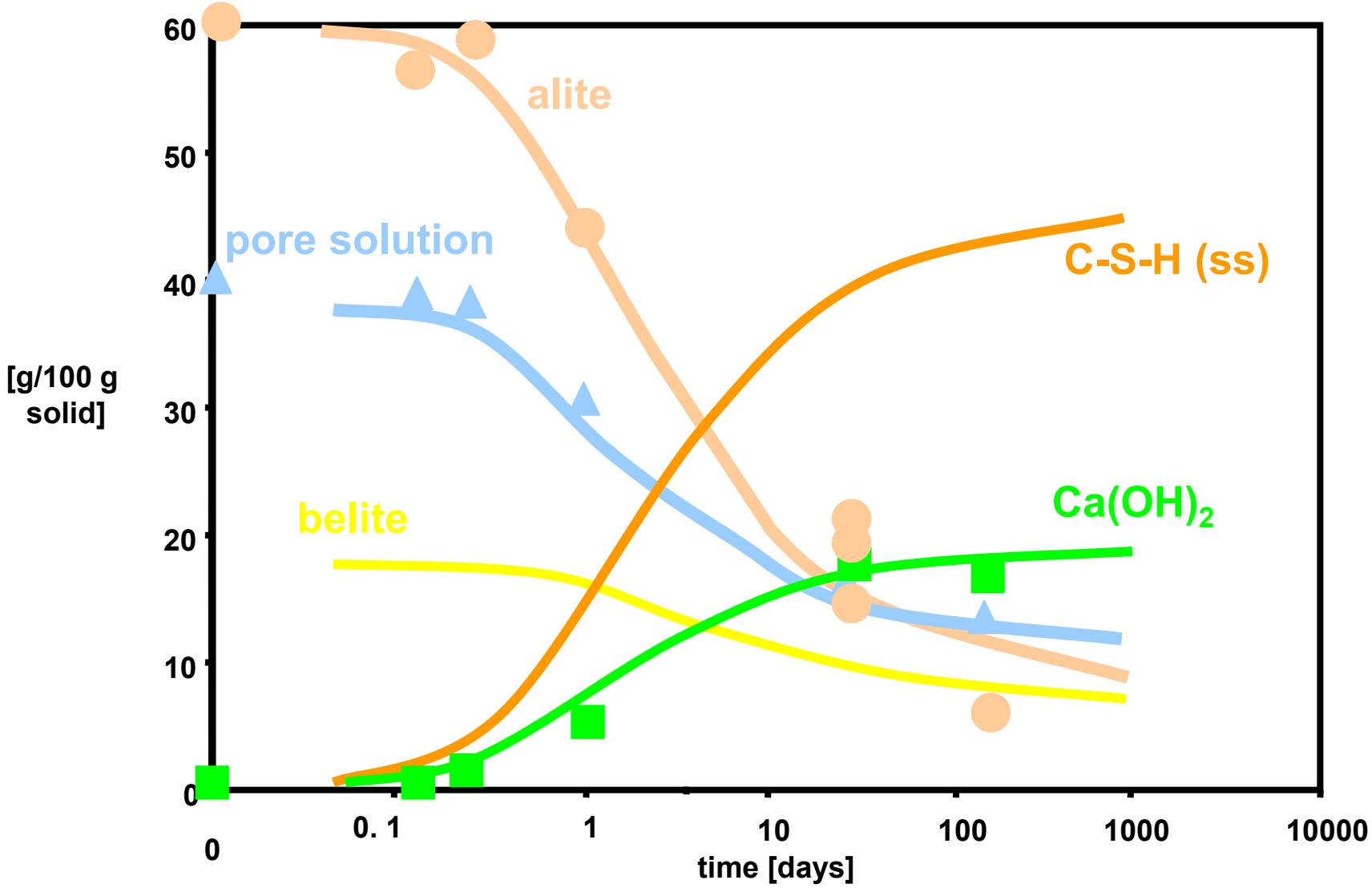
$$R_T = A\, e^{-\frac{E_a}{RT}}$$

E_a: literature

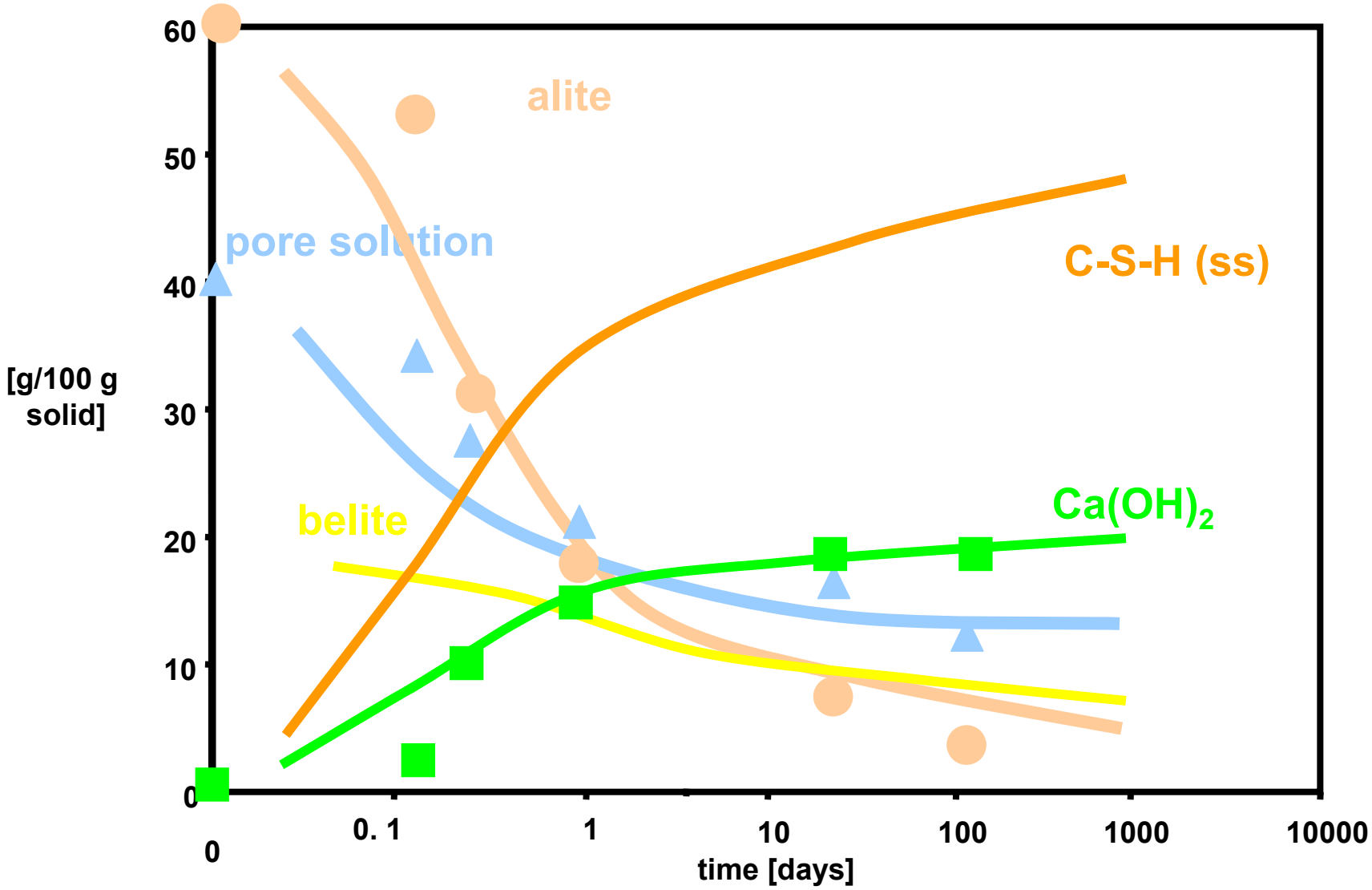


Lothenbach et al. (2008) CCR 38, 1-18

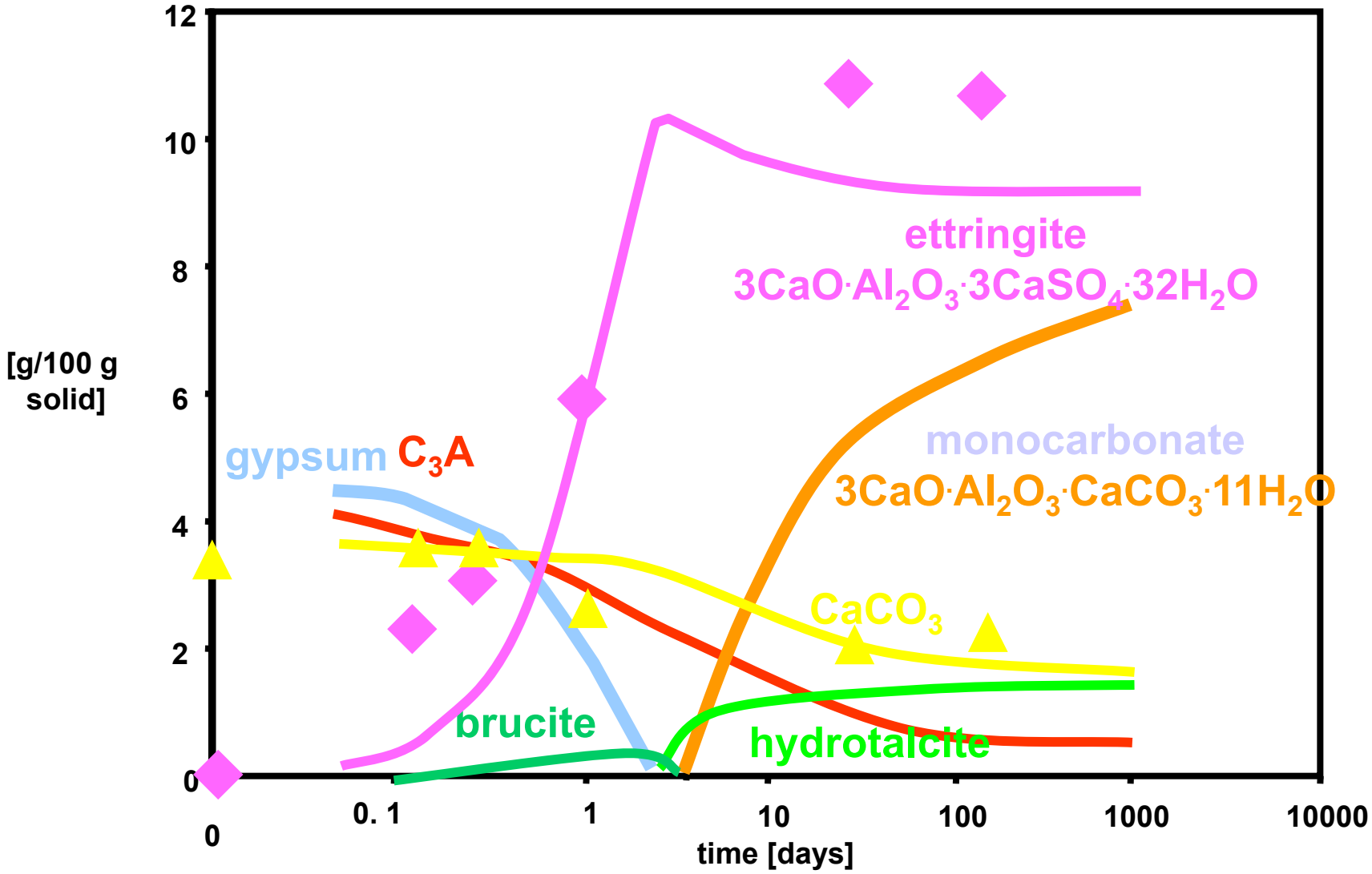
Ca- and Si-hydrates: 5 °C



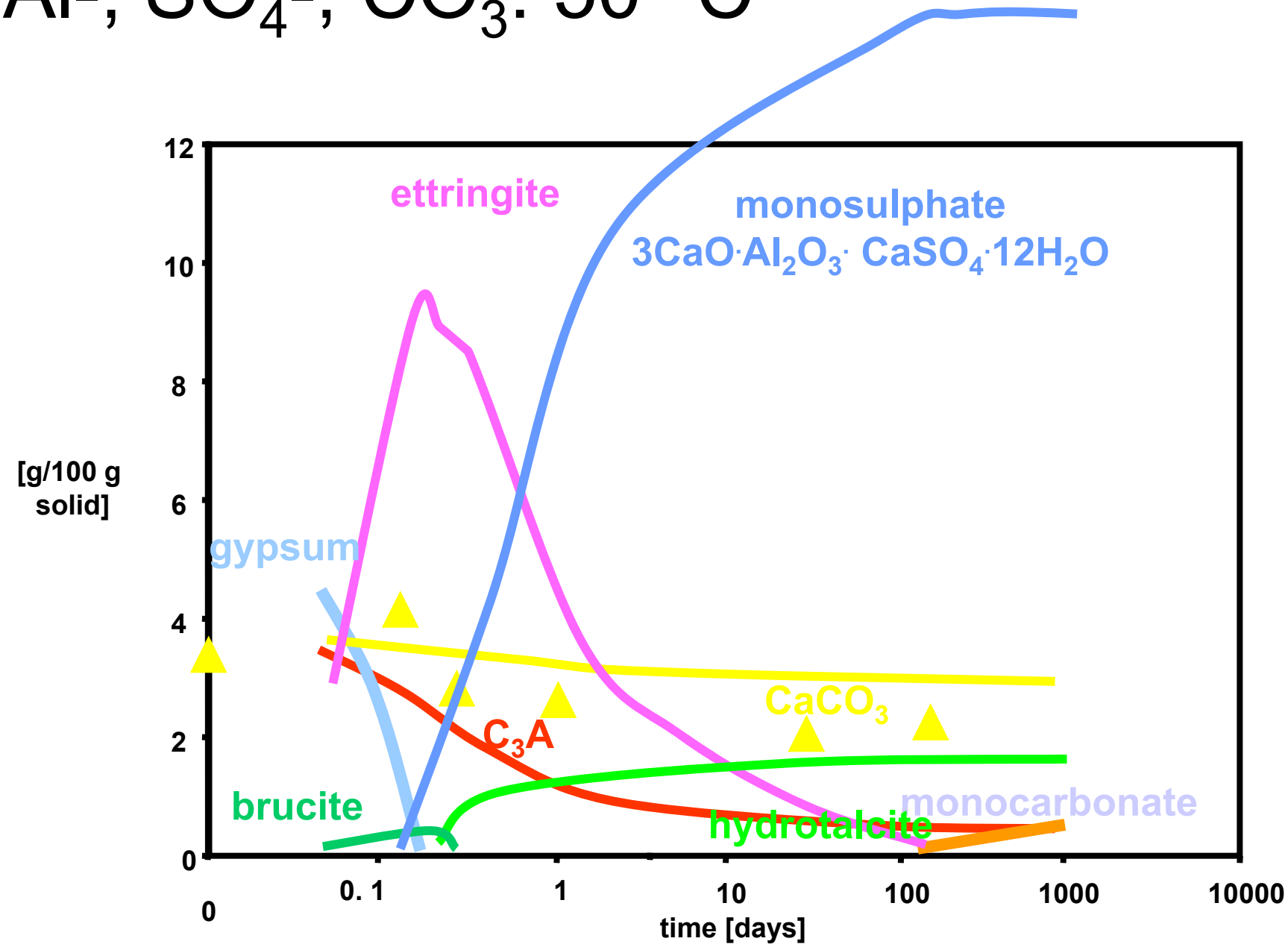
Ca- and Si-hydrates: 50 °C



Al-, SO_4-, CO_3: 5 °C


12
10
8
6
4
2
0
[g/100 g solid]
0
0. 1
1
10
100
1000
10000
time [days]
ettringite
3CaO·Al2O3·3CaSO4·32H2O
monocarbonate
3CaO·Al2O3·CaCO3·11H2O
gypsum
C3A
CaCO3
brucite
hydrotalcite

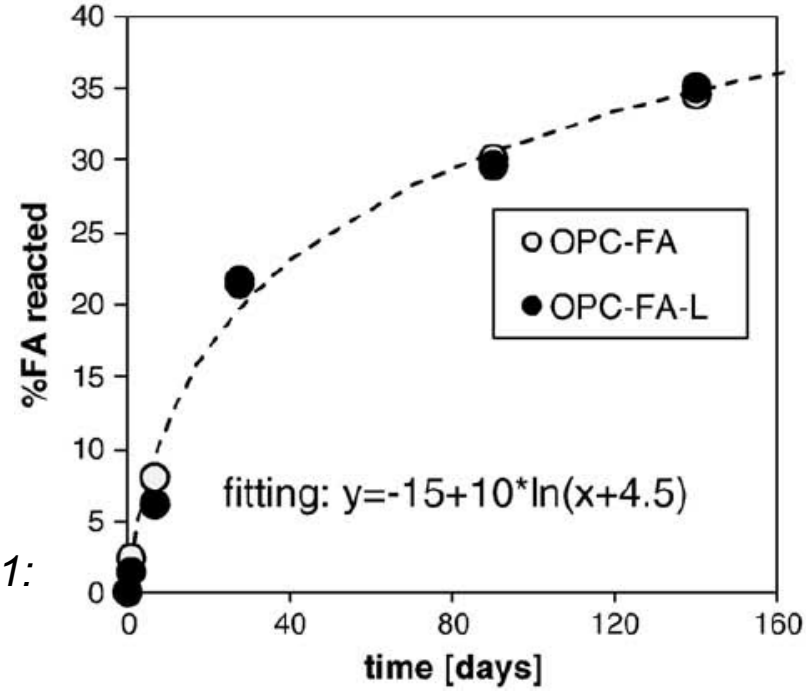
Al-, SO_4-, CO_3: 50 °C



Conclusion

- Empirical approach of P&K (adapted)
  - Describes observed dissolution (> 1 day) in OPC well
  - Simple to use
  - Influencing parameters: **surface area, w/c, temperature**
  - Purely empirical, other models can be used
  - Other influences: pH, composition of pore solution, … not included

- Other models can be used
  - Any (empirical) equation which describes the reaction of solid as a function of time



De Weerdt ea (2011) CCR 41: Reaction degree of fly ash

Modeling: Dissolution

$$R_{t,T} = \frac{K_1}{N_1}(1-\alpha_t)(-\ln(1-\alpha_t))^{(1-N_1)}\left(\frac{rh-0.55}{0.45}\right)^4 \frac{surface\ area}{385} e^{-\frac{E_a}{R}(\frac{1}{T}-\frac{1}{T_0})}$$

$$R_{t,T} = \frac{K_2 \times (1-\alpha_t)^{2/3}}{1-(1-\alpha_t)^{1/3}}\left(\frac{rh-0.55}{0.45}\right)^4 e^{-\frac{E_a}{R}(\frac{1}{T}-\frac{1}{T_0})}$$

$$R_{t,T} = K_3 \times (1-\alpha_t)^{N_3}\left(\frac{rh-0.55}{0.45}\right)^4 e^{-\frac{E_a}{R}(\frac{1}{T}-\frac{1}{T_0})}$$

Relative surface area factor used for „nucleation and growth“ only (relative to Dalziel & Gutteridge, 1986)

Influence of temperature Arrhenius equation Ea values: Lothenbach et al., 2008

Influence of the relative humidity as proposed in Parrot and Killoh, 1984

Hydration in closed systems: rh =1

Cement specific input: surface area [m²/kg], w/c, composition

Modeling: Dissolution

$$R_{t,T} = \frac{K_1}{N_1}(1-\alpha_t)(-\ln(1-\alpha_t))^{(1-N_1)}\left(\frac{rh-0.55}{0.45}\right)^4 \frac{surface\,area}{385} e^{-\frac{E_a}{R}(\frac{1}{T}-\frac{1}{T_0})}$$

$$R_{t,T} = \frac{K_2 \times (1-\alpha_t)^{2/3}}{1-(1-\alpha_t)^{1/3}}\left(\frac{rh-0.55}{0.45}\right)^4 e^{-\frac{E_a}{R}(\frac{1}{T}-\frac{1}{T_0})}$$

$$R_{t,T} = K_3 \times (1-\alpha_t)^{N_3}\left(\frac{rh-0.55}{0.45}\right)^4 e^{-\frac{E_a}{R}(\frac{1}{T}-\frac{1}{T_0})}$$

degree of hydration of each clinker phase

- *initial* $\alpha_t = \alpha_{t-1} + \Delta t \cdot R_{t-1}$
- *later, for* α_{t-1}(total) > *H·w/c;*
  *H·**w/c** = critical degree of hydration*

$$\alpha_t = \alpha_{t-1} + \Delta t \cdot R_{t-1} \cdot (1+3.333 \cdot (H \cdot w/c - \alpha_t))^4$$

Hydration is reduced with time at low w/c

Cement specific input: surface area [m²/kg], w/c, composition

Parrot and Killoh model as Excel file

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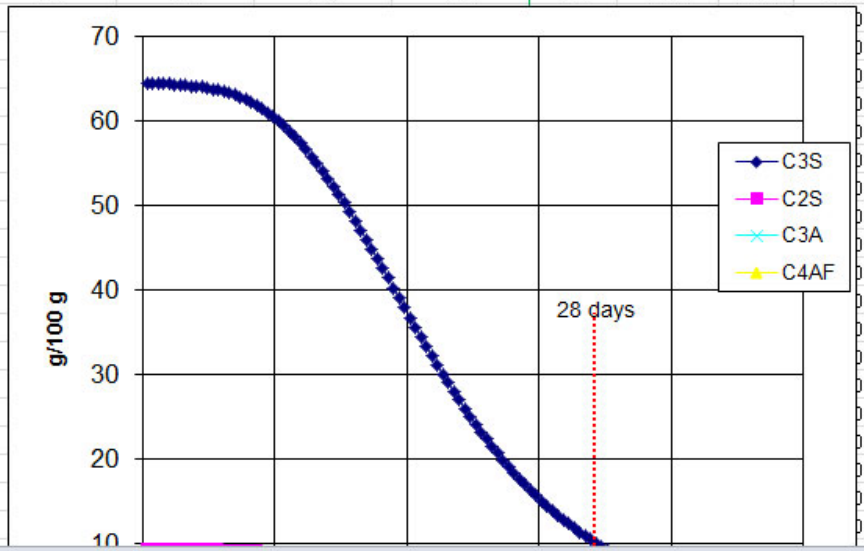
B21 =A21/24

	A	B	C	D	E	F	Y	Z	AA	AB	AC	AD	AE	AF	AG
1	**Modell Parrot and Killoh version 2014**				*Ea*										
2	surface area	413	C3S	64.6	*41570*										
3	Reference area	*385*	C2S	9.3	*20785*										
4	w/z	0.4	C3A	7.4	*54040*										
5	*Temperature*	20	C4AF	7.8	*34087*										
6		*293.15*													
7	reference temp	*293.15*	r.h.	1.0	*relative humidity (not tested for rh < 1!)*										
8	*R*	*8.314*													
9	**Notes**														
10	**Enter your values in the "yellow" boxes; if necessary adapt K,N and H values (ungroup rows)**														
11	**This calculation tool is not throughfully tested. In case of errors please contact barbara.lothenbach@empa.ch**														
12	**Original Model from Parrot and Killoh (1984) Br Ceram Proc 35, 41-53**														
13	**Ea and temperature dependence from Lothenbach et al (2008), Cem Concr Res 38, 1-18**														
14	**Adapted K,N and H from Lothenbach et al. (2008) Cem Conr Res 38, 848-860**														
15	**If you use this model cite the above publications**														
16															
17			**hydrated [g/100g unhydrated cement]**				**not hydrated [g/100 g unhydrated cement]**				**% hydrated (for each clinker)**				**Total degr**
18															**hydratio**
19		*time (days)*	**C3S**	**C2S**	**C3A**	**C4AF**	**C3S**	**C2S**	**C3A**	**C4AF**	**C3S**	**C2S**	**C3A**	**C4AF**	
20	time (hours)			[g/100g unhydrated cement]				[g/100 g unhydrated cement]				[% per clinker]			rel. to total clinke
21	**0.00**	*4.16667E-11*	6.46E-14	9.28E-15	7.42E-15	7.81E-15	64.6	9.3	7.4	7.8	0.00	0.00	0.00	0.00	**0.00**
22	**0.02**	*0.0010*	6.46E-14	9.28E-15	7.42E-15	7.81E-15									**0.00**
23	**0.03**	*0.0011*	4.6947E-07	0.000497745	5.26529E-06	1.40004E-08									**0.00**
24	**0.03**	*0.0012*	5.956E-05	0.001045236	0.000128439	1.17193E-06									**0.00**
25	**0.03**	*0.0013*	0.00033748	0.00164744	0.000347214	5.97927E-06									**0.00**
26	**0.04**	*0.0015*	0.00085187	0.002309822	0.000626573	1.46015E-05									**0.00**
27	**0.04**	*0.0016*	0.00159888	0.00303839	0.000962308	2.69992E-05									**0.00**
28	**0.04**	*0.0018*	0.00259141	0.003839751	0.00135615	4.33981E-05									**0.00**
29	**0.05**	*0.0019*	0.00385337	0.004721173	0.001812231	6.41972E-05									**0.00**
30	**0.05**	*0.0021*	0.00541697	0.005690644	0.002336189	8.99277E-05									**0.00**
31	**0.06**	*0.0024*	0.00732192	0.006756952	0.002934883	0.000121243									**0.00**
32	**0.06**	*0.0026*	0.00961556	0.007929755	0.003616323	0.00015892									**0.00**
33	**0.07**	*0.0029*	0.0123534	0.009219675	0.004389689	0.000203869									**0.00**
34	**0.08**	*0.0031*	0.01560002	0.01063839	0.005265399	0.000257149									**0.00**
35	**0.08**	*0.0035*	0.01943008	0.012198738	0.006255218	0.000319984									**0.00**
36	**0.09**	*0.0038*	0.02392976	0.013914831	0.00737238	0.000393788									**0.00**
37	**0.10**	*0.0042*	0.02919826	0.015802185	0.008631749	0.000480186									**0.00**
38	**0.11**	*0.0046*	0.03534969	0.01787785	0.010049994	0.000581051									**0.00**
39	**0.12**	*0.0051*	0.04251511	0.020160571	0.011645789	0.000698532									**0.00**
40	**0.13**	*0.0056*	0.05084504	0.022670945	0.013440042	0.0008351									**0.00**



Parrot

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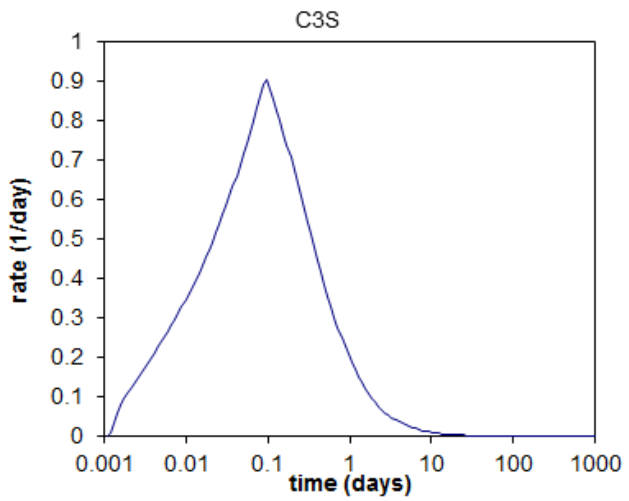
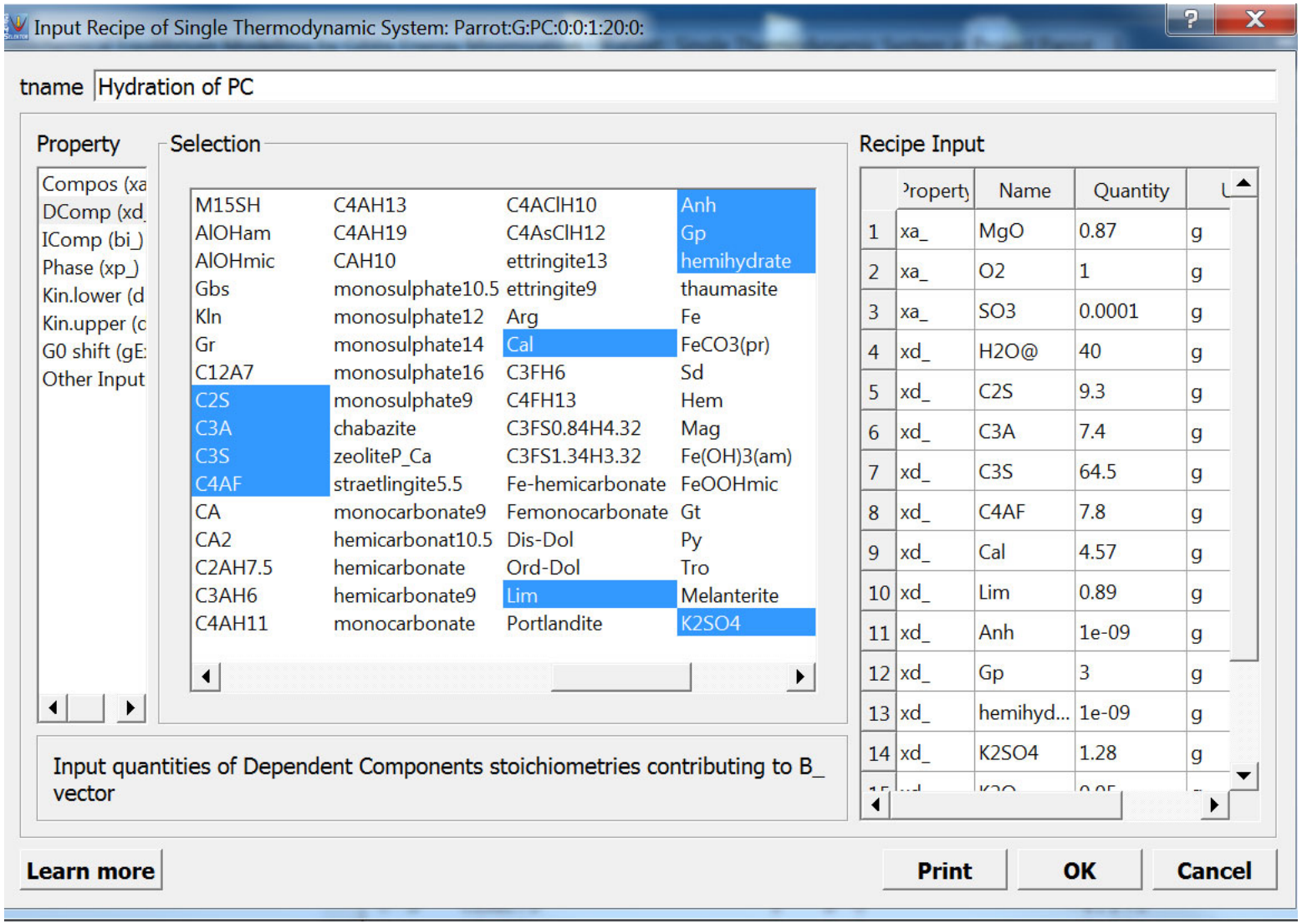
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
3	Reference area	385	C2S	9.3	20785								N	0.7		3.3			N	0
4	w/z	0.4	C3A	7.4	54040								H	1.33					H	
5	Temperature	20	C4AF	7.8	34087							C2S	K	0.5	0.006	0.2		C2S	K	0
6		293.15											N	1		5			N	
7	reference temp	293.15	r.h.	1.0	relative humidity (not tested for rh < 1!!)								H	1.33					H	1.5
8	R	8.314										C3A	K	1	0.04	1		C3A	K	
9	**Notes**												N	0.85		3.2			N	0.8
10	**Enter your values in the "yellow" boxes; if necessary adapt K,N and H values (ungroup rows)**												H	1.33					H	1.
11	**This calculation tool is not throughfully tested. In case of errors please contact barbara.lothenbach@empa.ch**											C4AF	K	0.37	0.015	0.4		C4AF	K	0.3
12	**Original Model from Parrot and Killoh (1984) Br Ceram Proc 35, 41-53**												N	0.7		3.7			N	0
13	**Ea and temperature dependence from Lothenbach et al (2008), Cem Concr Res 38, 1-18**												H	1.33					H	1.6
14	**Adapted K,N and H from Lothenbach et al. (2008) Cem Conr Res 38, 848-860**																			
15	**If you use this model cite the above publications**							C3S		2			C2S		1.55			C3A		1.8
16																				
17			hydrated [g/100g unhydrated cement)					1.5	1.1	0.05			0.5	0.7	0.02			1	1	0.04
18								0.7	3.3				1	5				0.85	3.2	
19		time (days)	C3S	C2S	C3A	C4AF	time function													
20	time (hours)		[g/100g unhydrated cement]					"Nucleation a	"Shell fo	"Diffusio	rate	degree	"Nucleati	"Shell forr	"Diffusio	degree		"Nuclea	"Shell fo	"Diffusi	degree
21	0.00	4.167E-11	6.46E-14	9.28E-15	7.42E-15	7.81E-15		0	0	0		1E-15	0	0	0	1E-15		0	0	0	1E-15
22	0.02	0.0010	6.46E-14	9.28E-15	7.42E-15	7.81E-15	0.00	7.27E-08	0.0011	######		1E-15	0.0005	0.0007	######	1E-15		####	0.0010	######	1E-15
23	0.03	0.0011	4.69E-07	0.00049775	5.2653E-06	1.4E-08	0.00	7.27E-09	0.00011	######	0.0001	7.27E-09	0.0001	0.0001	######	0.00005		####	0.0001	######	0.0000
24	0.03	0.0012	5.96E-05	0.00104524	0.00012844	1.1719E-06	0.00	9.15E-07	0.00012	######	0.0003	9.22E-07	0.0001	0.0001	0.1230	0.00011		####	0.0001	18.6018	0.0000
25	0.03	0.0013	0.000337	0.00164744	0.00034721	5.9793E-06	0.00	4.3E-06	0.000									####	0.0001	0.8388	0.0000
26	0.04	0.0015	0.000852	0.00230982	0.00062657	1.4602E-05	0.00	7.96E-06	0.000									####	0.0001	0.3413	0.0000
27	0.04	0.0016	0.001599	0.00303839	0.00096231	2.6999E-05	0.00	1.16E-05	0.000									####	0.0001	0.2080	0.0001
28	0.04	0.0018	0.002591	0.00383975	0.00135615	4.3398E-05	0.00	1.54E-05	0.000									).0001	0.0002	0.1490	0.0001
29	0.05	0.0019	0.003853	0.00472117	0.00181223	6.4197E-05	0.00	1.95E-05	0.000									).0001	0.0002	0.1163	0.0002
30	0.05	0.0021	0.005417	0.00569064	0.00233619	8.9928E-05	0.00	2.42E-05	0.000									).0001	0.0002	0.0957	0.0003
31	0.06	0.0024	0.007322	0.00675695	0.00293488	0.00012124	0.00	2.95E-05	0.000									).0001	0.0002	0.0817	0.0004
32	0.06	0.0026	0.009616	0.00792975	0.00361632	0.00015892	0.00	3.55E-05	0.000									).0001	0.0002	0.0715	0.0004
33	0.07	0.0029	0.012353	0.00921968	0.00438969	0.00020387	0.00	4.24E-05	0.000									).0001	0.0003	0.0638	0.0005
34	0.08	0.0031	0.0156	0.01063839	0.0052654	0.00025715	0.00	5.03E-05	0.000									).0001	0.0003	0.0578	0.0007
35	0.08	0.0035	0.01943	0.01219874	0.00625522	0.00031998	0.00	5.93E-05	0.000									).0001	0.0003	0.0530	0.0008
36	0.09	0.0038	0.02393	0.01391483	0.00737238	0.00039379	0.00	6.97E-05	0.000									####	0.0003	0.0491	0.0009
37	0.10	0.0042	0.029198	0.01580218	0.00863175	0.00048019	0.00	8.16E-05	0.000									####	0.0004	0.0458	0.0011
38	0.11	0.0046	0.03535	0.01787785	0.01004999	0.00058105	0.00	9.52E-05	0.000									####	0.0004	0.0430	0.0013
39	0.12	0.0051	0.042515	0.02016057	0.01164579	0.00069853	0.01	0.000111	0.000									####	0.0005	0.0407	0.0015
40	0.13	0.0056	0.050845	0.02267095	0.01344004	0.0008351	0.01	0.000129	0.000									####	0.0005	0.0386	0.0018
41	0.15	0.0061	0.060512	0.02543161	0.01545615	0.00099359	0.01	0.00015	0.000									####	0.0006	0.0368	0.0020
42	0.16	0.0067	0.071715	0.02846743	0.01772028	0.00117725	0.01	0.000173	0.000									####	0.0006	0.0352	0.0023
43	0.18	0.0074	0.08468	0.03180574	0.02026171	0.00138983	0.01	0.000201	0.000									####	0.0007	0.0337	0.0027
44	0.20	0.0081	0.099667	0.03547656	0.02311314	0.00163559	0.01	0.000232	0.000									####	0.0007	0.0324	0.0031
45	0.21	0.0090	0.116977	0.03951285	0.02631114	0.00191945	0.01	0.000268	0.00089	0.0790	0.3292	0.00181	0.0004	0.0006	0.0127	0.00426		####	0.0008	0.0313	0.0035
46	0.24	0.0098	0.13695	0.04395084	0.02989656	0.00224705	0.01	0.000309	0.00098	0.0740	0.3453	0.00212	0.0005	0.0006	0.0126	0.00474		####	0.0009	0.0302	0.0040
47	0.26	0.0108	0.159977	0.04883028	0.03391501	0.00262484	0.01	0.000356	0.00108	0.0695	0.3619	0.00248	0.0005	0.0007	0.0124	0.00526		####	0.0010	0.0292	0.0045

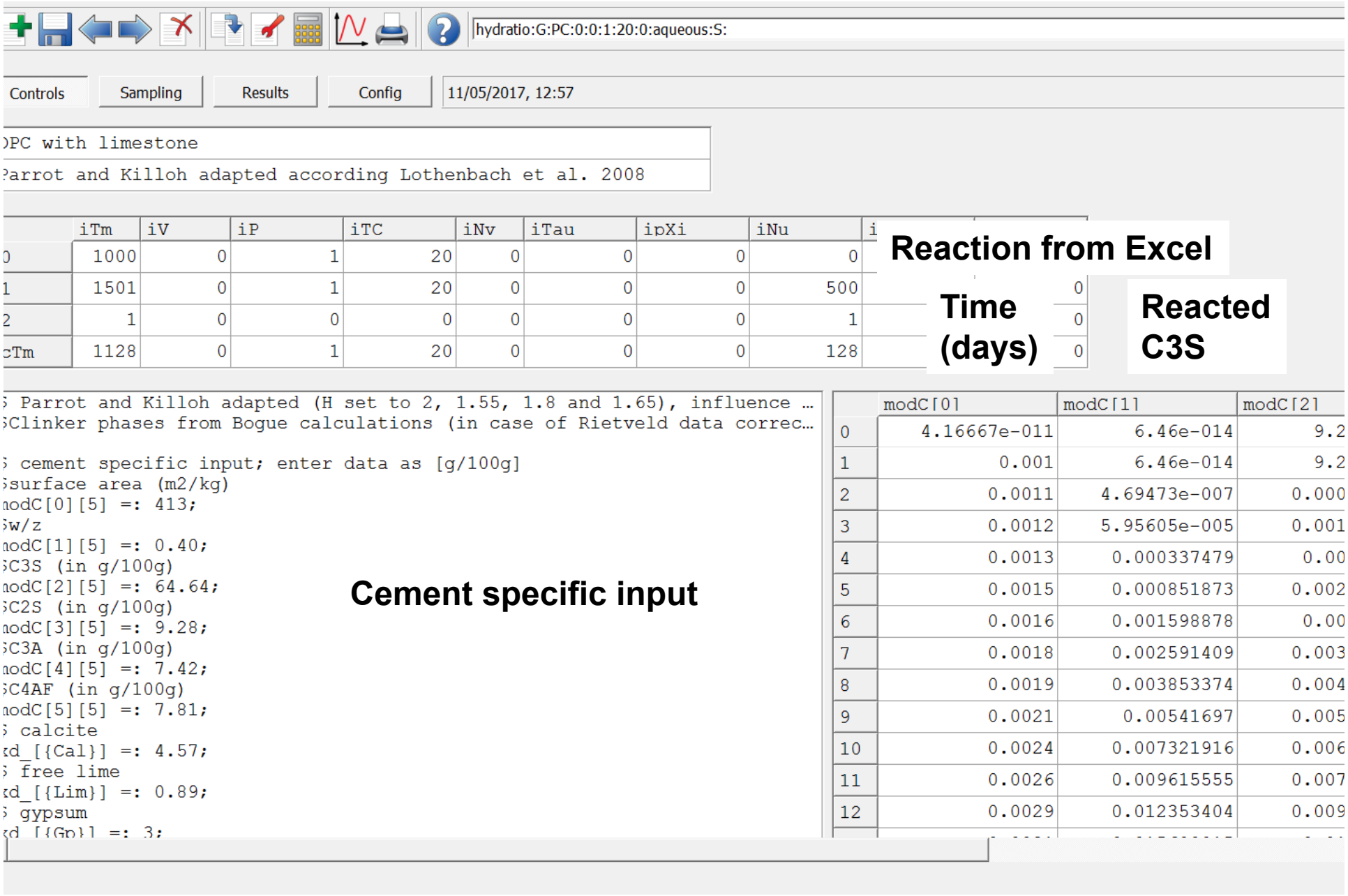


Hydration modelling EXCEL + GEMS

1. Open project Parrot



All input in g (100 g cement)



	iTm	iV	iP	iTC	iNv	iTau	ipXi	iNu	i
0	1000	0	1	20	0	0	0	0	
1	1501	0	1	20	0	0	0	500	0
2	1	0	0	0	0	0	0	1	0
cTm	1128	0	1	20	0	0	0	128	0

```
; Parrot and Killoh adapted (H set to 2, 1.55, 1.8 and 1.65), influence …
;Clinker phases from Bogue calculations (in case of Rietveld data correc…

; cement specific input; enter data as [g/100g]
;surface area (m2/kg)
modC[0][5] =: 413;
;w/z
modC[1][5] =: 0.40;
;C3S (in g/100g)
modC[2][5] =: 64.64;
;C2S (in g/100g)
modC[3][5] =: 9.28;
;C3A (in g/100g)
modC[4][5] =: 7.42;
;C4AF (in g/100g)
modC[5][5] =: 7.81;
; calcite
xd_[{Cal}] =: 4.57;
; free lime
xd_[{Lim}] =: 0.89;
; gypsum
xd_[{Gp}] =: 3;
```

	modC[0]	modC[1]	modC[2]
0	4.16667e-011	6.46e-014	9.2
1	0.001	6.46e-014	9.2
2	0.0011	4.69473e-007	0.000
3	0.0012	5.95605e-005	0.001
4	0.0013	0.000337479	0.00
5	0.0015	0.000851873	0.002
6	0.0016	0.001598878	0.00
7	0.0018	0.002591409	0.003
8	0.0019	0.003853374	0.004
9	0.0021	0.00541697	0.005
10	0.0024	0.007321916	0.006
11	0.0026	0.009615555	0.007
12	0.0029	0.012353404	0.009

Architecture of GEMS file

- Input always in g/100g
- The amount of clinker reacted copied from EXCEL file
- Inputs needed in GEMS:
  - surface area [m^2/kg]
  - w/c
  - C_3S, C_2S, C_3A, C_4AF (pure phases)
  - Calcite, free lime, gypsum, anhydrite, hemihydrate, periclase, Na_2SO_4 and K_2SO_4 (-> soluble alkalis)
  - Na_2O, K_2O, MgO and SO_3 in clinker (as g/g clinker) optional

Architecture of GEMS file

- Process: controls below input
  - Ea (activation energy)
  - Conversion of different input parameter
    - Correction factors for minor elements in clinker
    - Amount of input water
  - Calculations of the dissolution of minor elements

Do not change!

Architecture of GEMS file

- Process: sampling: definition of output
  - X-axis: log (time)
  - Mass in g/100 g of hydrated cement
    - All data corrected from g/100 g unhydrated cement to g/100 g hydrated cement (corresponds to conditions of XRD, TGA measurements); can easily be changed, but you will have to convert XRD/TGA data
    - Amount of clinkers (with impurities)
    - Amount of hydrates (! Check single system file for the presence of additional solids and include them in the list)
    - Amount of pore solution (including dissolved species)

Check single system file for additional solids

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Controls | Sampling | Results | Config | 29/04/2019, 12:37

cTau	0	cpXi	0	cXi	1	cNu
cpH	0	cpe	0	cEh	0	cT

```
$ Abscissa: log(time in days)
xp[J] =: lg(modC[J][0]);
$ Ordinates (in g/100 g unhydrated cement)
$ clinker unreacted;  include also minor elements
yp[J][0] =: phM[{Alite}]/modC[24][5];
yp[J][1] =: phM[{Belite}]/modC[25][5];
yp[J][2] =: phM[{Aluminate}]/modC[26][5];
yp[J][3] =: phM[{Ferrite}]/modC[27][5];
yp[J][4] =: phM[{CSHQ}];
yp[J][5] =: phM[{Portlandite}];
yp[J][6] =: phM[{Gypsum}];
yp[J][7] =: phM[{syngenite}];
yp[J][8] =: phM[{Calcite}];
yp[J][9] =: (phM[{ettringite}]+phM[{SO4_CO3_AFt}]+phM[{CO3_SO4_AFt}]+phM…
yp[J][10] =: (phM[{C4AsH16}]+phM[{C4AsH14}]+phM[{SO4_OH_AFm}]+phM[{OH_SO…
yp[J][11] =: phM[{C4AcH11}];
yp[J][12] =: phM[{C4Ac0.5H12}];
yp[J][13] =: phM[{straetlingite}];
yp[J][14] =: phM[{C3AH6}];
yp[J][15] =: phM[{OH-hydrotalcite}]+phM[{hydrotalc-pyro}];
yp[J][16] =: phM[{C3(AF)S0.84H}]+phM[{C3FS0.84H4.32}]+phM[{C3FS1.34H3.32…
yp[J][17] =: phM[{Brucite}];
yp[J][18] =: phM[{Ferrihydrite-mc}];
yp[J][19] =: phM[{aq_gen}];

$correction to hydrated cement possible
$ /(1+modC[1][5] -phM[{aq_gen}]/100) =1+0.4-mass H2O dissol
$ =mass hydrated cement (after removal of pore water)
```

= C3S not reacted at time t
modC[24][5] correction for presence of minor elements in clinker; = 0.99 here

phM[{Portlandite}] -> mass of portlandite in g per 100 g unhyrated cement
! Spelling has to correspond exactly to single component!

/(1+modC[1][5]-phM[{aq_gen}]/100)
=1+0.4-mass H_2O unreacted/100
= mass hydrated cement
(after removal of pore water)

For comparison with XRD/TGA

Controls | Sampling | Results | Config | 29/04/2019, 12:51

hydration of PC

pY_Nam: phM

Unit of x-axis

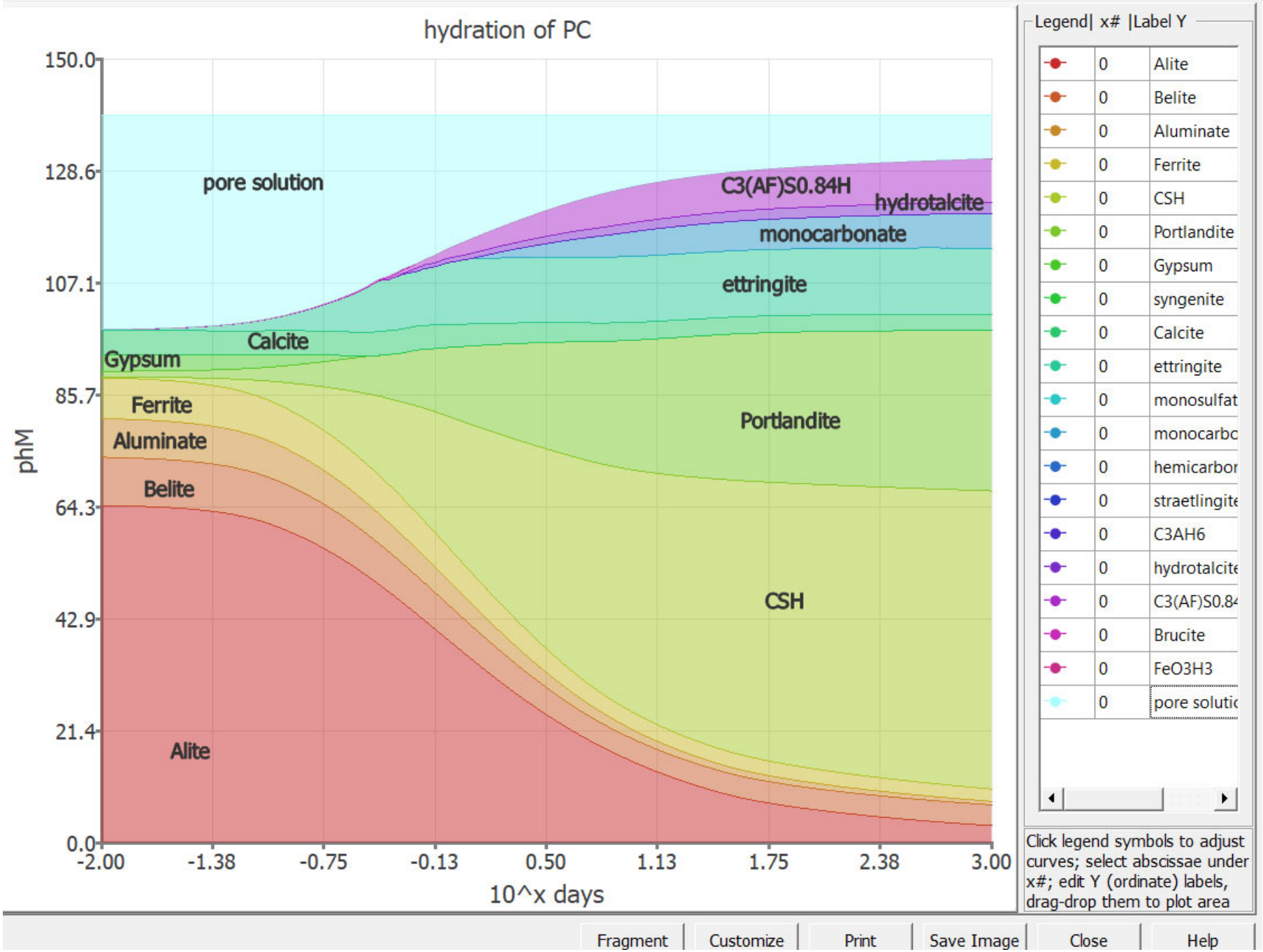
pX_Nam	10^x days	Alite	Belite	Aluminate	Ferrite
0	-10.380211	64.64	9.28	7.42	7.81
1	-3	64.64	9.28	7.42	7.81
2	-2.9586073	64.64	9.2795023	7.4199947	7.81
3	-2.9208187	64.63994	9.2789548	7.4198716	7.8099988
4	-2.8860566	64.639663	9.2783526	7.4196528	7.809994
5	-2.8239087	64.639148	9.2776902	7.4193734	7.8099854
6	-2.79588	64.638401	9.2769616	7.4190377	7.809973
7	-2.7447275	64.637409	9.2761602	7.4186438	7.8099566
8	-2.7212464	64.636147	9.2752788	7.4181878	7.8099358
9	-2.6777807	64.634583	9.2743094	7.4176638	7.8099101
10	-2.6197888	64.632678	9.273243	7.4170651	7.8098788
11	-2.5850266	64.630384	9.2720702	7.4163837	7.8098411
12	-2.537602	64.627647	9.2707803	7.4156103	7.8097961
13	-2.5086383	64.6244	9.2693616	7.4147346	7.8097429
14	-2.455932	64.62057	9.2678013	7.4137448	7.80968
15	-2.4202164	64.61607	9.2660852	7.4126276	7.8096062

y-axis labels

X-axis
Time
(10^x days)

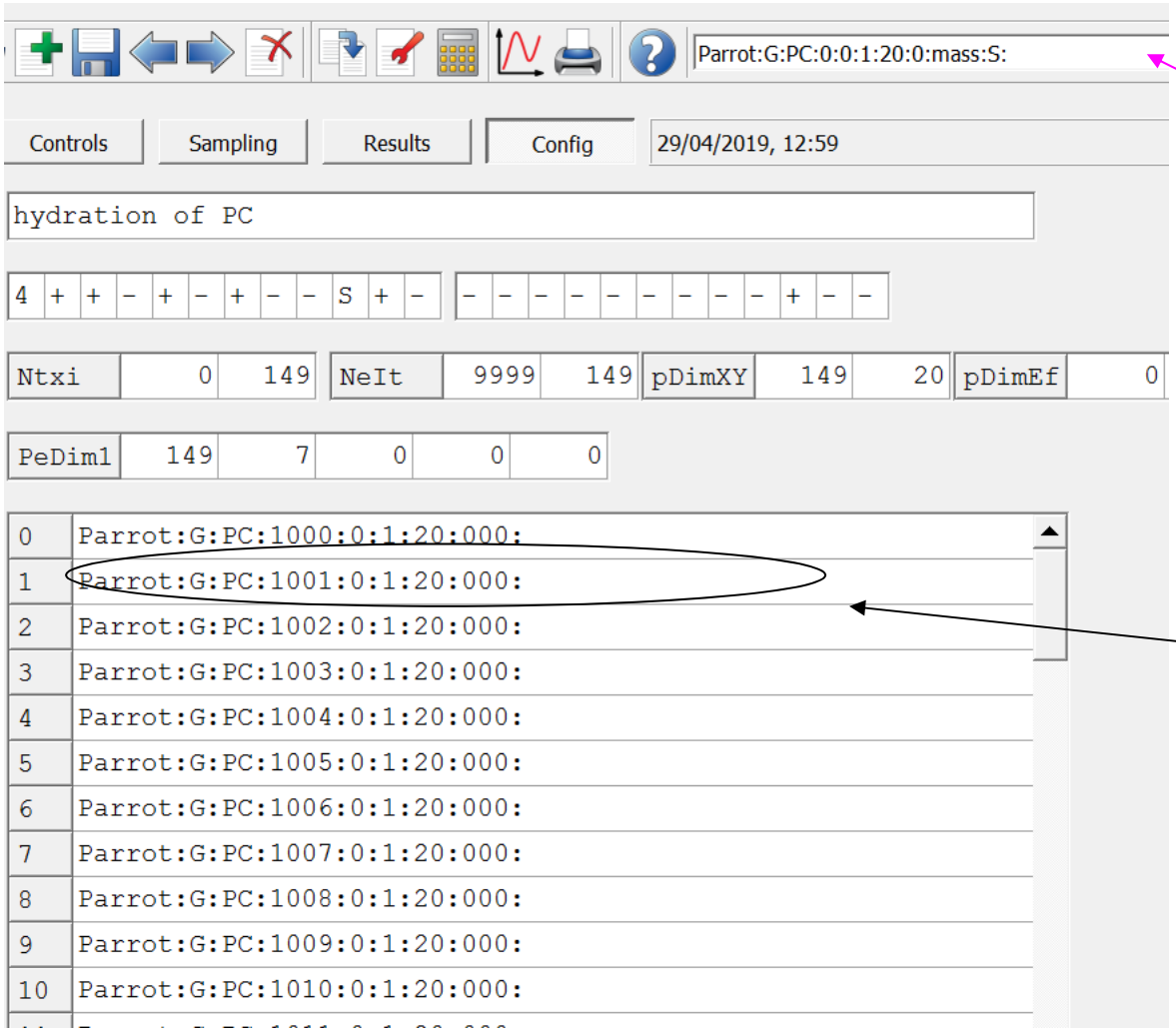
y-axis
e.g. unreacted clinker

(in g/100 g of unhydrated cement as defined in page sampling)


hydration of PC
150.0
128.6
107.1
85.7
64.3
42.9
21.4
0.0
phM
pore solution
C3(AF)S0.84H
hydrotalcite
monocarbonate
ettringite
Calcite
Gypsum
Ferrite
Aluminate
Belite
Alite
Portlandite
CSH
-2.00
-1.38
-0.75
-0.13
0.50
1.13
1.75
2.38
3.00
10^x days
Legend| x# |Label Y
0 Alite
0 Belite
0 Aluminate
0 Ferrite
0 CSH
0 Portlandite
0 Gypsum
0 syngenite
0 Calcite
0 ettringite
0 monosulfat
0 monocarbc
0 hemicarbor
0 straetlingite
0 C3AH6
0 hydrotalcite
0 C3(AF)S0.8
0 Brucite
0 FeO3H3
0 pore solutic
Click legend symbols to adjust curves; select abscissae under x#; edit Y (ordinate) labels, drag-drop them to plot area
Fragment
Customize
Print
Save Image
Close
Help

Architecture of GEMS file

- Process: Config: single system files



Name of the „parent file“ in „Single-System Equilibria“

Names of the „kid files“ produced:
The results of each calculation can be checked

Architecture of GEMS file

- Process: Results: output
- X-axis: log (time)
  - Y-axis Mass in g/100 g of hydrated cement
  - Experimental data, same format as calculated data
    - Number of data points can be adapted by „Record:Remake“
- Data used to prepare graph, can be exported to Excel or other softwares by copy/paste

Comparison with experimental data

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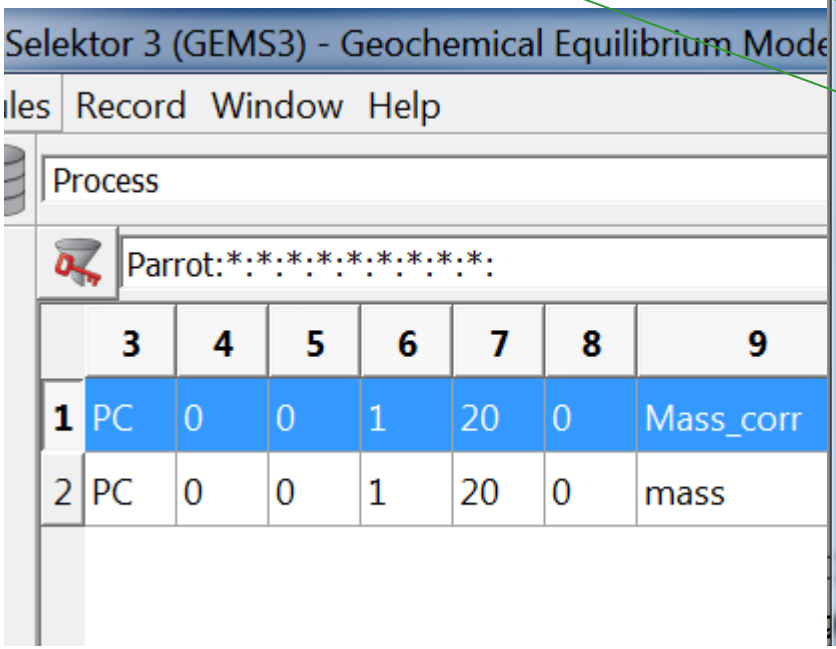
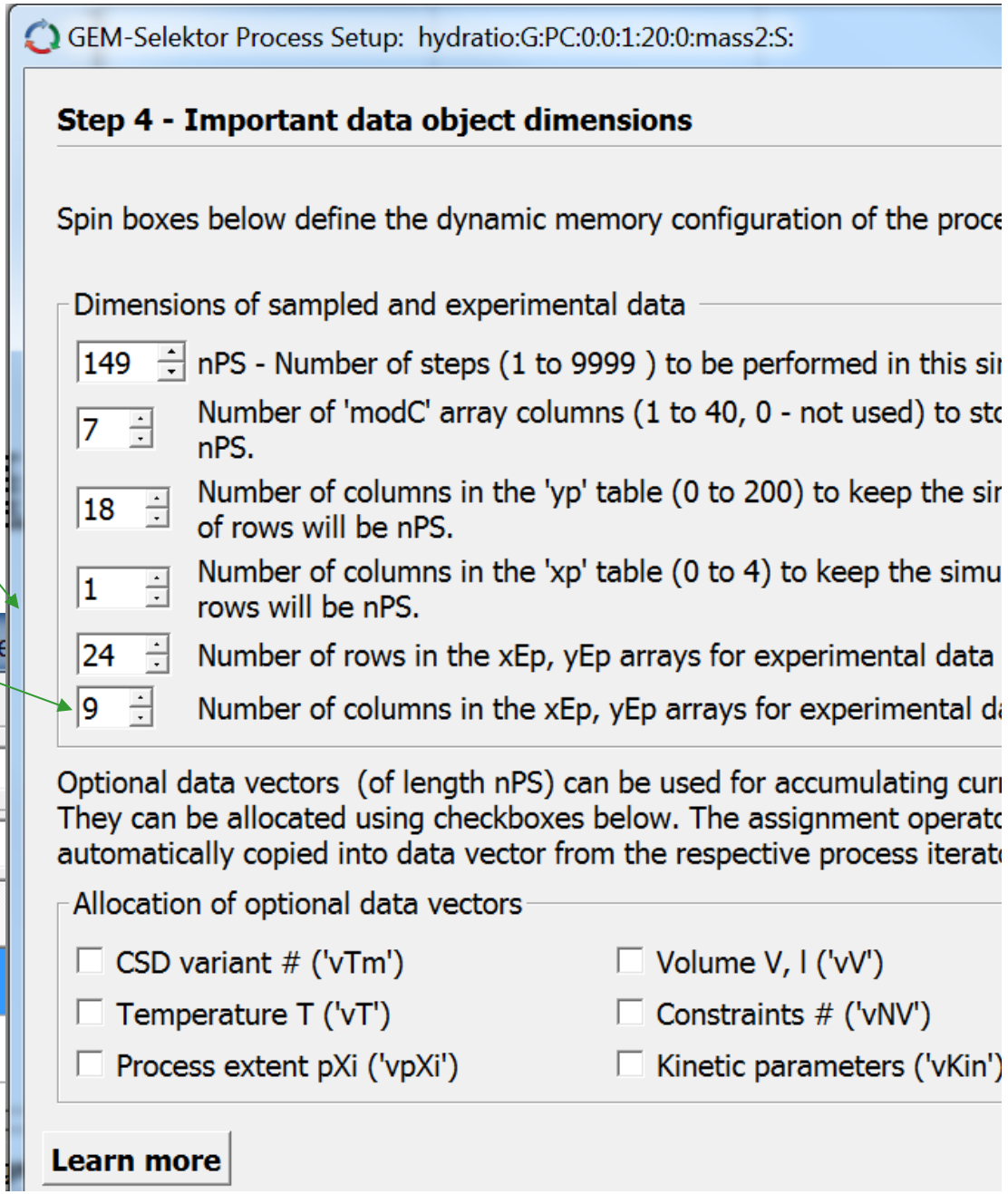
Remake

Number of experimental points

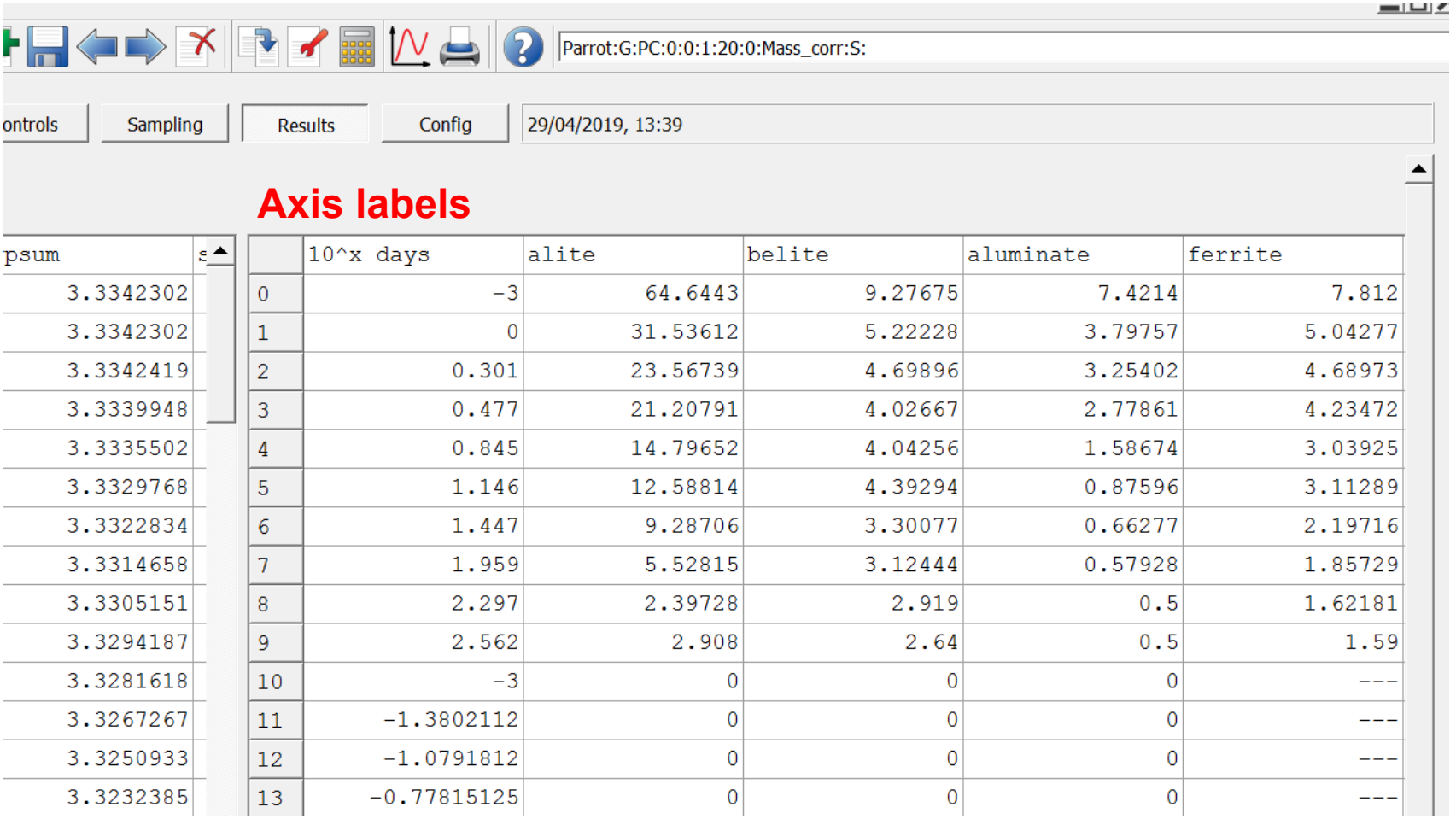
Number of data categories





Possibility to plot experimental data
See process Mass_corr

Experimental y-axis
(in g/100 g of unhydrated cement)



Axis labels

psum		10^x days	alite	belite	aluminate	ferrite
3.3342302	0	-3	64.6443	9.27675	7.4214	7.812
3.3342302	1	0	31.53612	5.22228	3.79757	5.04277
3.3342419	2	0.301	23.56739	4.69896	3.25402	4.68973
3.3339948	3	0.477	21.20791	4.02667	2.77861	4.23472
3.3335502	4	0.845	14.79652	4.04256	1.58674	3.03925
3.3329768	5	1.146	12.58814	4.39294	0.87596	3.11289
3.3322834	6	1.447	9.28706	3.30077	0.66277	2.19716
3.3314658	7	1.959	5.52815	3.12444	0.57928	1.85729
3.3305151	8	2.297	2.39728	2.919	0.5	1.62181
3.3294187	9	2.562	2.908	2.64	0.5	1.59
3.3281618	10	-3	0	0	0	---
3.3267267	11	-1.3802112	0	0	0	---
3.3250933	12	-1.0791812	0	0	0	---
3.3232385	13	-0.77815125	0	0	0	---

Experimental X-axis
Time (in log)

Comparison with experimental data

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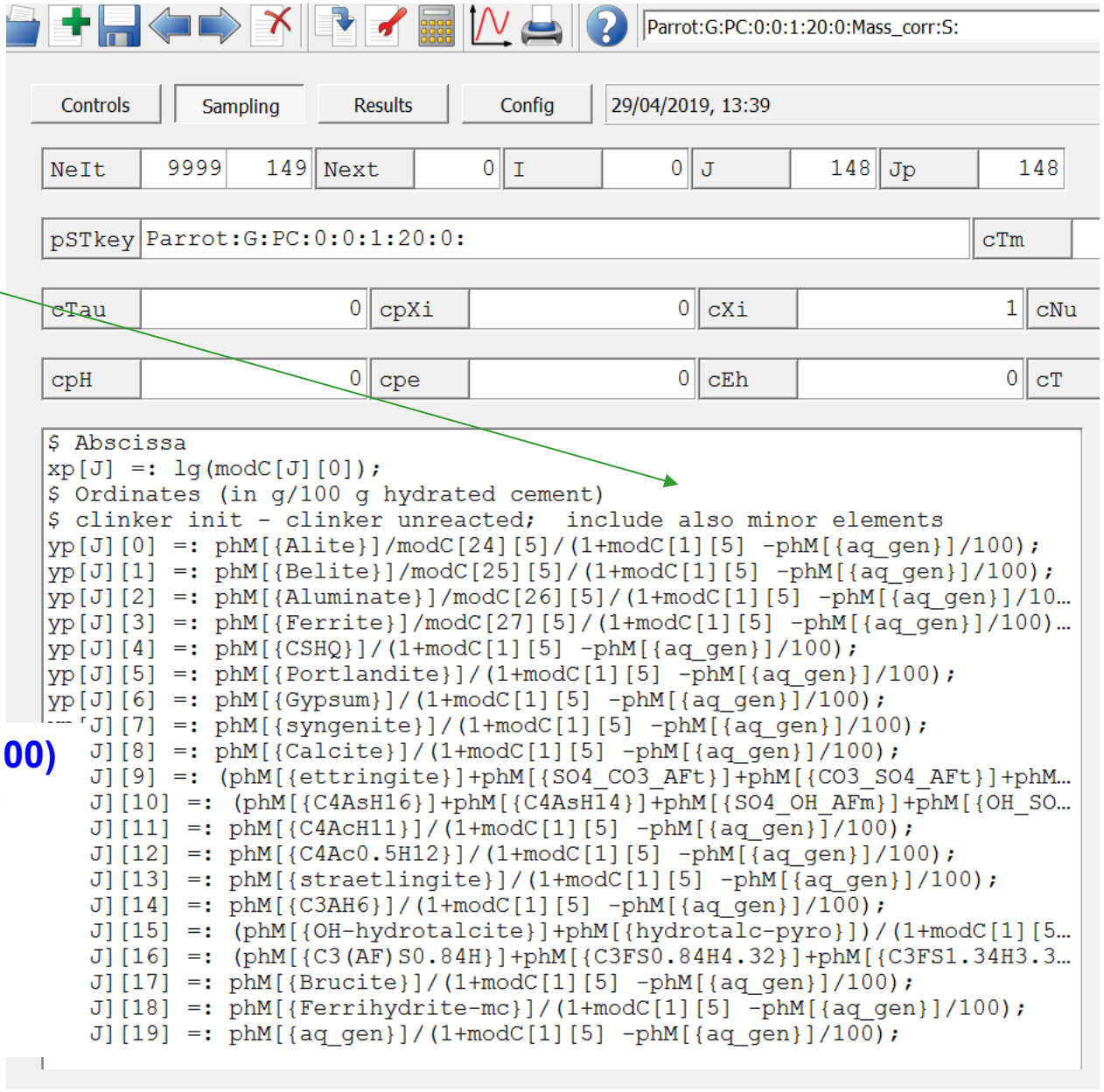
Same input
Modified output
Refers to hydrated cement



/(1+modC[1][5]-phM[{aq_gen}]/100)
=1+0.4-mass H_2O unreacted/100
= mass hydrated cement
(after removal of pore water)

For comparison with XRD/TGA

Different outputs possible

- Y-axis Mass in g/100 g of original cement

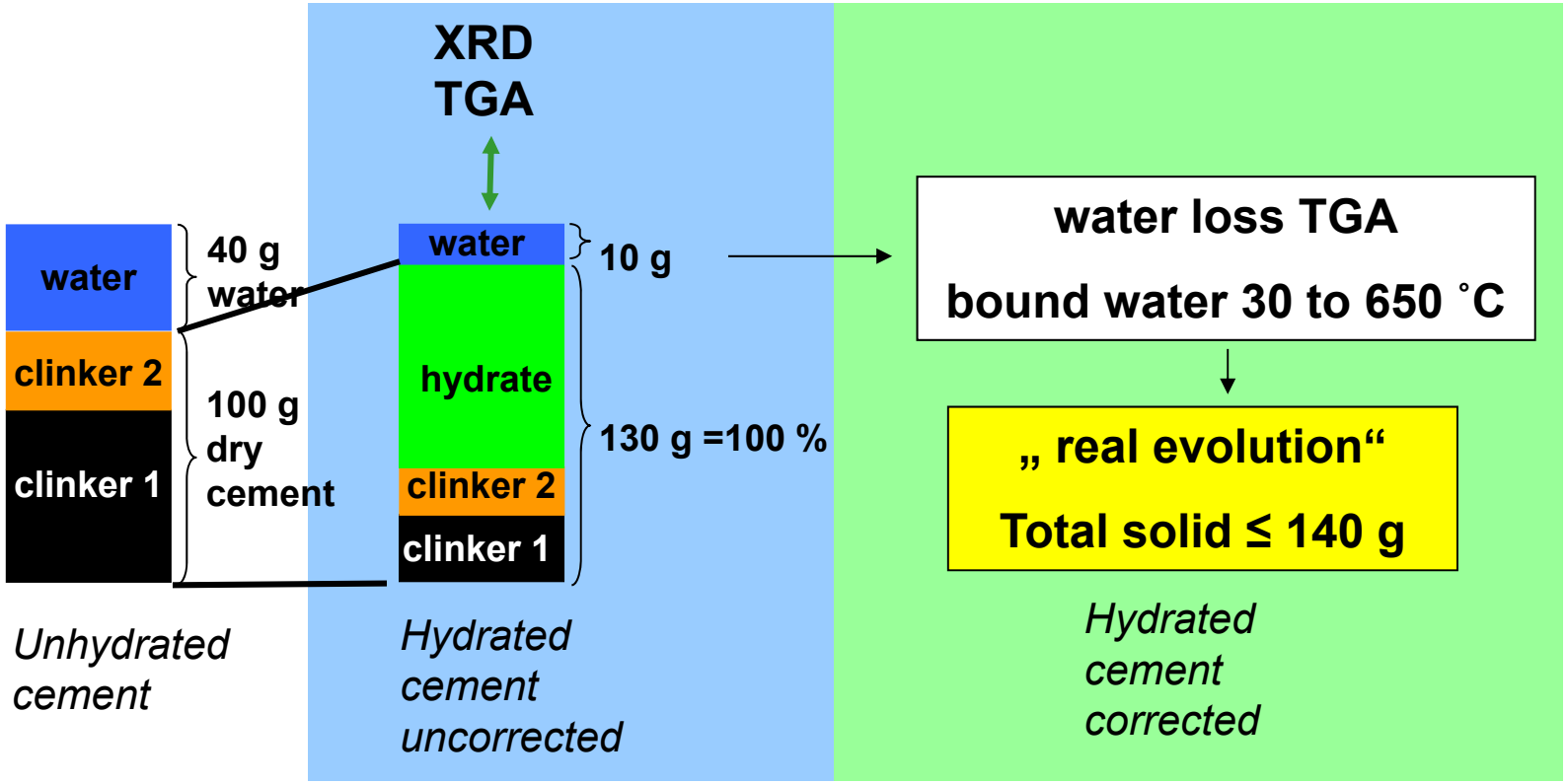
  phM[{Portlandite}] => correct measurements to 100 dry weight

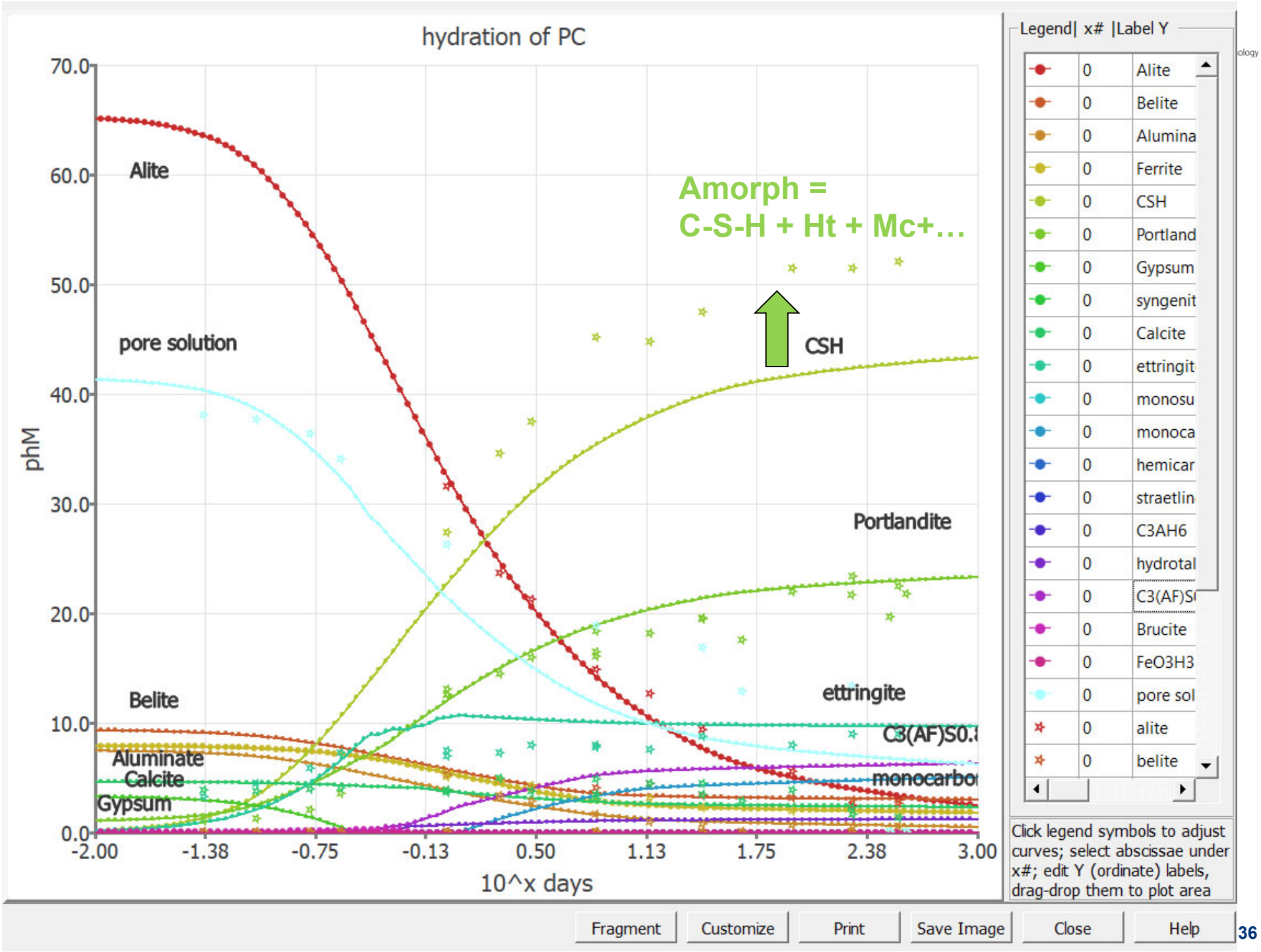
- Y-axis Mass in g/100 g of hydrated cement

  phM[{Portlandite}]/(1+modC[1][5]-phM[{aq_gen}]/100)

  correction of the output /(1+0.4-mass H_2O unreacted/100)

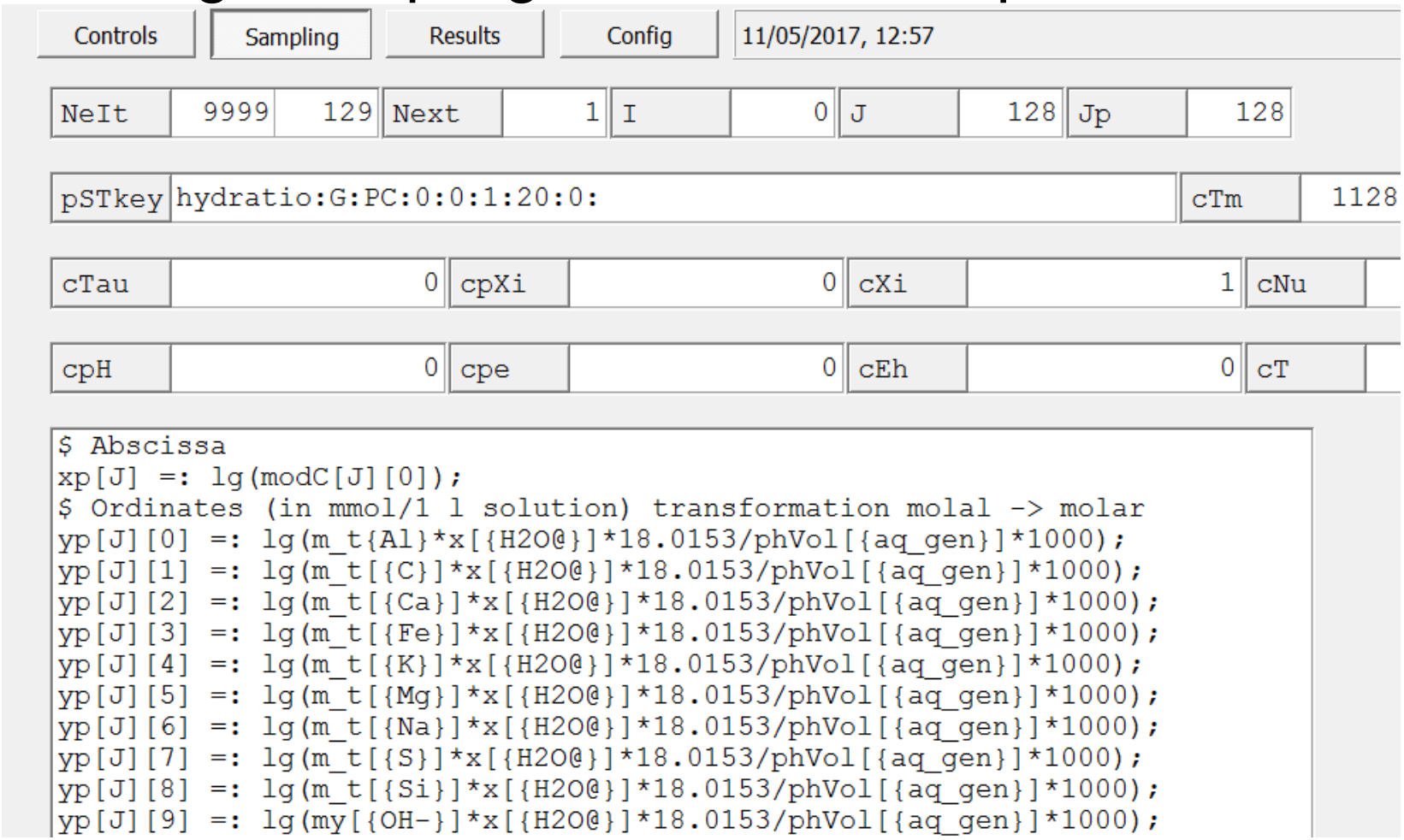
  => / mass hydrated cement (after removal of pore water)

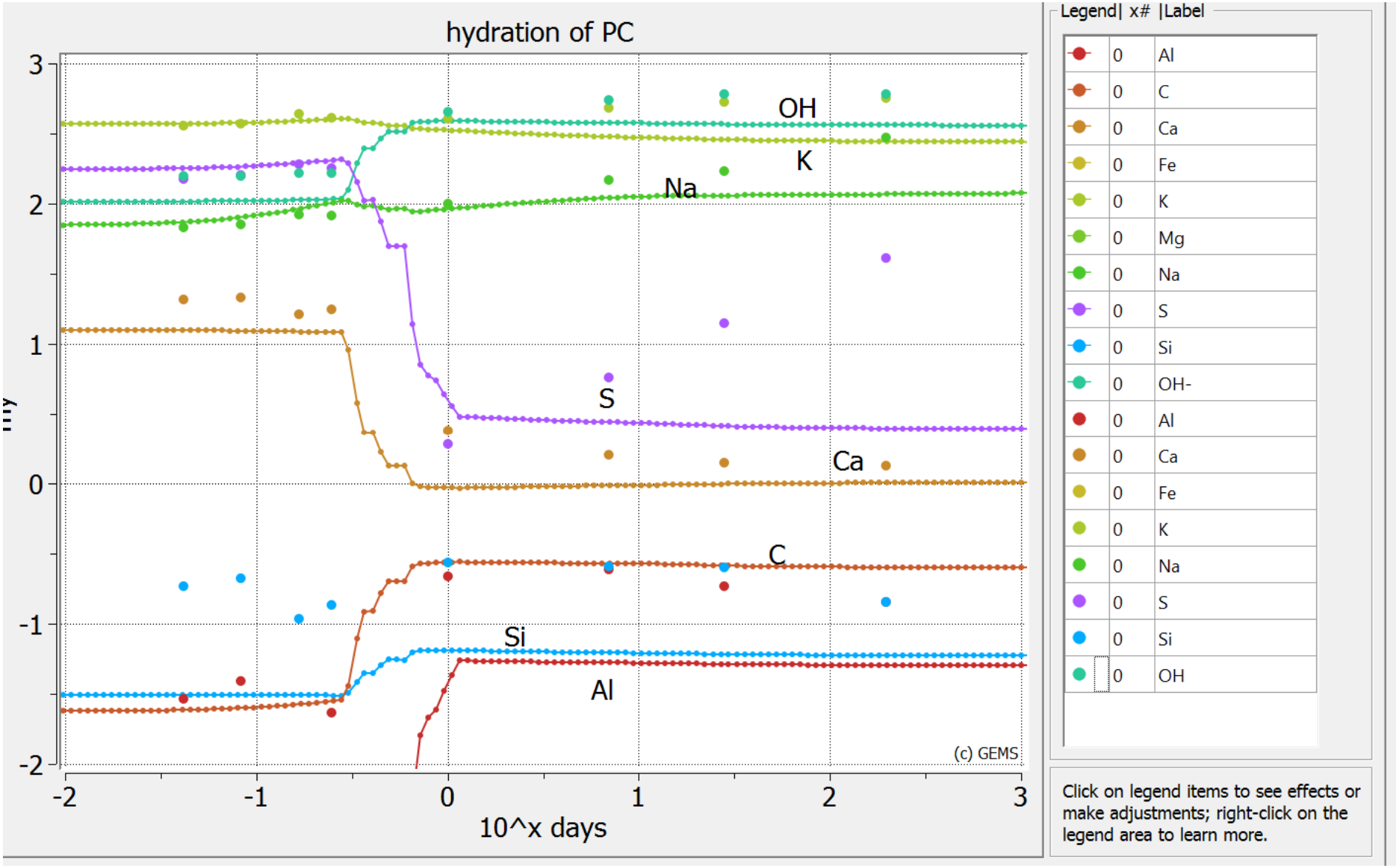



hydration of PC
Alite
pore solution
Belite
Aluminate
Calcite
Gypsum
Amorph =
C-S-H + Ht + Mc+…
CSH
Portlandite
ettringite
C3(AF)S0.
monocarbo
phM
10^x days
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0.0
-2.00
-1.38
-0.75
-0.13
0.50
1.13
1.75
2.38
3.00
Legend| x# |Label Y
0 Alite
0 Belite
0 Alumina
0 Ferrite
0 CSH
0 Portland
0 Gypsum
0 syngenit
0 Calcite
0 ettringit
0 monosu
0 monoca
0 hemicar
0 straetlin
0 C3AH6
0 hydrotal
0 C3(AF)S
0 Brucite
0 FeO3H3
0 pore sol
0 alite
0 belite
Click legend symbols to adjust curves; select abscissae under x#; edit Y (ordinate) labels, drag-drop them to plot area
Fragment
Customize
Print
Save Image
Close
Help

Sampling of aqueous concentrations

- Controls (= input) identical
- Page sampling and results adapted





Legend| x# |Label

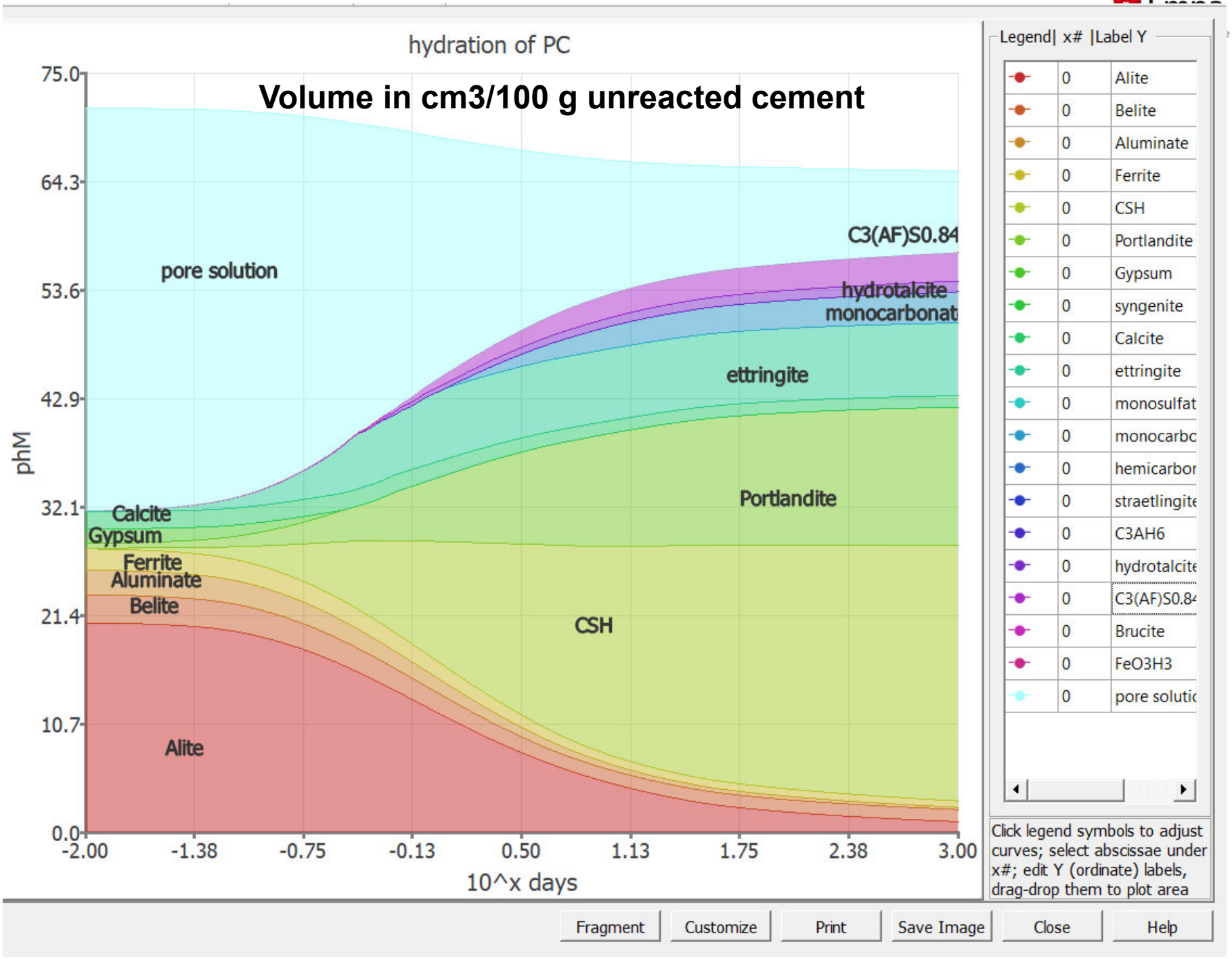
	0	Al
	0	C
	0	Ca
	0	Fe
	0	K
	0	Mg
	0	Na
	0	S
	0	Si
	0	OH-
	0	Al
	0	Ca
	0	Fe
	0	K
	0	Na
	0	S
	0	Si
	0	OH

Click on legend items to see effects or make adjustments; right-click on the legend area to learn more.

Common excercise

- Calculate volumes of the hydrating cement

- Hint:
  - Duplicate process «mass»
  - Exchange phM by phVol (use «word» to do that)
  - Equivalent expression:
    /mmDC[{C3S}]*vol[{C3S}]
    „mmDC[{}]“ Mass of component
    „vol[{}]“ Volume of component


hydration of PC
Volume in cm3/100 g unreacted cement
75.0
64.3
53.6
42.9
32.1
21.4
10.7
0.0
phM
-2.00
-1.38
-0.75
-0.13
0.50
1.13
1.75
2.38
3.00
10^x days
pore solution
C3(AF)S0.84
hydrotalcite
monocarbonat
ettringite
Portlandite
CSH
Calcite
Gypsum
Ferrite
Aluminate
Belite
Alite
Legend| x# |Label Y
0 Alite
0 Belite
0 Aluminate
0 Ferrite
0 CSH
0 Portlandite
0 Gypsum
0 syngenite
0 Calcite
0 ettringite
0 monosulfat
0 monocarbc
0 hemicarbor
0 straetlingite
0 C3AH6
0 hydrotalcite
0 C3(AF)S0.84
0 Brucite
0 FeO3H3
0 pore solutic
Click legend symbols to adjust curves; select abscissae under x#; edit Y (ordinate) labels, drag-drop them to plot area
Fragment
Customize
Print
Save Image
Close
Help