Oregon State University

Empa
Materials Science and Technology

Lecture 4
Hydrated Portland cement

Process calculations: Part 2

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Tutorial – process: hydration of Portland cement

Empa
Materials Science and Technology

Hydration of Portland cement

1) Hydration of PC - single system — Lecture 3

2) Influence of limestone on hydration of PC – process file
   a) Mass based output
   b) Volume based output
   c) Composition of aqueous phase

3) Influence of fly ash on hydration of PC – process file

Lecture 4

Process file - hydration of PC + limestone

Description of analytical problem

- Addition of increasing amounts of limestone to OPC
- We want to assess the chemical and mineralogical consequences of the addition of increasing amounts of limestone, as calcite, in a systematic way.
- Related phase changes
  a) mass changes
  b) volume changes
  c) changes in the aqueous phase composition

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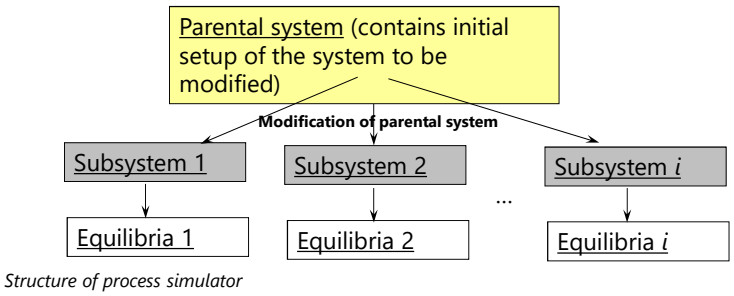
Process file - hydration of PC + limestone

Process simulations - Short introduction

- simulation of stepwise processes, e.g. dissolution, incremental addition, mixing, titration
- especially useful if a regular change of the bulk composition occurs in the process
- simulation of incremental temperature changes



Structure of process simulator

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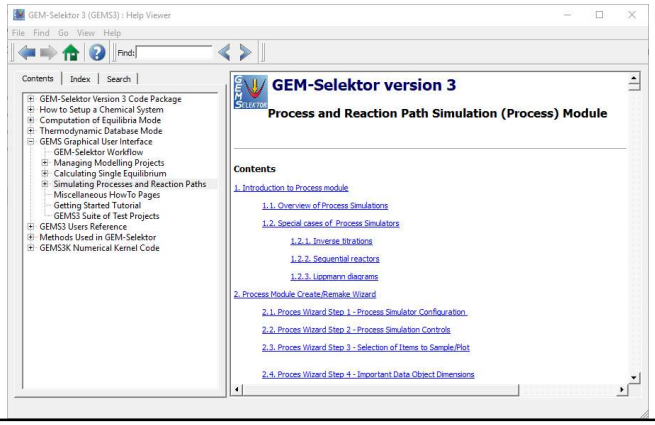
Process file - hydration of PC + limestone

Process simulations - Short introduction

- GEMS uses a built in math script interpreter to execute process simulations and other functions (similar to the macros in Excel)
- a description of the math script interpreter and used expressions can be found in the related GEMS help file



Process file - hydration of PC + limestone

Experimental problem:

Blending of the **hydrated cement** from the previous example ...

Normative phase composition [g/100 g]	
Alite [c]	66.5
Belite [c]	10.3
Aluminate [c]	7.5
Ferrite [c]	8.5
MgO(periclase) [c]	0.9
CaO (free) [d]	0.93
$CaCO_3$ [d]	0.6
$CaSO_4 \cdot 2H_2O$ [d]	3.1
K_2SO_4 [b]	1.3
Na_2SO_4 [b]	0.21
Present as solid solution in the clinker phases	
K_2O [d]	0.054
Na_2O [d]	0.33
MgO [d]	0.94
SO_3 [d]	0.11

B. Lothenbach et al. / Cement and Concrete Research 38 (2008) 848–860

Available in CEMDATA18 as predefined composition «PC»

Parental system

... with various amounts of **limestone**

Process file - hydration of PC + limestone

Experimental problem:

Addition of increasing amounts of limestone to PC up to 10% in steps of 0.2%)

Assumptions:

- initial amount of cement constant = 100 g "cement" = PC + limestone (= 100% $CaCO_3$)
- w/b ratio = 0.50 (50 g water), constant
- addition of 0.1 g O_2, constant
- 100% hydration

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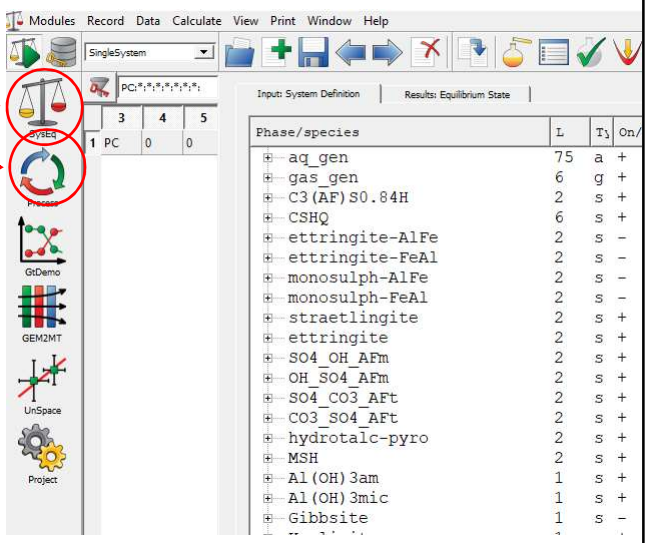
Process file - hydration of PC + limestone

We use the single file created previously now as parent file for the process simulation.

Single calculations →

Process calculations →



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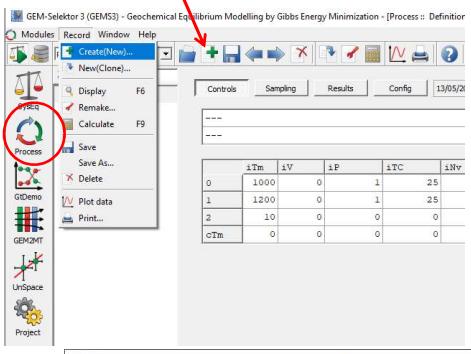
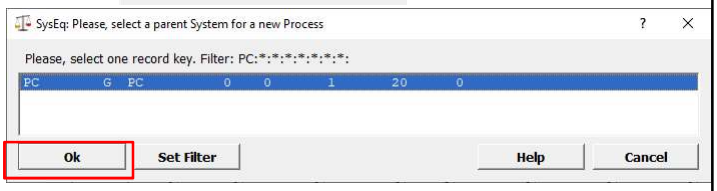
Process file - hydration of PC + limestone

Create new process file

or click here

1.





Select parent file

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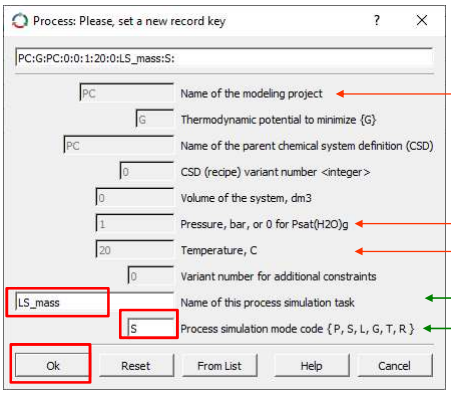
Process file - hydration of PC + limestone



project name

pressure

temperature

file name of process simulation

simulation type

user input

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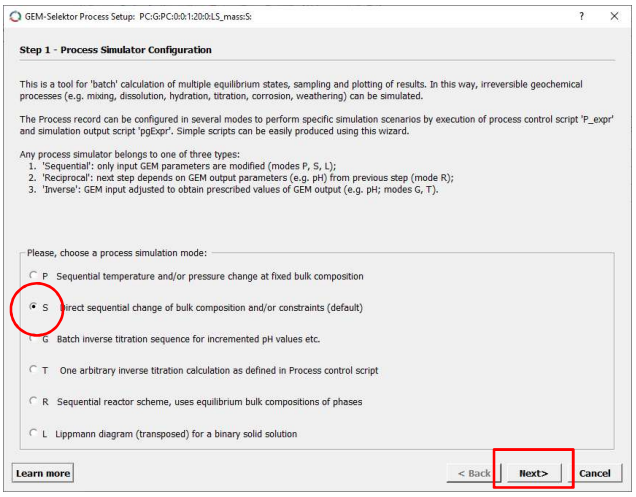
Process file - hydration of PC + limestone

Choice of simulation type:
In the case of incremental limestone addition we directly change the bulk composition

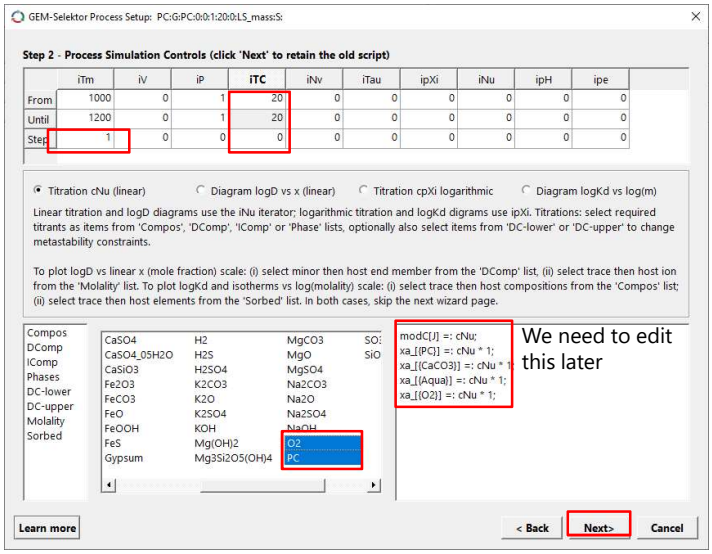
→ **Sequential change of bulk composition**



Process file - hydration of PC + limestone

Wizard available for process files

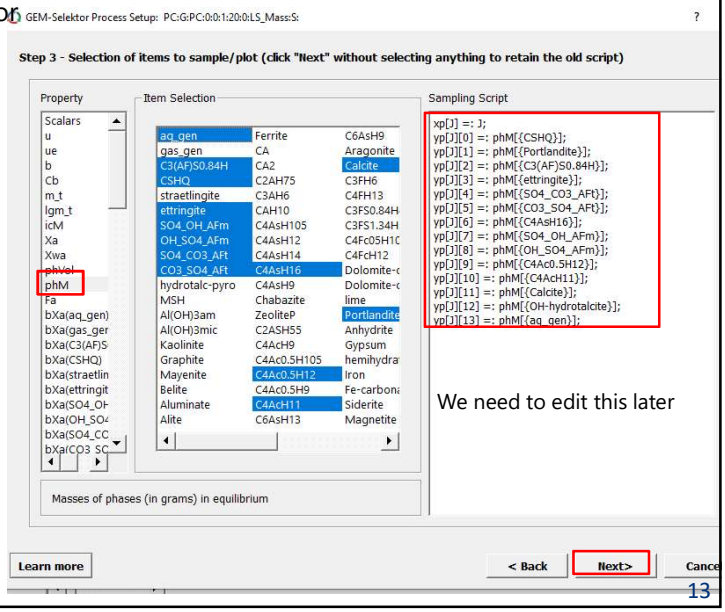
1. Adapt temperature and step size for stored individual calculations
2. Select PC and $CaCO_3$ (as we want to vary their relative amounts)
3. Select Aqua and O_2



Process file - hydration of PC + limestone

Wizard available for process files

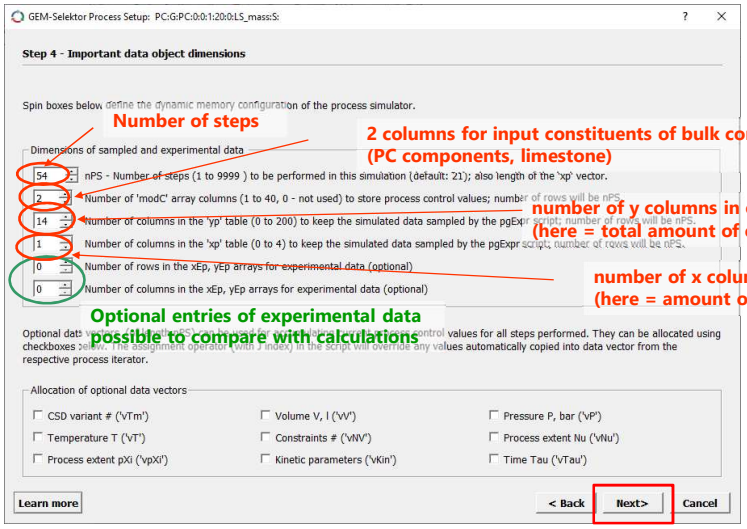
1. Select solids: choose
2. **phM** => **mass (in g)**; => we can adapt skript later



We need to edit this later

Process file - hydration of PC + limestone

Numerical settings of process simulation



Number of steps

2 columns for input constituents of bulk composition (PC components, limestone)

number of y columns in output file (here = total amount of expected phases = 14)

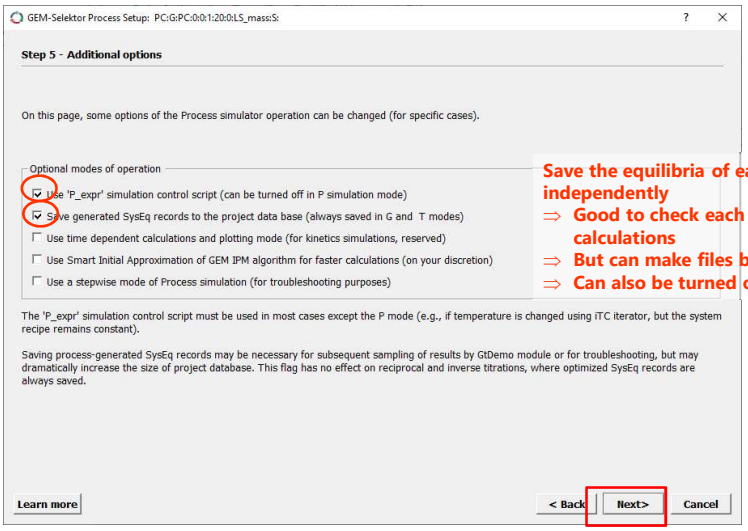
number of x columns in output file (here = amount of limestone)

Optional entries of experimental data possible to compare with calculations

Convenient to «overestimate» because maybe more phases occur than expected

Process file - hydration of PC + limestone

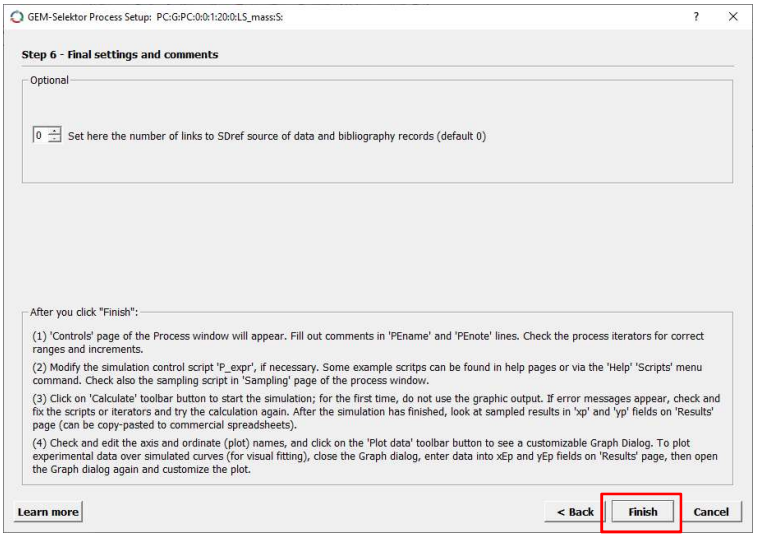
Additional settings



Save the equilibria of each step independently
⇒ Good to check each calculations
⇒ But can make files big
⇒ Can also be turned off

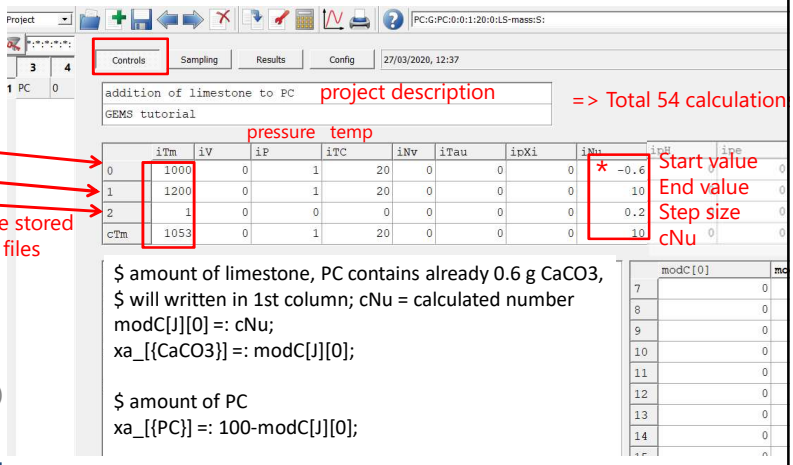
Process file - hydration of PC + limestone

Additional settings



Process file - hydration of PC + limes

cNu: running number
can be used for various calulation
here: fraction of $CaCO_3$




```
$ amount of limestone, PC contains already 0.6 g CaCO3,
$ will written in 1st column; cNu = calculated number
modC[J][0] =: cNu;
xa_[{CaCO3}] =: modC[J][0];

$ amount of PC
xa_[{PC}] =: 100-modC[J][0];

$ PC written in 2nd column;
modC[J][1] =: 100-modC[J][0];

$ water and oxygen
xa_[{Aqua}] =: 50;
xa_[{O2}] =: 0.1;
```

Modify text to
($ = comment)

When finished
Click somewhere
(outside active box)
=> else GEMS might
ignore changes

* *We start at -0.6 as our cement contains already 0.6% $CaCO_3$, and we want to model also the hydrates without any limestone*

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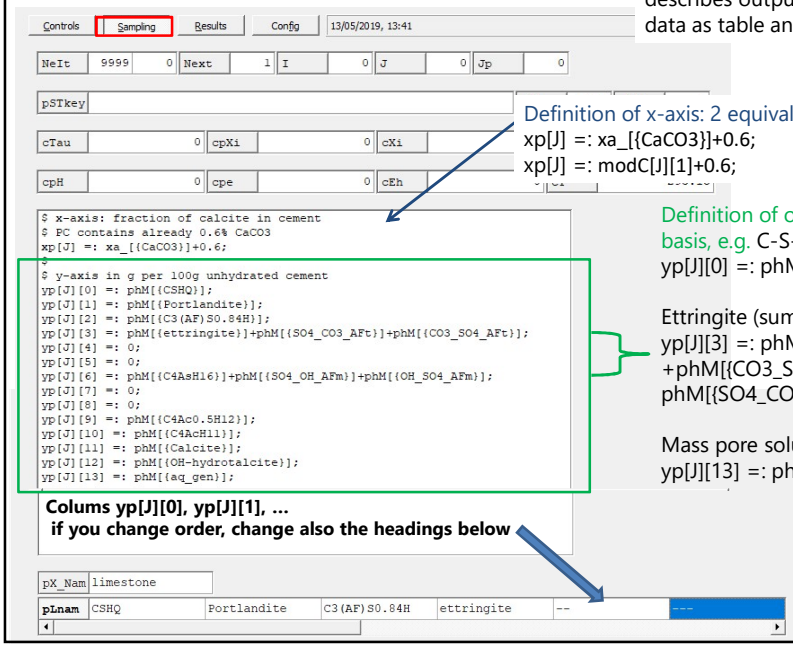
Process file - hydration of PC + limestone

Empa

describes output of calculated data as table and graph



Definition of x-axis: 2 equivalent options

```
xp[J] =: xa_[{CaCO3}]+0.6;
xp[J] =: modC[J][1]+0.6;
```

Definition of output on a mass basis, e.g. C-S-H

```
yp[J][0] =: phM[{CSHQ}];
```

Ettringite (summarized):

```
yp[J][3] =: phM[{ettringite}]
+phM[{CO3_SO4_AFt}]+
phM[{SO4_CO3_AFt}] ;
```

Mass pore solution:

```
yp[J][13] =: phM[{aq_gen}];
```

```
$ x-axis: fraction of calcite in cement
$ PC contains already 0.6% CaCO3
xp[J] =: xa_[{CaCO3}]+0.6;
$
$ y-axis in g per 100g unhydrated cement
yp[J][0] =: phM[{CSHQ}];
yp[J][1] =: phM[{Portlandite}];
yp[J][2] =: phM[{C3(AF)S0.84H}];
yp[J][3] =: phM[{ettringite}]+phM[{SO4_CO3_AFt}]+phM[{CO3_SO4_AFt}];
yp[J][4] =: 0;
yp[J][5] =: 0;
yp[J][6] =: phM[{C4AsH16}]+phM[{SO4_OH_AFm}]+phM[{OH_SO4_AFm}];
yp[J][7] =: 0;
yp[J][8] =: 0;
yp[J][9] =: phM[{C4Ac0.5H12}];
yp[J][10] =: phM[{C4AcH11}];
yp[J][11] =: phM[{Calcite}];
yp[J][12] =: phM[{OH-hydrotalcite}];
yp[J][13] =: phM[{aq_gen}];
```

Colums yp[J][0], yp[J][1], ...
if you change order, change also the headings below

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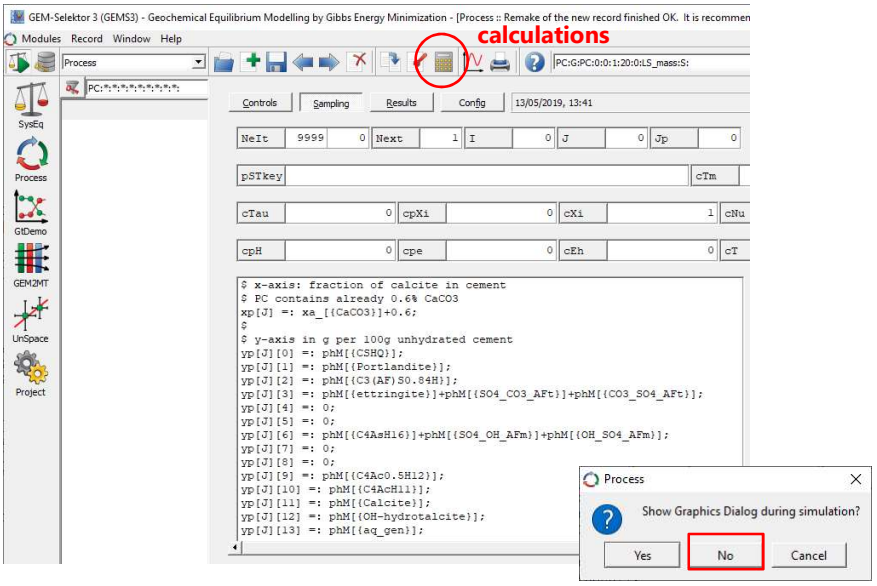
Process file - hydration of PC + limestone



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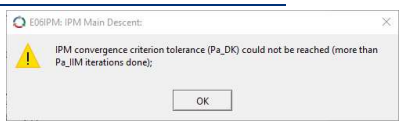
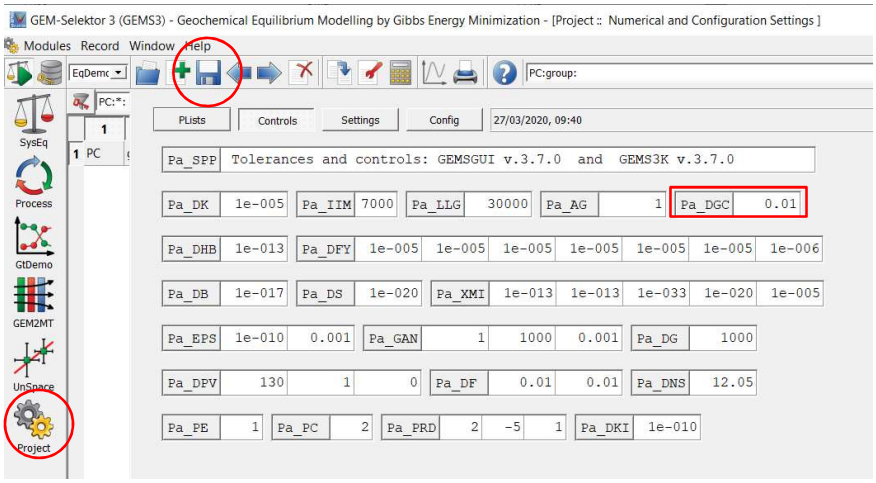
Process file - hydration of PC + limestone

In case the convergence error occurs ...





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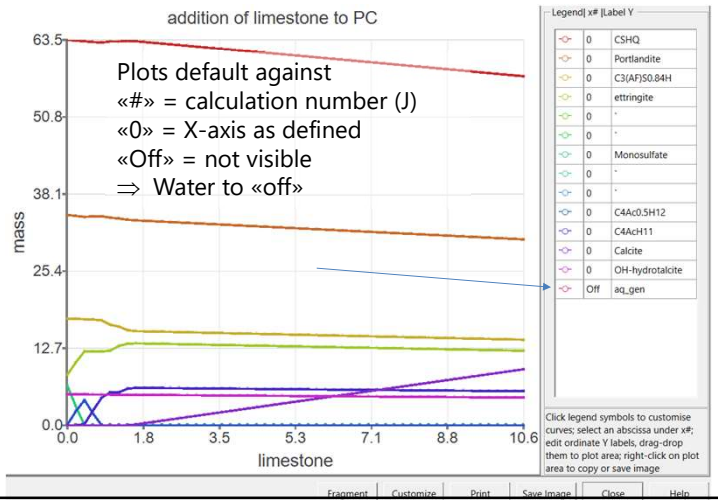
Process file - hydration of PC + limestone

1. open graph

2. label graph



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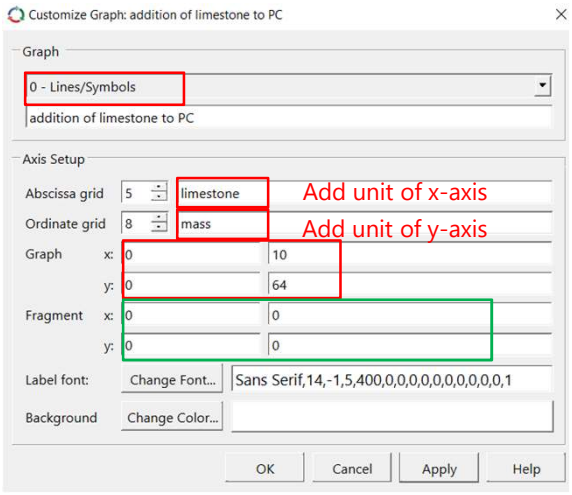
Process file - hydration of PC + limestone

Modify the graph as you prefer: example



Min - max

0 – 0: autoscale

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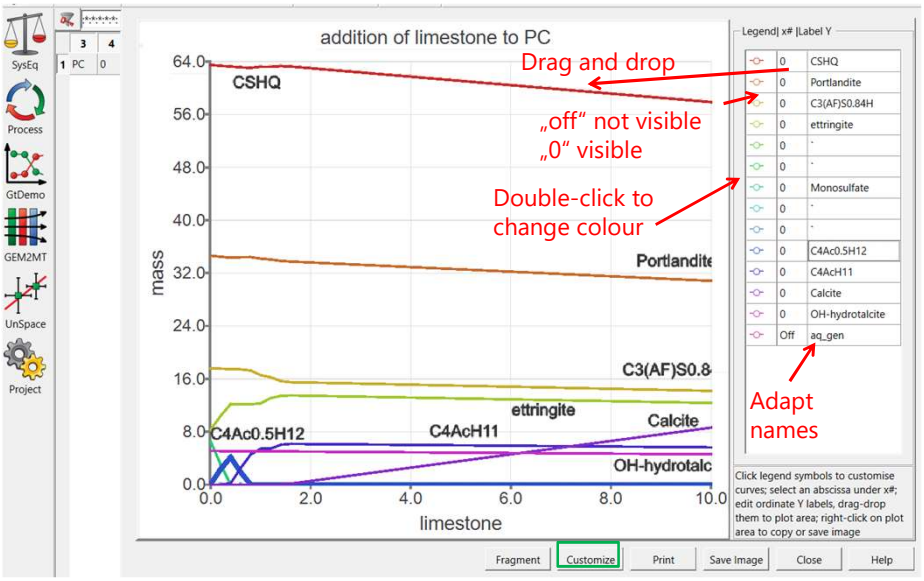
Process file - hydration of PC + limestone



To adapt scale / axis-labelling

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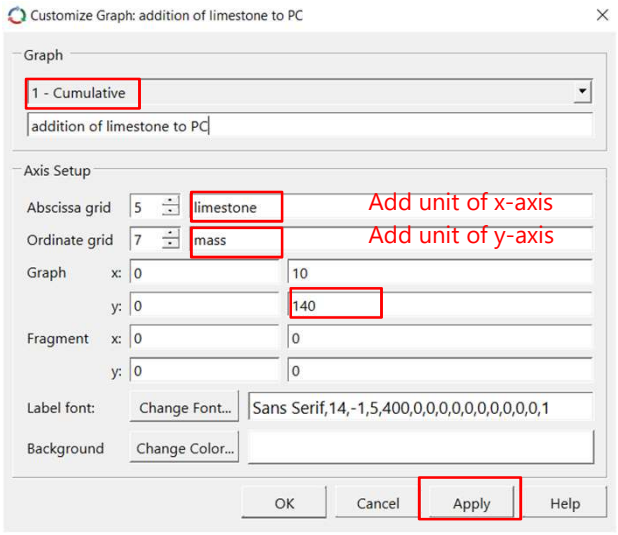
Process file - hydration of PC + limestone

Modify the graph as you prefer: example



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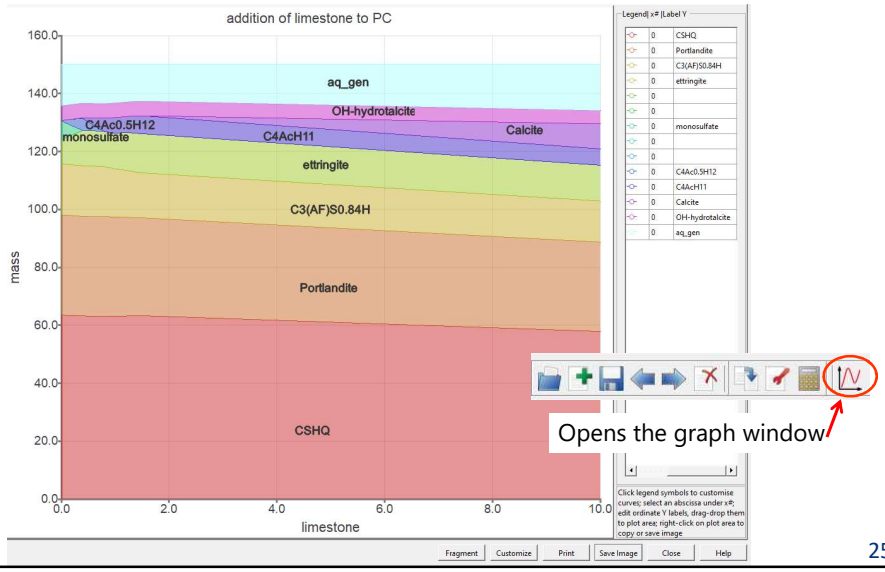
Process file - hydration of PC + limestone

Cumulative graph – good to check if a phase is missing in the output (as everything incl. water) needs to sum up to 150 g in this example)



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Process file - hydration of PC + limestone

Numerical output

Possibility of simple copy and paste of the data into other programs e.g. Excel or Origin

Controls | Sampling | Results | Config | 31/05/2023, 13:18

addition of limestone to PC | pY_Nam mass

pX_Nam	limestone	CSHQ	Portlandite	C3(AF)S0.84H	ettringite		
0	0	63.47953	34.63977	17.57782	8.325552	0	0
1	0.2	63.35415	34.47733	17.54284	10.38858	0	0
2	0.4	63.24718	34.32545	17.46471	12.19496	0	0
3	0.6	63.12069	34.40284	17.42985	12.17059	0	0
4	0.8	63.04952	34.42419	17.26622	12.1448	0	0
5	1	63.21118	34.18831	16.56108	12.31385	0	0
6	1.2	63.20575	34.05228	16.24585	13.08273	0	0
7	1.4	63.31221	33.84896	15.66943	13.42436	0	0
8	1.6	63.24648	33.74393	15.49346	13.503	0	0
9	1.8	63.11851	33.67438	15.4622	13.47583	0	0
10	2	62.99054	33.60484	15.43094	13.44865	0	0
11	2.2	62.86257	33.53529	15.39968	13.42148	0	0
12	2.4	62.7346	33.46576	15.36842	13.39431	0	0
13	2.6	62.60662	33.39622	15.33716	13.36714	0	0
14	2.8	62.47866	33.32669	15.3059	13.33996	0	0
15	3	62.35069	33.25716	15.27464	13.31279	0	0
16	3.2	62.22272	33.18764	15.24338	13.28562	0	0
17	3.4	62.09475	33.11812	15.21212	13.25845	0	0
18	3.6	61.96679	33.0486	15.18086	13.23127	0	0
19	3.8	61.83882	32.97909	15.1496	13.2041	0	0
20	4	61.71085	32.90958	15.11834	13.17693	0	0
21	4.2	61.58289	32.84008	15.08708	13.14976	0	0
22	4.4	61.45493	32.77058	15.05582	13.12258	0	0
23	4.6	61.32696	32.70108	15.02456	13.09541	0	0
24	4.8	61.199	32.63158	14.9933	13.06824	0	0

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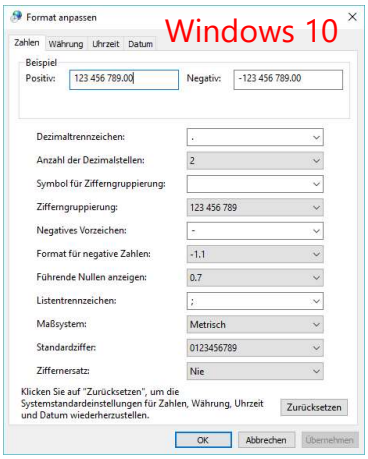
Process file - hydration of PC + limestone

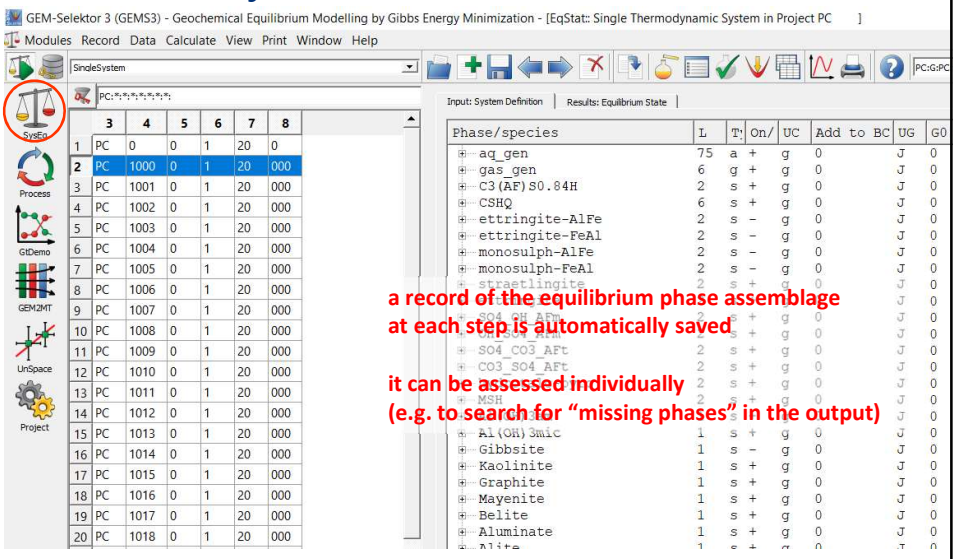
Copying data to or from Excel files

We need **decimal points**, **not commas** !

Change your excel to use „ . “ as a decimal point in the control panel of Windows



Process file - hydration of PC + limestone

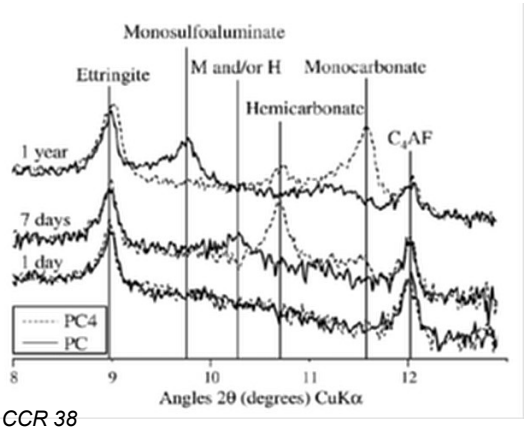


a record of the equilibrium phase assemblage at each step is automatically saved

it can be assessed individually (e.g. to search for “missing phases” in the output)

Background: Limestone addition to PC

Formation of monosulfoaluminate in carbonate free paste, whereas monocarboaluminate+AFt are predominant in calcite blended paste



Lothenbach ea 2008, CCR 38

Good agreement between experiments and calculations

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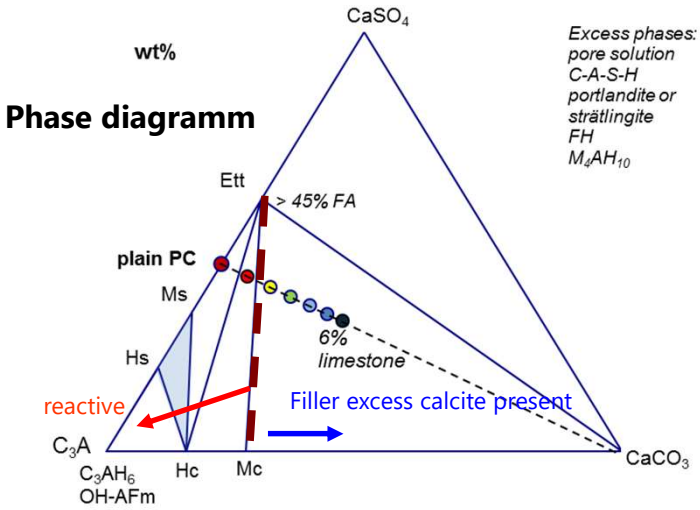
Background: Limestone addition to PC



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Process file - hydration of PC + limestone

The past example has shown that adding limestone causes significant mineralogical changes during cement hydration.

While these changes affect the qualitative composition of the phase assemblages they also affect the quantities of phases present.

Thus an influence on the specific volumes of the hydrated phases in dependence of the limestone content is likely.

Modification of the existing process to plot
- *specific volumes of the individual phases present in the chosen example*
- *composition of the liquid phase*

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Process file - hydration of PC + limestone

Example calculation of volume changes:

Modification of the existing process to plot specific volumes of the individual phases present in the chosen example

Calculation of volumes is based on individual molar volumes of each phase included in the database

Ettringite with 32 H2O			
((H2O)2)Ca6Al2(SO4)3(OH)12(H2O)24			
M0	1255.1108	Zz	0	ab	
V0d	70.703003	0	
G0d	-15205936	---	
H0d	-17535007	---	
S0d	1900	---	
Cp0d	2174.3604	0	
PrTr	1	25	
LamST	---	---	
BetAlp	---	---	
0	Lothenbach_ea:2008:pap:	logK -44.9; S
1	Ederova_ea:1979:pap:	Cp
2	Taylor:1997:book:	V0 (dens 1775 kg/m3)

For example ettringite:

Theor. density: 1.775 g/cm³ (derived from fitted unit cell size)

Molar volume

= 1255.11 g/mol / 1.775 g/cm³ = 707 cm³/mol

1cm³/mol = 10^{-1}J/bar → <u>70.7 J/bar</u>

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Process file - hydration of PC + limestone

Modification of the existing process to plot specific volumes of the individual phases present in the chosen example

Hints:

- **Clone "old" process (ensure that you are in process mode) and save it under a different name (suggested name: LS_Vol).**
- **Select same parent system.**
- **Only change the output part of the process file to calculate volume instead of mass.**
  example:

mass:
yp[J][0] =: phM[{CSHQ}];

volume:
yp[J][0] =: phVol[{CSHQ}];

- **Efficient: copy to word and use "replace"**

yp[J][0] =: Xa[{CSHQ}]; **=> *Moles***

- **Change y-axis labelling to "volume" and make a cumulative plot.**

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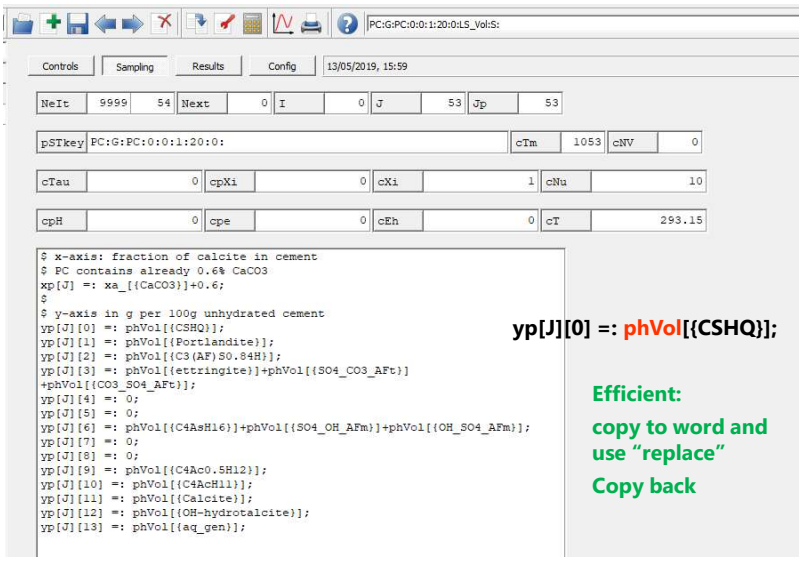
Process file - hydration of PC + limestone



yp[J][0] =: phVol[{CSHQ}];

Efficient:
copy to word and use "replace"
Copy back

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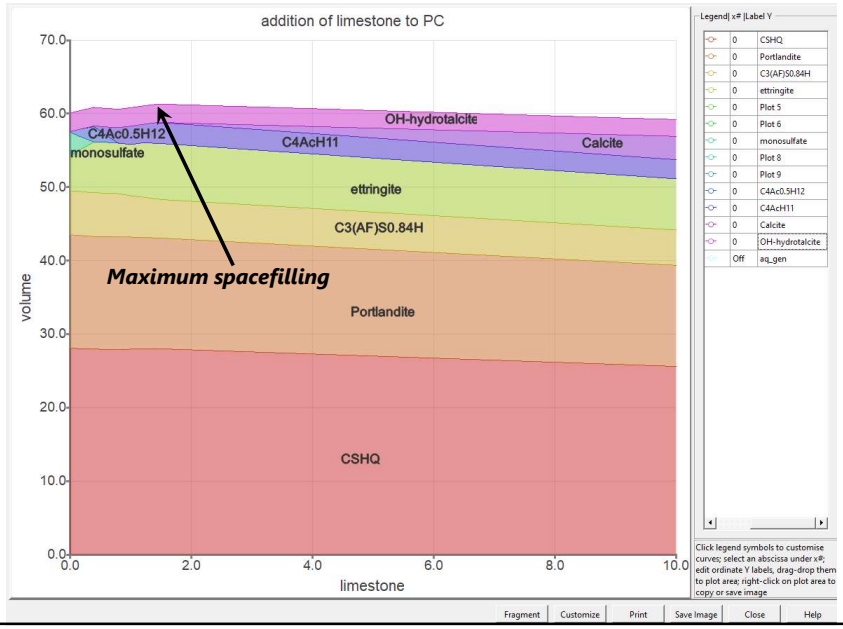
Process file - hydration of PC + limestone



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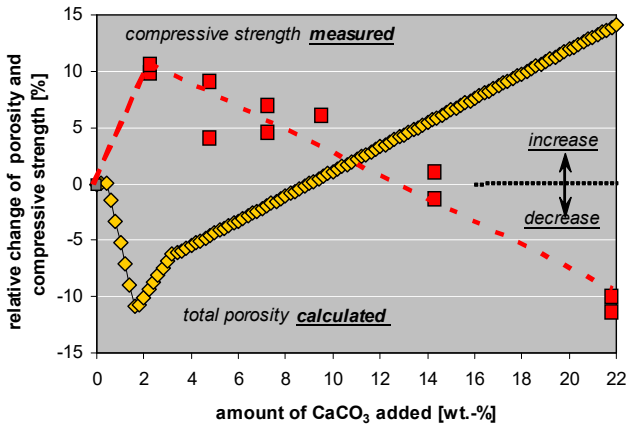
Process file - hydration of PC + limestone

Possible Links: **Thermodynamics vs. engineering properties**



one example of a good correlation between predicted changes of relative porosity and measured compressive strength

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Process file - hydration of PC + limestone

Example calculation of pore solution composition:

- Clone "old" process (ensure that you are in process mode) and save it under a different name (suggested name: LS_sol).
- Select same parent system.
- Only change the output part of the process file to calculate ionic concentrations. Use the recipe wizard.
- Plot aqueous composition as total molality [mmol/kg] and pH

Aqueous composition:

this example

yp[J][0] =: m_t[{Ca}];	***total concentration (as measured e.g. by ICP-OES or IC)***
yp[J][0] =: lgm_t[{Ca}];	***log total concentration (as measured e.g. by ICP-OES or IC)***
yp[J][0] =: my[{Ca+2}];	***species concentrations***
yp[J][0] =: 10^lga[{Ca+2}];	***species activity (as measured by ion selective electrode)***
yp[J][0] **=: pH;**	gives *pH ! Very sensitive to temperature*
yp[J][0] =: **IS;**	ionic strength
yp[J][0] =: **my[{OH-}];**	hydroxide concentration (molal)

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Process file - hydration of PC + limestone

Controls | Sampling | Results | Config | 27/03/2020, 13:55

NeIt	9999	0	Next	1	I	0	J	0	Jp	0

pSTkey	PC:G:PC:0:0:1:20:0:	cTm	1(

cTau	0	cpXi	0	cXi	1	cNu	

cpH	0	cpe	0	cEh	0	cT	

```
$$x axis: total fraction of CaCO3 in cement
$PC contains already 0.6 wt%
xp[J] =: xa_[{CaCO3}]+0.6;

yp[J][0] =: lgm_t[{Al}];
yp[J][1] =: lgm_t[{C}];
yp[J][2] =: lgm_t[{Ca}];
yp[J][3] =: lgm_t[{Fe}];
yp[J][4] =: lgm_t[{K}];
yp[J][5] =: lgm_t[{Mg}];
yp[J][6] =: lgm_t[{Na}];
yp[J][7] =: lgm_t[{S}];
yp[J][8] =: lgm_t[{Si}];
yp[J][9] =: pH;
```

yp[J][0] =: lgm_t[{Al}];
log total concentration
(as measured e.g. by ICP-OES or IC)

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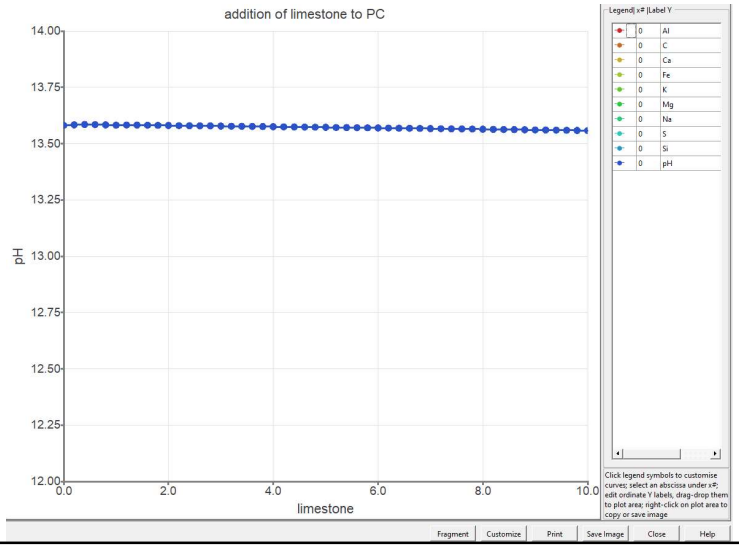
Process file - hydration of PC + limestone

pH - value



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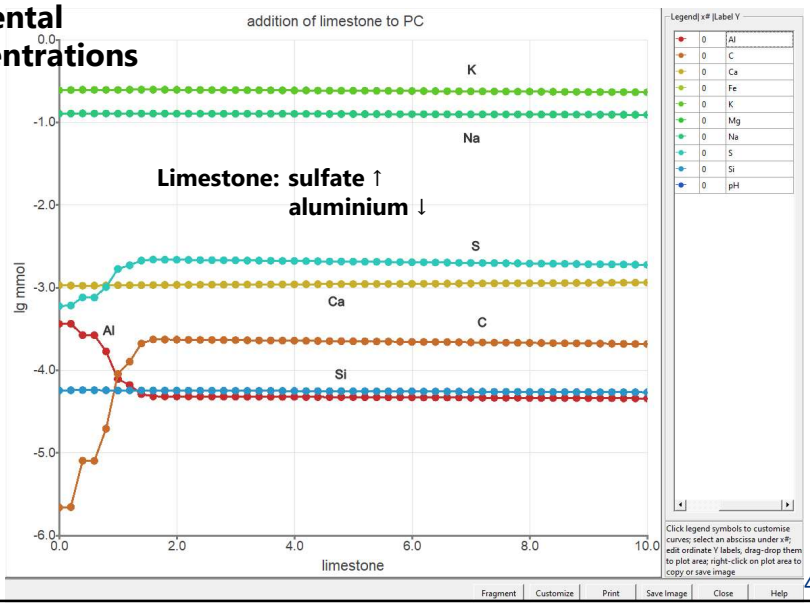
Process file - hydration of PC + limestone

Elemental concentrations



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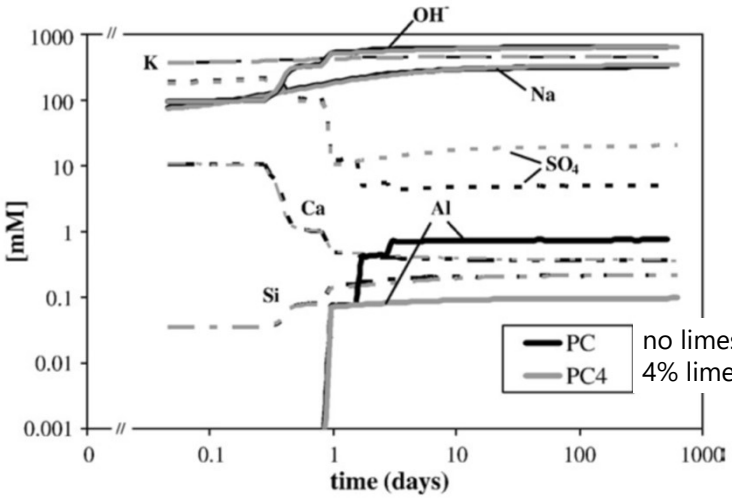
Process file - hydration of PC + limestone



Lothenbach ea 2008, CCR 38

Limestone: sulfate ↑
aluminium ↓

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Process file - hydration of PC + limestone

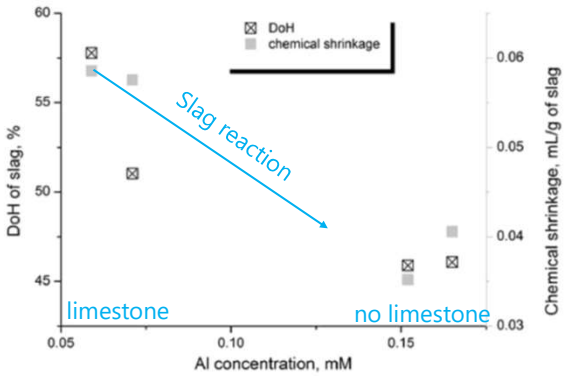

Fig. 21. The relationship between Al concentration in the pore solution and chemical shrinkage and degree of hydration of slag at 28 days. Note, there is ± 2% error associated with the method for measuring the DoH of slag.

Adu-Amankwah ea 2017, CCR 100

Limestone: sulfate ↑
aluminium ↓

⇒ **High Al suppresses slag and alite reaction**
⇒ **Limestone accelerates**

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Process file - hydration of PC + fly ash

The past example has shown that adding limestone causes significant mineralogical changes during cement hydration.

We now take a look what will happen when we use fly ash instead of limestone.

In a second step we replace 5% of PC by limestone in those blends

Modification of the existing process to plot
- *PC blended with fly ash (0-20 mass-% replacement in steps of 0.4 mass-%)*
- *PC blended with fly ash (0-20 mass-% replacement in steps of 0.4 mass-%), subtraction of 5 mass-% of PC by limestone*

Mass-based output only.

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Process file - hydration of PC + fly ash

Example:

- **Modification of the existing process to plot a) masses and b) specific volumes of the individual phases present in the chosen example**
- **Use an "artificial fly ash" with 100% glass content and simplified composition**
- **Assume 100% hydration of the fly ash and congruent dissolution**
- **Vary fly ash content between 0 and 20% in steps of 0.4%**
- **Create a predefined composition for fly ash (FA)**

Hints:

- **Clone the project with limestone addition (mass-based), name it e.g. FA_mass**
- **Modify the input part:**
  - **Vary fly ash content: modC[J][0] =: cNu*0.4;**
  - **Fly ash quantity as xa_[{FA}] =: ...**
  - **Remember that there is no limestone in the fly ash**
  - **Activate C_3AH_6 in the parent file**
- **Check for missing phases (look at the calculated single files). Add them to the output part. Label the graph correctly.**
- **When the mass-based file runs smoothly, clone the file, name it e.g. FA_Vol and modify the output part to display specific volumes (optional individual work)**

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Process file - hydrated of PC + fly ash

Composition of fly ash

average glass composition

XRF-analysis[a] [wt%]	F1
SiO_2	50.9
Al_2O_3	24.7
Fe_2O_3	7.3
CaO	3.7
MgO	1.8
K_2O	3.9
Na_2O	0.9
TiO_2	1.1
Mn_2O_3	0.1
P_2O_5	0.8
SO_3	0.4[c]
SrO	
LOI	3.5
C	2.7[d]
Sum	99.1

Mineralogical phase composition[b] [wt%]	F1
Mullite	8.2
Quartz	7.0
Hematite	0.7
Magnetite	0.8
Anhydrite	
Periclase	
Lime	
Amorphous	83.3
	100.0

Glass composition [wt%]	F1
SiO_2	54.4
Al_2O_3	24.8
Fe_2O_3	5.7
CaO	4.6
MgO	2.1
K_2O	4.9
Na_2O	1.1
TiO_2	1.4
Mn_2O_3	0.1
P_2O_5	0.9
SO_3	0.0
	100.0

We only consider the «big four» to make it simpler.

Deschner et al., Cem Concr. Res. 42 (2012), 1389-1400.

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Process file - hydrated PC + fly ash

Fly ash as predefined composition

Two options for input:

Glass composition [wt%]	F1
SiO_2	54.4
Al_2O_3	24.8
Fe_2O_3	5.7
CaO	4.6
MgO	2.1
K_2O	4.9
Na_2O	1.1
TiO_2	1.4
Mn_2O_3	0.1
P_2O_5	0.9
SO_3	0.0

Option 1: Input in g oxide

recalculation in mol-%

	in glass	normalised	molar mass	normalised
	g/100g	g/100g	g/mol	mol/100g
SiO2	54.4	60.6	60.08	1.00943076
Al2O3	24.8	27.6	101.96	0.27116236
Fe2O3	5.7	6.4	159.69	0.03979282
CaO	4.8	5.4	56.08	0.0954203
total	89.7	100		

recalculation in atom-%

	normalised
	mol/100g
Si	1.00943
Al	0.54232
Fe	0.07959
Ca	0.09542
O	3.04715

=> Different options for input in predefined composition

Option 2: Input in mol elements

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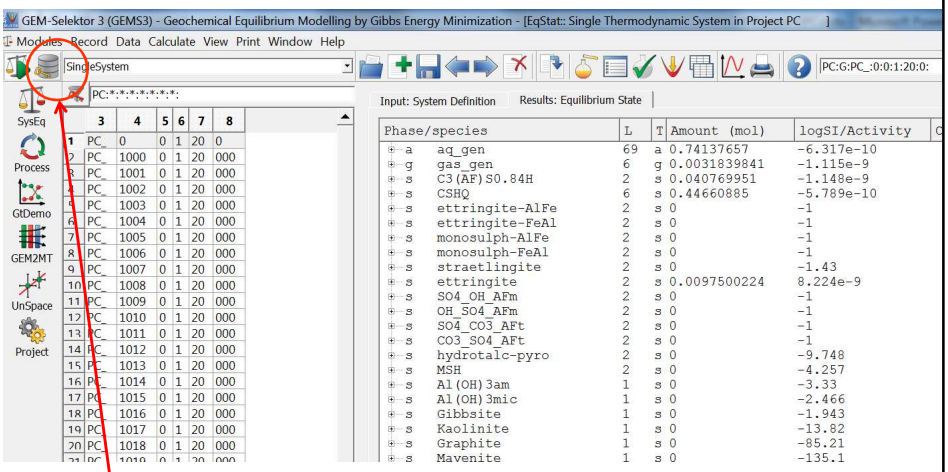
Process file - hydrated PC + fly ash

Make a predefined composition for fly ash



Click here to assess the copy of the database associated with this project

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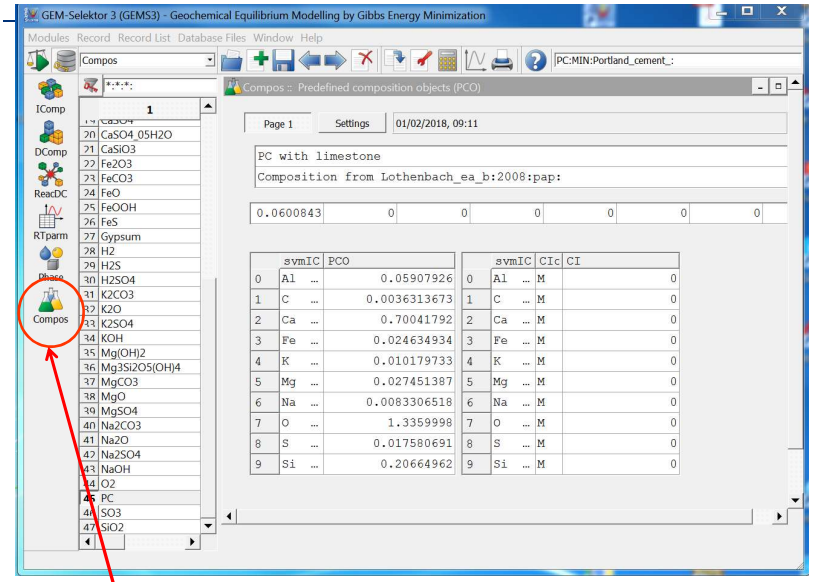
Make a predefined composition for fly ash



Click here to assess the list of predefined compositions and to create a new one

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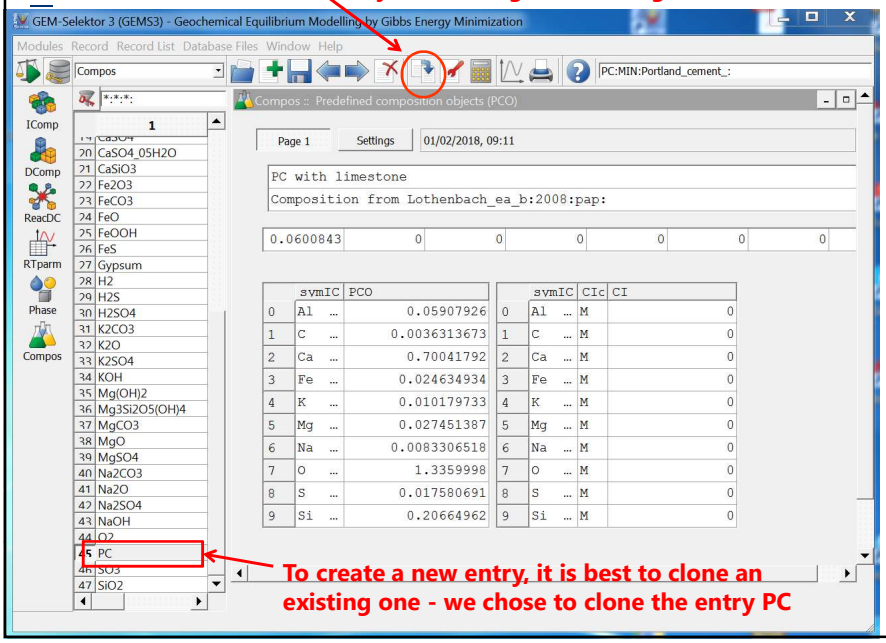
N

Use «Record – New(Clone)» from the pull-down menue or click here («Record – Remake» allows you to change an existing record)



To create a new entry, it is best to clone an existing one - we chose to clone the entry PC

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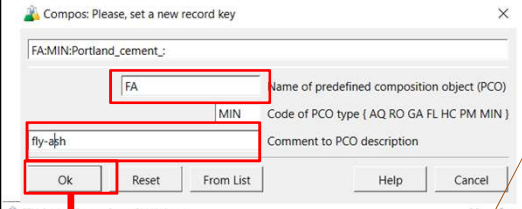
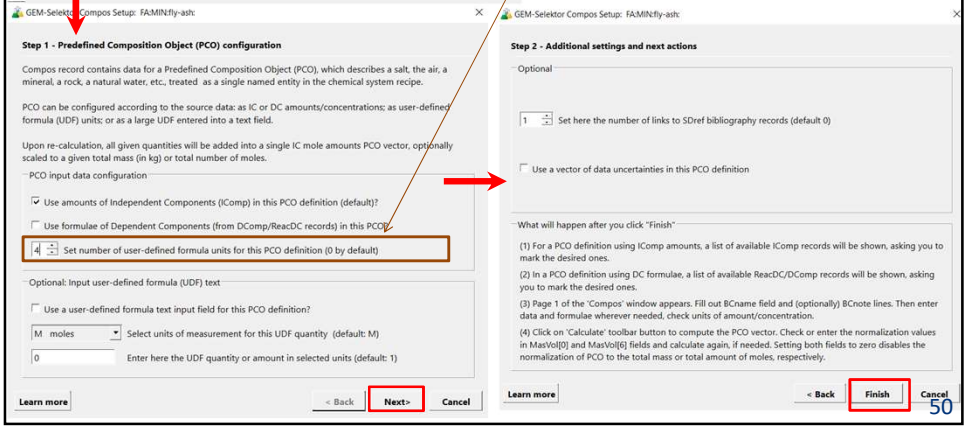
Make a predefined composition for fly ash: option 1, add g oxides



Can be used to add g oxides 4 as CaO, Al2O3, SiO2, Fe2O3

Will have to written manually



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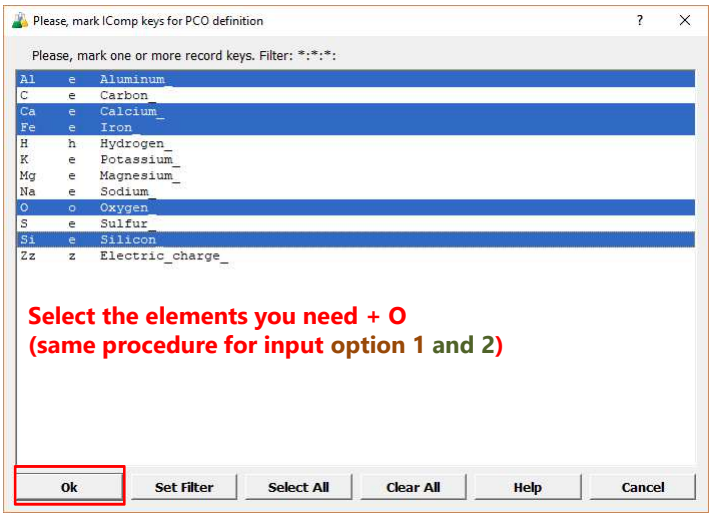
Make a predefined composition for fly ash: option 1 and 2



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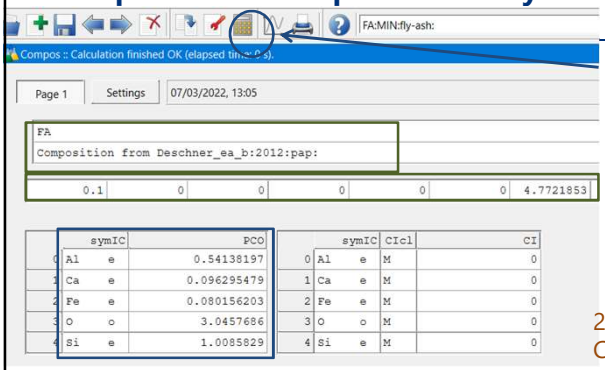
Make a predefined composition for fly ash: option 1, add g oxides

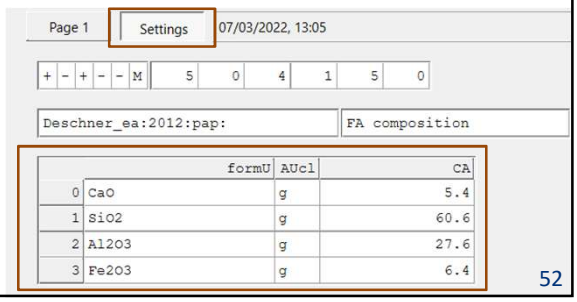


3) Once everthing is entered, recalculate ...

... and save new record.

1)
⇒ Enter 0.1
Normalises everything to 100 g (0.1 kg)

2) Enter values
Composition normalised to 100g



Write CaO, Al2O3, SiO2, Fe2O3

Case sensitive!

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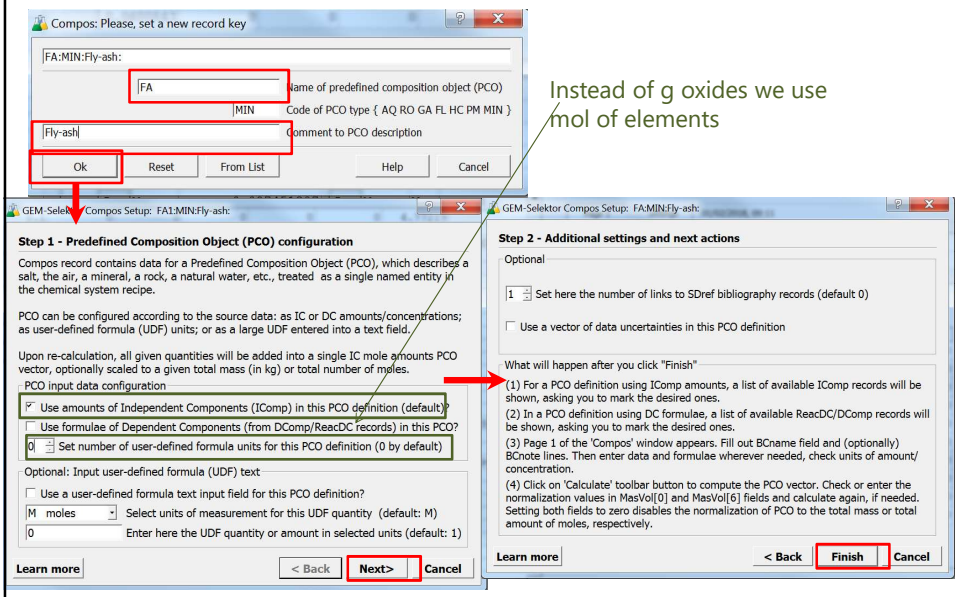
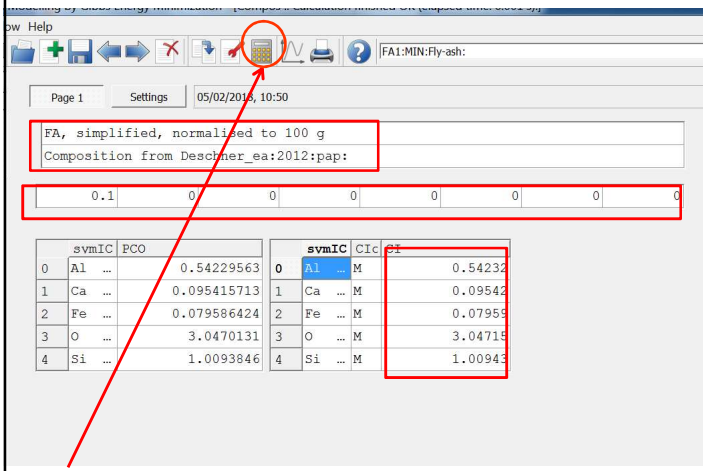
Make a predefined composition for fly ash: option 2, mol elements



Make a predefined composition for fly ash: option 2, mol elements



recalculation in atom-%

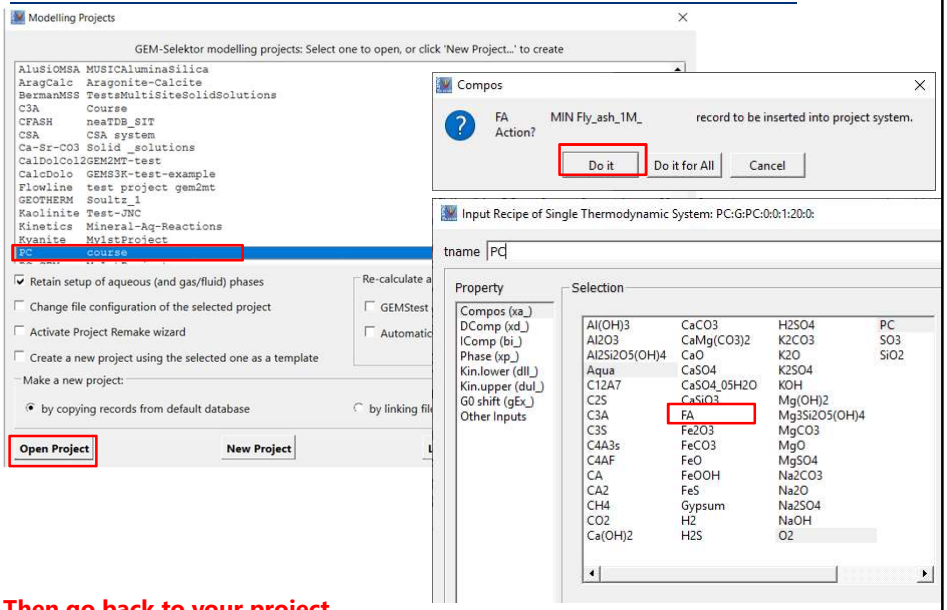
	normalised mol/100g
Si	1.00943
Al	0.54232
Fe	0.07959
Ca	0.09542
O	3.04715

=> Enter values

When everthing is entered, recalculate … **… and save new record.**

equivalent options, minor difference due rounding off (number of digits …

Single calculation - hydration of PC + fly ash



Then go back to your project

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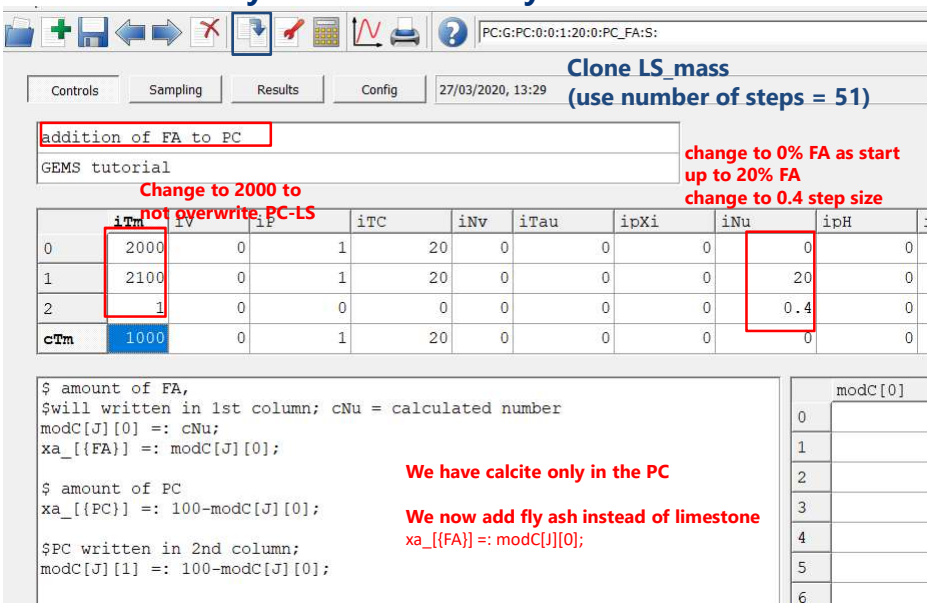
Process file - hydration of PC + fly ash



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Process file - hydration of PC + fly ash

Controls | Sampling | Results | Config | 31/05/2023, 17:42

NeIt	9999	51	Next	0	I	0	J	50	Jp	50

pSTkey	PC:G:PC:0:0:1:20:0:	cTm	2050

cTau	0	cpXi	0	cXi	1	cNu	

cpH	0	cpe	0	cEh	0	cT	

```
$ x-axis: fraction of FA in cement
xp[J] =: xa_[{FA}];
$
$ y-axis in g per 100 g unhydrated cement
yp[J][0] =: phM[{CSHQ}];
yp[J][1] =: phM[{Portlandite}];
yp[J][2] =: phM[{C3(AF)S0.84H}];
yp[J][3] =: phM[{ettringite}]+phM[{SO4_CO3_AFt}]+phM[{CO3_SO4_AFt}];
yp[J][4] =: phM[{straetlingite}];
yp[J][5] =: phM[{C3AH6}];
yp[J][6] =: phM[{C4AsH16}]+phM[{SO4_OH_AFm}]+phM[{OH_SO4_AFm}];
yp[J][7] =: 0;
yp[J][8] =: 0;
yp[J][9] =: phM[{C4Ac0.5H12}];
yp[J][10] =: phM[{C4AcH11}];
yp[J][11] =: phM[{Calcite}];
yp[J][12] =: phM[{OH-hydrotalcite}];
yp[J][13] =: phM[{aq_gen}];
```

Change comment, change x-axis

New phase: $(CaO)_2Al_2O_3SiO_2(H_2O)_{7\text{-}8}$

New phase: Katoite

=> Label also columns

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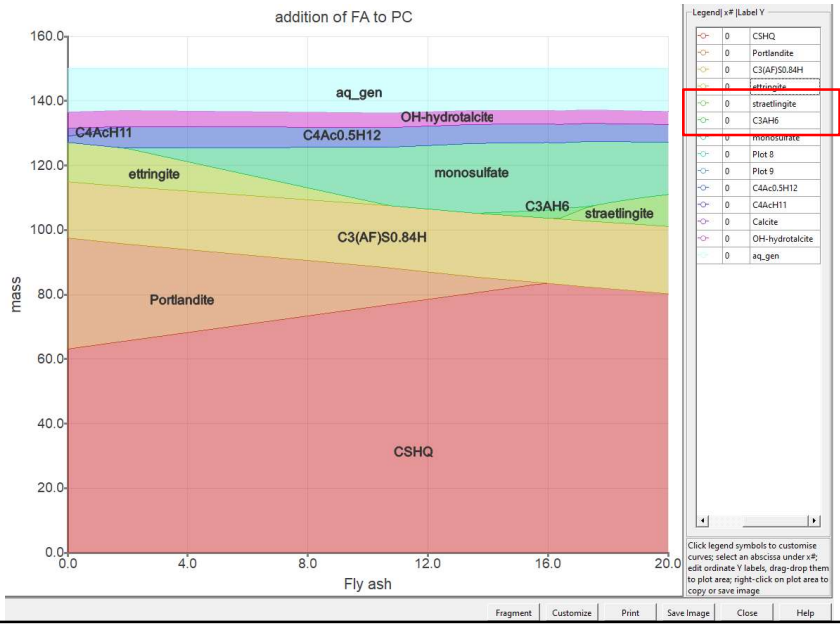
Process file - hydration of PC + fly ash



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Process file - hydration of PC + fly ash

What happens, when we replace 5% of PC by limestone?

Controls | Sampling | Results | Config | 27/03/2020, 15:27

addition of FA to PC+Cc
GEMS tutorial

	iTm	iV	iP	iTC	iNv	iTau	ipXi	iNu	ipH
0	2000	0	1	20	0	0	0	0	
1	2100	0	1	20	0	0	0	20	
2	1	0	0	0	0	0	0	0.4	
cTm	2000	0	1	20	0	0	0	0	

```
$ amount of FA,
$will written in 1st column; cNu = calculated number
modC[J][0] =: cNu;
xa_[{FA}] =: modC[J][0];

$ amount of PC
xa_[{PC}] =: 100-modC[J][0]-5;
xa_[{CaCO3}] =: 5;

$PC written in 2nd column;
modC[J][1] =: 100-modC[J][0]-5;
```

We substract the 5% LS from the PC ...

... and add 5% $CaCO_3$.

	mo
0	
1	
2	
3	
4	
5	
6	

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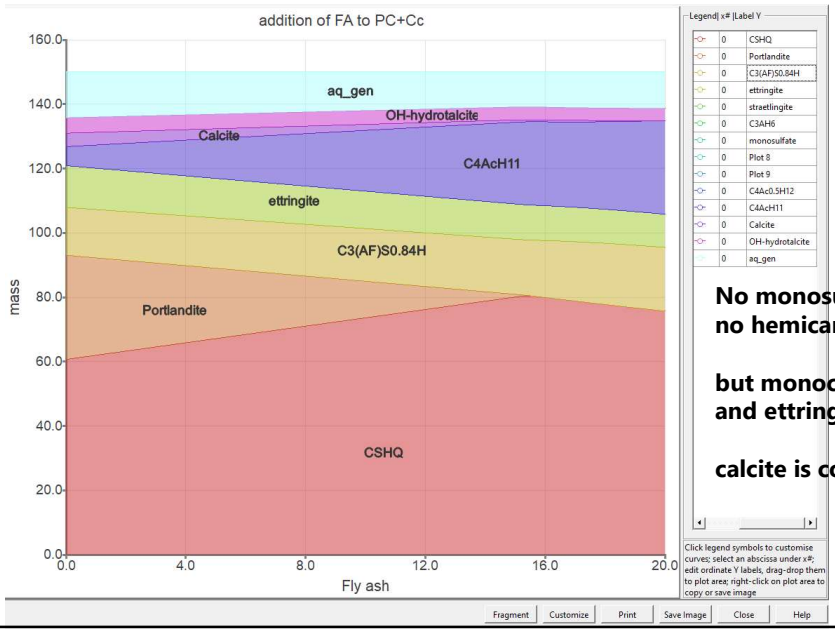
Process file - hydration of PC + fly ash



No monosulfate, no hemicarbonate

but monocarbonate and ettringite

calcite is consumed

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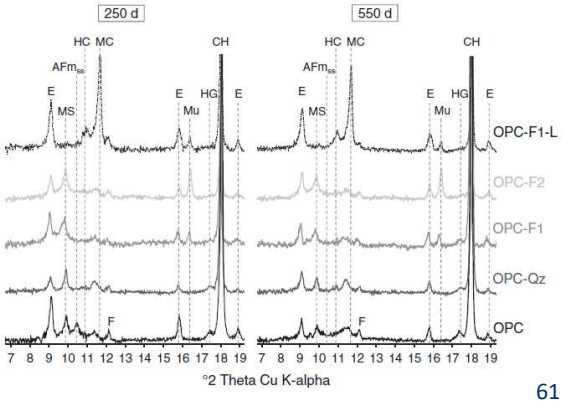
Process file - hydration of PC + fly ash

Addition of fly ash to PC:

- **Less portlandite, more C-S-H (Ca/Si of C-S-H decreases, not shown)**
- **Ettringite destabilized, formation of monosulfate**
  => ternary blends with fly ash and limestone favourable to stabilize ettringite (see e.g. de Weerdt et al., Cem. Concr. Res. 41 (2011), 279-291)
- **Strätlingite appears after consumption of portlandite**



Deschner et al., Cem Concr Res. 52 (2013), 169-181.

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