Oregon State University

NTNU – Trondheim
Norwegian University of Science and Technology

Empa
Materials Science and Technology

Lecture 05
Hydration

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

Barbara Lothenbach

GEM SELEKTOR

Software development/fitting tools/kinetic:
Dmitrii Kulik
Dan Miron

PAUL SCHERRER INSTITUT
PSI

1

Hydration

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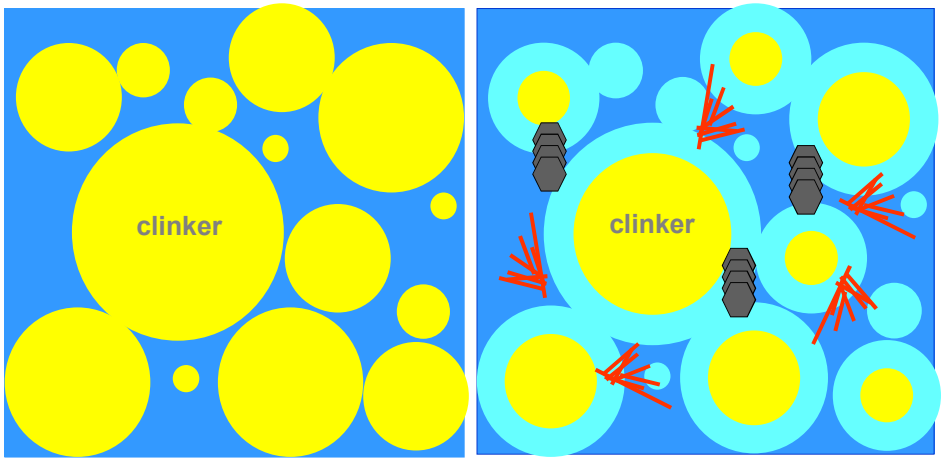


2

Modeling: Dissolution

Empa

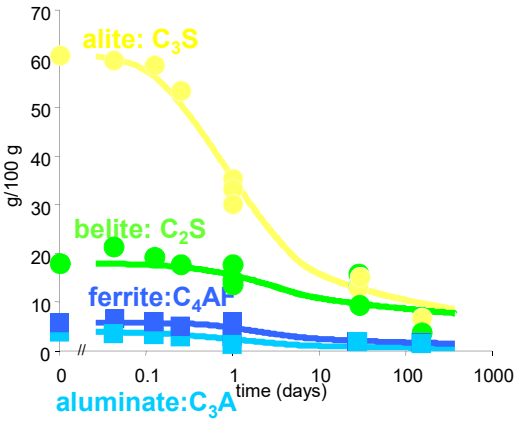
Empirical Approach: Parrot and Killoh (1984)

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

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

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

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



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

3

Modeling: Dissolution

Empa

Empirical Approach: Parrot and Killoh (1984)

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

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

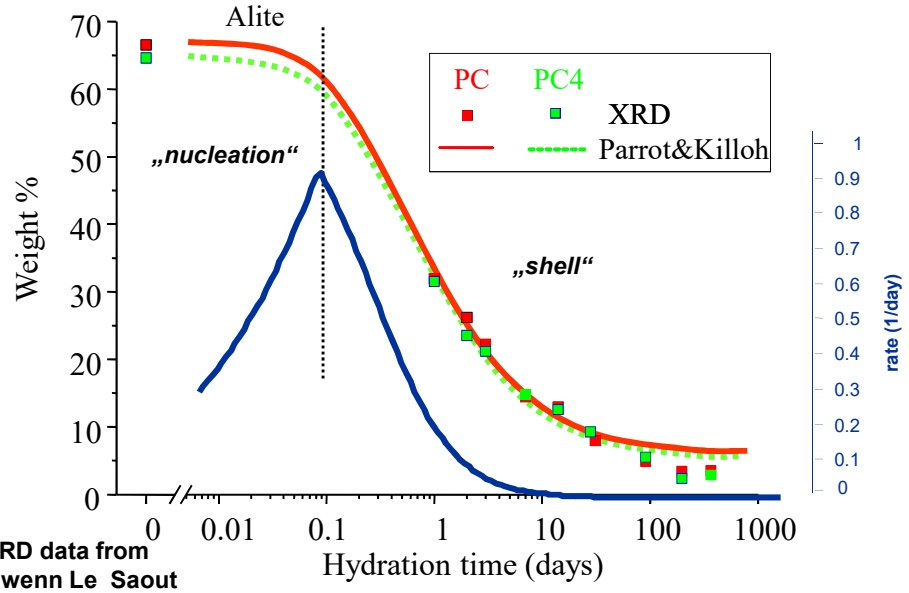
for $\alpha_t > H \cdot {}^{w}/_{c}$.

	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	0.006	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

4

Modeling: Dissolution



XRD data from
Gwenn Le Saout

5

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*

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degree of hydration

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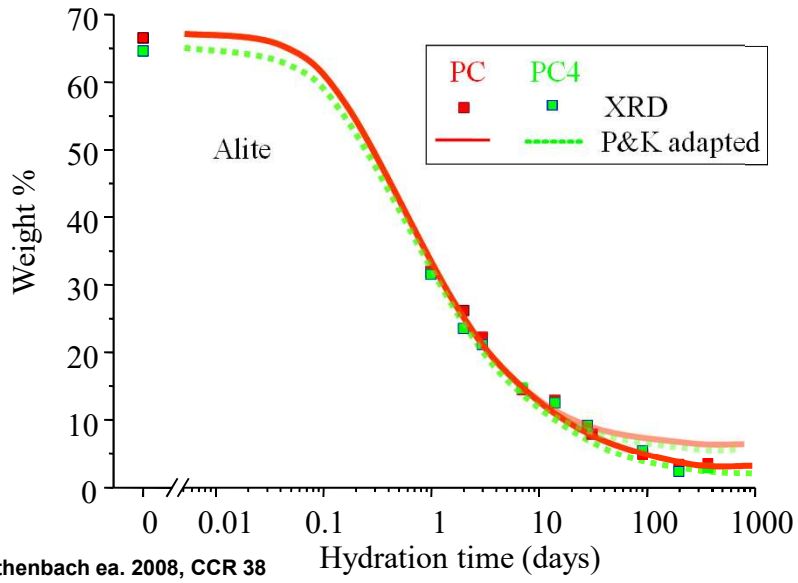
	alite	belite	alum.	ferrite
K_1	1.5	0.5	1.0	0.37
N_1	0.7	1.0	0.85	0.7
K_2	0.05	**0.02**	0.04	0.015
K_3	1.1	**0.7**	1.0	0.4
N_3	3.3	5.0	3.2	3.7
H	**2.0**	**1.55**	**1.8**	**1.65**

Cement specific input: surface area, w/c

6

Modeling: Dissolution



Lothenbach ea. 2008, CCR 38

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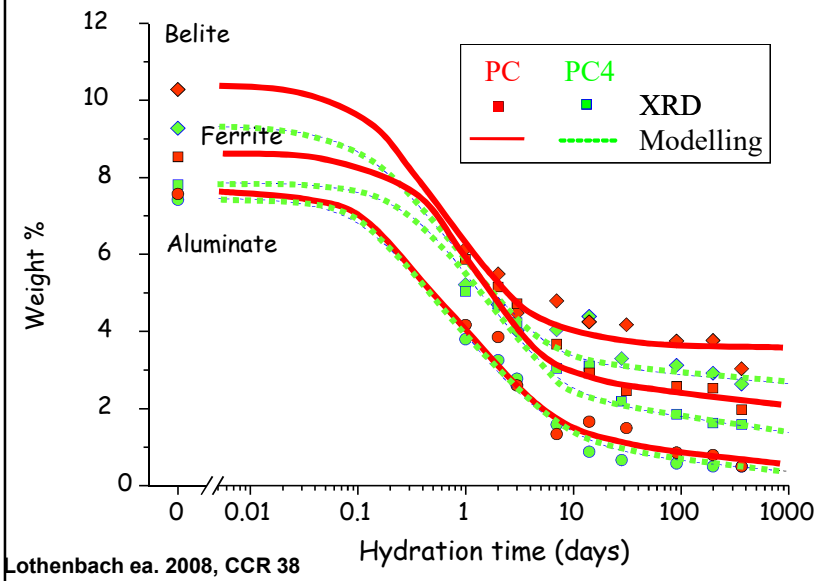
Modeling: Dissolution



Lothenbach ea. 2008, CCR 38

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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, ...

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Output data, Portlandite

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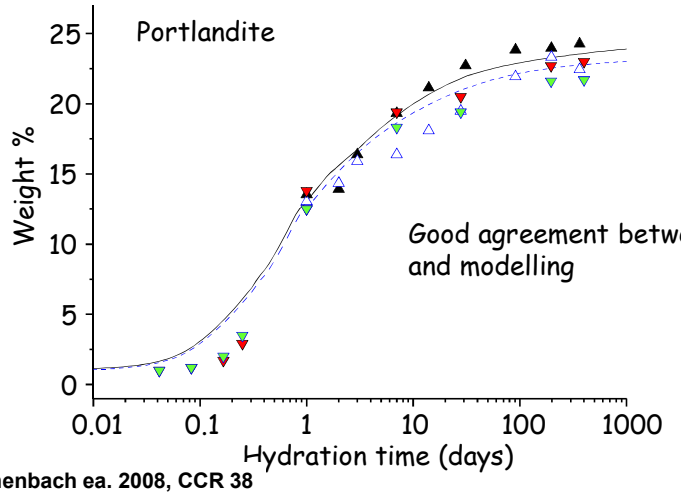
PC PC4
XRD, TGA
Thermodynamic modelling



Lothenbach ea. 2008, CCR 38

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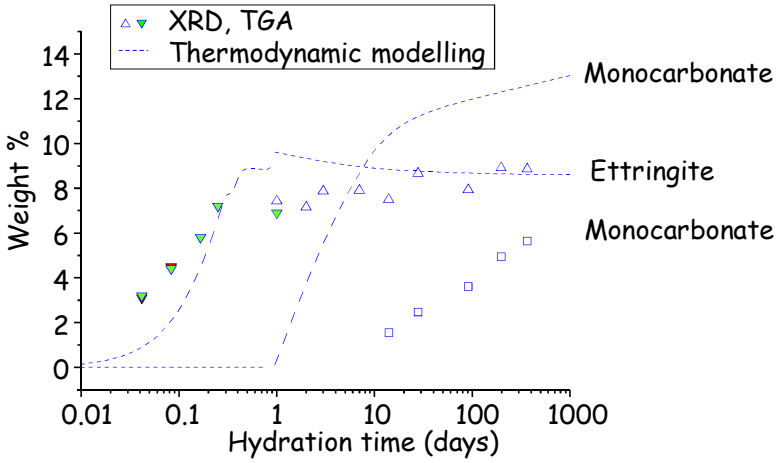
Output data, AFt, AFm phases



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

Lothenbach ea. 2008, CCR 38

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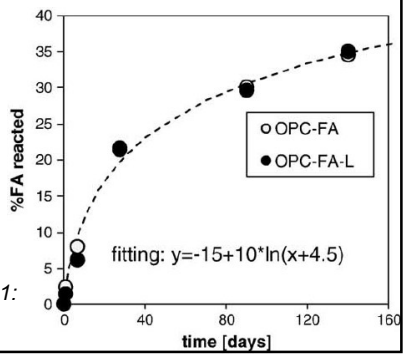
Conclusion

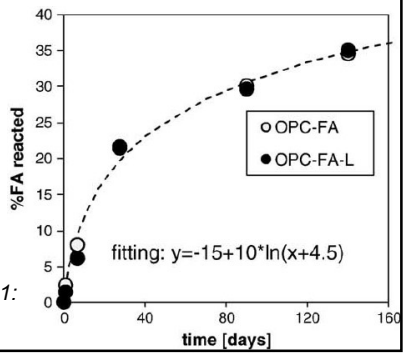
- Empirical approach of P&K (adapted)
  - Describes observed dissolution (> 1 day) in OPC well
  - Simple to use
  - Influencing parameters: **surface area, w/c, temperature**
  - Purely empirical, other models can be used
  - Other influences: pH, composition of pore solution, … not included
- Other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

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

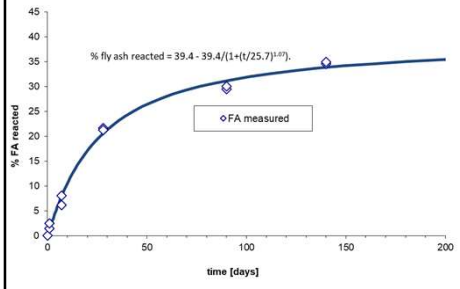


De Weerdt ea (2011) CCR 41: Reaction degree of fly ash

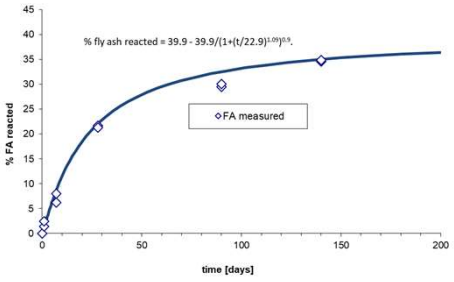
Alternative fits:

- four (4PL) five (5PL) parameter logistic fit

DoR= D+(A-D)/(1+(x/C)^B)
Symetric



DoR= D+(A-D)/(1+(x/C)^B)^G
Assymetric, sometimes overfitting



A	minimum
D	maximum
C	inflection point
B	steepness of curve
G	assymetry

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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

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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* $\alpha_{t-1}(total) > H \cdot w/c$; *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

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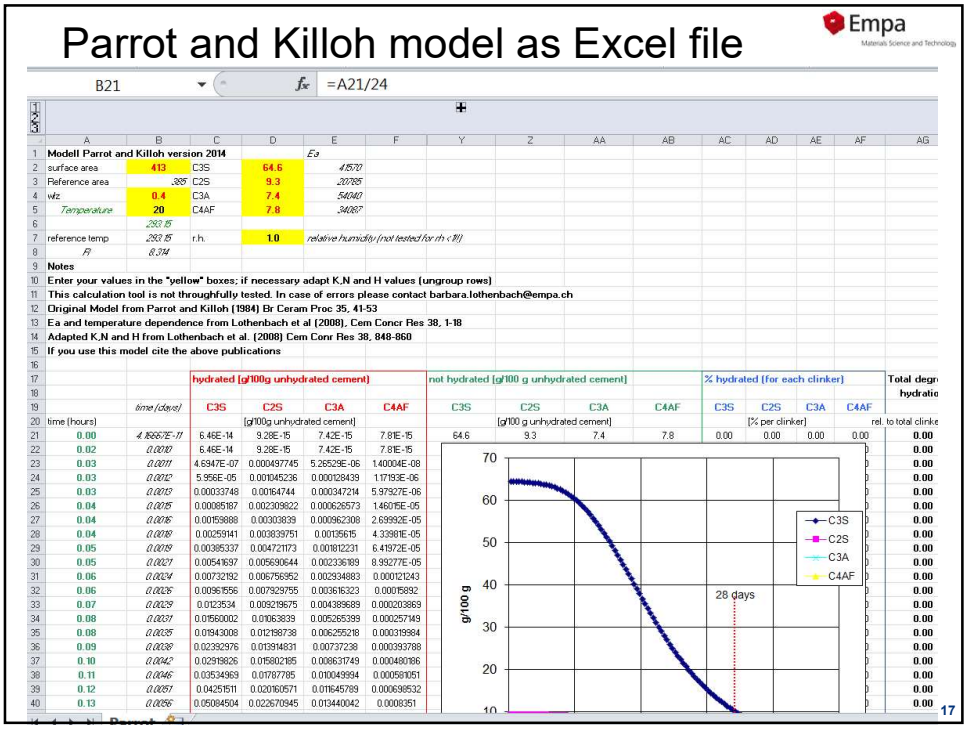
Parrot and Killoh model as Excel file



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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	wlz	**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	*Fl*	*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 hydratio**
18															
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**	*4.8667E-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*	4.694E-07	0.000497745	5.26529E-06	1.40004E-08									**0.00**
24	**0.03**	*0.0012*	5.95E-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	0.00472173	0.00181231	6.41972E-05									**0.00**
30	**0.05**	*0.0021*	0.00541697	0.00569044	0.002336189	8.93277E-05									**0.00**
31	**0.06**	*0.0024*	0.00732192	0.006756952	0.002934883	0.000121243									**0.00**
32	**0.06**	*0.0026*	0.00951556	0.007929755	0.003616323	0.00015892									**0.00**
33	**0.07**	*0.0028*	0.0123534	0.009219675	0.004389588	0.000203869									**0.00**
34	**0.08**	*0.0031*	0.01592002	0.01063839	0.005265399	0.000257149									**0.00**
35	**0.08**	*0.0035*	0.01943008	0.012198738	0.006255218	0.000319884									**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	0.000480786									**0.00**
38	**0.11**	*0.0046*	0.03534969	0.01787785	0.010049994	0.000581051									**0.00**
39	**0.12**	*0.0051*	0.0425151	0.020160571	0.011645789	0.000698532									**0.00**
40	**0.13**	*0.0056*	0.05084504	0.022670945	0.013440042	0.0008351									**0.00**

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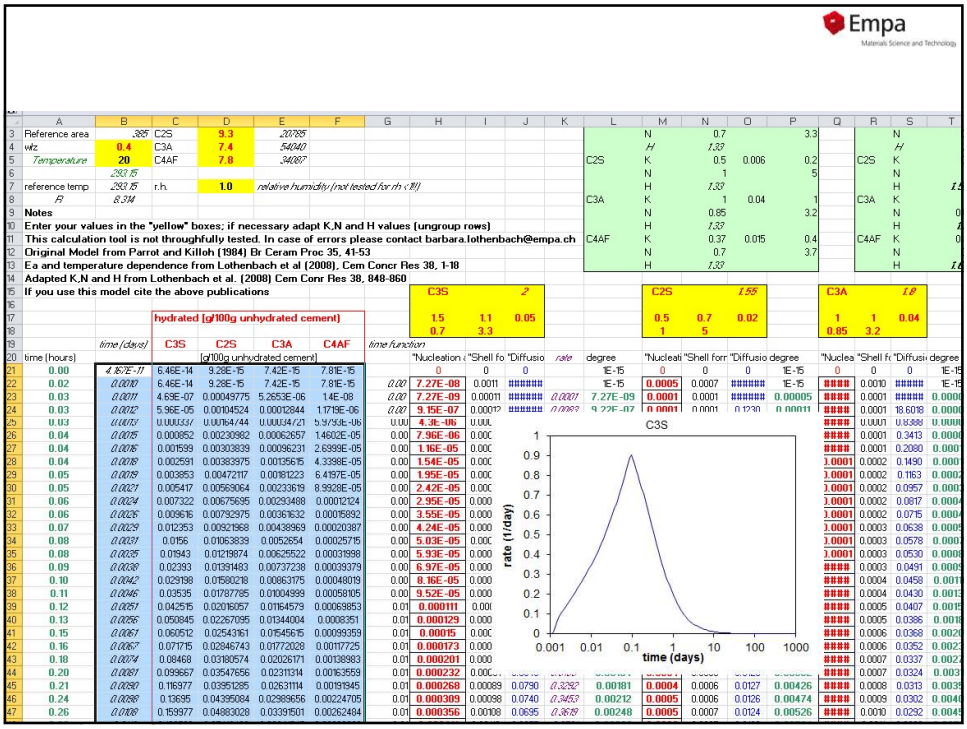

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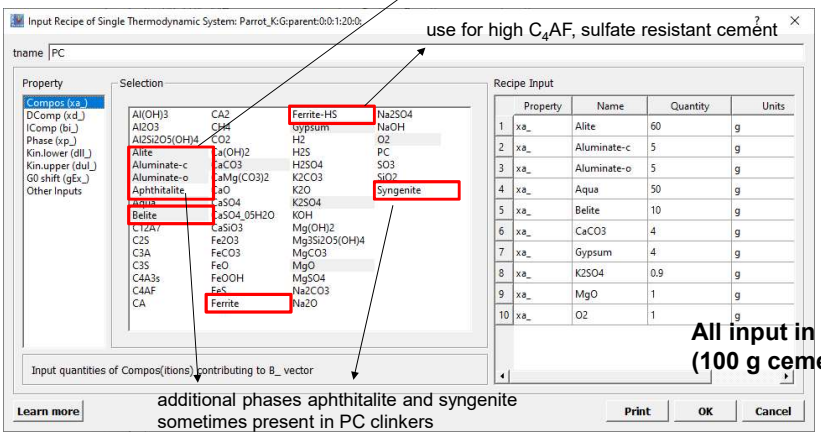
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
3	Reference area	*385*	C2S	**9.3**	*20785*								N	0.7		3.3			N	
4	wlz	**0.4**	C3A	**7.4**	*54040*								*H*	*1.33*					*H*	
5	*Temperature*	**20**	C4AF	**7.8**	*34087*							C2S	K	0.5	0.006	0.2		C2S	K	
6		*293.15*											N	1		5			N	
7	reference temp	*293.15*	r.h.	**1.0**	*relative humidity (not tested for rh < 1!)*								H	*1.33*					H	*1.5*
8	*Fl*	*8.314*										C3A	K	1	0.04	1		C3A	K	
9	**Notes**												N	0.85		3.2			N	0
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
12	**Original Model from Parrot and Killoh (1984) Br Ceram Proc 35, 41-53**												N	0.7		3.7			N	
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*					
16																				
17			**hydrated [g/100g unhydrated cement]**										1.5	1.1	0.05					
18													0.7	3.3						
19		*time (days)*	**C3S**	**C2S**	**C3A**	**C4AF**	*time function*													
20	time (hours)			[g/100g unhydrated cement]				*Nucleation r*	*Shell fo*	*Diffusio*	*rate*	degree	*Nucleati*	*Shell forr*	*Diffusio*	degree		*Nucleat*	*Shell fo*	*Diffusio*	degrees
21	**0.00**	*4.867E-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	*0.07*	**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	*0.07*	**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	*0.07*	**9.15E-07**	0.00012	#######	*0.0009*	9.22E-07	**0.0001**	0.0001	0.1230	0.00011		#####	0.0001	18.6018	0.0000
25	**0.03**	*0.0013*	0.00033747	0.00164744	0.00034721	5.97927E-06	0.00	**4.3E-06**	0.0001									#####	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	0.0000
28	**0.04**	*0.0018*	0.002591	0.00383975	0.00135615	4.3398E-05	0.00	**1.54E-05**	0.000									#####	0.0002	0.1490	0.0000
29	**0.05**	*0.0019*	0.003853	0.00472117	0.00181223	6.4197E-05	0.00	**1.95E-05**	0.000									#####	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									#####	0.0002	0.0957	0.0002
31	**0.06**	*0.0024*	0.007322	0.00675695	0.00293488	0.00012124	0.00	**2.95E-05**	0.000									#####	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									#####	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									#####	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									#####	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									#####	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**	*0.0089*	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. Copy folder **P_K** into C:\Users***\Library\Gems3\projects
2. Open GEMS and project P_K

Parent file

Clinker phases incl. minor elements as predefined compositions



All input in g (100 g cement)

additional phases aphthitalite and syngenite sometimes present in PC clinkers

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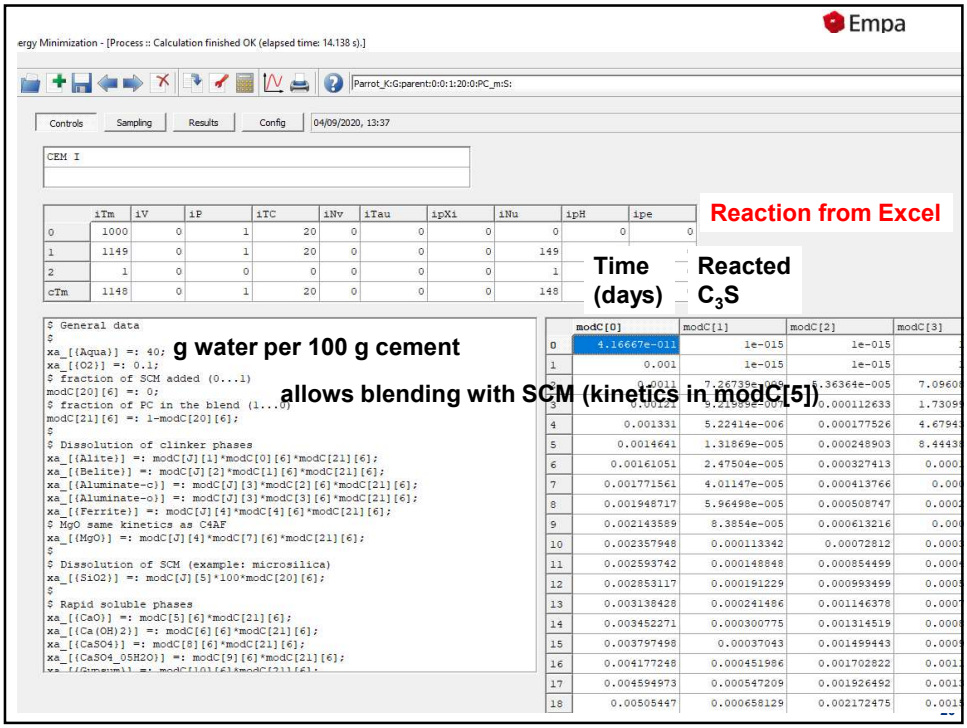

g water per 100 g cement

allows blending with SCM (kinetics in modC[5])

Cement composition in modC[6]

Reaction from Excel

Reaction degree
C_3S C_2S C_3A C_4AF SCM cement composition
MgO

	modC[1]	modC[2]	modC[3]	modC[4]	modC[5]	modC[6]
0	1e-015	1e-015	1e-015	1e-015	2.18727e-009	64.6
1	1e-015	1e-015	1e-015	1e-015	0.000749251	9.3
2	7.26739e-009	5.36364e-005	7.09608e-007	1.79262e-009	0.00080471	3.7
3	9.21989e-007	0.000112633	1.73099e-005	1.50055e-007	0.00086427	3.7
4	5.22414e-006	0.000177526	4.67943e-005	7.65592e-007	0.000928233	7.8
5	1.31869e-005	0.000248903	8.44438e-005	1.86959e-006	0.000996923	0.5
6	2.47504e-005	0.000327413	0.000129691	3.457e-006	0.001070689	0.4
7	4.01147e-005	0.000413766	0.00018277	5.55673e-006	0.001149905	0.9
8	5.96498e-005	0.000508747	0.000244236	8.21987e-006	0.001234972	3.1
9	8.3854e-005	0.000613216	0.00031485	1.15144e-005	0.001326321	0
10	0.000113342	0.00072812	0.000395537	1.55241e-005	0.001424414	0
11	0.000148848	0.000854499	0.000487375	2.03482e-005	0.001529747	1.2
12	0.000191229	0.000993499	0.000591602	2.61036e-005	0.001642852	0.2
13	0.000241486	0.001146378	0.000709623	3.29256e-005	0.001764301	0
14	0.000300775	0.001314519	0.000843021	4.09711e-005	0.001894704	0
15	0.00037043	0.001499443	0.000993582	5.04209e-005	0.00203472	4.6
16	0.000451986	0.001702822	0.001163308	6.14835e-005	0.002185052	0
17	0.000547209	0.001926492	0.001354447	7.43983e-005	0.002346457	0
18	0.000658129	0.002172475	0.001569513	8.94407e-005	0.002519744	0
19	0.000787075	0.00244299	0.001811326	0.000106927	0.002705782	0

C3S	64.6
C2S	9.3
C3A cubic	3.7
C3A orthorhombic	3.7
C4AF	7.8
CaO	0.5
Ca(OH)2	0.4
MgO	0.9
gypsum	3.1
hemihydrate	0
anhydrite	0
K2SO4	1.2
Na2SO4	0.2
Aphthitalite	0
Syngenite	0
Calcite	4.6
Dolomite	0
Quartz	0

Data adapted from Lothenbach et al., 2008

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Architecture of GEMS file

- Input always in g/100g
- The amount of clinker reacted copied from EXCEL file
- Inputs needed in GEMS:
  - w/c (as g water per 100 g cement)
  - Cement composition

C3S	64.6
C2S	9.3
C3A cubic	3.7
C3A orthorhombic	3.7
C4AF	7.8
CaO	0.5
Ca(OH)2	0.4
MgO	0.9
gypsum	3.1
hemihydrate	0
anhydrite	0
K2SO4	1.2
Na2SO4	0.2
Aphthitalite	0
Syngenite	0
Calcite	4.6
Dolomite	0
Quartz	0

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Architecture of GEMS file

- Process: sampling: definition of output
  - X-axis: log (time)
  - Mass in g/100 g of unhydrated cement
    - All data per 100 g unhydrated cement
      for comparison you will have to convert XRD/TGA data from g/100g hydrated paste to g/100g unhydrated cement
    - Amount of clinkers (with impurities)
    - Amount of hydrates (! Check single system file for the presence of additional solids and include them in the list)
    - Volumes in cm^3/100g unhydrated cement (conversion needed for experimental data)
    - Amount of pore solution (including dissolved species)

Check single system file for additional solids

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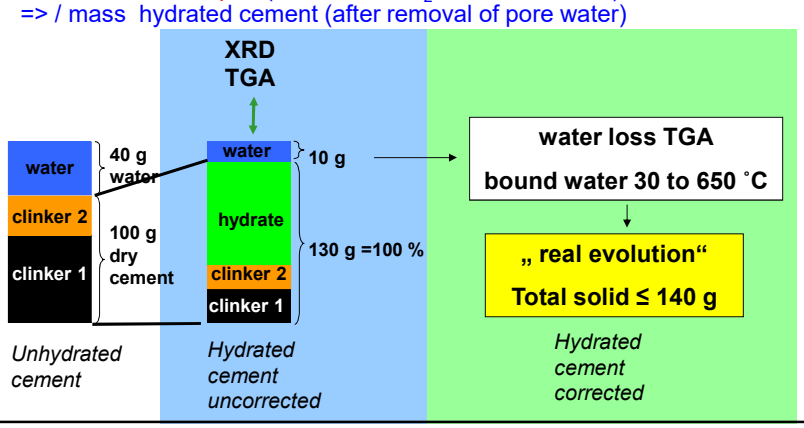
Different outputs possible

- 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)



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Different outputs possible

As the sample weight of the solid fraction of the sample is changing during hydration (see Figure 4.16 in Chapter 4 about XRD), the results need to be rescaled, to either paste or anhydrous, similarly as for the results of XRD-Rietveld analysis.

- Per 100 g paste:

$$Ca(OH)_{2,paste} = Ca(OH)_{2,measured}/[(1-H_2O_{bound})(1+w/c)] = \frac{Ca(OH)_{2,measured}}{\text{weight at } 600°C(1+w/c)} \quad (5.3)$$

- Per 100 g anhydrous:

$$Ca(OH)_{2,dry} = Ca(OH)_{2,measured}/(1-H_2O_{bound}) = \frac{Ca(OH)_{2,measured}}{\text{weight at } 600°C} \quad (5.4)$$

Lothenbach et al., Thermogravimetric analysis, in: Scrivener, Snellings, Lothenbach, A Practical Guide to Microstructural Analysis of Cementitious Materials, CRC Press, 2016

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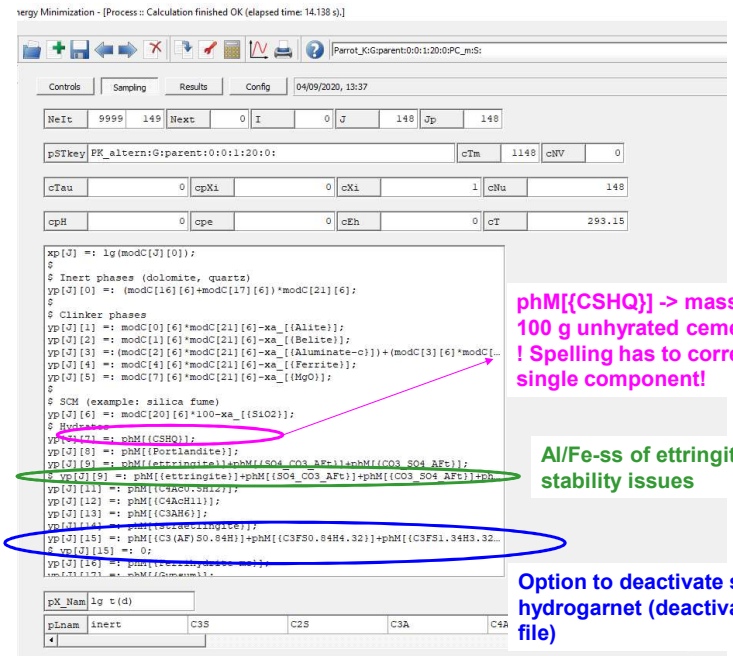

phM[{CSHQ}] -> mass of CSHQ in g per 100 g unhyrated cement
! Spelling has to correspond exactly to single component!

Al/Fe-ss of ettringite deactivated due to stability issues

Option to deactivate siliceous hydrogarnet (deactivate also in parent file)

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Empa

Controls | Sampling | Results | Config | 04/09/2020, 13:37

CEM I

Unit of x-axis

pY_Nam phM

pX_Nam	lg t(d)	inert	C3S	C2S	C3A	C4AF	MgO
0	-10.380211	0	64.6	9.3	7.4	7.8	0.9
1	-3	0	64.6	9.3	7.4	7.8	0.9
2	-2.9586073	0	64.6	9.2995012	7.3999947	7.8	0.9
3	-2.9172344	0	64.59994	9.2989525	7.3998719	7.7999988	0.89999986
4	-2.8758219	0	64.599663	9.298349	7.3996537	7.799994	0.89999931
5	-2.8344293	0	64.599148	9.2976652	7.3993751	7.7999854	0.89999832
6	-2.7930366	0	64.598401	9.2969551	7.3990403	7.799973	0.89999689
7	-2.7516439	0	64.597409	9.296152	7.3986475	7.7999567	0.899995
8	-2.7102512	0	64.596147	9.2952687	7.3981927	7.7999359	0.8999926
9	-2.6688585	0	64.594583	9.2942971	7.3976701	7.7999102	0.89998964
10	-2.6274658	0	64.592678	9.2932285	7.397073	7.7998789	0.89998603
11	-2.5860732	0	64.590384	9.2920532	7.3963934	7.7998413	0.89998169
12	-2.5446804	0	64.587647	9.2907605	7.3956221	7.7997964	0.89997651
13	-2.5032878	0	64.5844	9.2893387	7.3947488	7.7997432	0.89997037
14	-2.4618951	0	64.58057	9.287775	7.3937616	7.7996804	0.89996313
15	-2.4205024	0	64.57607	9.2860552	7.3926475	7.7996067	0.89995462
16	-2.3791097	0	64.570802	9.2841638	7.3913915	7.7995204	0.89994466
17	-2.337717	0	64.56465	9.2820836	7.3899771	7.7994197	0.89993304
18	-2.2963244	0	64.557485	9.279796	7.3883856	7.7993024	0.8999195
19	-2.2549317	0	64.549155	9.2771802	7.3865962	7.799166	0.89990377
20	-2.213539	0	64.539488	9.2745136	7.3845855	7.7990077	0.8998855
21	-2.1721463	0	64.528285	9.2714712	7.3823275	7.7988243	0.89986434
22	-2.1307536	0	64.51532	9.2681257	7.3797929	7.798612	0.89983984
23	-2.0893609	0	64.500333	9.264447	7.3769492	7.7983665	0.89981152
24	-2.0479683	0	64.483023	9.260402	7.3737598	7.798083	0.89977881

lg t(d)

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)

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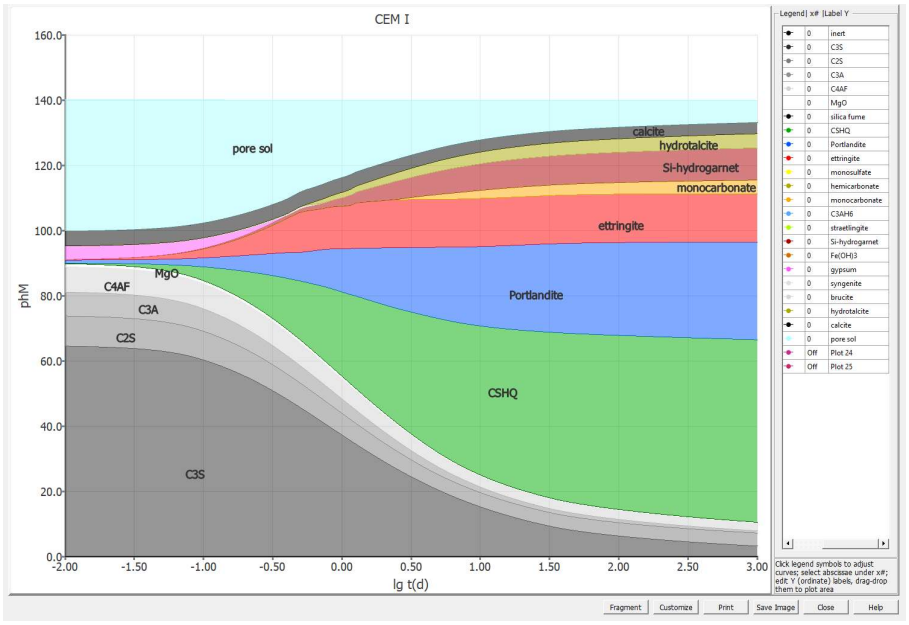
Empa



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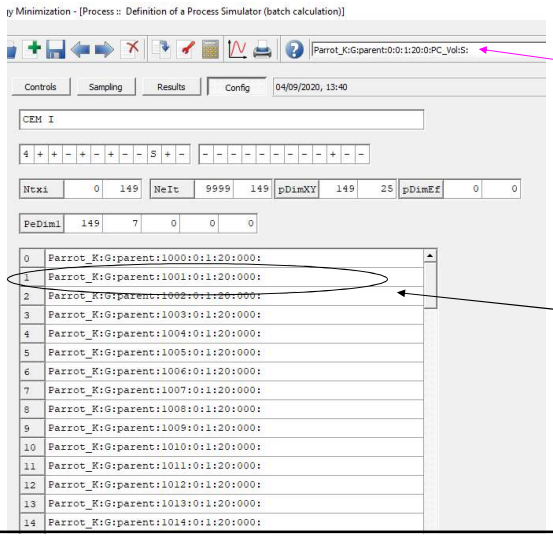
Architecture of GEMS file

- 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

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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

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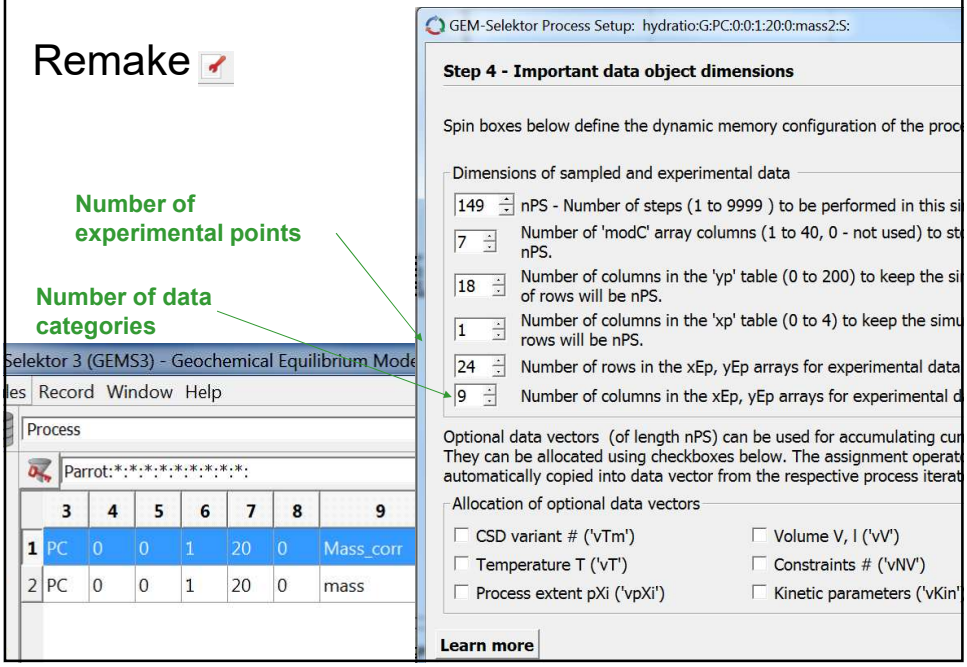
Comparison with experimental data

Empa

Remake

Number of experimental points

Number of data categories



Comparison with experimental data

Empa

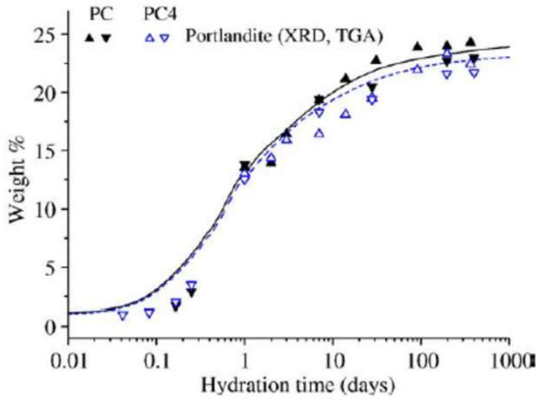


Fig. 11. Amounts of portlandite deduced by XRD/Rietveld analysis and thermal analysis as a function of hydration time. Lines refer to the results of thermodynamic modelling.

Lothenbach et al., 2008

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Comparison with experimental data

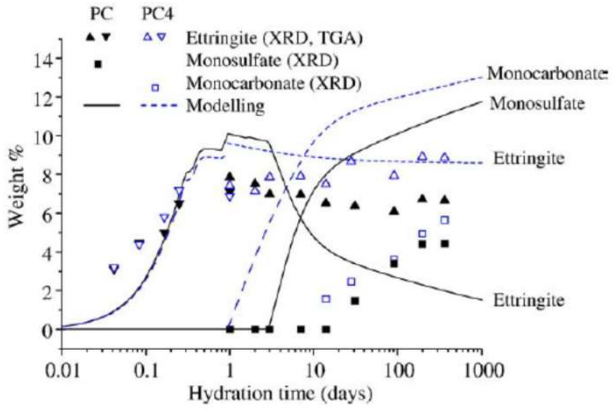

Fig. 12. Amounts of hydrated crystalline products deduced by XRD/ Rietveld analysis as a function of hydration time. Lines refer to the results of thermodynamic modelling.

Lothenbach et al., 2008

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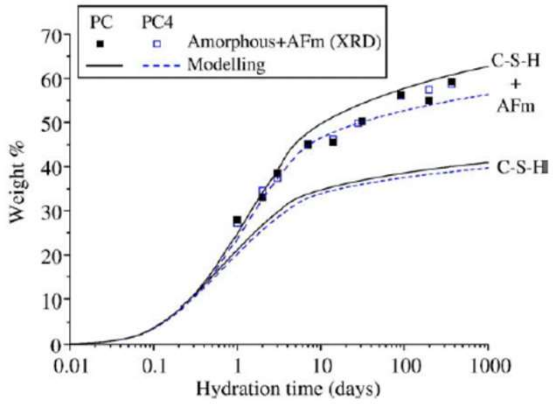
Comparison with experimental data



Amorph =
C-S-H + Ht + Mc+…

Fig. 13. Amounts of amorphous hydrated products deduced by XRD/ Rietveld analysis as a function of hydration time. Lines refer to the results of thermodynamic modelling.

Lothenbach et al., 2008

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Sampling of aqueous concentrations

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

Controls | Sampling | Results | Config | 04/09/2020, 13:37

NeIt	9999	149	Next	0	I	0	J	148	Jp	148	
pSTkey	PK_altern:G:parent:0:0:1:20:0:								cTm	1148	cNV 0
cTau	0		cpXi	0			cXi	1	cNu	148	
cpH	0		cpe	0			cEh	0	cT	293.15	

```
xp[J] =: lg(modC[J][0]);
$
$ Concentration (in mmol/l l solution)
$ re-calculation from molal (mol/kg H2O) -> molar (mol/l solution)
yp[J][0] =: lg(m_t{Al}*x[{H2O@}]*18.0153/phVol[{aq_gen}]*1000);
yp[J][1] =: lg(m_t[{C}]*x[{H2O@}]*18.0153/phVol[{aq_gen}]*1000);
yp[J][2] =: lg(m_t[{Ca}]*x[{H2O@}]*18.0153/phVol[{aq_gen}]*1000);
yp[J][3] =: lg(m_t[{Fe}]*x[{H2O@}]*18.0153/phVol[{aq_gen}]*1000);
yp[J][4] =: lg(m_t[{K}]*x[{H2O@}]*18.0153/phVol[{aq_gen}]*1000);
yp[J][5] =: lg(m_t[{Mg}]*x[{H2O@}]*18.0153/phVol[{aq_gen}]*1000);
yp[J][6] =: lg(m_t[{Na}]*x[{H2O@}]*18.0153/phVol[{aq_gen}]*1000);
yp[J][7] =: lg(m_t[{S}]*x[{H2O@}]*18.0153/phVol[{aq_gen}]*1000);
yp[J][8] =: lg(m_t[{Si}]*x[{H2O@}]*18.0153/phVol[{aq_gen}]*1000);
yp[J][9] =: lg(my[{OH-}]*x[{H2O@}]*18.0153/phVol[{aq_gen}]*1000);
```

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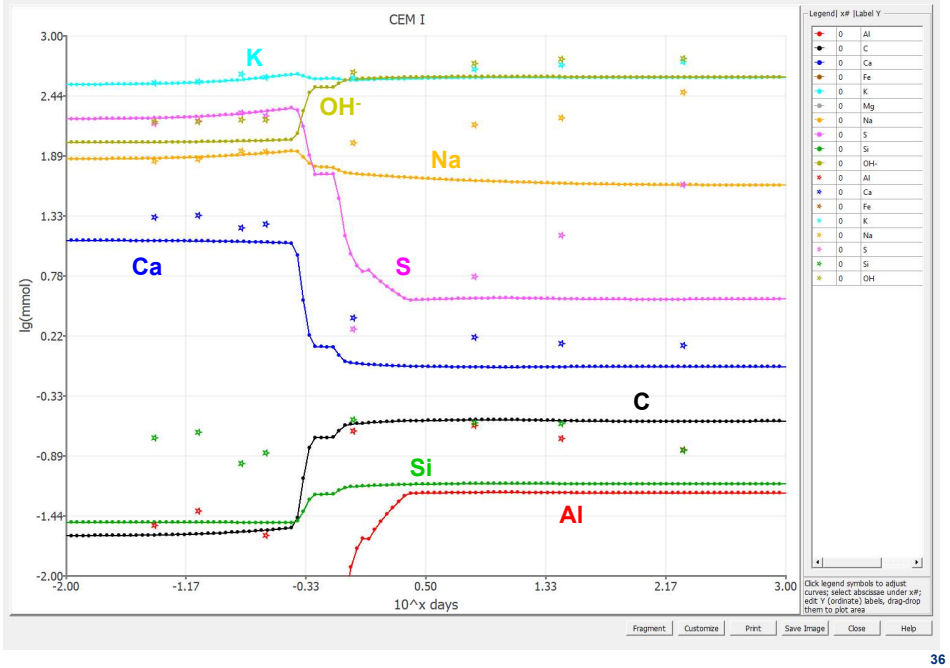

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Excercise

- Calculate volumes of the hydrating cement
- Hint:
  - Duplicate process «mass»
  - Exchange phM by phVol
- Use density to calculate volume of unreacted clinker:
  yp[J][1] =: (modC[0][6]*modC[21][6]-xa_[{Alite}])/**3.15**;
- yp[J][2] =: (modC[1][6]*modC[21][6]-xa_[{Belite}])/3.30;
- yp[J][3] =:(modC[2][6]*modC[21][6]-xa_[{Aluminate-c}])/3.064+(modC[3][6]*modC[21][6]-xa_[{Aluminate-o}])/3.052;
- yp[J][4] =: (modC[4][6]*modC[21][6]-xa_[{Ferrite}])/3.57;
- yp[J][5] =: (modC[7][6]*modC[21][6]-xa_[{MgO}])/3.58;

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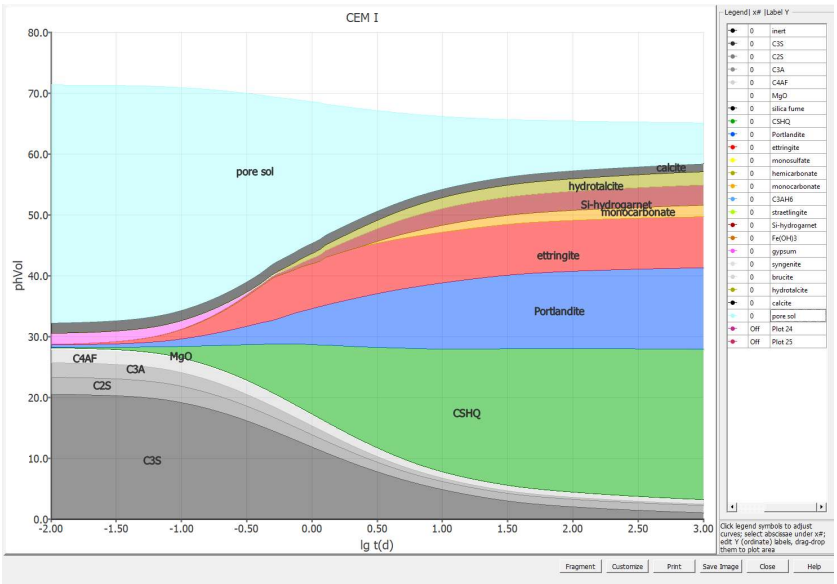
Volume in cm3/100 g unreacted cement



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