Oregon State University

Empa
Materials Science and Technology

Lecture 07
Interaction with the environment

Klaartje De Weerdt, NTNU
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Software development/fitting tools/kinetic:
Dmitrii Kulik
Dan Miron

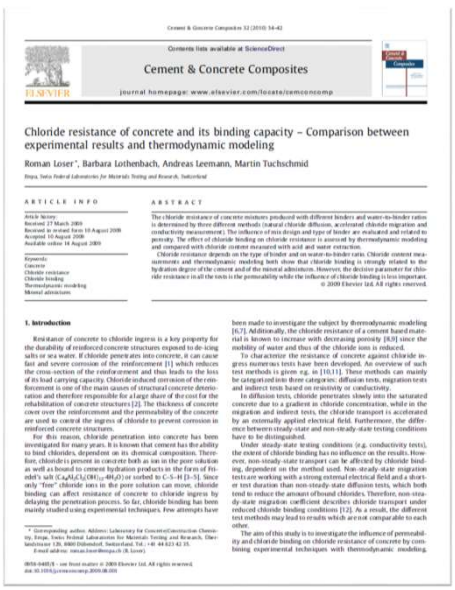
PAUL SCHERRER INSTITUT
PSI

NTNU – Trondheim
Norwegian University of Science and Technology

Cement and Concrete Research

Comparing chloride ingress from seawater and NaCl solution in Portland cement mortar

K. De Weerdt, B. Lothenbach, M.R. Geiker



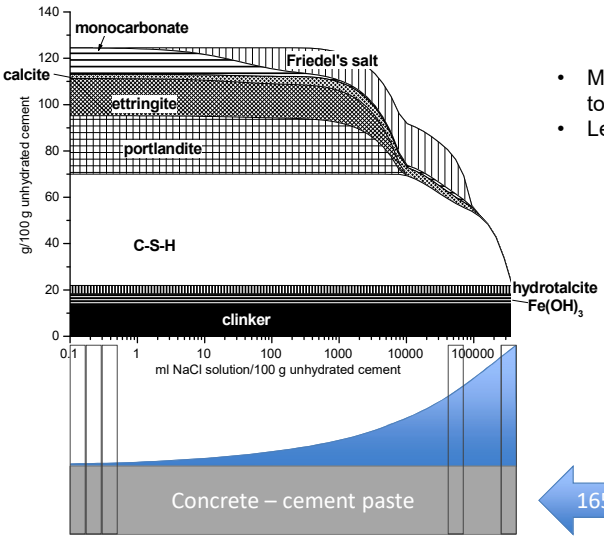
Cement & Concrete Composites

Chloride resistance of concrete and its binding capacity – Comparison between experimental results and thermodynamic modeling

Roman Loser, Barbara Lothenbach, Andreas Leemann, Martin Tuchschmid

Simple modelling approach

Loser ea 2010, CCC 32



- Monocarbonate transforms to Friedel's salt
- Leaching at surface

165 g/L NaCl

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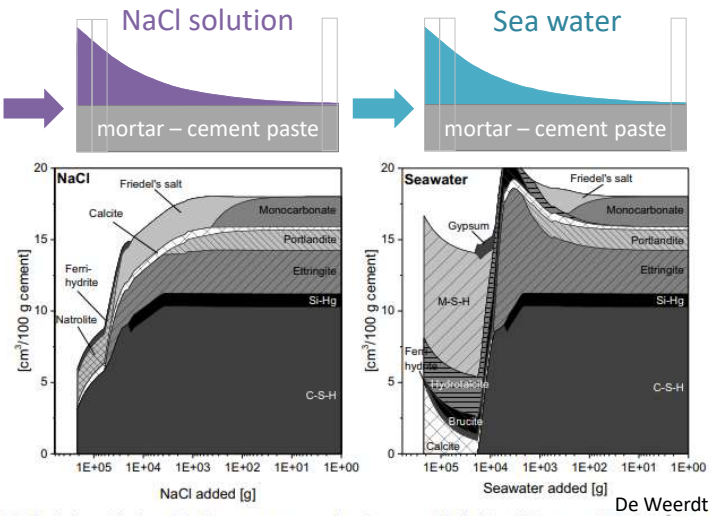
GOAL:

Predict phase changes when adding an increasing amount of ..



De Weerdt ea 2010, CCR

Fig. 10. Predicted volume of the phases in the PC paste upon exposure to increasing amounts of NaCl solution (left) or seawater (right) in [cm³/100 g cement].

4

Learning goals

GEMS-skills:

- Building a SysEq file from scratch
- Editing a Proces file
- Insert predefined compositions (OPC)

Content

Example: calculate the phase changes in PC paste exposed to NaCl solution

1. Create Single System – SysEq ☺
2. Make predefined composition of PC
3. Make Process

Task: calculate the phase changes in PC paste exposed to sea water

Content

Example: calculate the phase changes in PC paste exposed to NaCl solution

1. Create Single System – SysEq ☺
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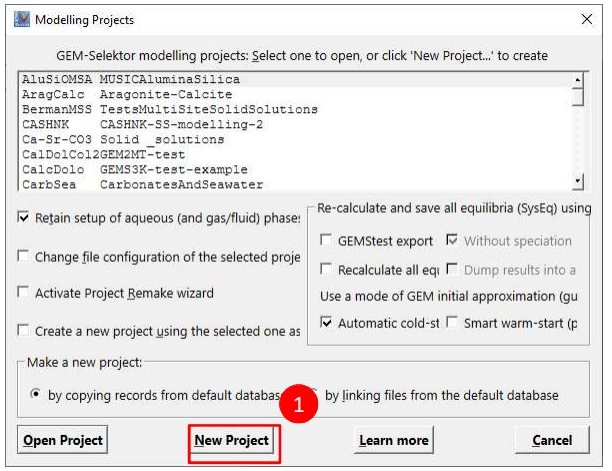
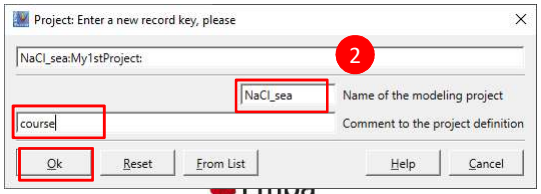
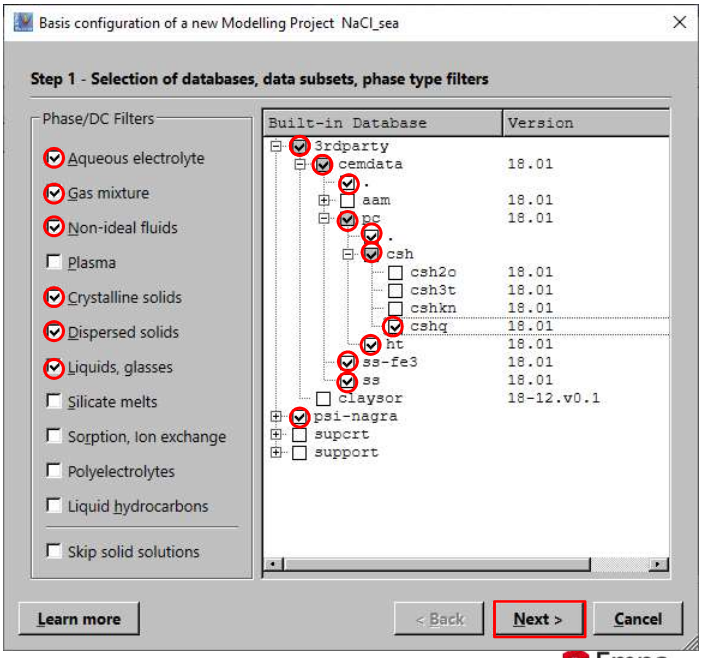
Task: calculate the phase changes in PC paste exposed to sea water



Create a new file





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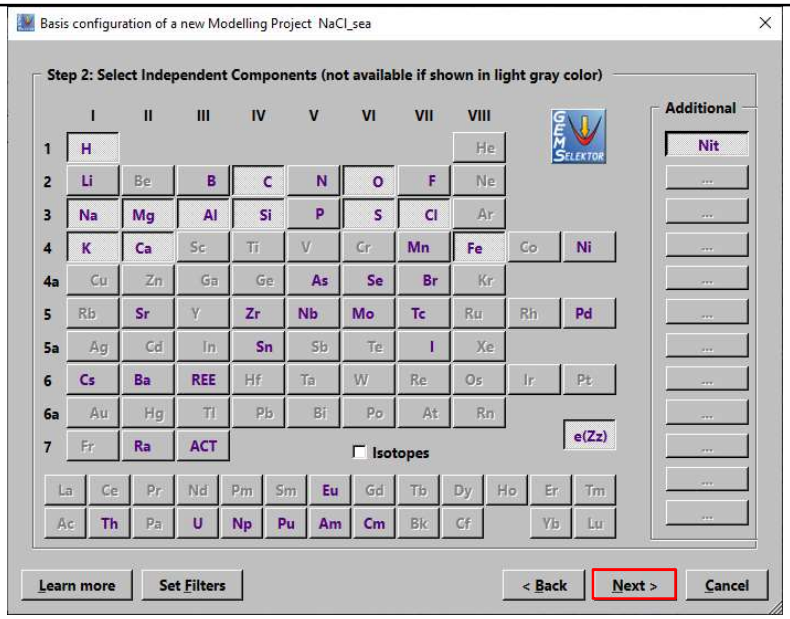

Choose the elements you will have in your system

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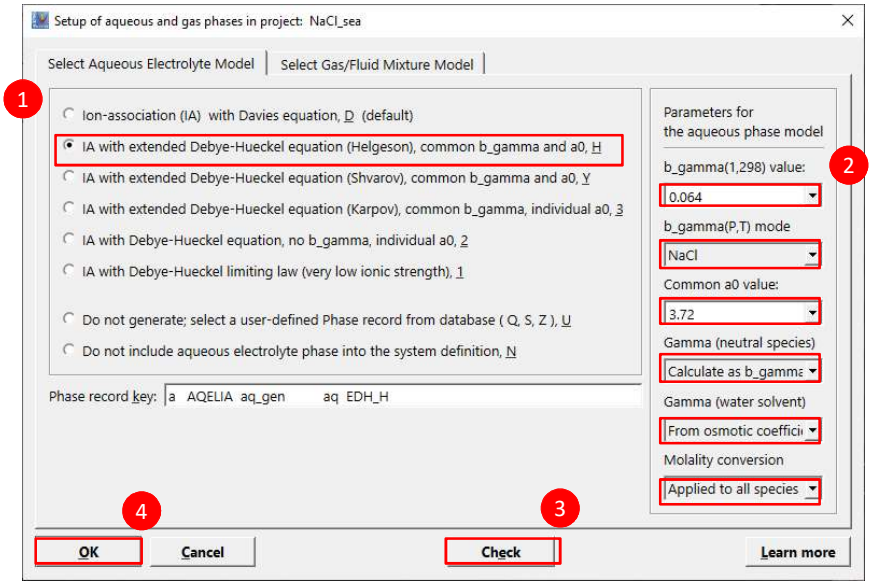

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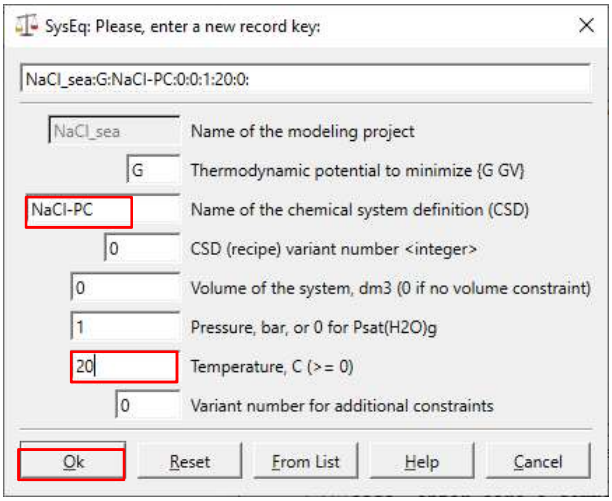
Name your single file

Temperature



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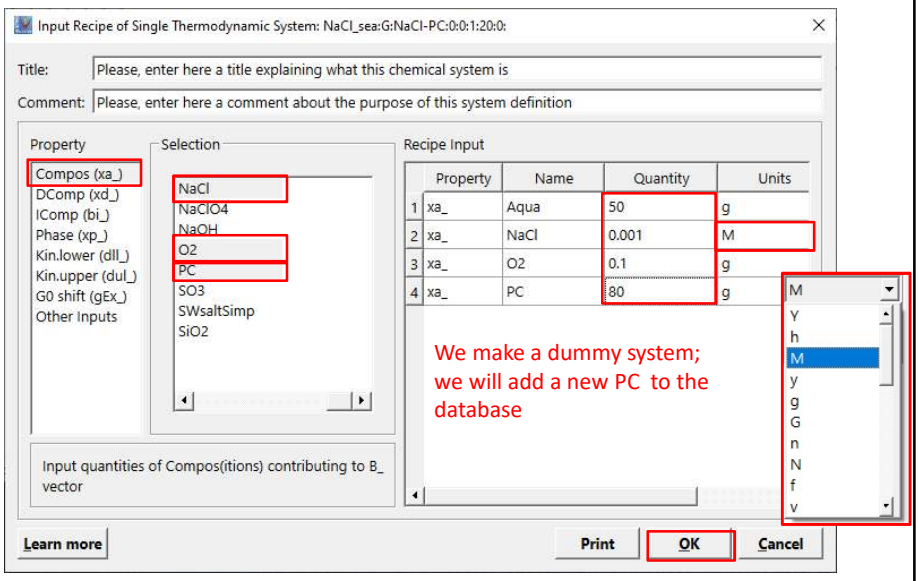

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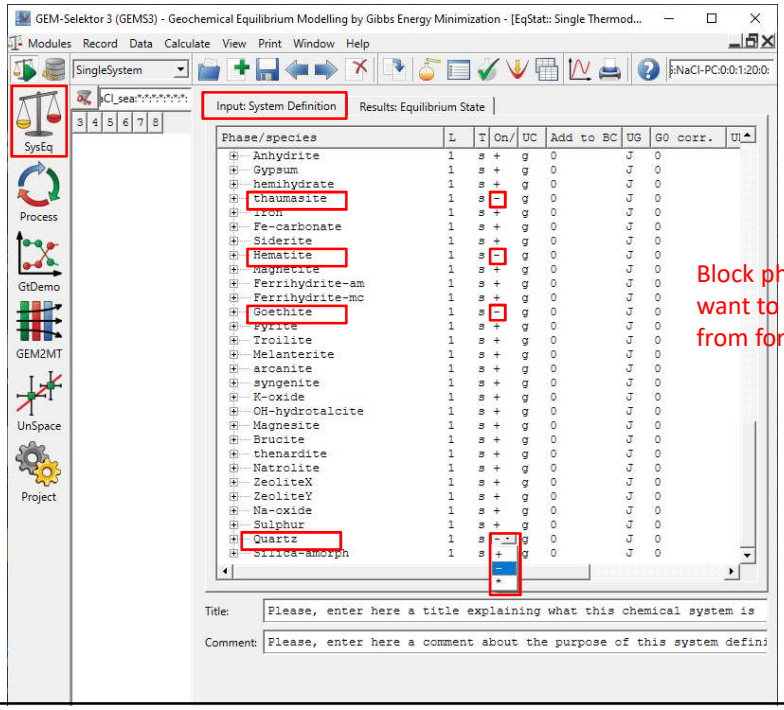
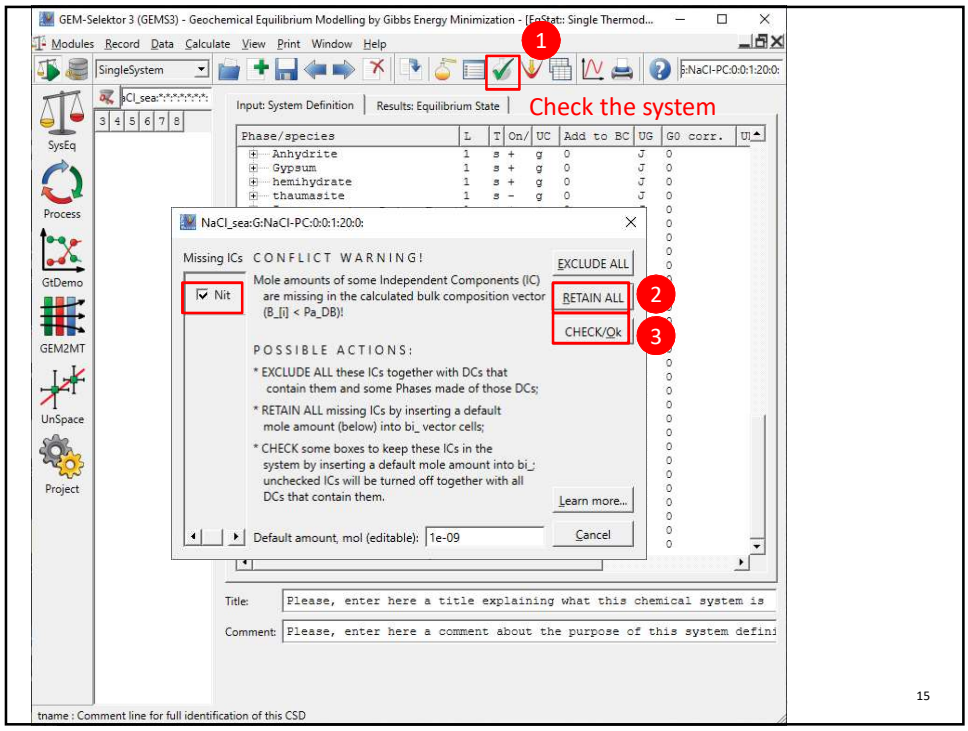
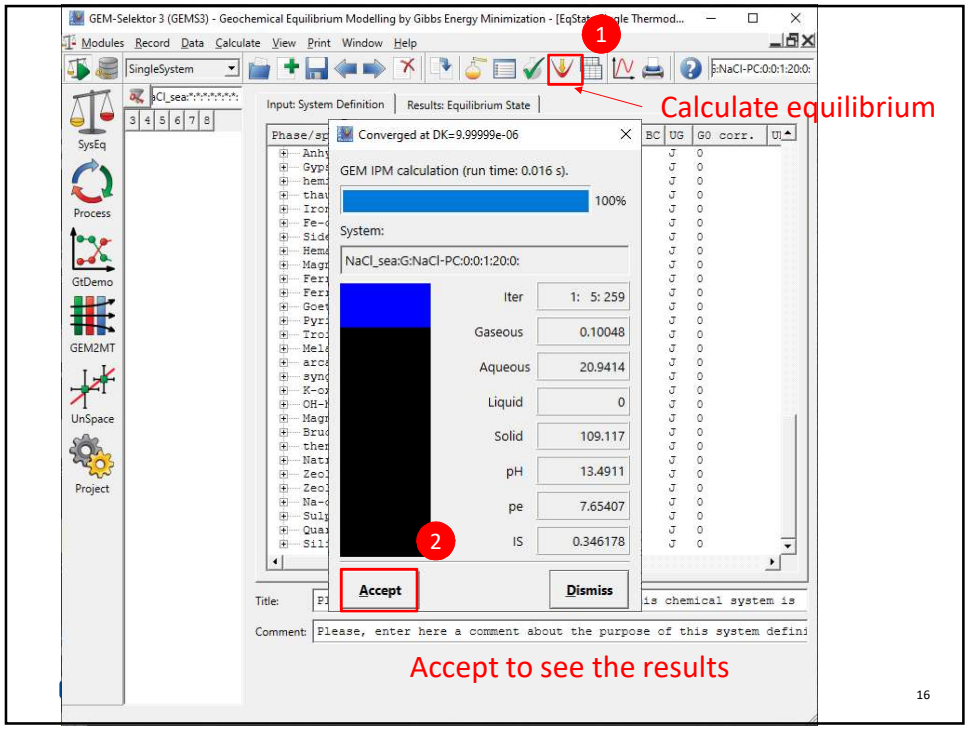
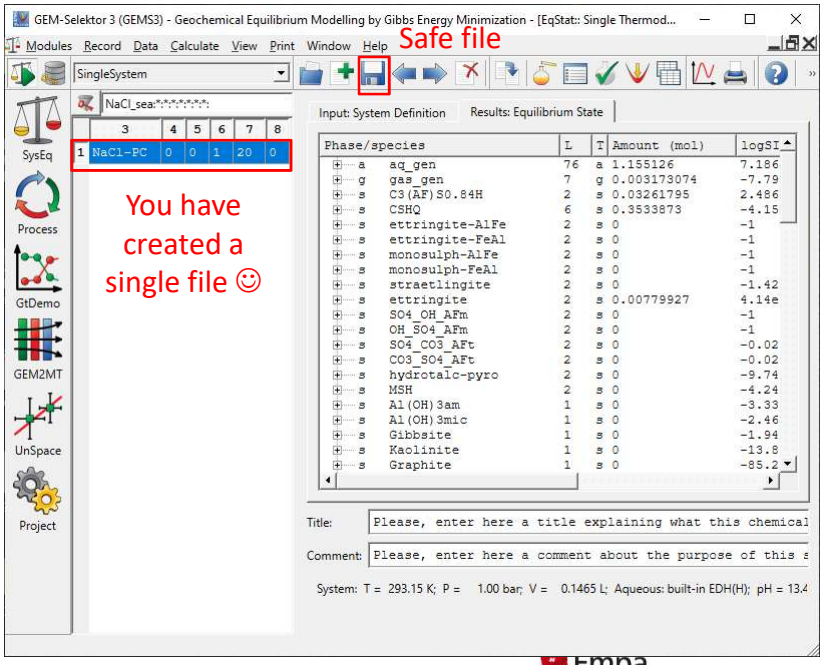


Block phases you want to prevent from forming


GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization
Modules Record Data Calculate View Print Window Help
1
Check the system
Input: System Definition
Results: Equilibrium State
Phase/species
Anhydrite
Gypsum
hemihydrate
thaumasite
NaCl_sea:G:NaCl-PC:0:0:1:20:0:
Missing ICs
CONFLICT WARNING!
Mole amounts of some Independent Components (IC) are missing in the calculated bulk composition vector (B_[i] < Pa_DB)!
Nit
EXCLUDE ALL
RETAIN ALL
CHECK/Ok
2
3
POSSIBLE ACTIONS:
* EXCLUDE ALL these ICs together with DCs that contain them and some Phases made of those DCs;
* RETAIN ALL missing ICs by inserting a default mole amount (below) into bi_ vector cells;
* CHECK some boxes to keep these ICs in the system by inserting a default mole amount into bi_; unchecked ICs will be turned off together with all DCs that contain them.
Learn more...
Default amount, mol (editable): 1e-09
Cancel
Title: Please, enter here a title explaining what this chemical system is
Comment: Please, enter here a comment about the purpose of this system defini
SysEq
Process
GtDemo
GEM2MT
UnSpace
Project
tname : Comment line for full identification of this CSD
15


GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization
Modules Record Data Calculate View Print Window Help
1
Calculate equilibrium
Converged at DK=9.99999e-06
GEM IPM calculation (run time: 0.016 s).
100%
System:
NaCl_sea:G:NaCl-PC:0:0:1:20:0:
Iter 1: 5: 259
Gaseous 0.10048
Aqueous 20.9414
Liquid 0
Solid 109.117
pH 13.4911
pe 7.65407
IS 0.346178
2
Accept
Dismiss
Title:
Comment: Please, enter here a comment about the purpose of this system defini
Accept to see the results
SysEq
Process
GtDemo
GEM2MT
UnSpace
Project
16

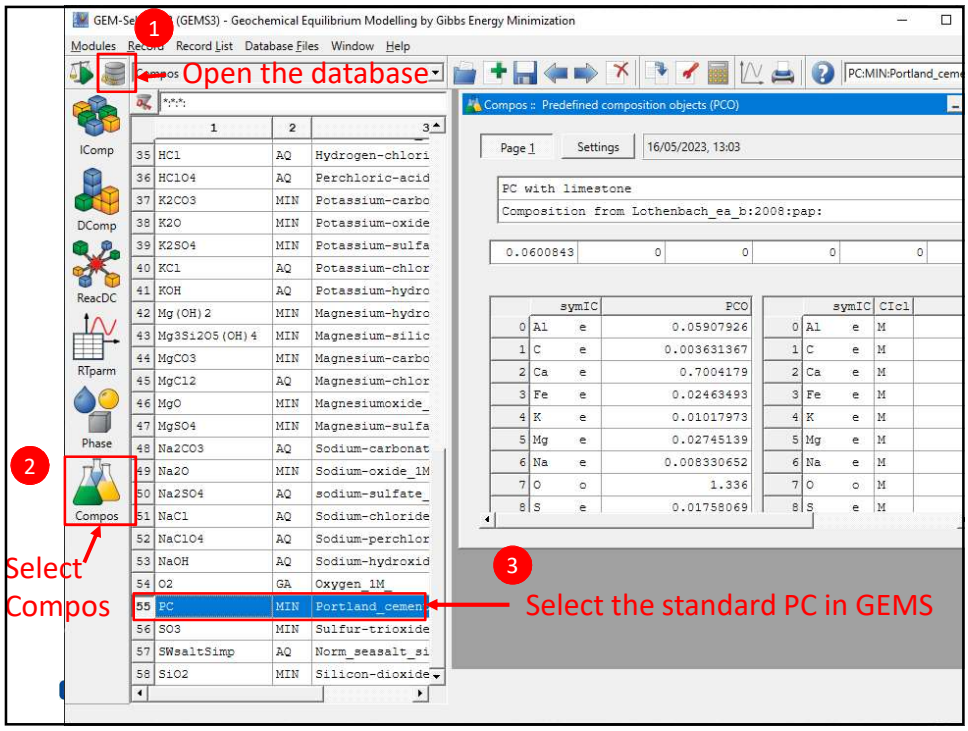


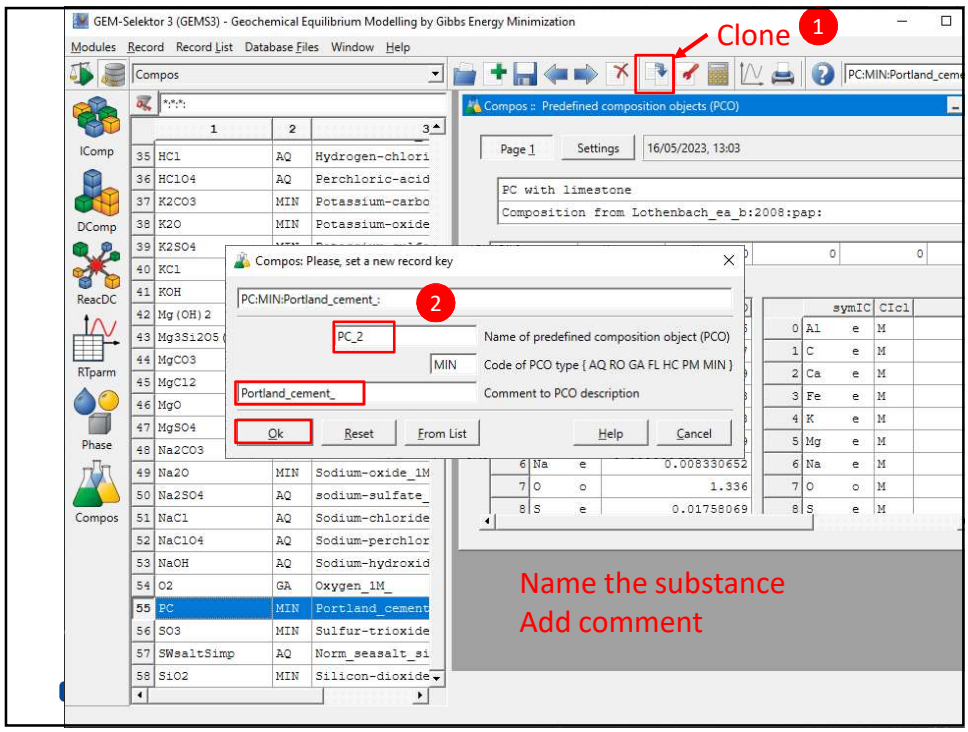
Content

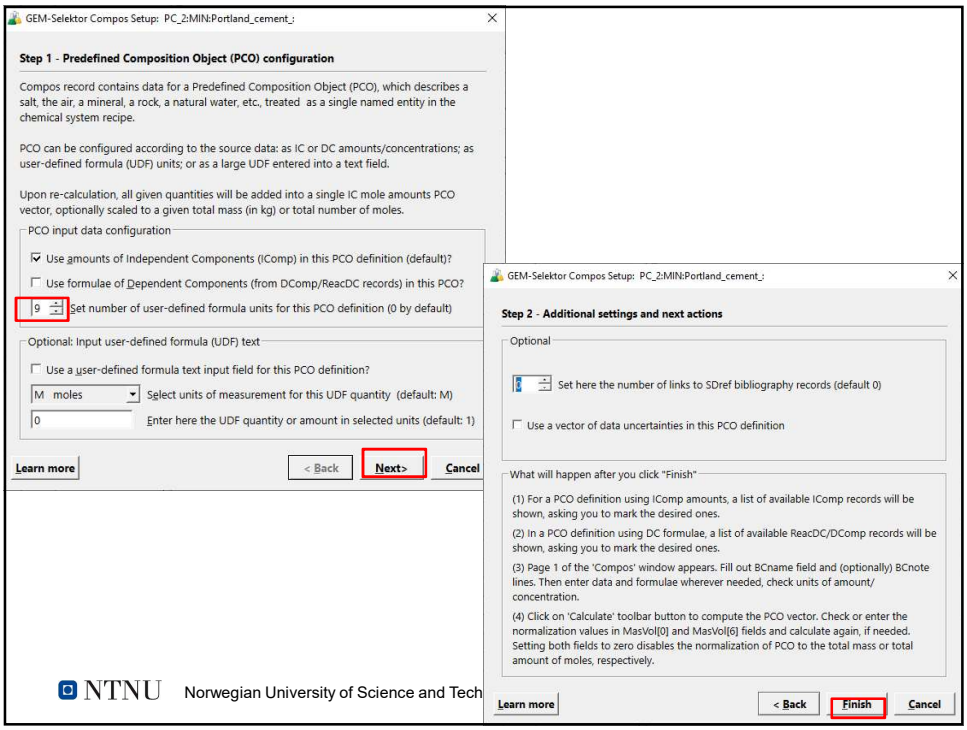
Example: calculate the phase changes in PC paste exposed to NaCl solution

1. Create Single System – SysEq ☺
2. Make predefined composition of PC
3. Make Process

Task: calculate the phase changes in PC paste exposed to sea water


1
Open the database
2
Select Compos
3
Select the standard PC in GEMS


Clone
1
2
Name the substance
Add comment


GEM-Selektor Compos Setup: PC_2:MIN:Portland_cement_:
Step 1 - Predefined Composition Object (PCO) configuration
Compos record contains data for a Predefined Composition Object (PCO), which describes a salt, the air, a mineral, a rock, a natural water, etc., treated as a single named entity in the chemical system recipe.
PCO can be configured according to the source data: as IC or DC amounts/concentrations; as user-defined formula (UDF) units; or as a large UDF entered into a text field.
Upon re-calculation, all given quantities will be added into a single IC mole amounts PCO vector, optionally scaled to a given total mass (in kg) or total number of moles.
PCO input data configuration
Use amounts of Independent Components (IComp) in this PCO definition (default)?
Use formulae of Dependent Components (from DComp/ReacDC records) in this PCO?
9
Set number of user-defined formula units for this PCO definition (0 by default)
Optional: Input user-defined formula (UDF) text
Use a user-defined formula text input field for this PCO definition?
M moles
Select units of measurement for this UDF quantity (default: M)
0
Enter here the UDF quantity or amount in selected units (default: 1)
Learn more
< Back
Next>
Cancel
GEM-Selektor Compos Setup: PC_2:MIN:Portland_cement_:
Step 2 - Additional settings and next actions
Optional
Set here the number of links to SDref bibliography records (default 0)
Use a vector of data uncertainties in this PCO definition
What will happen after you click "Finish"
(1) For a PCO definition using IComp amounts, a list of available IComp records will be shown, asking you to mark the desired ones.
(2) In a PCO definition using DC formulae, a list of available ReacDC/DComp records will be shown, asking you to mark the desired ones.
(3) Page 1 of the 'Compos' window appears. Fill out BCname field and (optionally) BCnote lines. Then enter data and formulae wherever needed, check units of amount/ concentration.
(4) Click on 'Calculate' toolbar button to compute the PCO vector. Check or enter the normalization values in MasVol[0] and MasVol[6] fields and calculate again, if needed. Setting both fields to zero disables the normalization of PCO to the total mass or total amount of moles, respectively.
Learn more
< Back
Finish
Cancel
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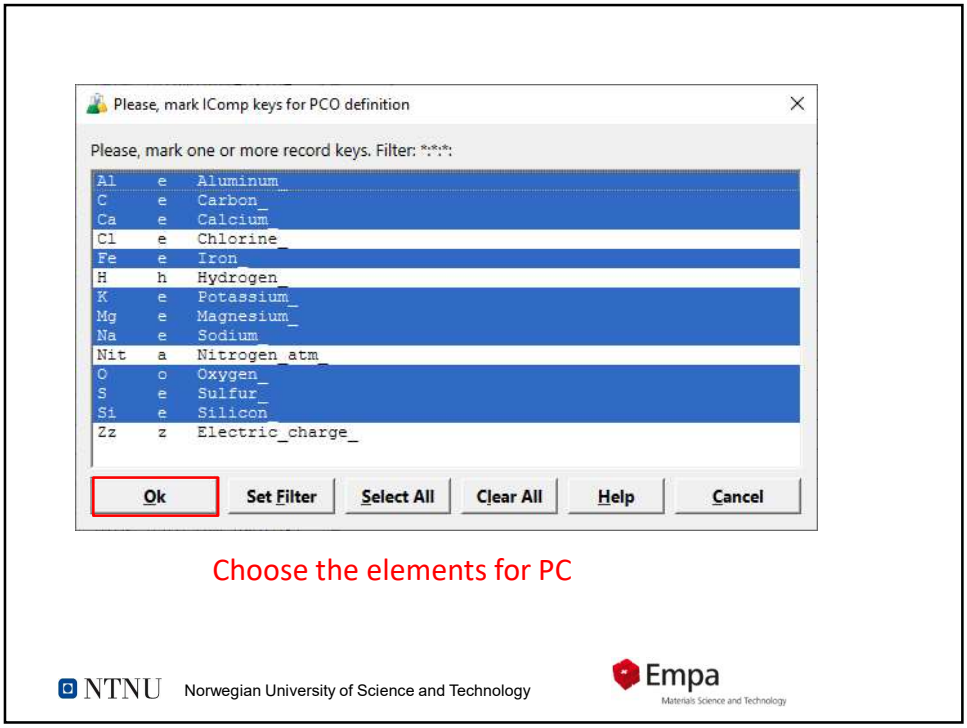
Please, mark IComp keys for PCO definition
Please, mark one or more record keys. Filter: *:*:*:
Al e Aluminum_
C e Carbon_
Ca e Calcium_
Cl e Chlorine_
Fe e Iron_
H h Hydrogen_
K e Potassium_
Mg e Magnesium_
Na e Sodium_
Nit a Nitrogen_atm_
O o Oxygen_
S e Sulfur_
Si e Silicon_
Zz z Electric_charge_
Ok
Set Filter
Select All
Clear All
Help
Cancel
Choose the elements for PC
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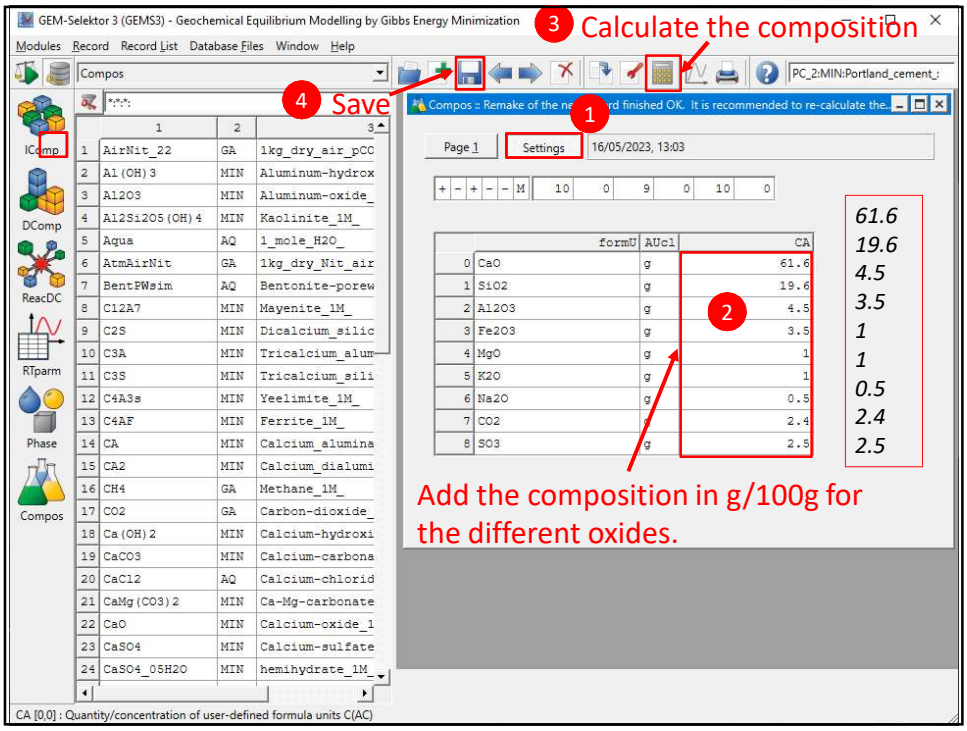
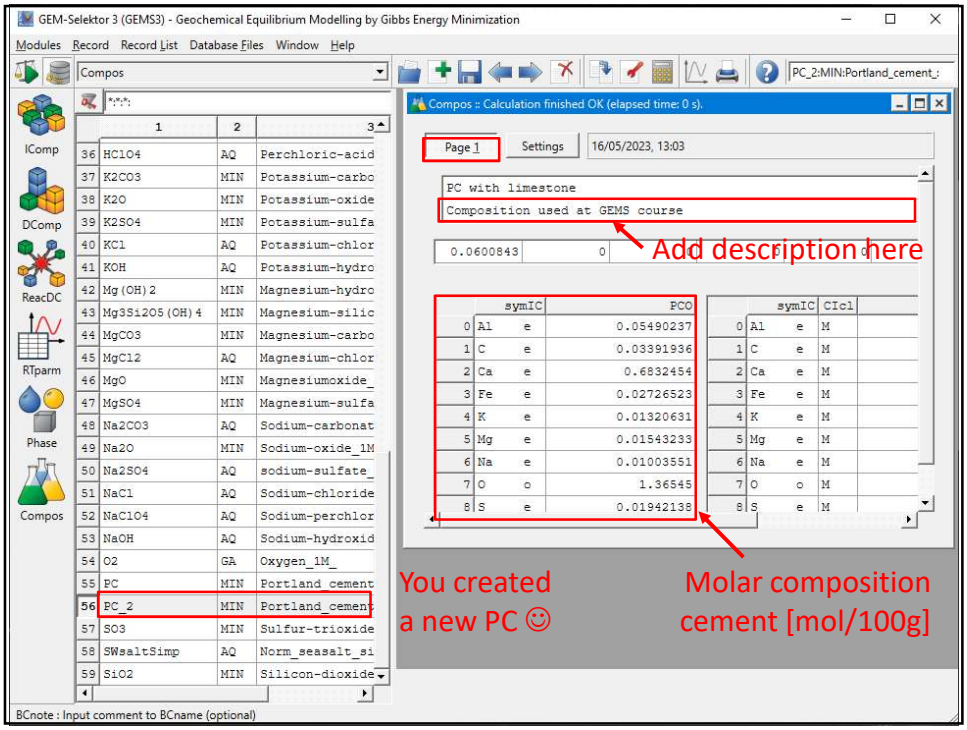

GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization
Modules Record Record List Database Files Window Help
Compos
PC_2:MIN:Portland_cement_:
3 Calculate the composition
4 Save
1
Page 1
Settings
16/05/2023, 13:03
2
61.6
19.6
4.5
3.5
1
1
0.5
2.4
2.5
Add the composition in g/100g for the different oxides.
CA [0,0] : Quantity/concentration of user-defined formula units C(AC)


GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization
Modules Record Record List Database Files Window Help
Compos
PC_2:MIN:Portland_cement_:
Compos :: Calculation finished OK (elapsed time: 0 s).
Page 1
Settings
16/05/2023, 13:03
PC with limestone
Composition used at GEMS course
Add description here
You created a new PC ☺
Molar composition cement [mol/100g]
BCnote : Input comment to BCname (optional)

Calculation input Compos - OPC

From cement producer

Input GEMS

OPC

	XRF %	XRF* %	g/100g OPC	molar mass g/mol	mol/100gOPC
SiO2	19.60	20.3	20.3	60.1	0.338
Al2O3	4.50	4.7	4.7	102.0	0.046
Fe2O3	3.50	3.6	3.6	159.7	0.023
CaO	61.60	63.8	63.8	56.1	1.137
MgO	1.00	1.0	1.0	40.3	0.026
SO3	2.50	2.6	2.6	80.1	0.032
K2O	1.00	1.0	1.0	94.2	0.011
Na2O	0.50	0.5	0.5	62.0	0.008
Co2	2.40	2.5	2.5	44.0	0.056
	96.6	*100.0*	*100.0*		

	mol/100g OPC
Al	0.09138
C	0.05645
Ca	1.13714
Fe	0.04538
K	0.02198
Mg	0.02568
Na	0.01670
O	2.27256
S	0.03232
Si	0.33769
	4.03729

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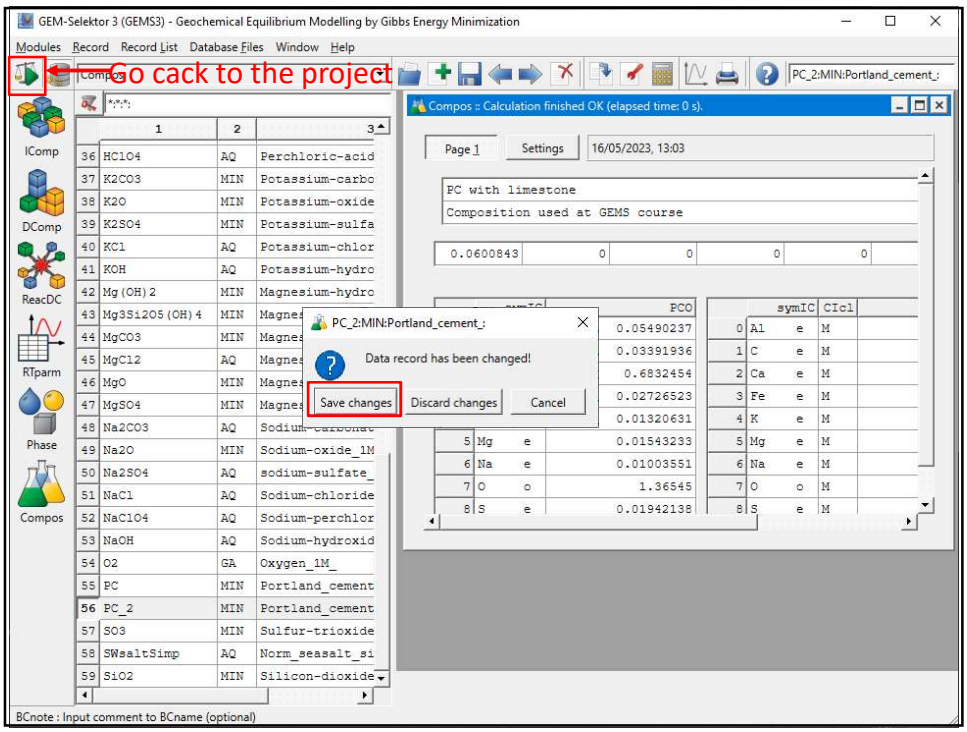
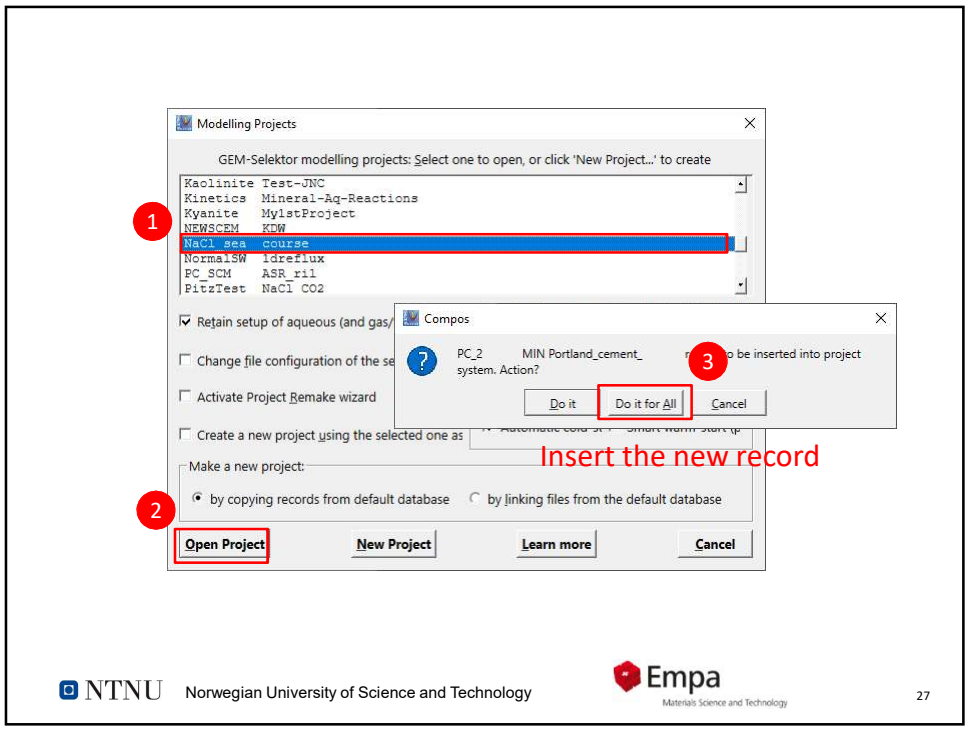
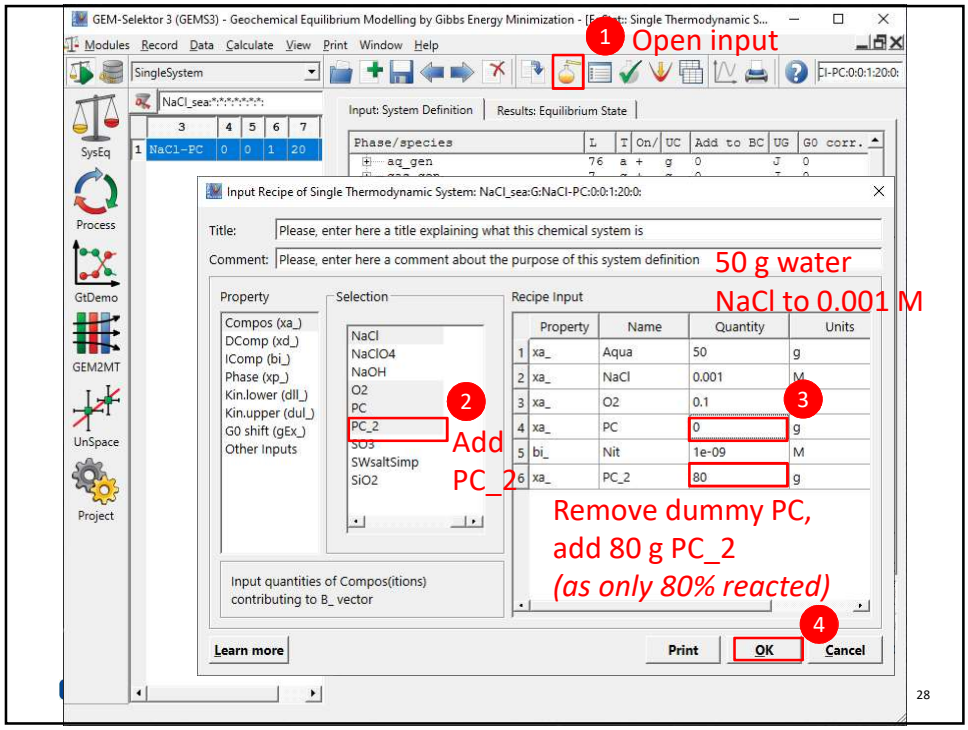
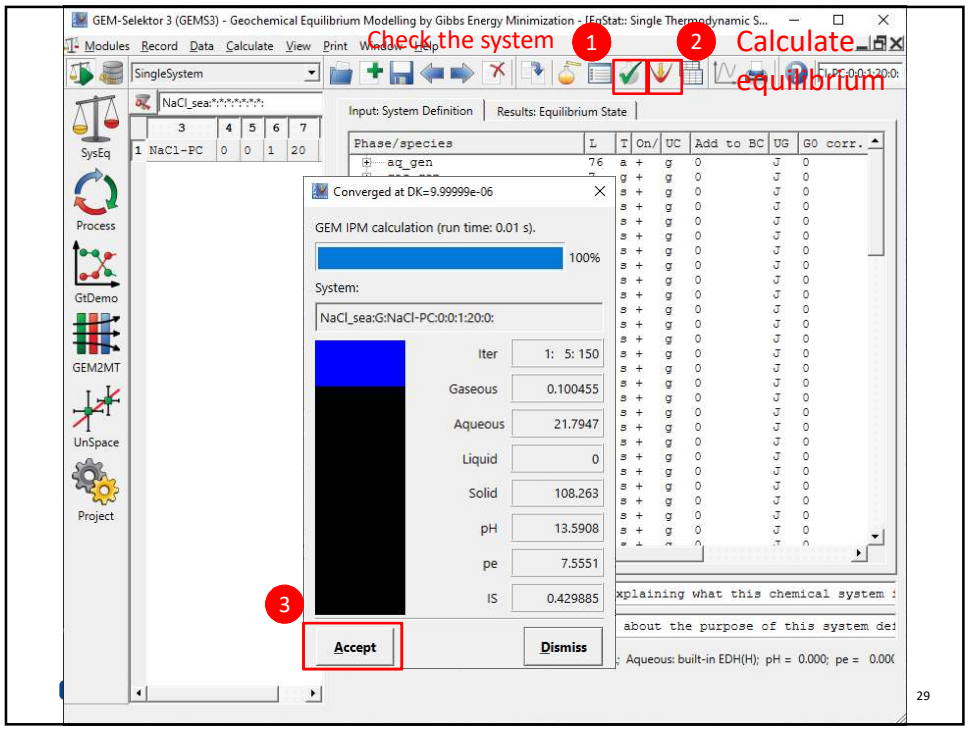
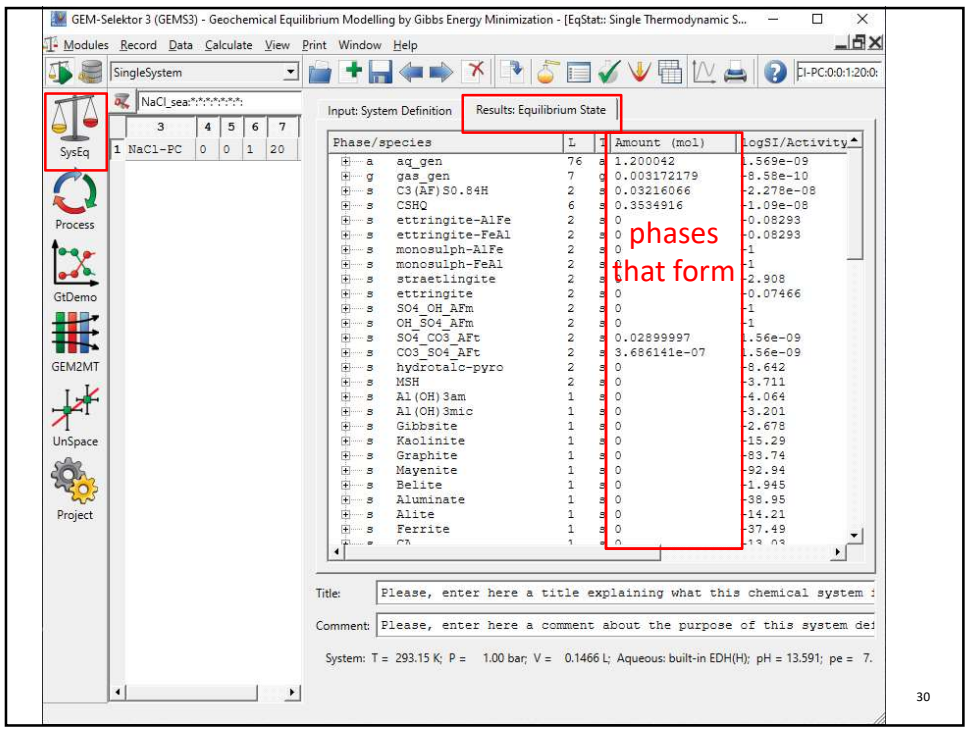
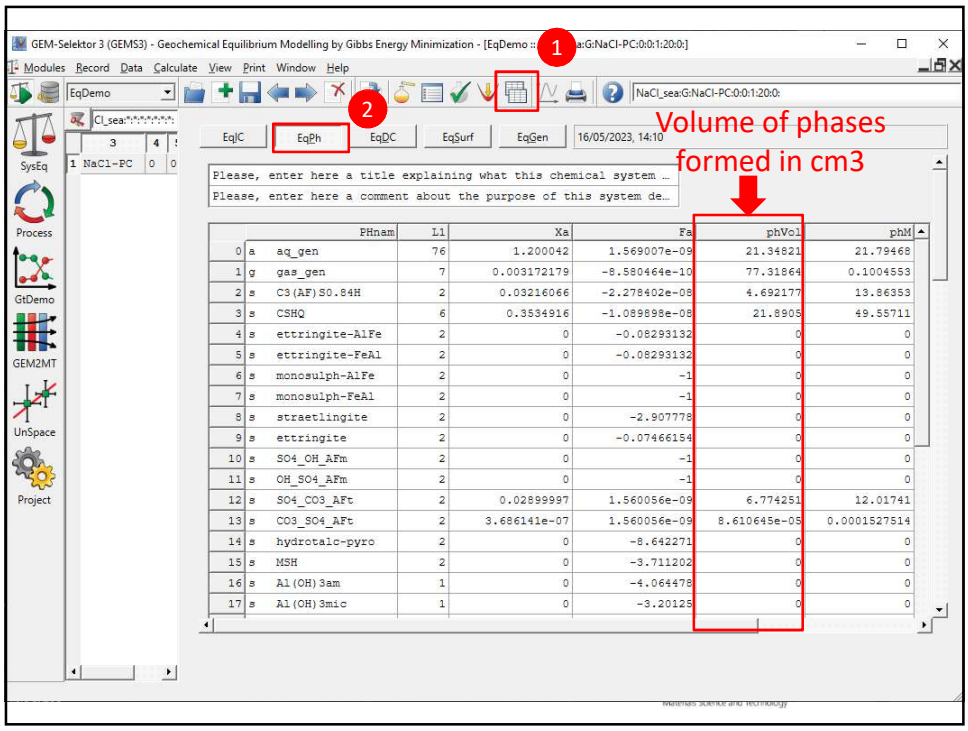



Modelling Projects
GEM-Selektor modelling projects: Select one to open, or click 'New Project...' to create
Kaolinite Test-JNC
Kinetics Mineral-Aq-Reactions
Kyanite MylstProject
NEWSCEM KDW
NaCl_sea course
NormalSW 1dreflux
PC_SCM ASR_ril
PitzTest NaCl CO2
Retain setup of aqueous (and gas/
Change file configuration of the se
Activate Project Remake wizard
Create a new project using the selected one as
Make a new project:
by copying records from default database
by linking files from the default database
Open Project
New Project
Learn more
Cancel
Compos
PC_2 MIN Portland_cement_
system. Action?
Do it
Do it for All
Cancel
Insert the new record
1
2
3


GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization
Modules Record Data Calculate View Print Window Help
SingleSystem
Input: System Definition
Results: Equilibrium State
Input Recipe of Single Thermodynamic System: NaCl_sea:G:NaCl-PC:0:0:1:20:0:
Title: Please, enter here a title explaining what this chemical system is
Comment: Please, enter here a comment about the purpose of this system definition
Property
Selection
Recipe Input
Compos (xa_)
DComp (xd_)
IComp (bi_)
Phase (xp_)
Kin.lower (dll_)
Kin.upper (dul_)
G0 shift (gEx_)
Other Inputs
NaCl
NaClO4
NaOH
O2
PC
PC_2
SO3
SWsaltSimp
SiO2
Property Name Quantity Units
1 xa_ Aqua 50 g
2 xa_ NaCl 0.001 M
3 xa_ O2 0.1
4 xa_ PC 0
5 bi_ Nit 1e-09 M
6 xa_ PC_2 80 g
Input quantities of Compos(itions) contributing to B_ vector
Learn more
Print
OK
Cancel
Open input
50 g water
NaCl to 0.001 M
Add PC_2
Remove dummy PC, add 80 g PC_2
(as only 80% reacted)
1
2
3
4


Check the system
1
2
Calculate equilibrium
Converged at DK=9.99999e-06
GEM IPM calculation (run time: 0.01 s).
100%
System:
NaCl_sea:G:NaCl-PC:0:0:1:20:0:
Iter 1: 5: 150
Gaseous 0.100455
Aqueous 21.7947
Liquid 0
Solid 108.263
pH 13.5908
pe 7.5551
IS 0.429885
3
Accept
Dismiss
29


phases that form
30



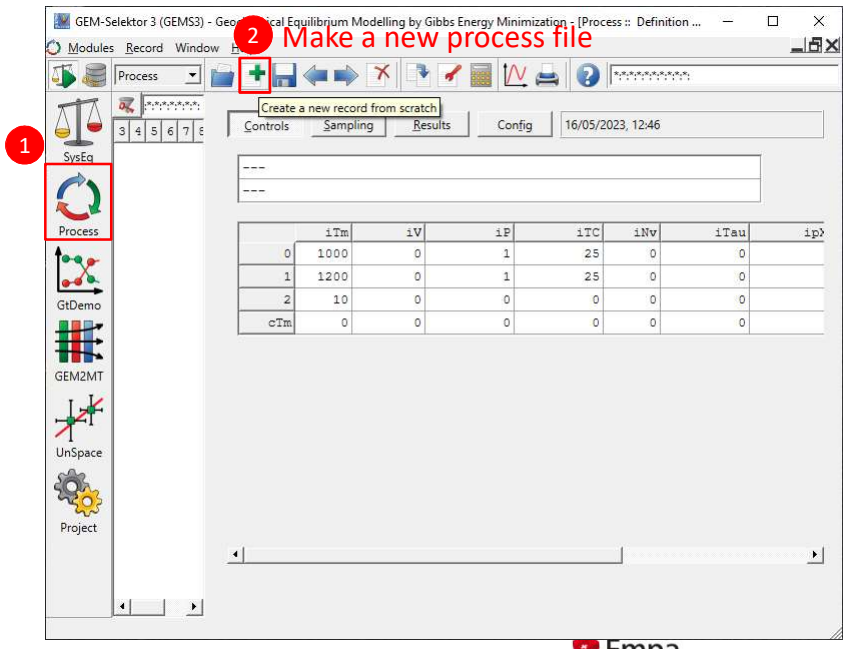
		PHnam	L1	Xa	Fa	phVol	phM
0	a	aq_gen	76	1.200042	1.569007e-09	21.34821	21.79468
1	g	gas_gen	7	0.003172179	-8.580464e-10	77.31864	0.1004553
2	s	C3(AF)S0.84H	2	0.03216066	-2.278402e-08	4.692177	13.86353
3	s	CSHQ	6	0.3534916	-1.089898e-08	21.8905	49.55711
4	s	ettringite-AlFe	2	0	-0.08293132	0	0
5	s	ettringite-FeAl	2	0	-0.08293132	0	0
6	s	monosulph-AlFe	2	0	-1	0	0
7	s	monosulph-FeAl	2	0	-1	0	0
8	s	straetlingite	2	0	-2.907778	0	0
9	s	ettringite	2	0	-0.07466154	0	0
10	s	SO4_OH_AFm	2	0	-1	0	0
11	s	OH_SO4_AFm	2	0	-1	0	0
12	s	SO4_CO3_AFt	2	0.02899997	1.560056e-09	6.774251	12.01741
13	s	CO3_SO4_AFt	2	3.686141e-07	1.560056e-09	8.610645e-05	0.0001527514
14	s	hydrotalc-pyro	2	0	-8.642271	0	0
15	s	MSH	2	0	-3.711202	0	0
16	s	Al(OH)3am	1	0	-4.064478	0	0
17	s	Al(OH)3mic	1	0	-3.20125	0	0

Content

Example: calculate the phase changes in PC paste exposed to NaCl solution

1. Create Single System – SysEq ☺
2. Make predefined composition of PC
3. Make Process

Task: calculate the phase changes in PC paste exposed to sea water



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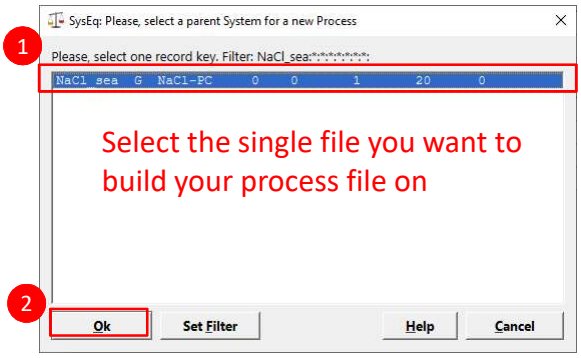

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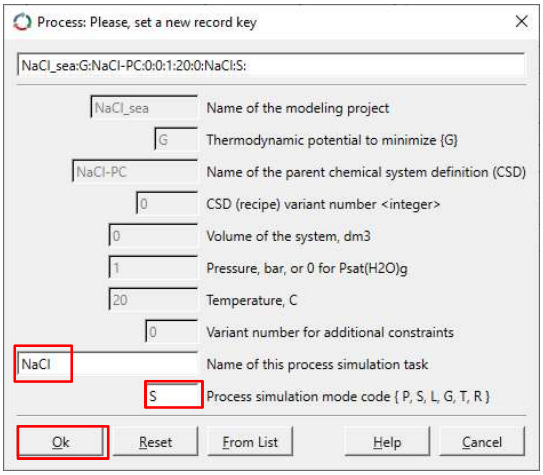
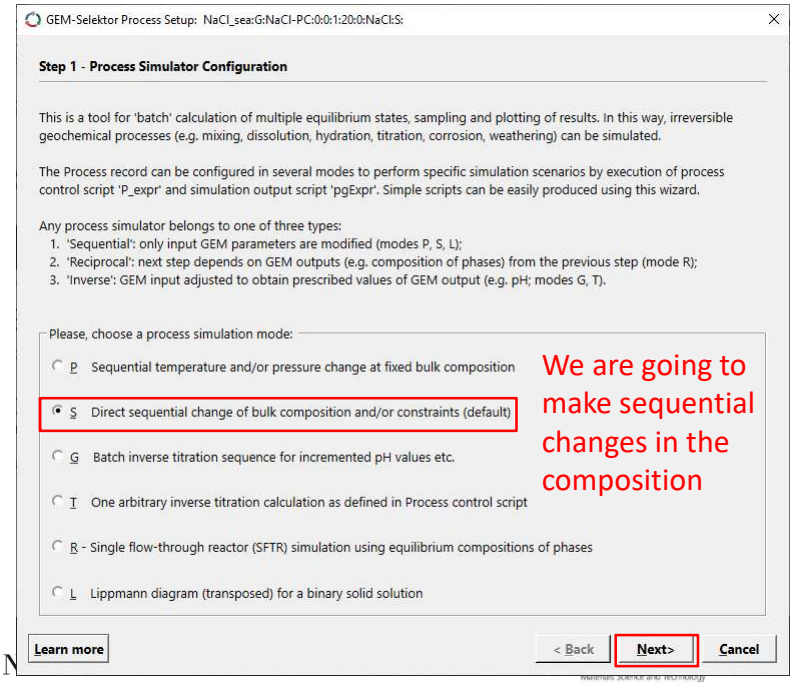
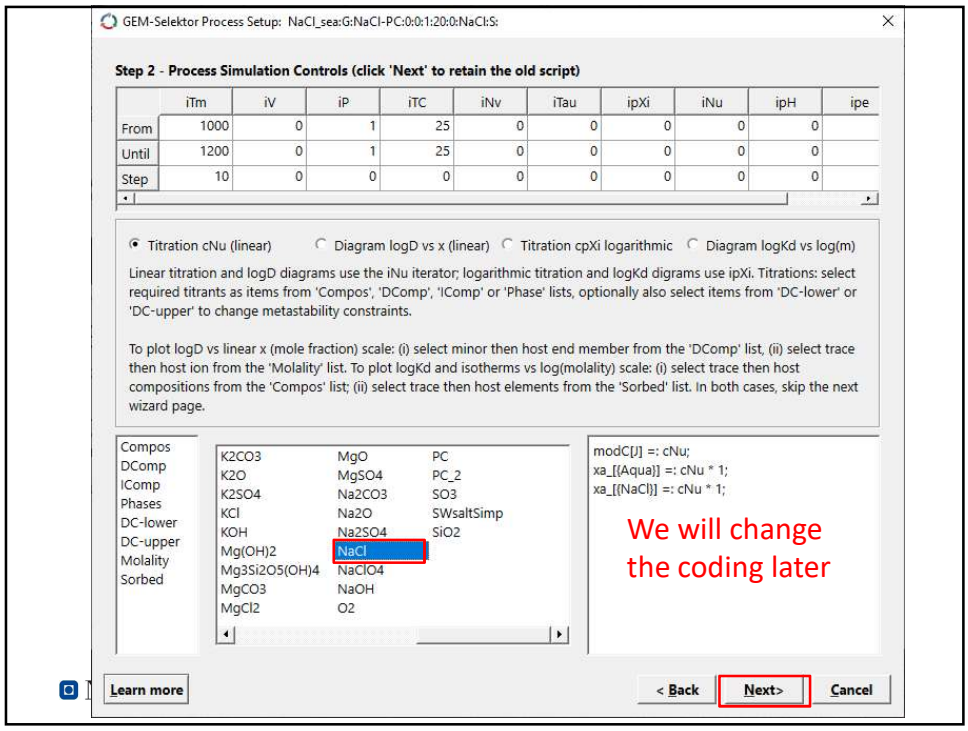
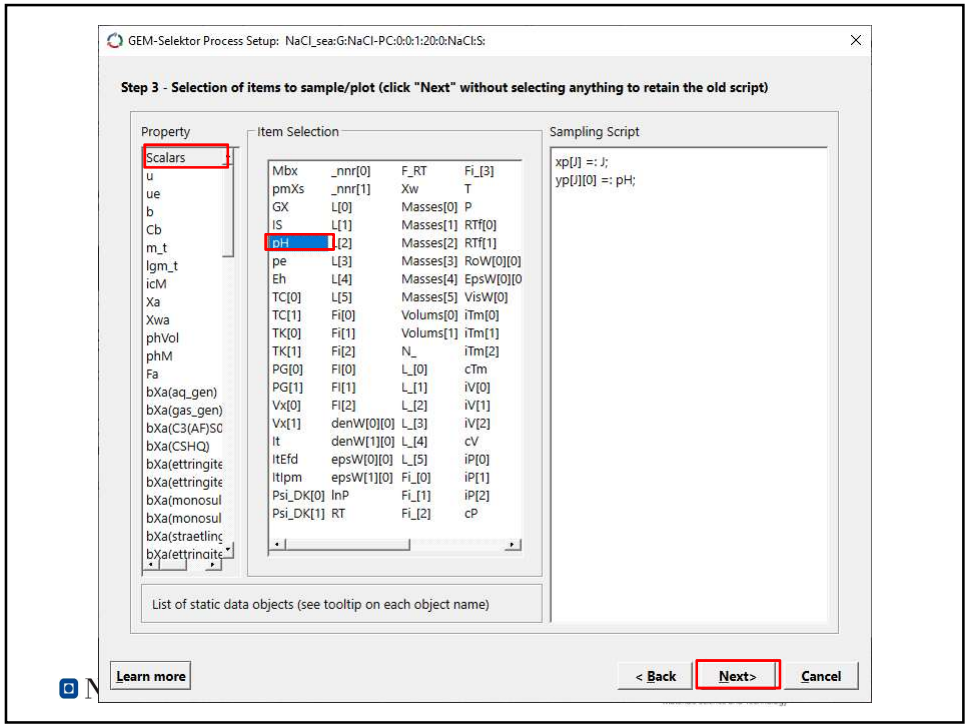


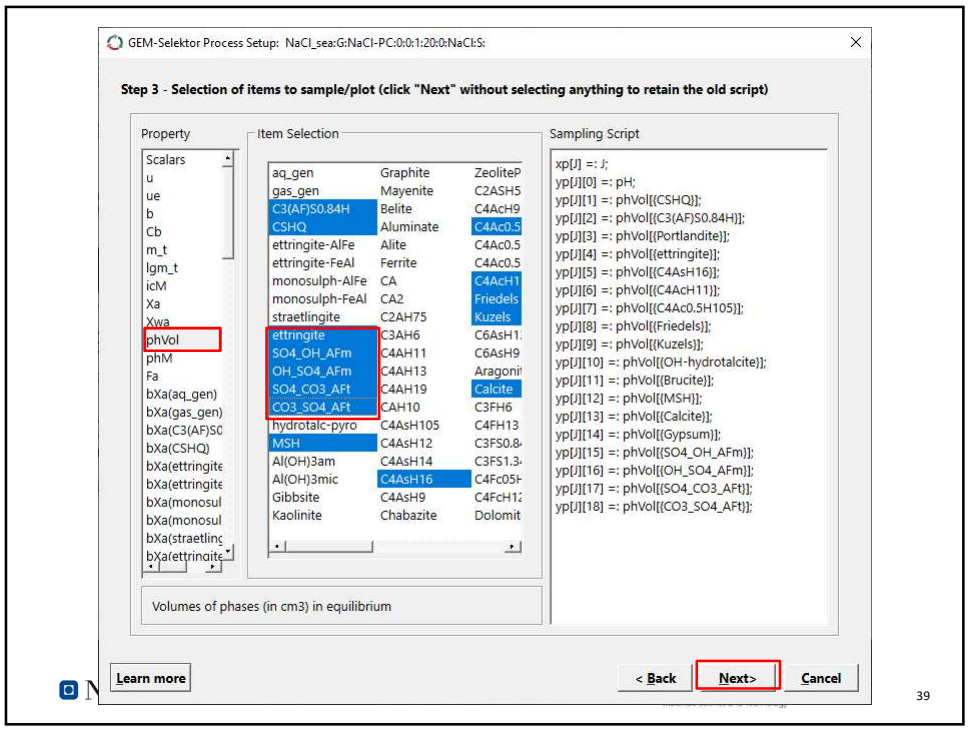
Name your process file
S → sequential changes

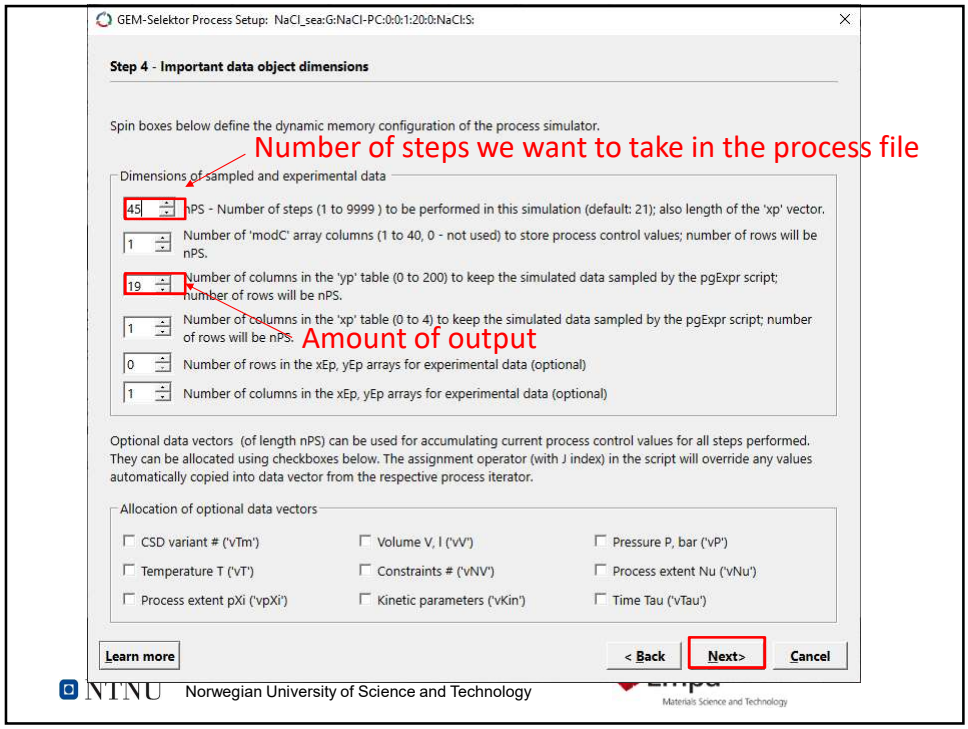


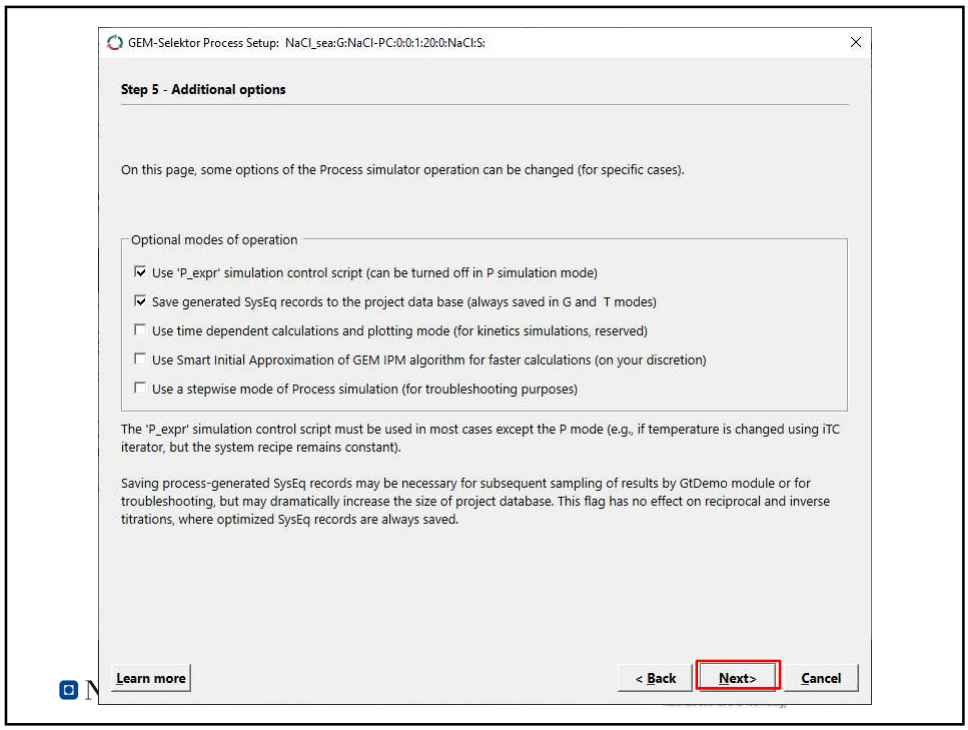
We are going to make sequential changes in the composition


GEM-Selektor Process Setup: NaCl_sea:G:NaCl-PC:0:0:1:20:0:NaCl:S:
Step 2 - Process Simulation Controls (click 'Next' to retain the old script)
iTm iV iP iTC iNv iTau ipXi iNu ipH ipe
From 1000 0 1 25 0 0 0 0 0
Until 1200 0 1 25 0 0 0 0 0
Step 10 0 0 0 0 0 0 0 0
Titration cNu (linear)
Diagram logD vs x (linear)
Titration cpXi logarithmic
Diagram logKd vs log(m)
Linear titration and logD diagrams use the iNu iterator; logarithmic titration and logKd digrams use ipXi. Titrations: select required titrants as items from 'Compos', 'DComp', 'IComp' or 'Phase' lists, optionally also select items from 'DC-lower' or 'DC-upper' to change metastability constraints.
To plot logD vs linear x (mole fraction) scale: (i) select minor then host end member from the 'DComp' list, (ii) select trace then host ion from the 'Molality' list. To plot logKd and isotherms vs log(molality) scale: (i) select trace then host compositions from the 'Compos' list; (ii) select trace then host elements from the 'Sorbed' list. In both cases, skip the next wizard page.
Compos
DComp
IComp
Phases
DC-lower
DC-upper
Molality
Sorbed
K2CO3 MgO PC
K2O MgSO4 PC_2
K2SO4 Na2CO3 SO3
KCl Na2O SWsaltSimp
KOH Na2SO4 SiO2
Mg(OH)2 NaCl
Mg3Si2O5(OH)4 NaClO4
MgCO3 NaOH
MgCl2 O2
modC[J] =: cNu;
xa_[(Aqua)] =: cNu * 1;
xa_[(NaCl)] =: cNu * 1;
We will change the coding later
Learn more
< Back
Next>
Cancel


GEM-Selektor Process Setup: NaCl_sea:G:NaCl-PC:0:0:1:20:0:NaCl:S:
Step 3 - Selection of items to sample/plot (click "Next" without selecting anything to retain the old script)
Property
Item Selection
Sampling Script
Scalars
u
ue
b
Cb
m_t
lgm_t
icM
Xa
Xwa
phVol
phM
Fa
bXa(aq_gen)
bXa(gas_gen)
bXa(C3(AF)SO
bXa(CSHQ)
bXa(ettringite
bXa(ettringite
bXa(monosul
bXa(monosul
bXa(straetling
bXa(ettringite
Mbx _nnr[0] F_RT Fi_[3]
pmXs _nnr[1] Xw T
GX L[0] Masses[0] P
IS L[1] Masses[1] RTf[0]
pH L[2] Masses[2] RTf[1]
pe L[3] Masses[3] RoW[0][0]
Eh L[4] Masses[4] EpsW[0][0
TC[0] L[5] Masses[5] VisW[0]
TC[1] Fi[0] Volums[0] iTm[0]
TK[0] Fi[1] Volums[1] iTm[1]
TK[1] Fi[2] N_ iTm[2]
PG[0] FI[0] L_[0] cTm
PG[1] FI[1] L_[1] iV[0]
Vx[0] FI[2] L_[2] iV[1]
Vx[1] denW[0][0] L_[3] iV[2]
It denW[1][0] L_[4] cV
ItEfd epsW[0][0] L_[5] iP[0]
ItIpm epsW[1][0] Fi_[0] iP[1]
Psi_DK[0] lnP Fi_[1] iP[2]
Psi_DK[1] RT Fi_[2] cP
xp[J] =: J;
yp[J][0] =: pH;
List of static data objects (see tooltip on each object name)
Learn more
< Back
Next>
Cancel


GEM-Selektor Process Setup: NaCl_sea:G:NaCl-PC:0:0:1:20:0:NaCl:S:
Step 3 - Selection of items to sample/plot (click "Next" without selecting anything to retain the old script)
Property
Item Selection
Sampling Script
Scalars
u
ue
b
Cb
m_t
lgm_t
icM
Xa
Xwa
phVol
phM
Fa
bXa(aq_gen)
bXa(gas_gen)
bXa(C3(AF)S0
bXa(CSHQ)
bXa(ettringite
bXa(ettringite
bXa(monosul
bXa(monosul
bXa(straetling
bXa(ettringite
aq_gen
gas_gen
C3(AF)S0.84H
CSHQ
ettringite-AlFe
ettringite-FeAl
monosulph-AlFe
monosulph-FeAl
straetlingite
ettringite
SO4_OH_AFm
OH_SO4_AFm
SO4_CO3_AFt
CO3_SO4_AFt
hydrotalc-pyro
MSH
Al(OH)3am
Al(OH)3mic
Gibbsite
Kaolinite
Graphite
Mayenite
Belite
Aluminate
Alite
Ferrite
CA
CA2
C2AH75
C3AH6
C4AH11
C4AH13
C4AH19
CAH10
C4AsH105
C4AsH12
C4AsH14
C4AsH16
C4AsH9
Chabazite
ZeoliteP
C2ASH5
C4AcH9
C4Ac0.5
C4Ac0.5
C4Ac0.5
C4AcH1
Friedels
Kuzels
C6AsH1
C6AsH9
Aragonit
Calcite
C3FH6
C4FH13
C3FS0.8
C3FS1.3
C4Fc05H
C4FcH1
Dolomit
xp[J] =: J;
yp[J][0] =: pH;
yp[J][1] =: phVol[{CSHQ}];
yp[J][2] =: phVol[{C3(AF)S0.84H}];
yp[J][3] =: phVol[{Portlandite}];
yp[J][4] =: phVol[{ettringite}];
yp[J][5] =: phVol[{C4AsH16}];
yp[J][6] =: phVol[{C4AcH11}];
yp[J][7] =: phVol[{C4Ac0.5H105}];
yp[J][8] =: phVol[{Friedels}];
yp[J][9] =: phVol[{Kuzels}];
yp[J][10] =: phVol[{OH-hydrotalcite}];
yp[J][11] =: phVol[{Brucite}];
yp[J][12] =: phVol[{MSH}];
yp[J][13] =: phVol[{Calcite}];
yp[J][14] =: phVol[{Gypsum}];
yp[J][15] =: phVol[{SO4_OH_AFm}];
yp[J][16] =: phVol[{OH_SO4_AFm}];
yp[J][17] =: phVol[{SO4_CO3_AFt}];
yp[J][18] =: phVol[{CO3_SO4_AFt}];
Volumes of phases (in cm3) in equilibrium
Learn more
< Back
Next>
Cancel


GEM-Selektor Process Setup: NaCl_sea:G:NaCl-PC:0:0:1:20:0:NaCl:S:
Step 4 - Important data object dimensions
Spin boxes below define the dynamic memory configuration of the process simulator.
Number of steps we want to take in the process file
Dimensions of sampled and experimental data
45
nPS - Number of steps (1 to 9999) to be performed in this simulation (default: 21); also length of the 'xp' vector.
1
Number of 'modC' array columns (1 to 40, 0 - not used) to store process control values; number of rows will be nPS.
19
Number of columns in the 'yp' table (0 to 200) to keep the simulated data sampled by the pgExpr script; number of rows will be nPS.
Amount of output
1
Number of columns in the 'xp' table (0 to 4) to keep the simulated data sampled by the pgExpr script; number of rows will be nPS.
0
Number of rows in the xEp, yEp arrays for experimental data (optional)
1
Number of columns in the xEp, yEp arrays for experimental data (optional)
Optional data vectors (of length nPS) can be used for accumulating current process control values for all steps performed. They can be allocated using checkboxes below. The assignment operator (with J index) in the script will override any values automatically copied into data vector from the respective process iterator.
Allocation of optional data vectors
CSD variant # ('vTm')
Volume V, l ('vV')
Pressure P, bar ('vP')
Temperature T ('vT')
Constraints # ('vNV')
Process extent Nu ('vNu')
Process extent pXi ('vpXi')
Kinetic parameters ('vKin')
Time Tau ('vTau')
Learn more
< Back
Next>
Cancel


GEM-Selektor Process Setup: NaCl_sea:G:NaCl-PC:0:0:1:20:0:NaCl:S:
Step 5 - Additional options
On this page, some options of the Process simulator operation can be changed (for specific cases).
Optional modes of operation
Use 'P_expr' simulation control script (can be turned off in P simulation mode)
Save generated SysEq records to the project data base (always saved in G and T modes)
Use time dependent calculations and plotting mode (for kinetics simulations, reserved)
Use Smart Initial Approximation of GEM IPM algorithm for faster calculations (on your discretion)
Use a stepwise mode of Process simulation (for troubleshooting purposes)
The 'P_expr' simulation control script must be used in most cases except the P mode (e.g., if temperature is changed using iTC iterator, but the system recipe remains constant).
Saving process-generated SysEq records may be necessary for subsequent sampling of results by GtDemo module or for troubleshooting, but may dramatically increase the size of project database. This flag has no effect on reciprocal and inverse titrations, where optimized SysEq records are always saved.
Learn more
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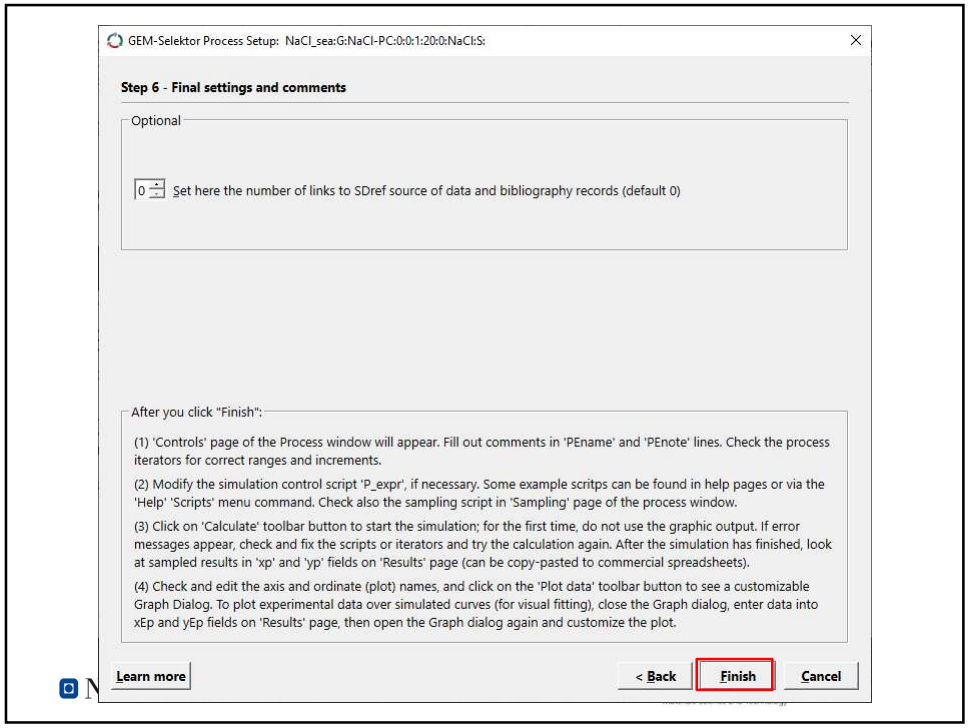
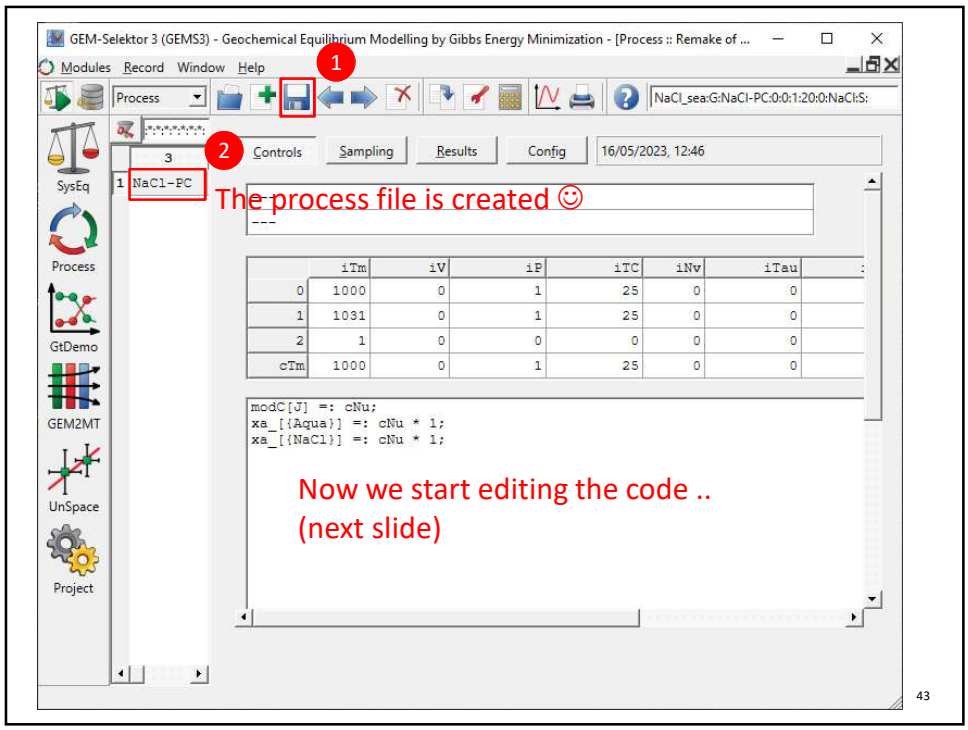
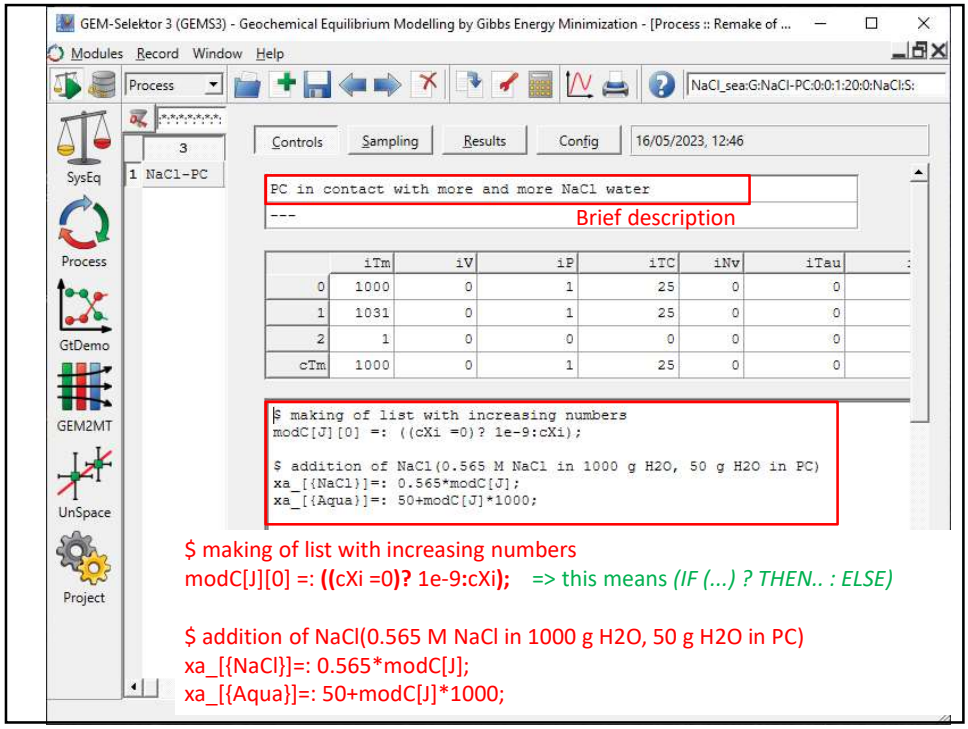
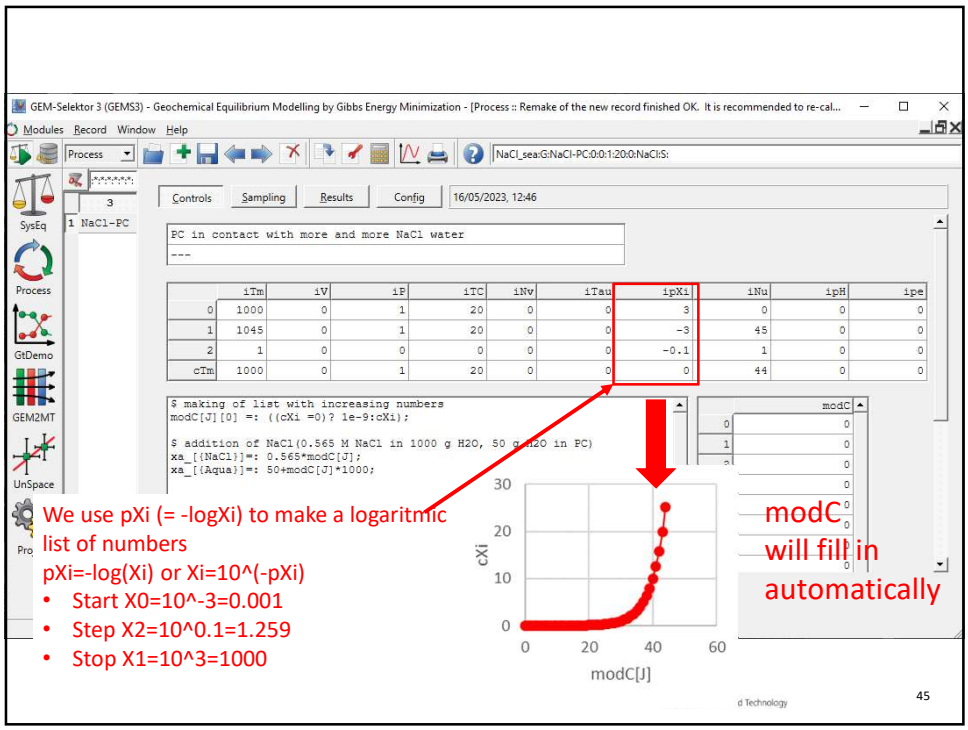
Next>
Cancel


GEM-Selektor Process Setup: NaCl_sea:G:NaCl-PC:0:0:1:20:0:NaCl:S:
Step 6 - Final settings and comments
Optional
0
Set here the number of links to SDref source of data and bibliography records (default 0)
After you click "Finish":
(1) 'Controls' page of the Process window will appear. Fill out comments in 'PEname' and 'PEnote' lines. Check the process iterators for correct ranges and increments.
(2) Modify the simulation control script 'P_expr', if necessary. Some example scritps can be found in help pages or via the 'Help' 'Scripts' menu command. Check also the sampling script in 'Sampling' page of the process window.
(3) Click on 'Calculate' toolbar button to start the simulation; for the first time, do not use the graphic output. If error messages appear, check and fix the scripts or iterators and try the calculation again. After the simulation has finished, look at sampled results in 'xp' and 'yp' fields on 'Results' page (can be copy-pasted to commercial spreadsheets).
(4) Check and edit the axis and ordinate (plot) names, and click on the 'Plot data' toolbar button to see a customizable Graph Dialog. To plot experimental data over simulated curves (for visual fitting), close the Graph dialog, enter data into xEp and yEp fields on 'Results' page, then open the Graph dialog again and customize the plot.
Learn more
< Back
Finish
Cancel

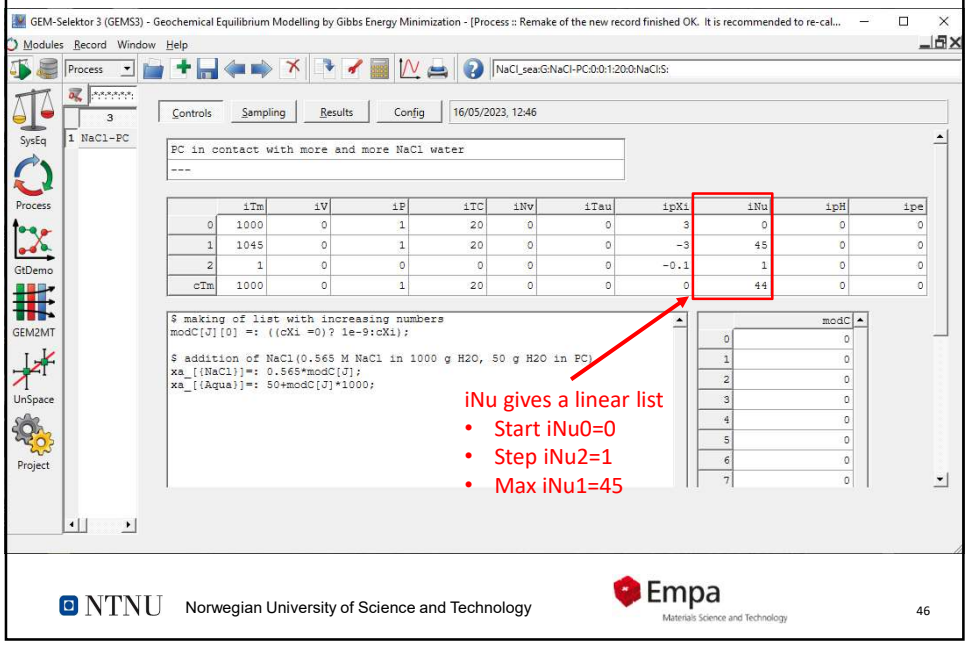

GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [Process :: Remake of ...
Modules Record Window Help
Process
NaCl_sea:G:NaCl-PC:0:0:1:20:0:NaCl:S:
1
2
Controls Sampling Results Config 16/05/2023, 12:46
SysEq
Process
GtDemo
GEM2MT
UnSpace
Project
3
1 NaCl-PC
The process file is created ☺
---
iTm iV iP iTC iNv iTau
0 1000 0 1 25 0 0
1 1031 0 1 25 0 0
2 1 0 0 0 0 0
cTm 1000 0 1 25 0 0
modC[J] =: cNu;
xa_[{Aqua}] =: cNu * 1;
xa_[{NaCl}] =: cNu * 1;
Now we start editing the code ..
(next slide)
43


GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [Process :: Remake of ...
Modules Record Window Help
Process
NaCl_sea:G:NaCl-PC:0:0:1:20:0:NaCl:S:
Controls Sampling Results Config 16/05/2023, 12:46
SysEq
Process
GtDemo
GEM2MT
UnSpace
Project
3
1 NaCl-PC
PC in contact with more and more NaCl water

Brief description
iTm iV iP iTC iNv iTau
0 1000 0 1 25 0 0
1 1031 0 1 25 0 0
2 1 0 0 0 0 0
cTm 1000 0 1 25 0 0
$ making of list with increasing numbers
modC[J][0] =: ((cXi =0)? 1e-9:cXi);
$ addition of NaCl(0.565 M NaCl in 1000 g H2O, 50 g H2O in PC)
xa_[{NaCl}]=: 0.565*modC[J];
xa_[{Aqua}]=: 50+modC[J]*1000;
$ making of list with increasing numbers
modC[J][0] =: ((cXi =0)? 1e-9:cXi); => this means (IF (...) ? THEN.. : ELSE)
$ addition of NaCl(0.565 M NaCl in 1000 g H2O, 50 g H2O in PC)
xa_[{NaCl}]=: 0.565*modC[J];
xa_[{Aqua}]=: 50+modC[J]*1000;


GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [Process :: Remake of the new record finished OK. It is recommended to re-cal...
Modules Record Window Help
Process
Controls Sampling Results Config 16/05/2023, 12:46
PC in contact with more and more NaCl water

$ making of list with increasing numbers
modC[J][0] =: ((cXi =0)? 1e-9:cXi);
$ addition of NaCl(0.565 M NaCl in 1000 g H2O, 50 g H2O in PC)
xa_[(NaCl)]=: 0.565*modC[J];
xa_[(Aqua)]=: 50+modC[J]*1000;
cXi
modC[J]
We use pXi (= -logXi) to make a logaritmic list of numbers
pXi=-log(Xi) or Xi=10^(-pXi)
• Start X0=10^-3=0.001
• Step X2=10^0.1=1.259
• Stop X1=10^3=1000
modC will fill in automatically
45


GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [Process :: Remake of the new record finished OK. It is recommended to re-cal...
Modules Record Window Help
Process
Controls Sampling Results Config 16/05/2023, 12:46
PC in contact with more and more NaCl water

$ making of list with increasing numbers
modC[J][0] =: ((cXi =0)? 1e-9:cXi);
$ addition of NaCl(0.565 M NaCl in 1000 g H2O, 50 g H2O in PC)
xa_[(NaCl)]=: 0.565*modC[J];
xa_[(Aqua)]=: 50+modC[J]*1000;
iNu gives a linear list
• Start iNu0=0
• Step iNu2=1
• Max iNu1=45
NTNU Norwegian University of Science and Technology
Empa Materials Science and Technology
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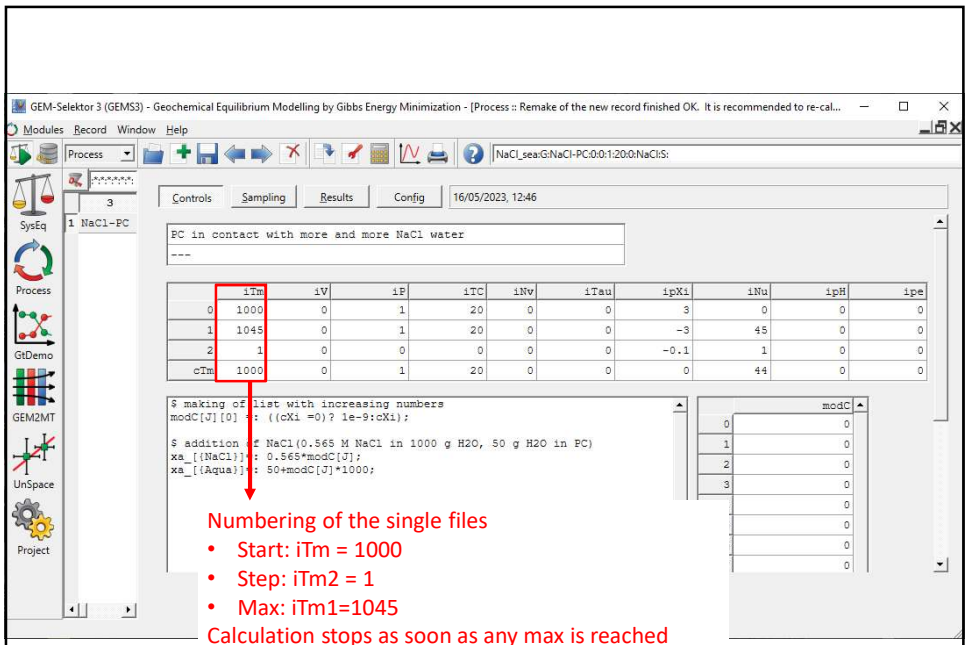
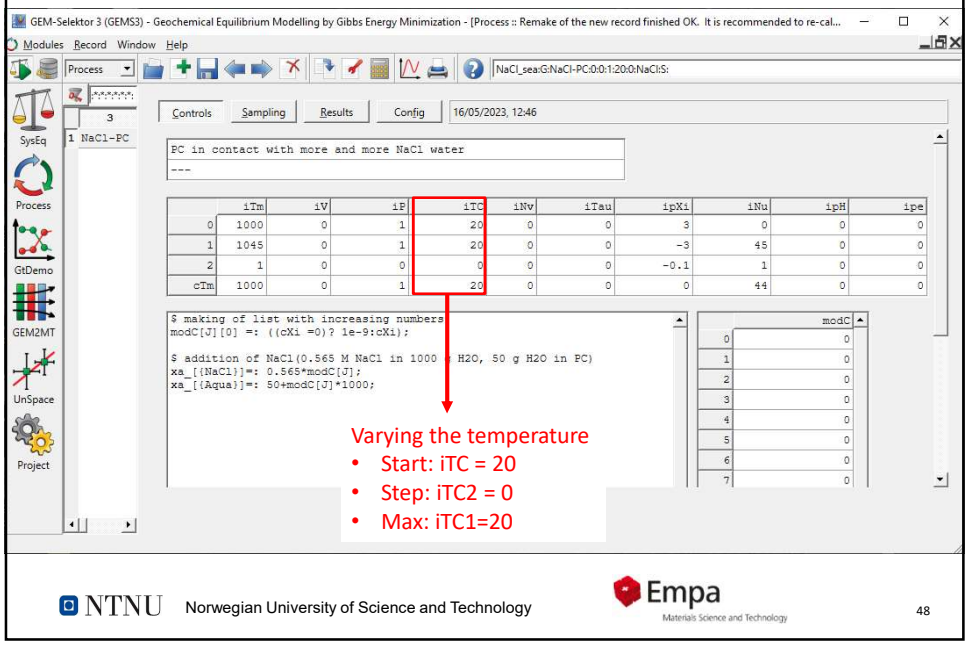
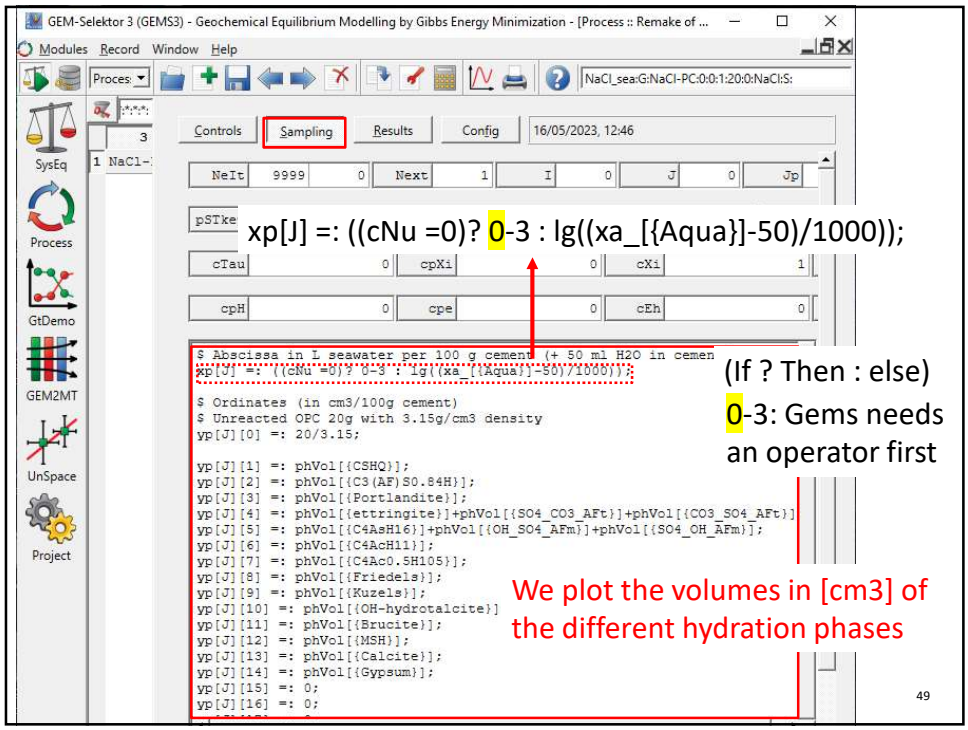

GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [Process :: Remake of the new record finished OK. It is recommended to re-cal...
Modules Record Window Help
Process
Controls Sampling Results Config 16/05/2023, 12:46
PC in contact with more and more NaCl water
---
iTm iV iP iTC iNv iTau ipXi iNu ipH ipe
0 1000 0 1 20 0 0 3 0 0 0
1 1045 0 1 20 0 0 -3 45 0 0
2 1 0 0 0 0 0 -0.1 1 0 0
cTm 1000 0 1 20 0 0 0 44 0 0
$ making of list with increasing numbers
modC[J][0] =: ((cXi =0)? 1e-9:cXi);
$ addition of NaCl(0.565 M NaCl in 1000 g H2O, 50 g H2O in PC)
xa_[(NaCl)]=: 0.565*modC[J];
xa_[(Aqua)]=: 50+modC[J]*1000;
modC
Numbering of the single files
• Start: iTm = 1000
• Step: iTm2 = 1
• Max: iTm1=1045
Calculation stops as soon as any max is reached
SysEq
Process
GtDemo
GEM2MT
UnSpace
Project


GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [Process :: Remake of the new record finished OK. It is recommended to re-cal...
Modules Record Window Help
Process
Controls Sampling Results Config 16/05/2023, 12:46
PC in contact with more and more NaCl water
---
iTm iV iP iTC iNv iTau ipXi iNu ipH ipe
0 1000 0 1 20 0 0 3 0 0 0
1 1045 0 1 20 0 0 -3 45 0 0
2 1 0 0 0 0 0 -0.1 1 0 0
cTm 1000 0 1 20 0 0 0 44 0 0
$ making of list with increasing numbers
modC[J][0] =: ((cXi =0)? 1e-9:cXi);
$ addition of NaCl(0.565 M NaCl in 1000 g H2O, 50 g H2O in PC)
xa_[(NaCl)]=: 0.565*modC[J];
xa_[(Aqua)]=: 50+modC[J]*1000;
modC
Varying the temperature
• Start: iTC = 20
• Step: iTC2 = 0
• Max: iTC1=20
SysEq
Process
GtDemo
GEM2MT
UnSpace
Project


GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [Process :: Remake of ...
Modules Record Window Help
Controls Sampling Results Config 16/05/2023, 12:46
xp[J] =: ((cNu =0)? 0-3 : lg((xa_[{Aqua}]-50)/1000));
$ Abscissa in L seawater per 100 g cement (+ 50 ml H2O in cemen
$ Ordinates (in cm3/100g cement)
$ Unreacted OPC 20g with 3.15g/cm3 density
yp[J][0] =: 20/3.15;
yp[J][1] =: phVol[{CSHQ}];
yp[J][2] =: phVol[{C3(AF)S0.84H}];
yp[J][3] =: phVol[{Portlandite}];
yp[J][4] =: phVol[{ettringite}]+phVol[{SO4_CO3_AFt}]+phVol[{CO3_SO4_AFt}]
yp[J][5] =: phVol[{C4AsH16}]+phVol[{OH_SO4_AFm}]+phVol[{SO4_OH_AFm}];
yp[J][6] =: phVol[{C4AcH11}];
yp[J][7] =: phVol[{C4Ac0.5H105}];
yp[J][8] =: phVol[{Friedels}];
yp[J][9] =: phVol[{Kuzels}];
yp[J][10] =: phVol[{OH-hydrotalcite}]
yp[J][11] =: phVol[{Brucite}];
yp[J][12] =: phVol[{MSH}];
yp[J][13] =: phVol[{Calcite}];
yp[J][14] =: phVol[{Gypsum}];
yp[J][15] =: 0;
yp[J][16] =: 0;
(If ? Then : else)
0-3: Gems needs an operator first
We plot the volumes in [cm3] of the different hydration phases
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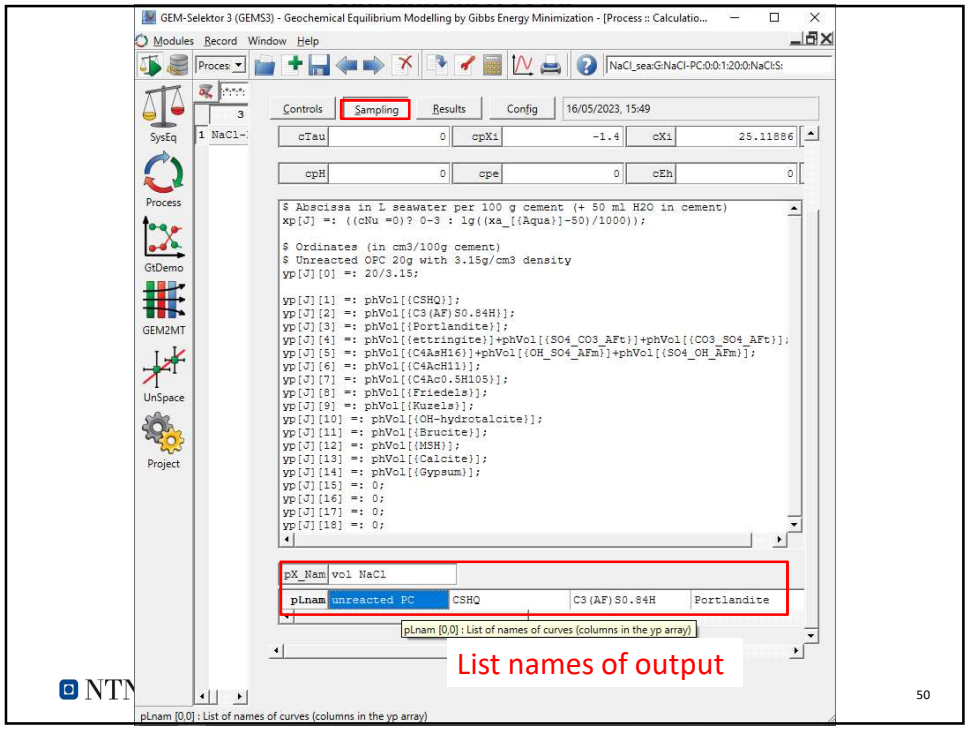
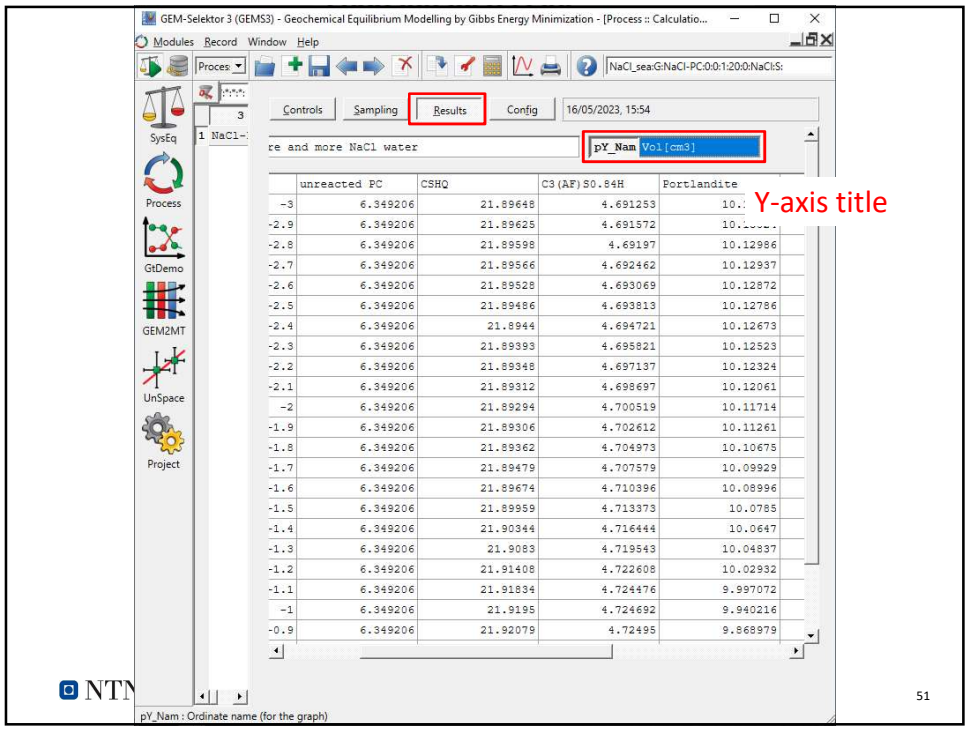
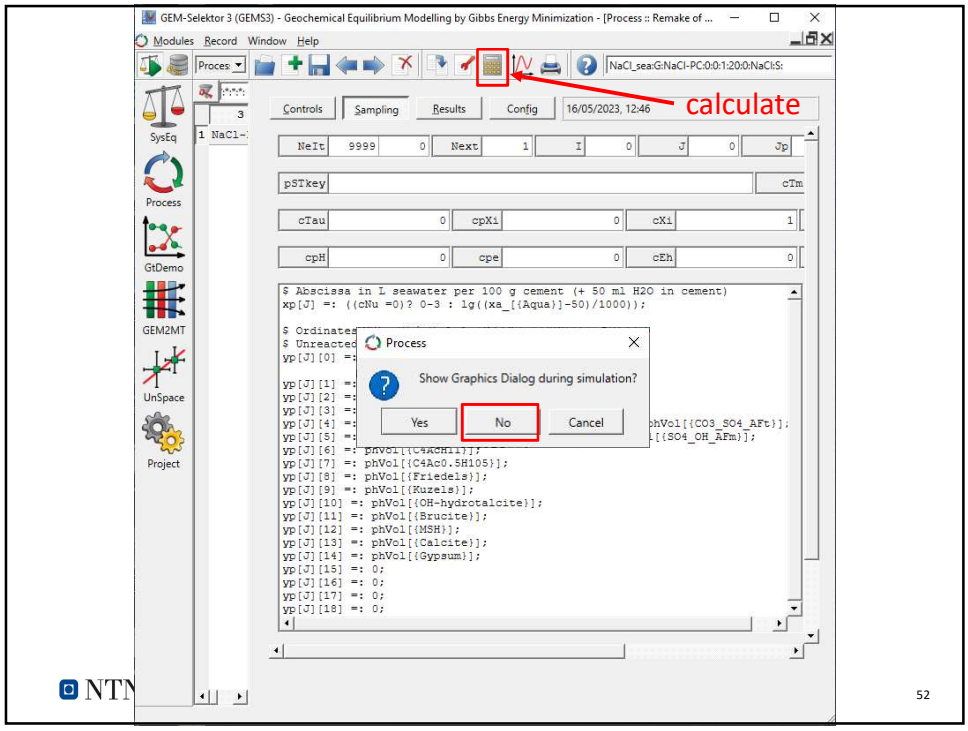
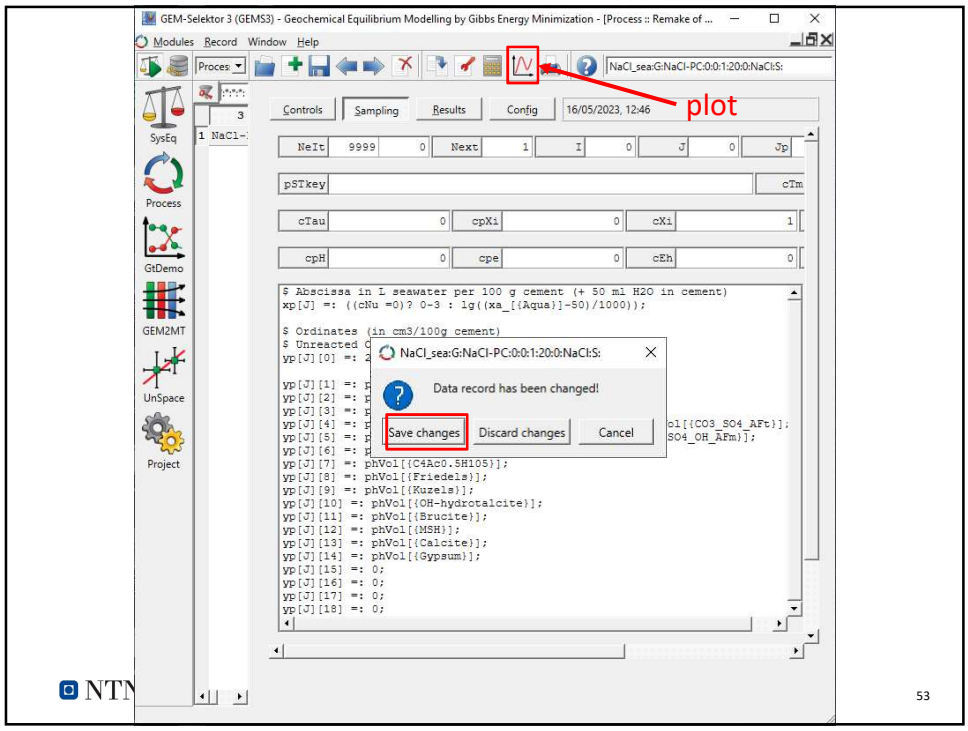
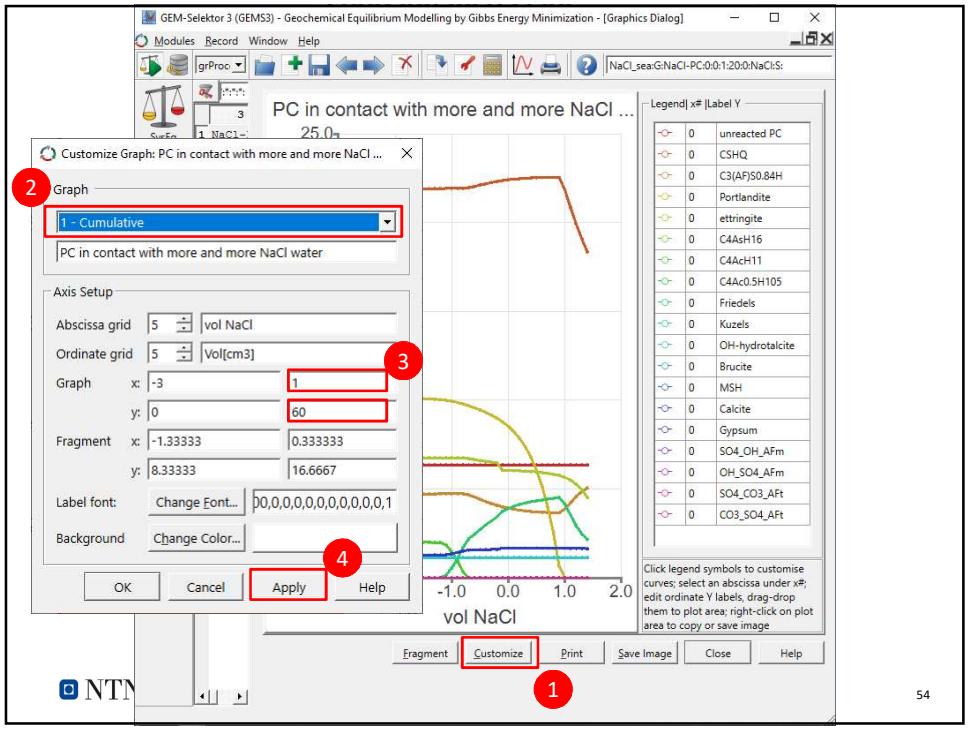
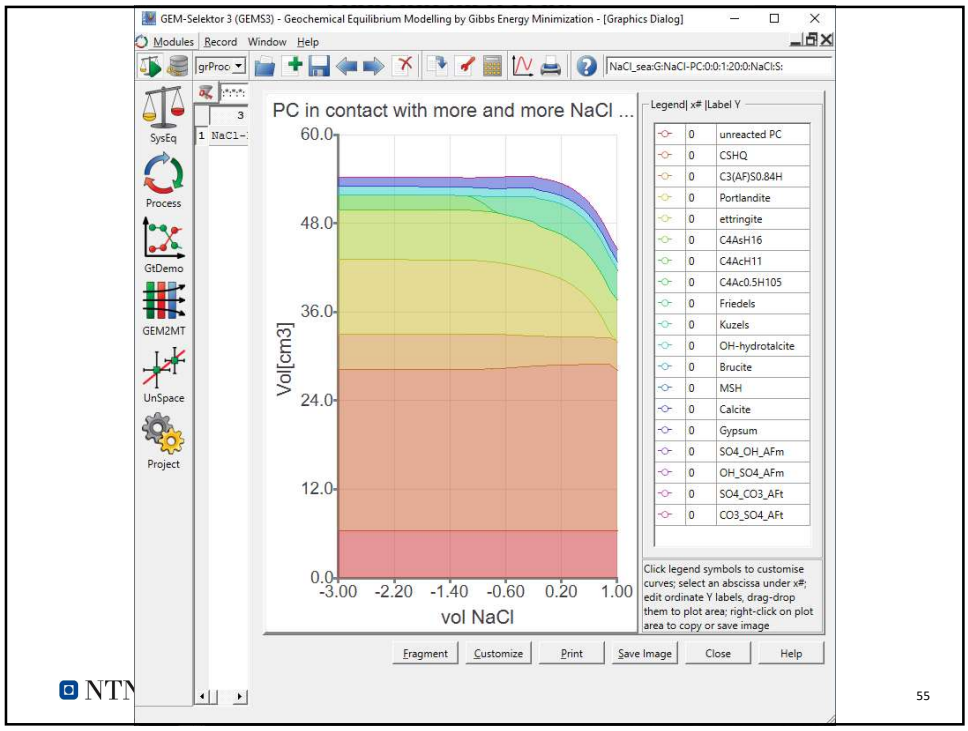

GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [Process :: Calculatio...
Modules Record Window Help
Controls Sampling Results Config 16/05/2023, 15:49
$ Abscissa in L seawater per 100 g cement (+ 50 ml H2O in cement)
xp[J] =: ((cNu =0)? 0-3 : lg((xa_[{Aqua}]-50)/1000));
$ Ordinates (in cm3/100g cement)
$ Unreacted OPC 20g with 3.15g/cm3 density
yp[J][0] =: 20/3.15;
yp[J][1] =: phVol[{CSHQ}];
yp[J][2] =: phVol[{C3(AF)S0.84H}];
yp[J][3] =: phVol[{Portlandite}];
yp[J][4] =: phVol[{ettringite}]+phVol[{SO4_CO3_AFt}]+phVol[{CO3_SO4_AFt}];
yp[J][5] =: phVol[{C4AsH16}]+phVol[{OH_SO4_AFm}]+phVol[{SO4_OH_AFm}];
yp[J][6] =: phVol[{C4AcH11}];
yp[J][7] =: phVol[{C4Ac0.5H105}];
yp[J][8] =: phVol[{Friedels}];
yp[J][9] =: phVol[{Kuzels}];
yp[J][10] =: phVol[{OH-hydrotalcite}];
yp[J][11] =: phVol[{Brucite}];
yp[J][12] =: phVol[{MSH}];
yp[J][13] =: phVol[{Calcite}];
yp[J][14] =: phVol[{Gypsum}];
yp[J][15] =: 0;
yp[J][16] =: 0;
yp[J][17] =: 0;
yp[J][18] =: 0;
pX_Nam vol NaCl
pLnam unreacted PC CSHQ C3(AF)S0.84H Portlandite
pLnam [0,0] : List of names of curves (columns in the yp array)
List names of output
50

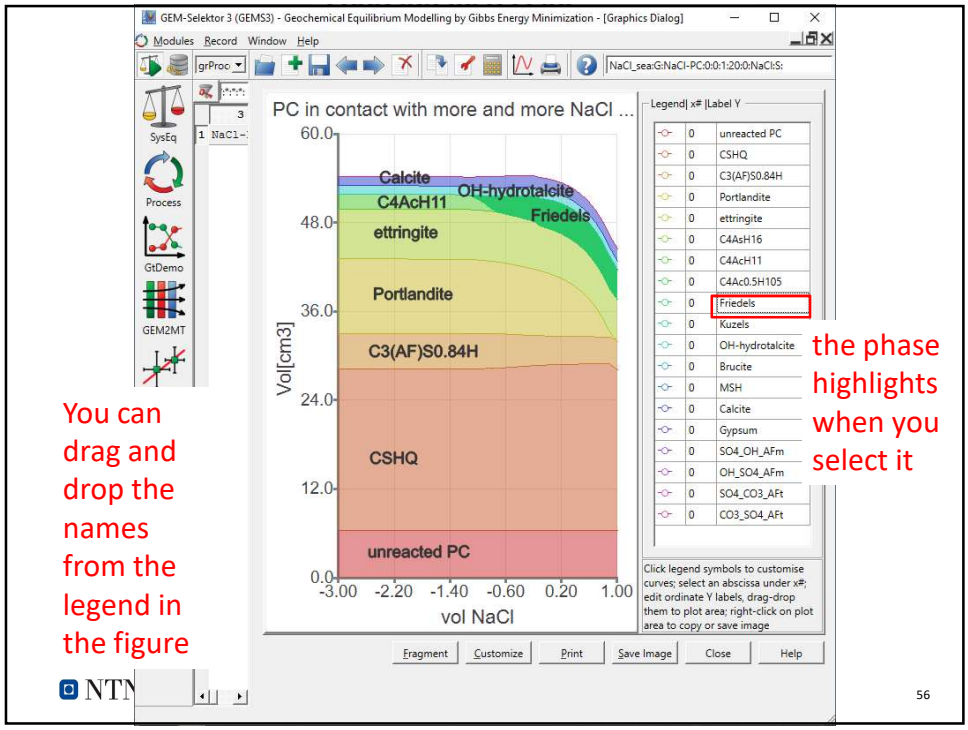

GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [Process :: Calculatio...
Modules Record Window Help
Controls Sampling Results Config 16/05/2023, 15:54
pY_Nam Vol[cm3]
Y-axis title
unreacted PC CSHQ C3(AF)S0.84H Portlandite
pY_Nam : Ordinate name (for the graph)
51

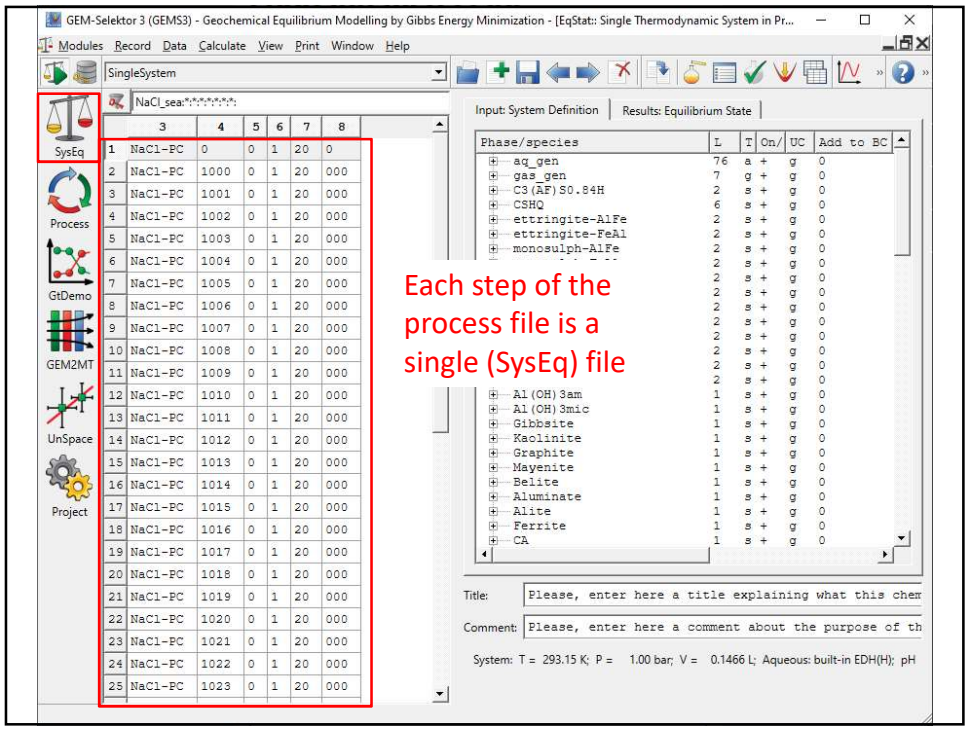

GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [Process :: Remake of ...
Modules Record Window Help
calculate
Controls Sampling Results Config 16/05/2023, 12:46
Process
Show Graphics Dialog during simulation?
Yes No Cancel
52

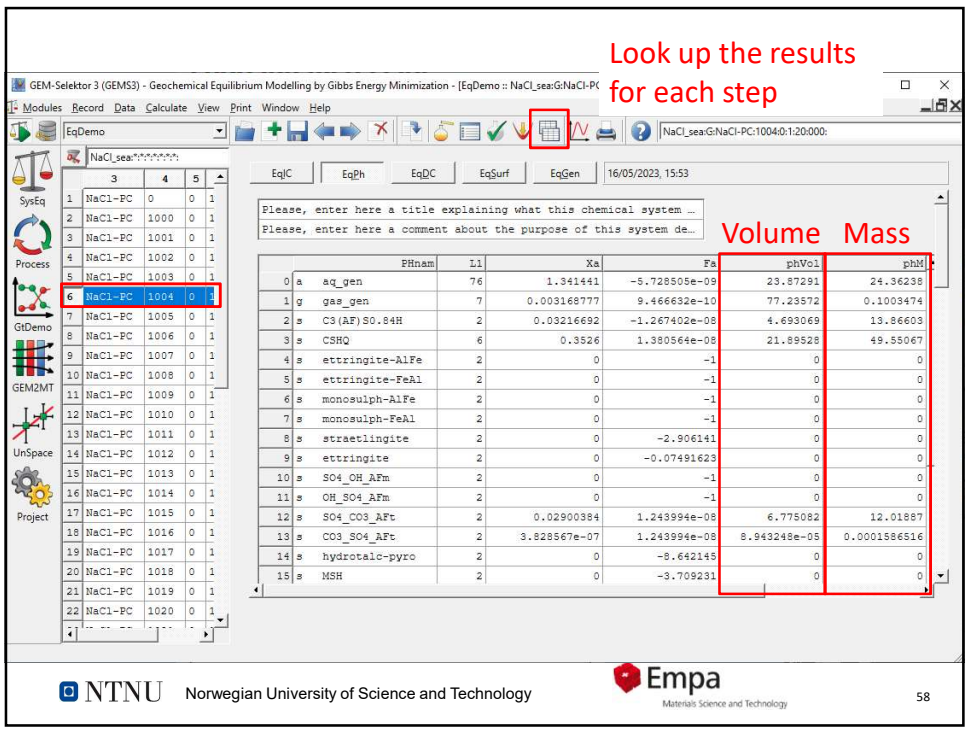

GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [Process :: Remake of ...
Modules Record Window Help
plot
Controls Sampling Results Config 16/05/2023, 12:46
NaCl_sea:G:NaCl-PC:0:0:1:20:0:NaCl:S:
Data record has been changed!
Save changes
Discard changes
Cancel
SysEq
Process
GtDemo
GEM2MT
UnSpace
Project


GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [Graphics Dialog]
Modules Record Window Help
PC in contact with more and more NaCl ...
Customize Graph: PC in contact with more and more NaCl ...
2
Graph
1 - Cumulative
PC in contact with more and more NaCl water
Axis Setup
Abscissa grid 5 vol NaCl
Ordinate grid 5 Vol[cm3]
3
Graph x: -3 1
y: 0 60
Fragment x: -1.33333 0.333333
y: 8.33333 16.6667
Label font: Change Font... 0,0,0,0,0,0,0,0,0,0,0,1
Background Change Color...
4
OK Cancel Apply Help
vol NaCl
Legend| x≠ |Label Y
unreacted PC
CSHQ
C3(AF)S0.84H
Portlandite
ettringite
C4AsH16
C4AcH11
C4Ac0.5H105
Friedels
Kuzels
OH-hydrotalcite
Brucite
MSH
Calcite
Gypsum
SO4_OH_AFm
OH_SO4_AFm
SO4_CO3_AFt
CO3_SO4_AFt
Click legend symbols to customise curves; select an abscissa under x≠; edit ordinate Y labels, drag-drop them to plot area; right-click on plot area to copy or save image
Fragment Customize Print Save Image Close Help
1


GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [Graphics Dialog]
Modules Record Window Help
PC in contact with more and more NaCl ...
Vol[cm3]
vol NaCl
Legend| x# |Label Y
unreacted PC
CSHQ
C3(AF)S0.84H
Portlandite
ettringite
C4AsH16
C4AcH11
C4Ac0.5H105
Friedels
Kuzels
OH-hydrotalcite
Brucite
MSH
Calcite
Gypsum
SO4_OH_AFm
OH_SO4_AFm
SO4_CO3_AFt
CO3_SO4_AFt
Click legend symbols to customise curves; select an abscissa under x#; edit ordinate Y labels, drag-drop them to plot area; right-click on plot area to copy or save image
Fragment Customize Print Save Image Close Help
SysEq Process GtDemo GEM2MT UnSpace Project
55


GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [Graphics Dialog]
PC in contact with more and more NaCl ...
Calcite
C4AcH11
OH-hydrotalcite
Friedels
ettringite
Portlandite
C3(AF)S0.84H
CSHQ
unreacted PC
Vol[cm3]
vol NaCl
You can drag and drop the names from the legend in the figure
the phase highlights when you select it
56


GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [EqStat:: Single Thermodynamic System in Pr...
Modules Record Data Calculate View Print Window Help
SingleSystem
SysEq
Process
GtDemo
GEM2MT
UnSpace
Project
Input: System Definition
Results: Equilibrium State
Phase/species
aq_gen
gas_gen
C3(AF)S0.84H
CSHQ
ettringite-AlFe
ettringite-FeAl
monosulph-AlFe
Al(OH)3am
Al(OH)3mic
Gibbsite
Kaolinite
Graphite
Mayenite
Belite
Aluminate
Alite
Ferrite
CA
Title:
Please, enter here a title explaining what this chem
Comment:
Please, enter here a comment about the purpose of th
System: T = 293.15 K; P = 1.00 bar; V = 0.1466 L; Aqueous: built-in EDH(H); pH
Each step of the process file is a single (SysEq) file


Look up the results for each step
GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [EqDemo :: NaCl_sea:G:NaCl-PC
Modules Record Data Calculate View Print Window Help
EqDemo
NaCl_sea:G:NaCl-PC:1004:0:1:20:000:
EqIC
EqPh
EqDC
EqSurf
EqGen
16/05/2023, 15:53
Please, enter here a title explaining what this chemical system ...
Please, enter here a comment about the purpose of this system de...
Volume
Mass
PHnam
aq_gen
gas_gen
CSHQ
ettringite-AlFe
ettringite-FeAl
monosulph-AlFe
monosulph-FeAl
straetlingite
ettringite
SO4_OH_AFm
OH_SO4_AFm
SO4_CO3_AFt
CO3_SO4_AFt
hydrotalc-pyro
MSH
NTNU
Norwegian University of Science and Technology
Empa
Materials Science and Technology
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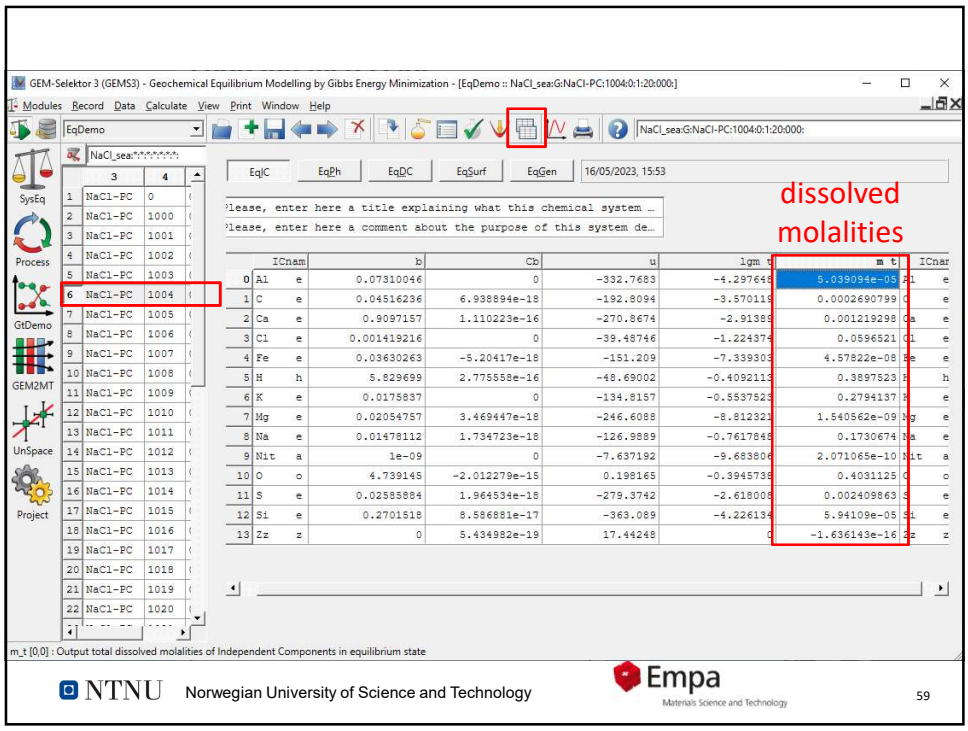
GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [EqDemo :: NaCl_sea:G:NaCl-PC:1004:0:1:20:000:]
dissolved molalities
m_t [0,0] : Output total dissolved molalities of Independent Components in equilibrium state
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Empa
Materials Science and Technology
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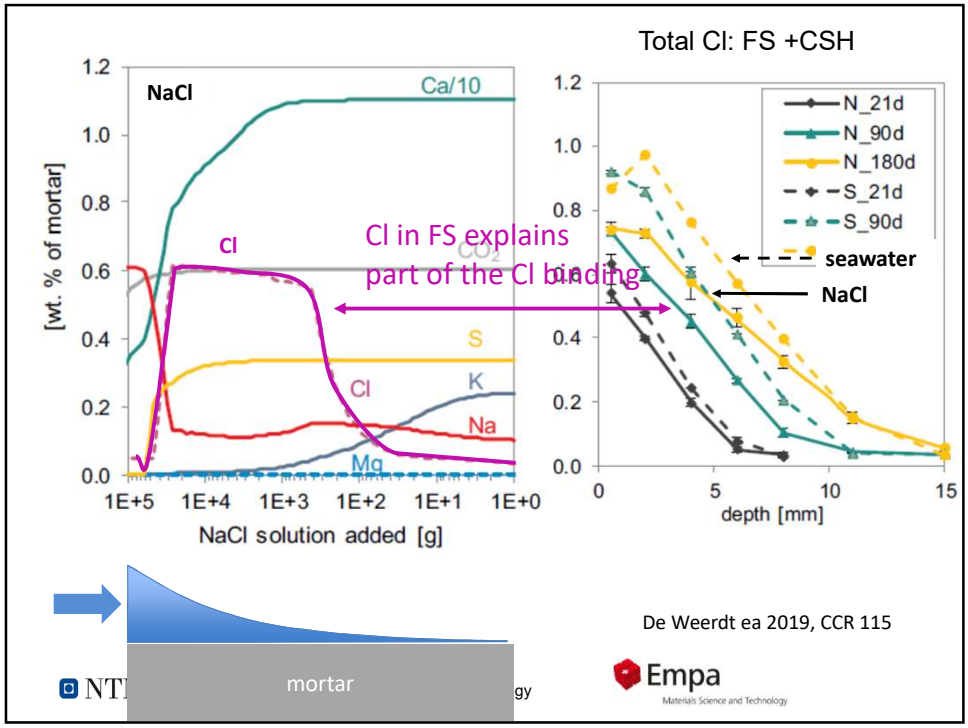
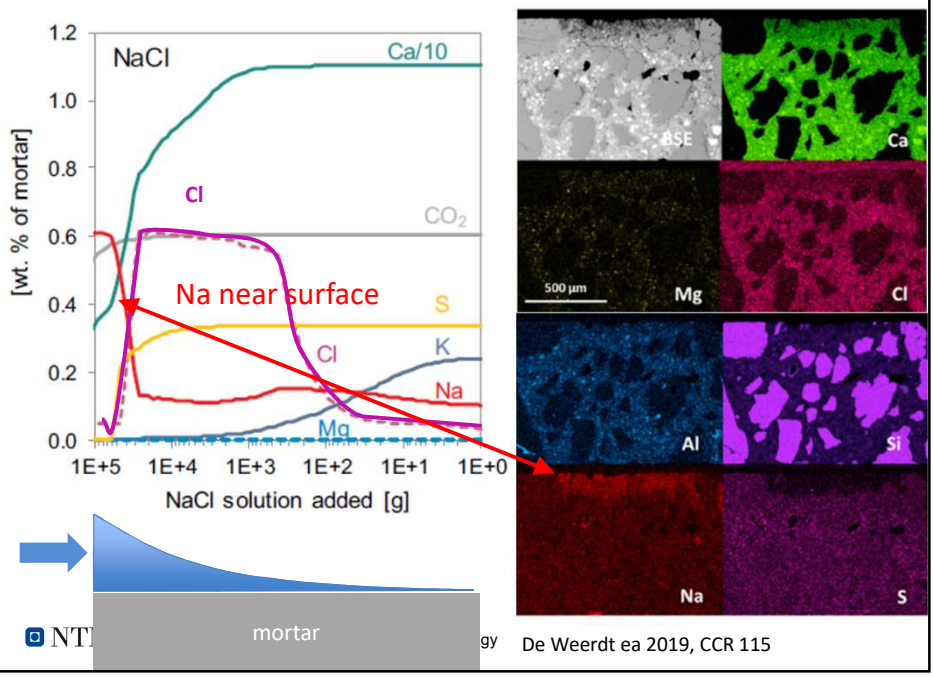
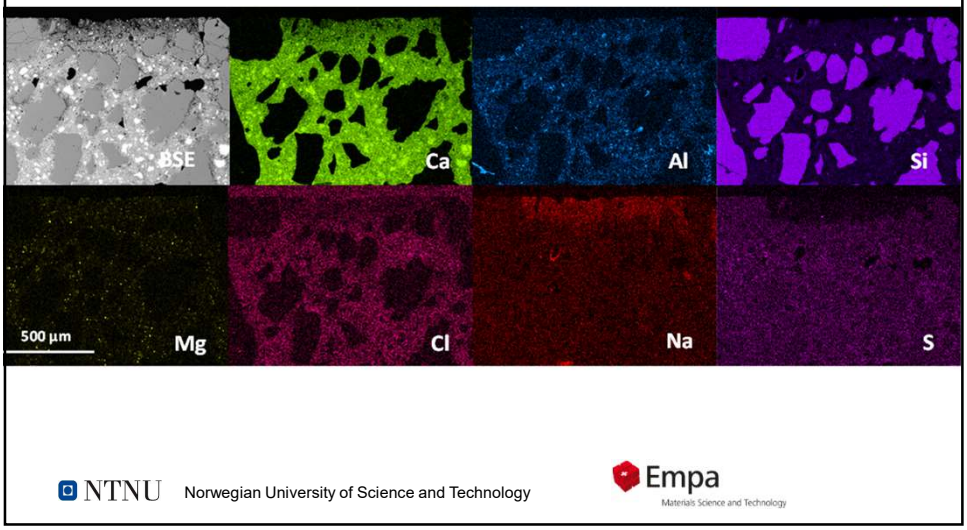

Total Cl: FS +CSH
NaCl
Ca/10
Cl
Cl in FS explains part of the Cl binding
S
K
Na
Mg
[wt. % of mortar]
NaCl solution added [g]
depth [mm]
N_21d
N_90d
N_180d
S_21d
S_90d
seawater
NaCl
mortar
De Weerdt ea 2019, CCR 115
Empa
Materials Science and Technology



De Weerdt ea 2019, CCR 115



NTNU Norwegian University of Science and Technology

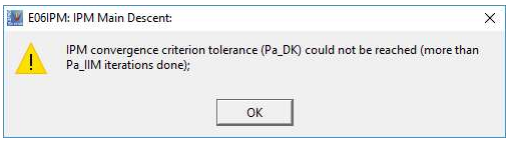
Empa Materials Science and Technology

We might encounter some instability problems on the way.
Please adapt the project controls ☺

GEMS – Convergence problem

Empa Materials Science and Technology

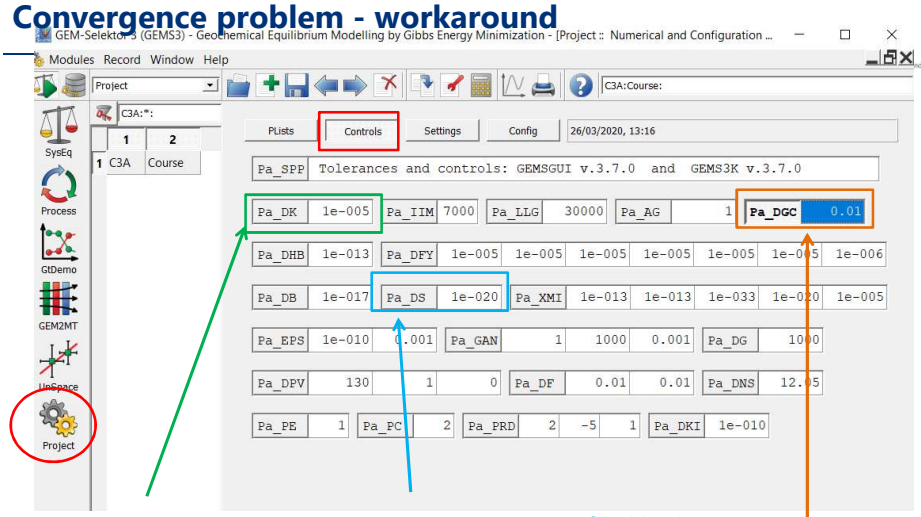
This error message might occur :



The reason is the current solid solution model, e.g. for Al-Fe-AFt.
As a workaround there are two possible solutions:

1) Do not use this solid solution. Use the single phases instead.
2) Modify the some of the settings of GEMS as shown on the next slide.
   In most cases this should work.

Convergence problem - workaround



2. Covergence tolerance parameter:
use higher value, e.g. 1e-004,
maximum seems to be 5e-003

3. Minimum amount of stable phases:
use lower value, e.g. 1e-023

1. Smoothing parameter:
use low positive value, e.g. 0.01
E => 0.01 works

Do not touch the other values !!!

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