

Lecture 02a What is GEMS



first tutorials

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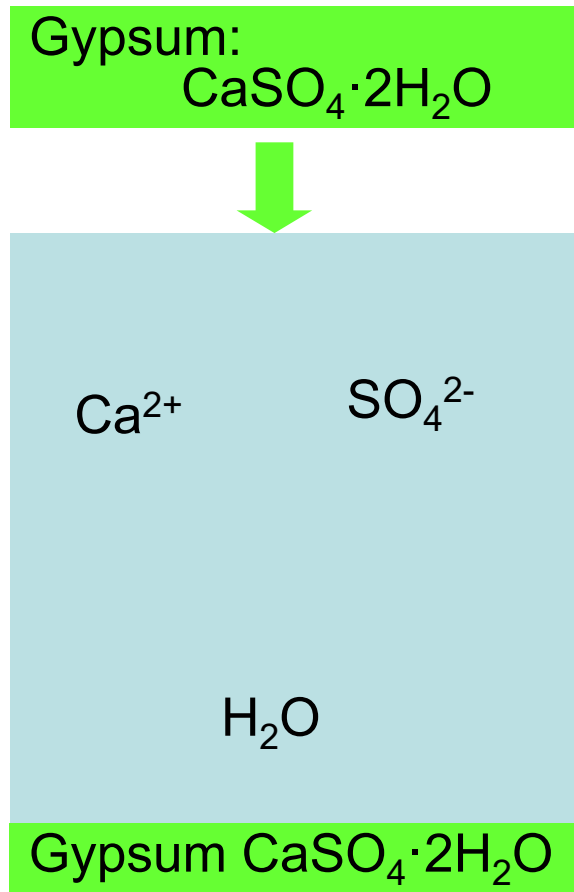
Thermodynamic modelling

1. Short overview thermodynamic modelling
 - a. chemical equilibrium
 - b. modelling software
 - c. databases

2. What is GEMS?
3. Installation of GEMS
4. First tutorials
 - Calculation of single systems:
 - Equilibrium C_3A , gypsum, portlandite
 - Parameter variations (*process*)
 - calcite, temperature, ...

2 Thermodynamic modelling

Example chemical equilibria: Gypsum in a glass of water



Reaction:



Solubility product

$$K_{\text{S}0} = \{\text{Ca}^{2+}\} \cdot \{\text{SO}_4^{2-}\} \cdot \{\text{H}_2\text{O}\}^2 / \{\text{CaSO}_4 \cdot 2\text{H}_2\text{O}\}$$

$$K_{\text{S}0} = \{\text{Ca}^{2+}\} \cdot \{\text{SO}_4^{2-}\} = 10^{-4.58}$$

{ } : activity; []: concentration

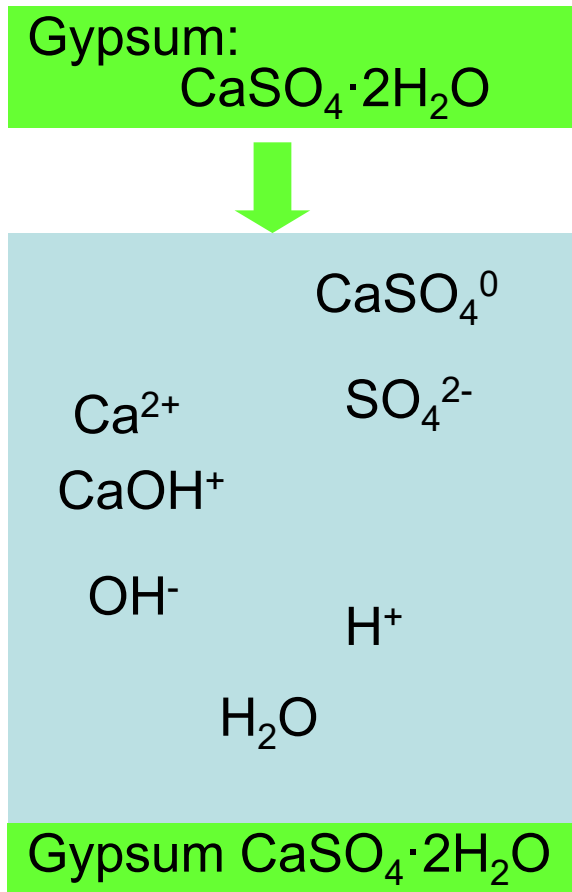
$$\{\text{Ca}^{2+}\} = [\text{Ca}^{2+}] \gamma_{\text{Ca}^{2+}} \quad \gamma \text{ Activity coefficient}$$

$$\log \gamma_{\text{Ca}^{2+}} = \frac{-AZ^2\sqrt{I}}{1 + Ba\sqrt{I}} + bI$$

extended Debye-Hückel

2 Thermodynamic modelling

Example chemical equilibria: Gypsum in a glass of water



Reaction:



Solubility product

$$K_{\text{S0}} = \{\text{Ca}^{2+}\} \cdot \{\text{SO}_4^{2-}\} = 10^{-4.58}$$

Complex formation: Equilibrium constants

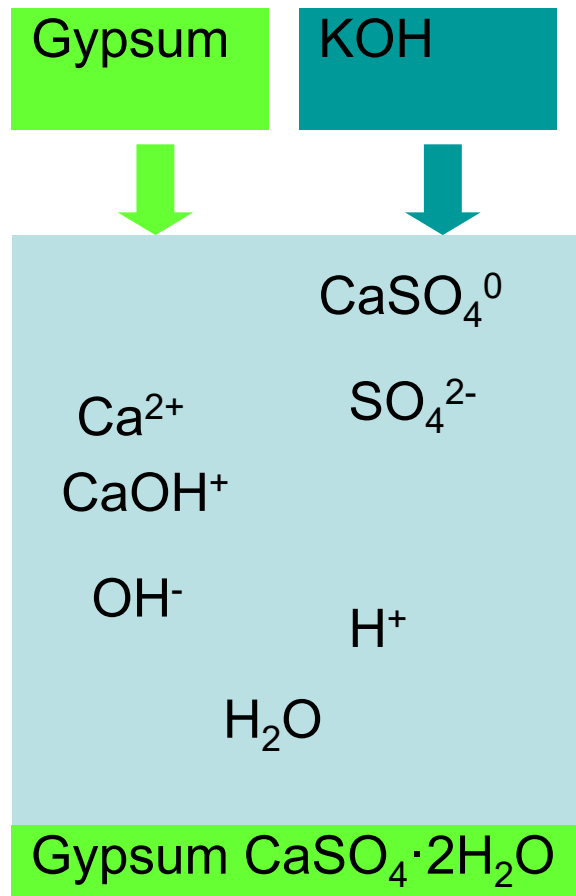
$$K = \{\text{CaOH}^+\} / \{\text{Ca}^{2+}\} \cdot \{\text{OH}^-\} = 10^{1.22}$$

$$K = \{\text{CaSO}_4^0\} / \{\text{Ca}^{2+}\} \cdot \{\text{SO}_4^{2-}\} = 10^{2.3}$$

$$K = \{\text{H}^+\} \cdot \{\text{OH}^-\} = 10^{-14.00}$$

2 Thermodynamic modelling

Chemical equilibria:



1 Concentration of Ca, SO₄?

2 What happens if we add KOH?

?

Solubility products

$$K_{S0} = \{Ca^{2+}\} \cdot \{SO_4^{2-}\} = 10^{-4.58}$$

$$K_{S0} = \{Ca^{2+}\} \cdot \{OH^{-}\}^2 = 10^{-5.20}$$

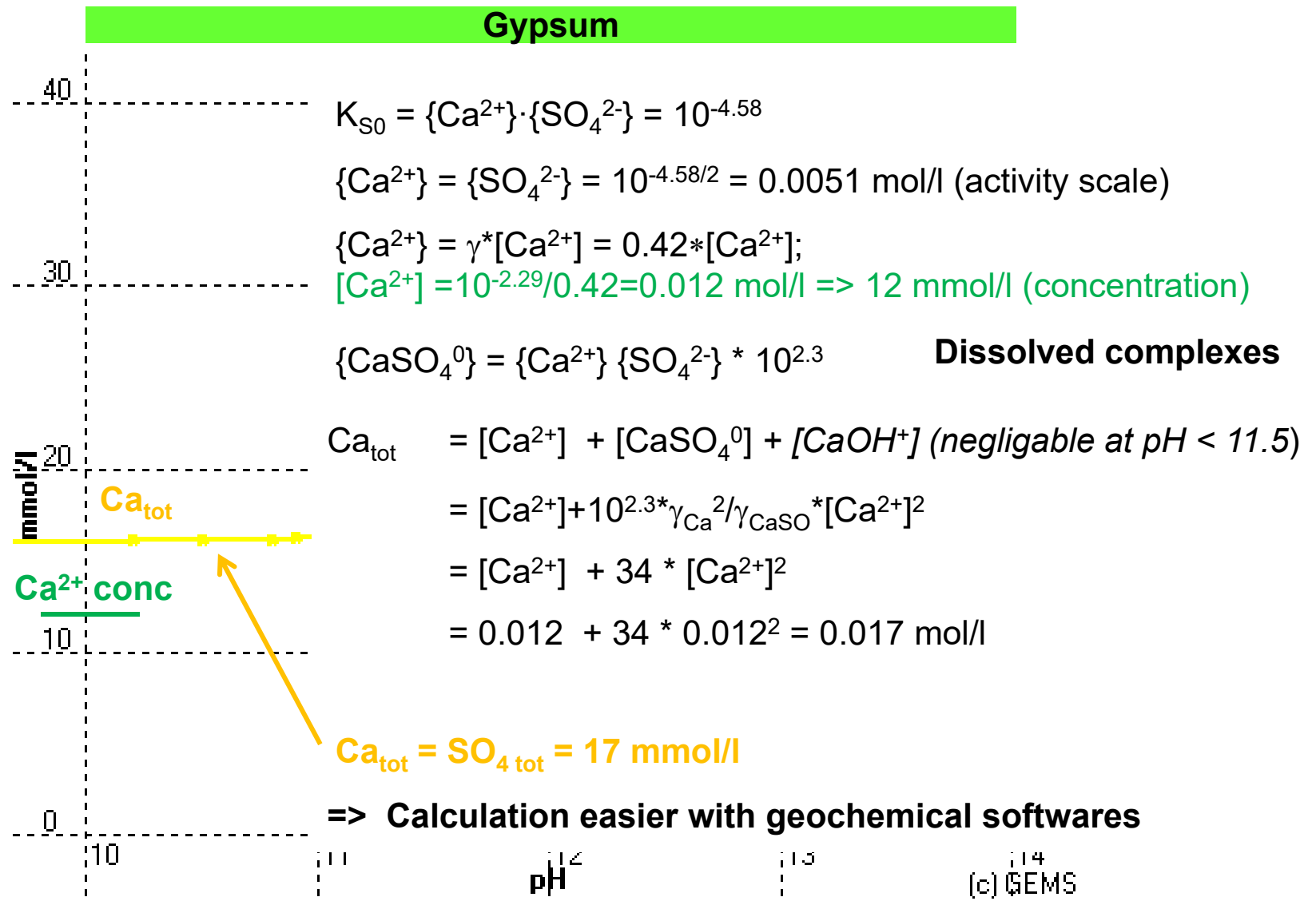
Equilibrium constants

$$K = \{CaOH^{+}\} / \{Ca^{2+}\} \cdot \{OH^{-}\} = 10^{1.22}$$

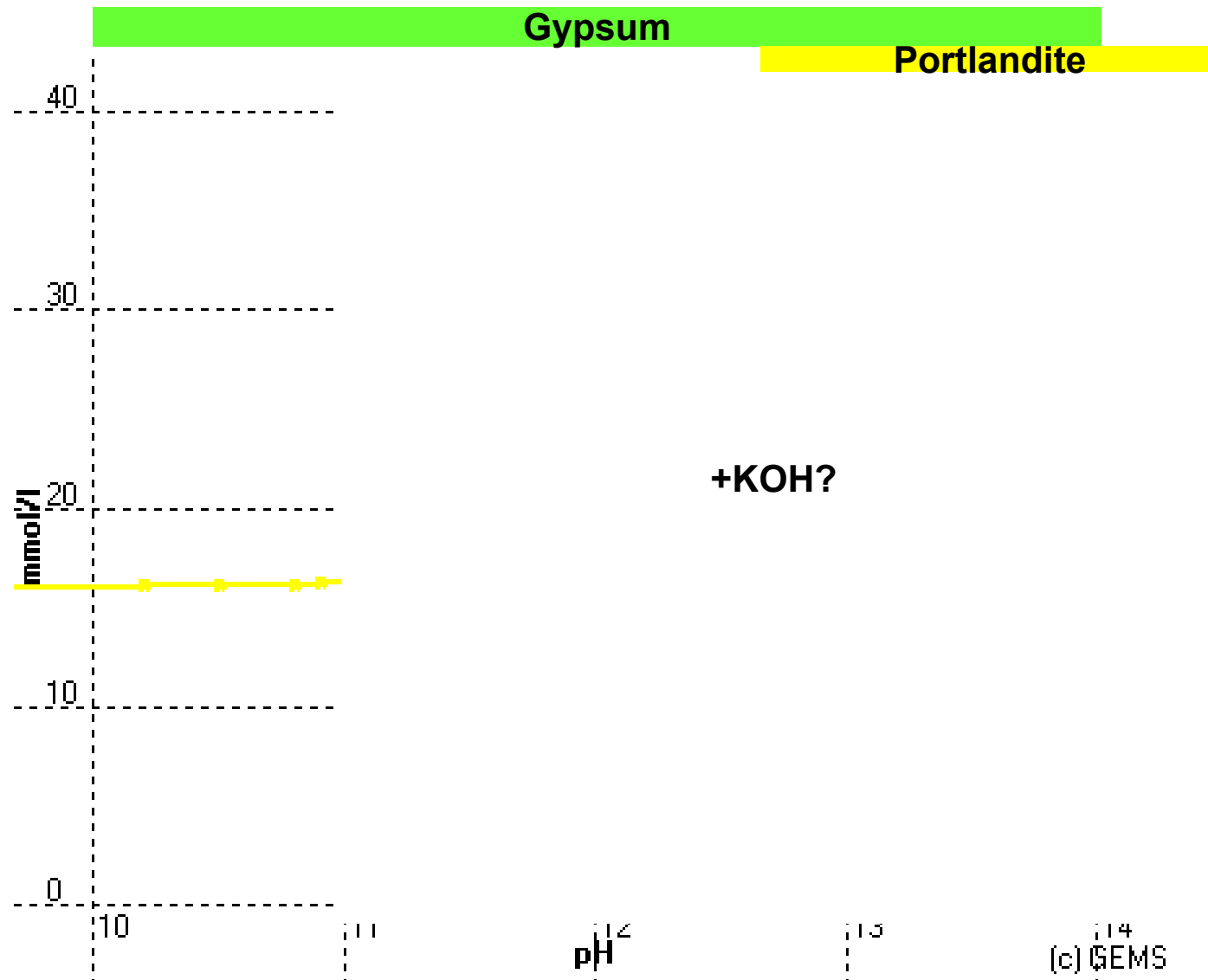
$$K = \{CaSO_4^0\} / \{Ca^{2+}\} \cdot \{SO_4^{2-}\} = 10^{2.3}$$

$$K = \{H^{+}\} \cdot \{OH^{-}\} = 10^{-14.00}$$

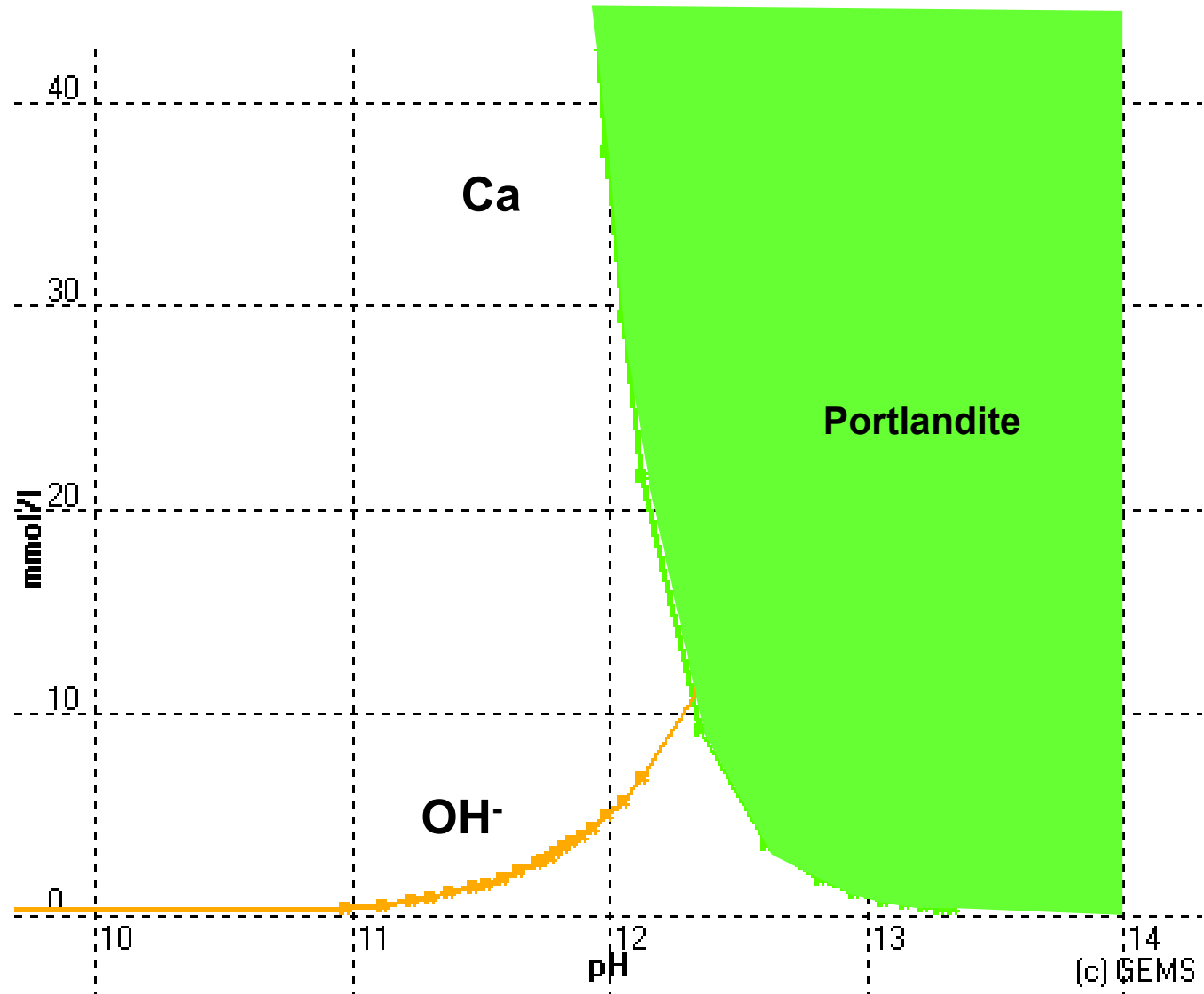
Solubility of gypsum



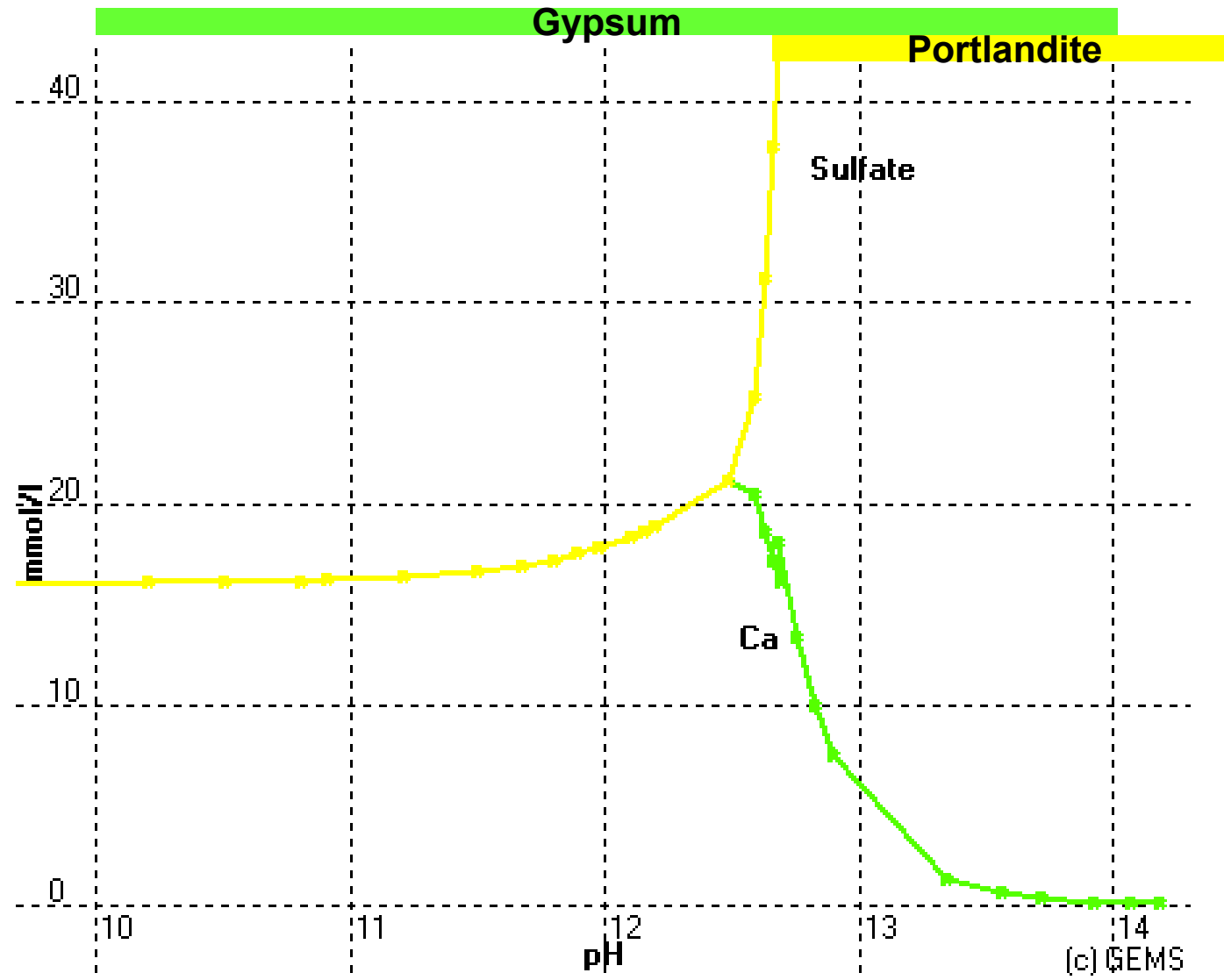
Solubility of gypsum



Solubility of portlandite



Solubility of gypsum



Codes

Complex systems



Geochemical codes needed for calculation:

- Geochemical database
- User interface: problem formulation
- Problem solving

Geochemical Codes

Freeware

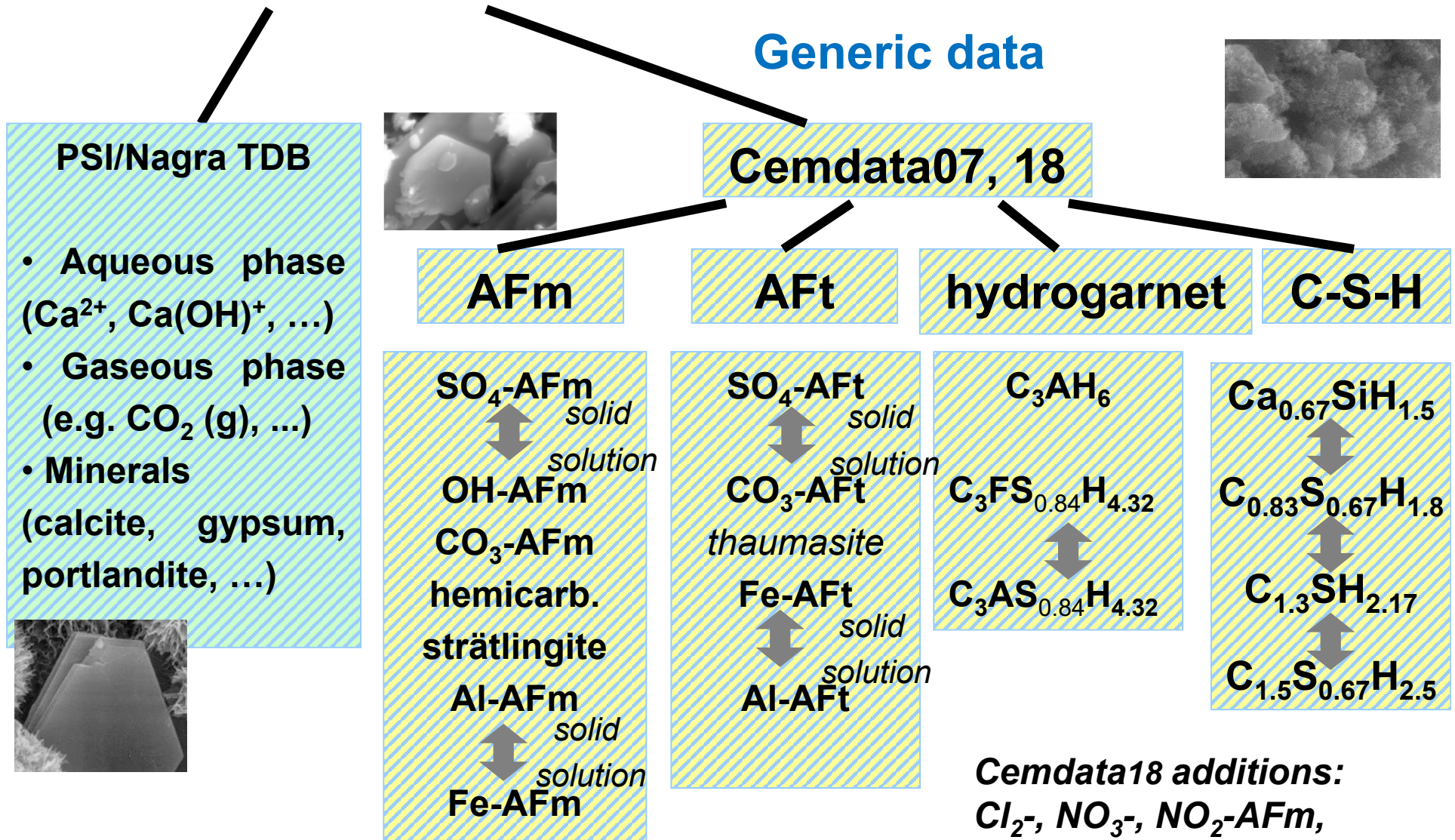
- **GEMS 3.7** <http://gems.web.psi.ch/>
solid solutions, kinetics, fitting, transport modelling
(Used in this course)
- **PHREEQC** <http://www.hydrochemistry.eu/>
transport modelling
- **MINTEQA2** <https://www.epa.gov/ceam/minteqa2-equilibrium-speciation-model>

Commercial products

- **MINEQL+** <http://www.mineql.com/>
- **CHESS**

**Comparable results
differences in database!**

Thermodynamic database



Data based on solubility measurements at different temperatures + solid phase characterisation

Cemdata18 additions:
 Cl_2^- , NO_3^- , $\text{NO}_2\text{-AFm}$,
 relative humidity, M-S-H ,
 zeolites, C-N-A-S-H , ...

Thermodynamic modelling

1. Geochemical programme ✓

2. Thermodynamic data ✓

3. Problem formulation:

Define quantities of

- water,
- solids: gypsum, calcite, C_3A , C_3S , ...
- liquids: H_2SO_4 , ...
- gas: CO_2 , N_2 , ...

... at the user interface of the respective programme

Input

Input Recipe of Single Thermodynamic System: portlandit:G:CO2:0:0:1:25:0:

tname

Property

- Compos (xa_)
- DComp (xd_)
- IComp (bi_)
- Phase (xp_)
- Kin.lower (dll_)
- Kin.upper (dul_)
- G0 shift (gEx_)
- Other Inputs

Selection

- Aqua
- CH4
- CO2
- Ca(OH)2
- CaCO3
- CaO
- CaSO4
- Gypsum
- H2
- H2S
- H2SO4
- O2
- SO3

Recipe Input

	Property	Name	Quantity	Units
1	xa_	Aqua	1000	g
2	xa_	CO2	1	g
3	xa_	Ca(OH)2	10	g
4	xa_	Gypsum	8	g
5	xa_	O2	.1	g

Input quantities of Compos(itions) contributing to B_ vector

[Learn more](#)

O₂ added to ensure oxidising conditions

Results 1

Solids: amount in g, mol, cm³,...

3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [EqDemo :: portlandit:G:CO2:0:0:1:25:0:]

ord Data Calculate View Print Window Help

portlandit:G:CO2:0:0:1:25:0:

portlandit:*,*,*,*,*,*,*,*:

4	5	6	7	8	
2	0	0	1	25	0

EqIC EqPh EqDC EqSurf EqGen 29/08/2012, 12:44

	PHnam	Xa	Fa	phVol	phM
0	a aq_gen	55.631449	4.049238e-010	1003.4458	1004.0869
1	g gas_gen	0.0018093475	-3.6160014e-011	44.853204	0.057896951
2	s Graphite	0	-82.225695	0	0
3	s Aragonite	0	-0.14383216	0	0
4	s Calcite	0.022715807	9.9544516e-010	0.8389856	2.273557
5	s lime	0	-9.7759048	0	0
6	s Portlandite	0.092888665	4.112154e-008	3.0708992	6.8823719
7	s Anhydrite	0	-0.22276489	0	0
8	s Gypsum	0.033682935	2.9568298e-008	2.5157783	5.7992987
9	s Hemihydrate	0	-0.98902801	0	0
10	s Sulphur	0	-116.25094	0	0

pmXs 14.955228

Results 2

Aqueous concentrations (mg/l, mM, ...)

m Modelling by Gibbs Energy Minimization - [EqDemo :: portlandit:G:CO2:0:0:1:25:0:]

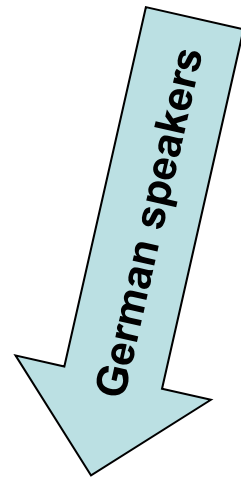
Window Help

EqIC EqPh EqDC EqSurf EqGen 29/08/2012, 12:44

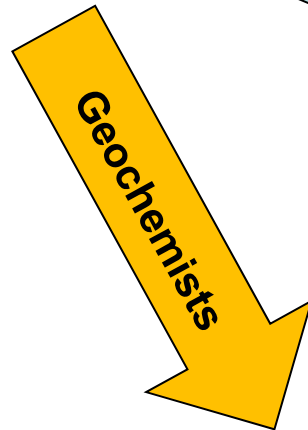
	ICnam b	Cb	u	lgm t	m t	ICnam	
0	C ...	0.022722315	0	-189.33166	-5.1869589	6.5019116e-006	C ...
1	Ca ...	0.1814309	1.8633089e-017	-266.17021	-1.4932845	0.032115559	Ca ...
2	H ...	111.47254	1.3788486e-014	-47.839341	-1.4125525	0.038676534	H ...
3	O ...	56.108789	-5.2917973e-015	-4.1667698e-011	-1.0342882	0.092408466	O ...
4	S ...	0.046464839	0	-267.67769	-1.8937821	0.012770795	S ...
5	Zz ...	0	6.0791121e-019	19.220318	0	2.6947074e-018	Zz ...

3 GEMS

What is GEMS?



Gemse (*chamois*)



Gemstone



GEMS TM:

**Gibbs Energy Minimization Software
for Thermodynamic Modelling**

Installation of GEMS 3

1) <http://gems.web.psi.ch/>

3) Click on «download»,
«click here to register...»,
give your details and

4)

2)

PAUL SCHERRER INSTITUT
PSI
GEM Software (GEMS) Home
Paul Scherrer Institut | 5232 Villigen PSI, Schweiz | Tel. +41 (0)56 310 21 11 | Fax +41 (0) 56 310 21 12

GEM Software Home
GEM-Selektor v.3
GEMS3K Code
GEMSFIT Code (coming soon)
Terms & Licen...
GEMS Default TDB
TSolMod Library
Publications

GEMS:
Gibbs Energy Minimization Software for Geochemical Modeling

[See presentation \(pdf\). Why GEM-Selektor and GEM Software?](#) [See a...](#)

Currently, GEM Software includes three code packages and a default thermodynamic data base:

- [GEM-Selektor v.3 \(GEMS3\)](#): the interactive code package for geochemical modeling
- [GEMS3K](#): the standalone code for solving for geochemical equilibria (with TSolMod)
- [GEMSFIT](#): the generic parameter-fitting code coupled with the GEMS3K code
- [GEMS TDB](#): the default chemical thermodynamic database of GEM-Selektor packa...



GEM-Selektor v.3 HTTP Download Page

Your GEMS3.7.x GEM-Selektor package download registration form has been submitted successfully.

For more information about installing GEM-Selektor on various operation systems, please download the [Installation instructions \(pdf\)](#) or check the [Technical Info page](#).

Please, use an appropriate direct link below to download the actual revision of the package (to save the installer archive file to disk):

[GEMS3.7.0 for Windows-64](#)

[GEMS3.7.0 for MacOS](#)

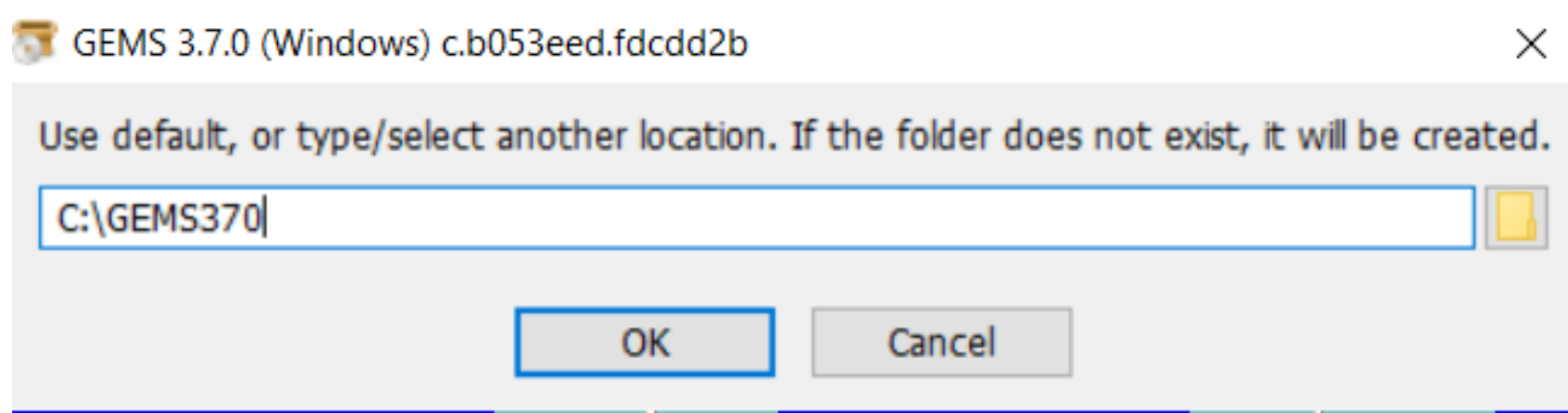
[GEMS3.7.0 for Ubuntu Linux-64](#)

Attention! There were relevant improvements and functionality additions in GEM-Selektor version 3.7 compared to previous versions. It is recommended to upgrade as soon as possible.

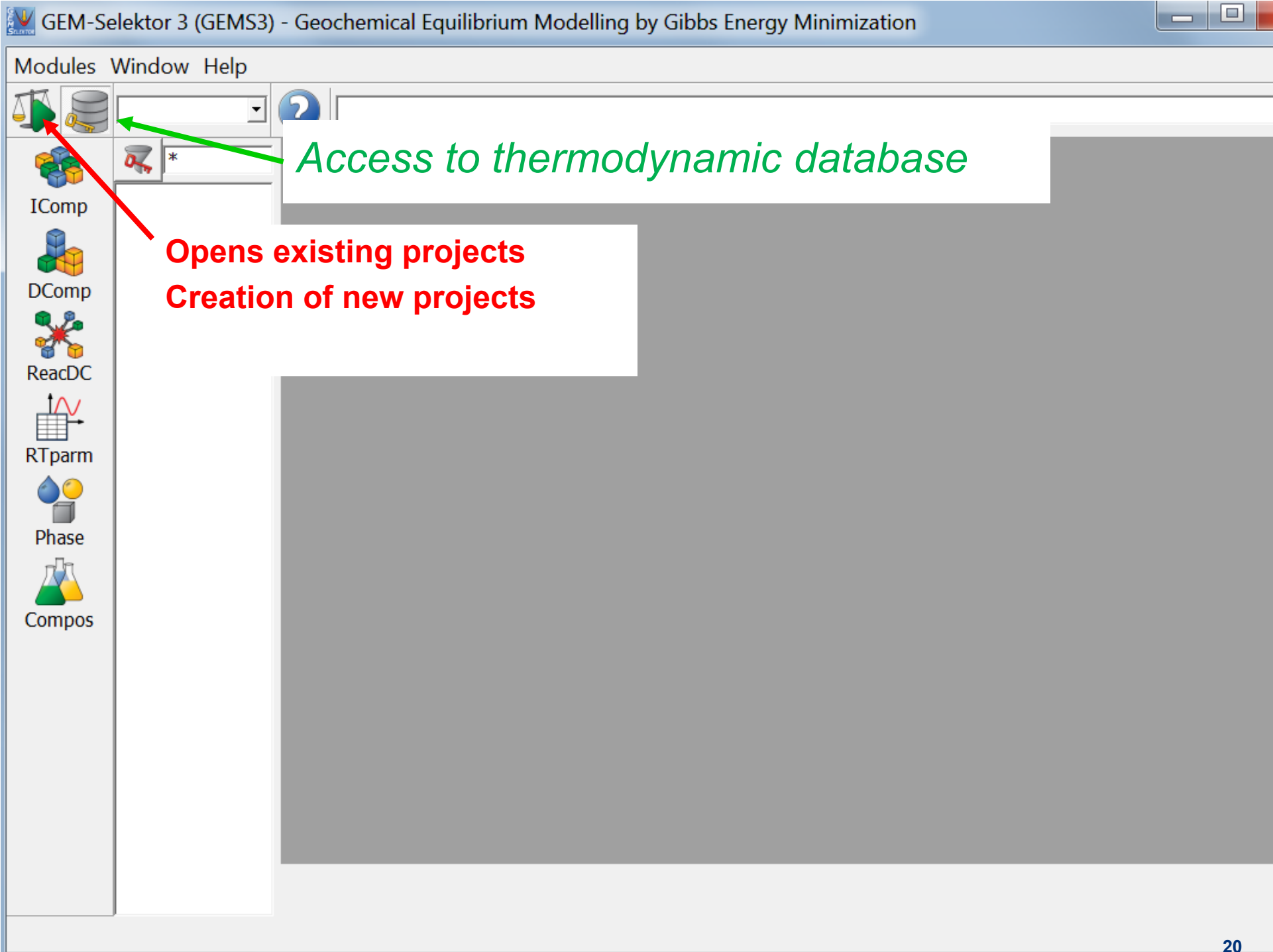
Attention! There is a lot of improved functionality in GEM-Selektor v.3.3 or higher compared with v.3.2. For backward compatibility, all modelling projects created in GEM-Selektor v.3.2.x or earlier, will open and work normally in GEM-Selektor v.3.3.x; accordingly, GEMS3K I/O files exported from GEM-Selektor v.3.2.x are readable and will work in coupled codes and examples using GEMS3K v.3.3.x.

Immediate extension of old modeling projects in GEM-Selektor v.3.3.x with newly created Phase records, remaking existing Phase records, or via Project remake/extension wizard is possible. Before doing that, the user needs only once to open the project; switch to Database Mode; open the Phase window; and remake one-by-one all Phase records available in the project (saving each record back after remake).

Installation Windows



- Install the programme in C:\GEMS370
The creation of a new folder avoids, for those who had GEMS previously installed, problems with older versions of the thermodynamic databases (tdb).
- ! Do **NOT** install it in the programme folder !
Problems with administrator rights in windows





IComp



DComp



ReactDC



RTparm



Phase



Compos

Modelling Projects

Selektor modelling projects: Select one to open, or click 'New Project...' to create a new project.

- AluSiOMSA MUSICALuminaSilica
- AragCalc Aragonite-Calcite
- BermanMSS TestsMultiSiteSolidSolutions
- Ca-Sr-CO3 Solid_solutions
- CalDolCol2GEM2MT-test
- CarbSea CarbonatesAndSeawater
- Flowline test project gem2mt
- GEO THERM Soultz_1
- Kaolinite Test-JNC
- Kinetics Mineral-Aq-Reactions
- Kyanite MylstProject
- SIT_port1 BU181104
- Solvus test project solvus
- TestPNTDB Test-PSI-Nagra-TDB-07-12
- TestPR test project PRSV fluid
- TestSIP98 Test-SUPCRT98-linked

Retain setup of aqueous (and gas/ Activate Project Remake wizard
 Change file configuration of the selected project Re-calculate and save all equilibria (including gas)
 Create a new project using the selected project AIA mode (single Smart IA mode

Make a new project:

by copying records from default database by linking files from the default database

Installation of cement database

1. Close GEMS

2. Get cemdata18 at <https://www.empa.ch/web/s308/thermodynamic-data>

istbesucht Erste Schritte

Empa > 700 - Functional Materials > 308 - Concrete / Construction Chemistry > Research > Cement Hydration > CEMDATA > Thermodynamic data

Thermodynamic data

Cemdata

Thermodynamic data for hydrated solids in Portland cement system (CaO-Al₂O₃-SiO₂-CaSO₄-CaCO₃-Fe₂O₃-MgO-H₂O)

- New version CEMDATA 18.1 available -

The first version of the cement specific cement database Cemdata was published in 2007-2009. Since then it was updated several times; the last update has been published in 2019 (Lothenbach et al. 2019)

Cemdata18: A chemical thermodynamic database for hydrated Portland cements and alkali-activated materials

Cemdata18 database has been developed specifically for hydrated Portland, calcium aluminate, calcium sulfoaluminate and blended cements, as well as for alkali-activated materials. It is available in GEMS and PHREEQC computer program formats, and includes thermodynamic properties determined from various experimental data published in recent years. Cemdata18 contains thermodynamic data for common cement hydrates such as C-S-H, AFm and Aft phases, hydrogarnet, hydrotalcite, zeolites, and M-S-H that are valid over temperatures ranging from 0 to at least 100°C. Solid solution models for AFm, Aft, C-S-H, and M-S-H are also included in the

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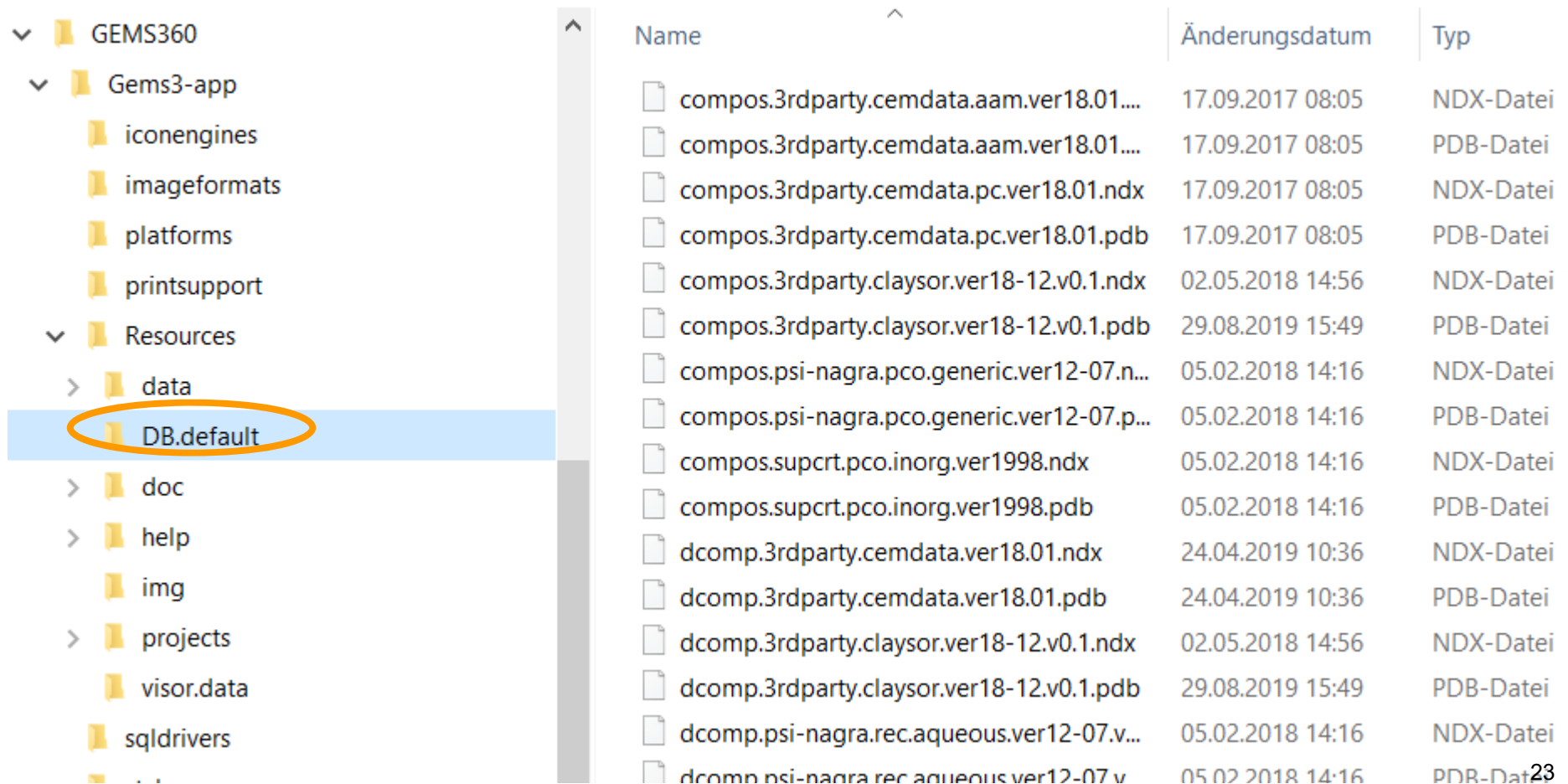
Downloads and Links

- GEMS PSI
- **Cemdata18.1 for GEMS**
- Cemdata18.1 for PHREEQC
- CEMDATA 14.01
- CEMDATA 14.01 overview

3. unzip cemdata18 database

Installation of cement database

1. **Close GEMS**
2. Get cemdata18 and unzip folder
3. Copy all files (*without folder!*) from the folder Cemdata18 into the directory C:\GEMS345/GEMS3-app/Resources/DB.default
4. Open GEMS and cemdatabase will be available for «new projects»



Name	Änderungsdatum	Typ
compos.3rdparty.cemdata.aam.ver18.01....	17.09.2017 08:05	NDX-Datei
compos.3rdparty.cemdata.aam.ver18.01....	17.09.2017 08:05	PDB-Datei
compos.3rdparty.cemdata.pc.ver18.01.ndx	17.09.2017 08:05	NDX-Datei
compos.3rdparty.cemdata.pc.ver18.01.pdb	17.09.2017 08:05	PDB-Datei
compos.3rdparty.claysor.ver18-12.v0.1.ndx	02.05.2018 14:56	NDX-Datei
compos.3rdparty.claysor.ver18-12.v0.1.pdb	29.08.2019 15:49	PDB-Datei
compos.psi-nagra.pco.generic.ver12-07.n...	05.02.2018 14:16	NDX-Datei
compos.psi-nagra.pco.generic.ver12-07.p...	05.02.2018 14:16	PDB-Datei
compos.supcrt.pco.inorg.ver1998.ndx	05.02.2018 14:16	NDX-Datei
compos.supcrt.pco.inorg.ver1998.pdb	05.02.2018 14:16	PDB-Datei
dcomp.3rdparty.cemdata.ver18.01.ndx	24.04.2019 10:36	NDX-Datei
dcomp.3rdparty.cemdata.ver18.01.pdb	24.04.2019 10:36	PDB-Datei
dcomp.3rdparty.claysor.ver18-12.v0.1.ndx	02.05.2018 14:56	NDX-Datei
dcomp.3rdparty.claysor.ver18-12.v0.1.pdb	29.08.2019 15:49	PDB-Datei
dcomp.psi-nagra.rec.aqueous.ver12-07.v...	05.02.2018 14:16	NDX-Datei
dcomp.psi-nagra.rec.aqueous.ver12-07.v...	05.02.2018 14:16	PDB-Datei

GEMS structure

calculations



Thermodynamic database
for experienced users

GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [EqStat: S

Modules Record Data Calculate View Print Window Help

SingleSystem

portlandit:*,*,*,*,*,*,*,*

	3	4	5	6	7	8
1	CO2	0	0	1	25	0

Input: System Definition Results: Equilibrium State

Phase/species	L	T
a aq_gen	22	a
g gas_gen	5	g
s Graphite	1	s
s Aragonite	1	s
s Calcite	1	s
s lime	1	s
s Portlandite	1	s
s Anhydrite	1	s
s Gypsum	1	s
s hemihydrate	1	s
s Sulphur	1	s

Single calculations

GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [DComp :: Thermochemical/EOS data fo...

Modules Record Record List Database Files Window Help

DComp

,,*,*,*

	1	2	3	4
1	g	S-2	H2S	en_
2	s	CO	Gr	dn_
3	s	CaCO	Arg	dn_
4	s	CaCO	Cal	dn_
5	s	CaO	Lim	ce_
6	s	CaOH	Portlandite	dn_
7	s	CaSO	Anh	dn_
8	s	CaSO	Gp	dn_
9	a	w_	H+	an_
10	a	w_	H2O@	an_

Page 1 Page 2 29/08/2012, 12:38

Portlandite
Ca (OH) 2

M0	74.0927	Zz	0	ab	--
----	---------	----	---	----	----

V0d	3.306	0
G0d	-897013	---
H0d	-984675	---

Clone record

Next/previous single calculation

Check for conflicts

tooltips

Create new record

save

delete

recipe

calculate

results

Single calculations

Active single calculation

Phase/species	L	T	Amount (mol)	logSI/Activity
a aq_gen	22	a	55.631449	-1.754e-11
g gas_gen	5	g	0.0018093475	-3.616e-11
s Graphite	1	s	0	-82.23
s Aragonite	1	s	0	-0.1438
s Calcite	1	s	0.022715807	9.954e-10
s lime	1	s	0	-9.776
s Portlandite	1	s	0.092888665	4.112e-08
s Anhydrite	1	s	0	-0.2228
s Gypsum	1	s	0.033682935	2.957e-08
s hemihydrate	1	s	0	-0.989
s Sulphur	1	s	0	-116.3

Continue with tutorial C3A

Hydration of C_3A ($Ca_3Al_2O_6$)^a

1) Simulation of reaction $C_3A + CaO + CaSO_4$ Guided tutorial

2) Simulation of reaction $C_3A + CaO + CaCO_3$

3) Simulation of reaction $C_3A + CaCO_3$

4) Simulation of reaction $C_3A + C + CaSO_4 + CaCO_3$

} Individual
work

See Seligmann & Greening ICCI 1969 and various papers by Kuzel et al. (Kuzel & Pöllmann CCR 1991, Kuzel et. al CCR 1996) for experimental verification

^a cement notation

C => CaO

A => Al_2O_3

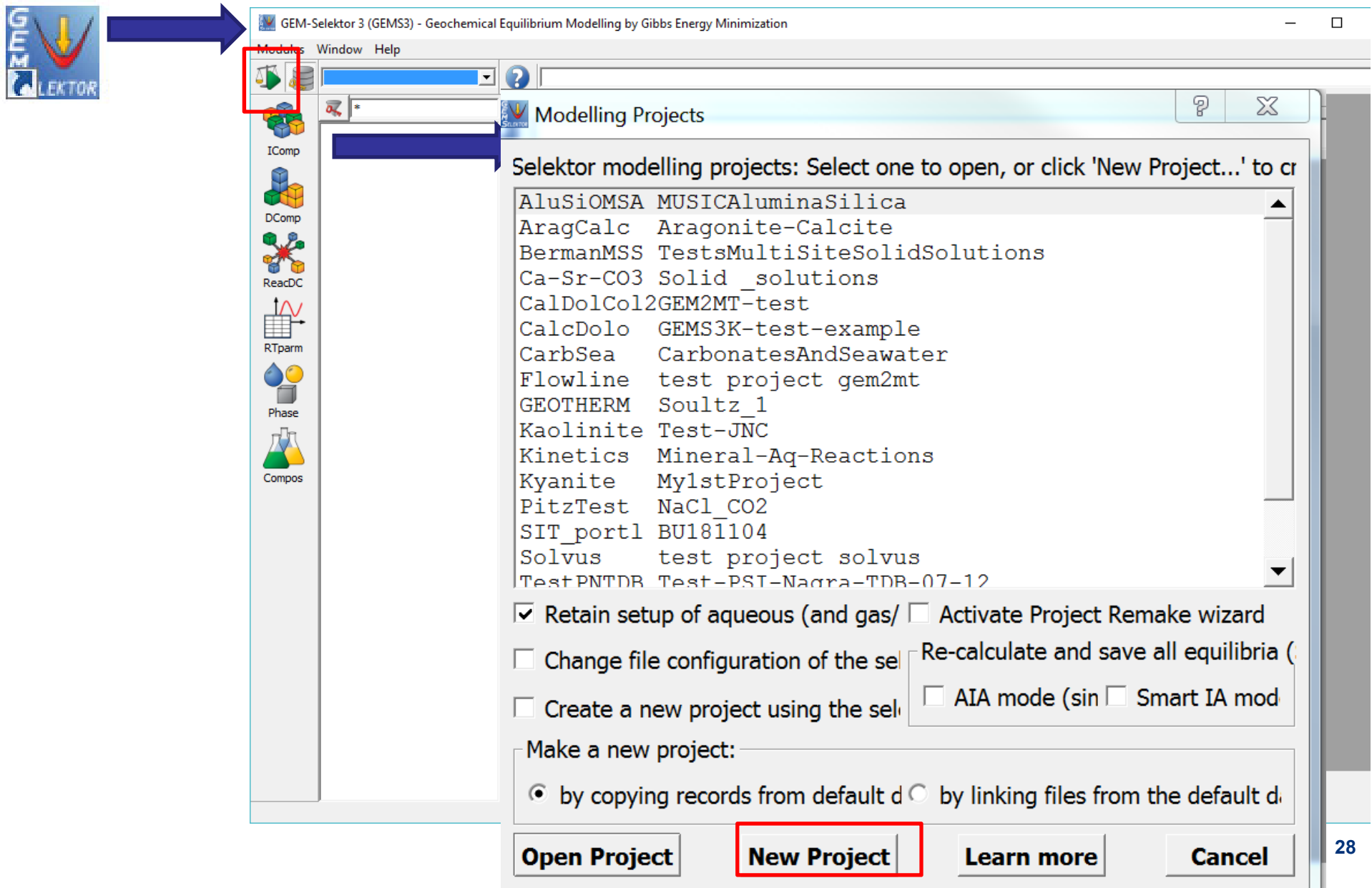
S => SiO_2

H => H_2O

s => SO_3

c => CO_2

Hydration of $C_3A + CaO + CaSO_4$ – project setup



The screenshot shows the GEM-Selektor 3 (GEMS3) software interface. A blue arrow points from the Lektor icon to the software window. A red box highlights the 'New Project' button at the bottom of the dialog.

Modelling Projects

Selektor modelling projects: Select one to open, or click 'New Project...' to cr

AluSiOMSA	MUSICAluminaSilica
AragCalc	Aragonite-Calcite
BermanMSS	TestsMultiSiteSolidSolutions
Ca-Sr-CO3	Solid_solutions
CalDolCol2	GEM2MT-test
CalcDolo	GEMS3K-test-example
CarbSea	CarbonatesAndSeawater
Flowline	test project gem2mt
GEO THERM	Soultz_1
Kaolinite	Test-JNC
Kinetics	Mineral-Aq-Reactions
Kyanite	MylstProject
PitzTest	NaCl_CO2
SIT_port1	BU181104
Solvus	test project solvus
TestPNTDR	Test-PST-Nagra-TDR-07-12

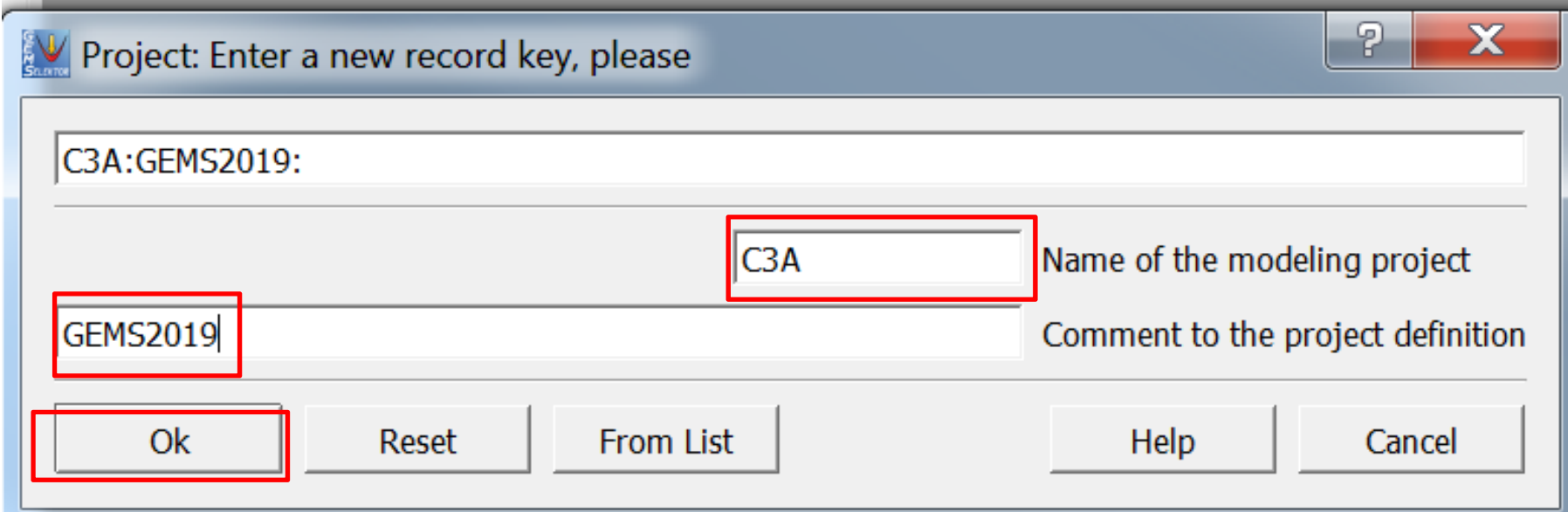
Retain setup of aqueous (and gas/ Activate Project Remake wizard
 Change file configuration of the sel Re-calculate and save all equilibria (
 Create a new project using the sel AIA mode (sin Smart IA mod

Make a new project:

by copying records from default d by linking files from the default d

Open Project **New Project** **Learn more** **Cancel**

Hydration of $C_3A + CaO + CaSO_4$ – project setup



Project: Enter a new record key, please

C3A:GEMS2019:

C3A Name of the modeling project

GEMS2019 Comment to the project definition

Ok Reset From List Help Cancel

Hydration of $C_3A + CaO + CaSO_4$ – project setup

Select CEMDATA18 (3rd party data base)

Basis configuration of a new Modelling Project C3A

Step 1 - Selection of databases, data subsets, phase type filters

Phase/DC Filters

- Aqueous electrolyte
- Gas mixture
- Non-ideal fluids
- Plasma
- Crystalline solids
- Dispersed solids
- Liquids, glasses
- Silicate melts
- Sorption, Ion exchange
- Polyelectrolytes
- Liquid hydrocarbons
- Skip solid solutions

Built-in Database	Version
<input checked="" type="checkbox"/> 3rdparty	
<input checked="" type="checkbox"/> cemdata	18.01
<input checked="" type="checkbox"/> .	
<input type="checkbox"/> aam	18.01
<input checked="" type="checkbox"/> pc	18.01
<input checked="" type="checkbox"/> .	
<input checked="" type="checkbox"/> csh	
<input type="checkbox"/> csh2o	18.01
<input type="checkbox"/> csh3t	18.01
<input type="checkbox"/> cshkn	18.01
<input checked="" type="checkbox"/> cshq	18.01
<input checked="" type="checkbox"/> ht	18.01
<input checked="" type="checkbox"/> ss-fe3	18.01
<input checked="" type="checkbox"/> ss	18.01
<input type="checkbox"/> claysor	18-12.v0.1
<input checked="" type="checkbox"/> psi-nagra	
<input type="checkbox"/> supcrt	
<input type="checkbox"/> support	

Cement database

General psi-nagra database

Learn more < Back **Next >** Cancel

Recommended selection for PC and blended cements

Hydration of $C_3A + CaO + CaSO_4$ – project setup

Select elements necessary to model C_3A hydration

Step 2: Select Independent Components (not available if shown in light gray color)

	I	II	III	IV	V	VI	VII	VIII	
1	H							He	
2	Li	Be	B	C	N	O	F	Ne	
3	Na	Mg	Al	Si	P	S	Cl	Ar	
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Cu
4a									Ni
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh
5a									Pd
6	Cs	Ba	REE	Hf	Ta	W	Re	Os	Ir
6a									Pt
7	Fr	Ra	ACT						

Additional

- Nit
- ...
- ...
- ...
- ...
- ...
- ...
- ...
- ...
- ...
- ...
- ...
- Vol

Isotopes

Learn more Set Filters < Back **Next >** Cancel

„reactive N“
(don't use here)

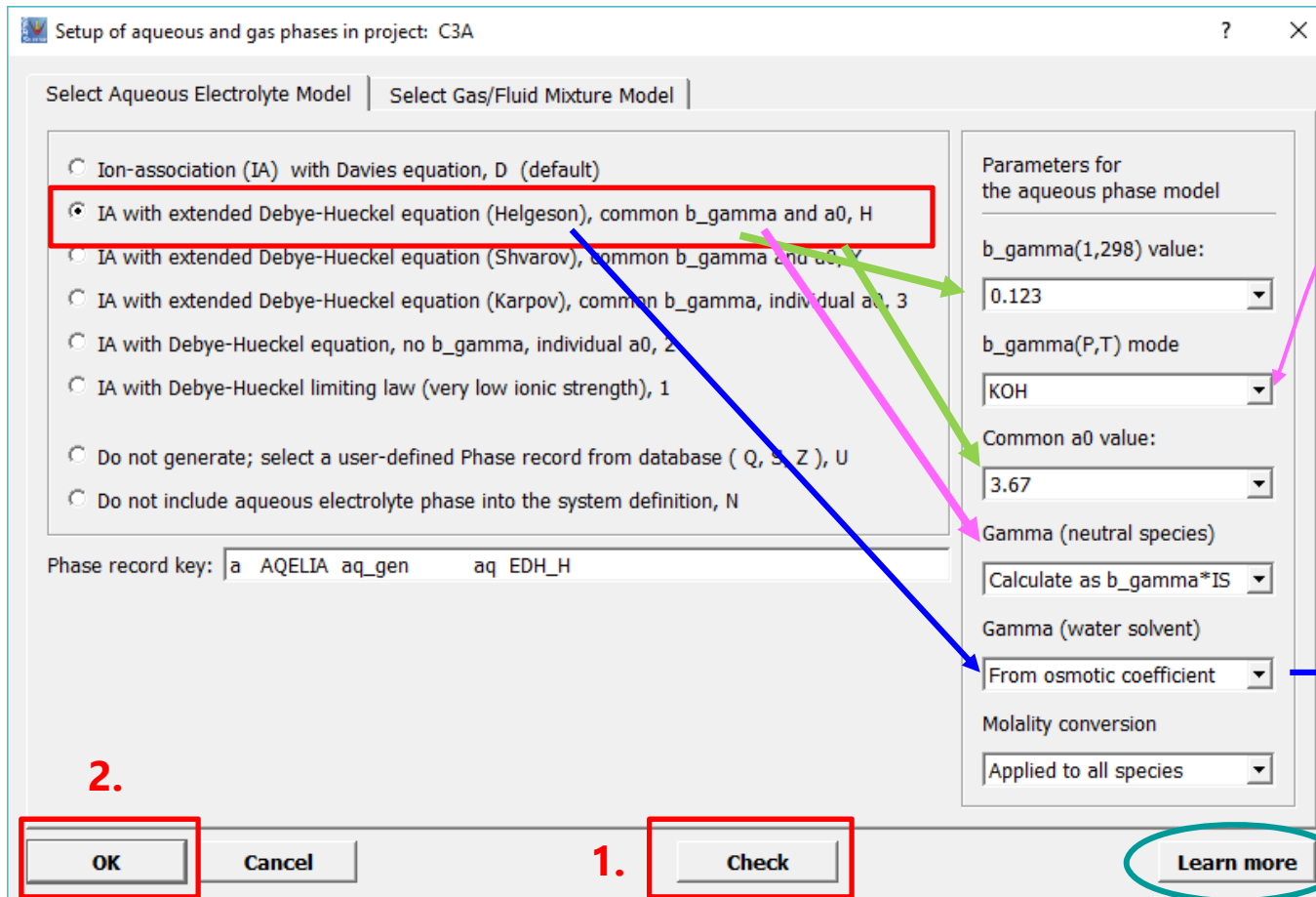
Air: O_2 , N_2 , etc.
(no reducing conditions,
 N_2 not reactive)

we can also use just oxygen (O_2)

needed for parts 2+3 of the tutorial

Hydration of $C_3A + CaO + CaSO_4$ – project setup

Select model for calculation of the aqueous phase



1) KOH good for cements

2) f(pressure, temp) -> electrolyte

a0=3.67 for KOH
b0= 0.123

Calculates activity of water

More details

2.

1.

Activity coefficients

Solubility product e. g. of gypsum

$$K_{S0} = \{Ca^{2+}\} \cdot \{SO_4^{2-}\} \cdot \{H_2O\}^2 / \{CaSO_4 \cdot 2H_2O\}$$

$$K_{S0} = \{Ca^{2+}\} \cdot \{SO_4^{2-}\} = 10^{-4.58}$$

{ } : activity; [] : concentration

$$\{Ca^{2+}\} = [Ca^{2+}] \cdot \gamma_{Ca^{2+}} \longleftarrow \text{Activity coefficient}$$

Correction of concentrations by activity coefficients, as the ions „feel“ their neighbours (other ions, solvent).

Activity coefficients depend mainly on:

- ionic strength
- other ionic species
- temperature

Activity vs. ionic strength

– selecting the right aqueous electrolyte model

Debye-Hückel $\log \gamma_{Ca^{2+}} = \frac{-AZ^2\sqrt{I}}{1 + Ba\sqrt{I}}$ **ionic strength $I < 0.1 \text{ M}$**

Extended Debye-Hückel $\log \gamma_{Ca^{2+}} = \frac{-AZ^2\sqrt{I}}{1 + Ba\sqrt{I}} + bI$

common a, common b (Helgeson)

$I < 1-2 \text{ M}$

individual a, common b (Truesdell-Jones)

$I < 1 \text{ M}$

individual a, no b

$I < 0.3 \text{ M}$

Davies $\log \gamma_{Ca^{2+}} = -AZ^2 \left(\frac{\sqrt{I}}{1 + \sqrt{I}} - 0.3I \right)$

$0.1 < I < 0.5 \text{ M}$

SIT $\log \gamma_{Ca^{2+}} = \frac{-AZ^2\sqrt{I}}{1 + 1.5\sqrt{I}} + \sum \varepsilon m_k$

$I < 3 \text{ M}$

The calculation of activity coefficients is available as built-in function in the GEMS code.

For a detailed overview of different activity coefficients see:

C:\GEMS36\Gems3-app\Resources\doc\pdf\Activity-Coeffs.pdf and references therein

Hydration of $C_3A + CaO + CaSO_4$ – project setup

SysEq: Please, enter a new record key:

C3A:G:C3A-Cs:0:0:1:25:0:

<input type="text" value="C3A"/>	Name of the modeling project
<input type="text" value="G"/>	Thermodynamic potential to minimize {G GV}
<input type="text" value="C3A-Cs"/>	Name of the chemical system definition (CSD)
<input type="text" value="0"/>	CSD (recipe) variant number <integer>
<input type="text" value="0"/>	Volume of the system, dm3 (0 if no volume constraint)
<input type="text" value="1"/>	Pressure, bar, or 0 for Psat(H2O)g
<input type="text" value="25"/>	Temperature, C (>= 0)
<input type="text" value="0"/>	Variant number for additional constraints

Project name

Method (Gibbs energy minimization)

System definition

Integer (default 0)

System volume unconstrained

Pressure (bar)

Temperature (°C)

Avoid special signs such as \$ & % ä ö ü æ å ø 好 ...

Hydration of $C_3A + CaO + CaSO_4$ – system creation (recipe)

We need a recipe

Input Recipe of Single Thermodynamic System: C3A-tut:G:C3A-Cs:0:0:1:25:0

tname **C3A + CaSO4** **comments**

Property	Selection	Recipe Input			
		Property	Name	Quantity	Units
Compos (xa)	Al(OH)3 C3A				
DComp (xd)	Al2O3 C4A				
IComp (bi_)	Aqua CA				
Phase (xp_)	C12A7 CA2				
Kin.lower (d)					
Kin.upper (c)					
G0 shift (gE)					
Other Input					

Input quantities of Compos(itions) contributing to B_ vector

Learn more Print OK Cancel

1 Reaction of C_3A with calcium sulfate

5 g C_3A + 2.52 g $CaSO_4$ + 2.5 g CaO + 50 g H_2O

+ 0.1 g O_2 (oxidizing conditions, CO_2 -free = no carbonation)

molar ratio $SO_3/Al_2O_3 = 1$, molar ratio $CO_2/Al_2O_3 = 0$

Reaction products?

Expectation: monosulfate



No ettringite



> Recipe >



> Equilibrium speciation

Hydration of $C_3A + CaO + CaSO_4$ – system creation (recipe)

Input Recipe of Single Thermodynamic System: C3A:G:C3A-Cs:0:0:1:25:0:

tname **C3A + CaSO4**

Property	Selection	Property	Selection	Property	Selection	Property	Selection
Compos (xa)							
DComp (xd)	Al(OH)3	C3A	CH4	CaO	H2	SO3	
IComp (bi)	Al2O3	C4A3s	CO2	CaSO4	H2S		
Phase (xp)	Aqua	CA	Ca(OH)2	CaSO4_05H2O	H2SO4		
Kin.lower (d)	C12A7	CA2	CaCO3	Gypsum	O2		

Input quantities of Compos(itions) contributing to B_ vector

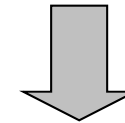
Property	Name	Quantity	Units
1 xa_	Aqua	50	g
2 xa_	C3A	5	g
3 xa_	CaO	2.5	g
4 xa_	CaSO4	2.52	g
5 xa_	O2	0.1	g

A bit of O₂ to guarantee oxidizing conditions

Learn more Print **OK** Cancel

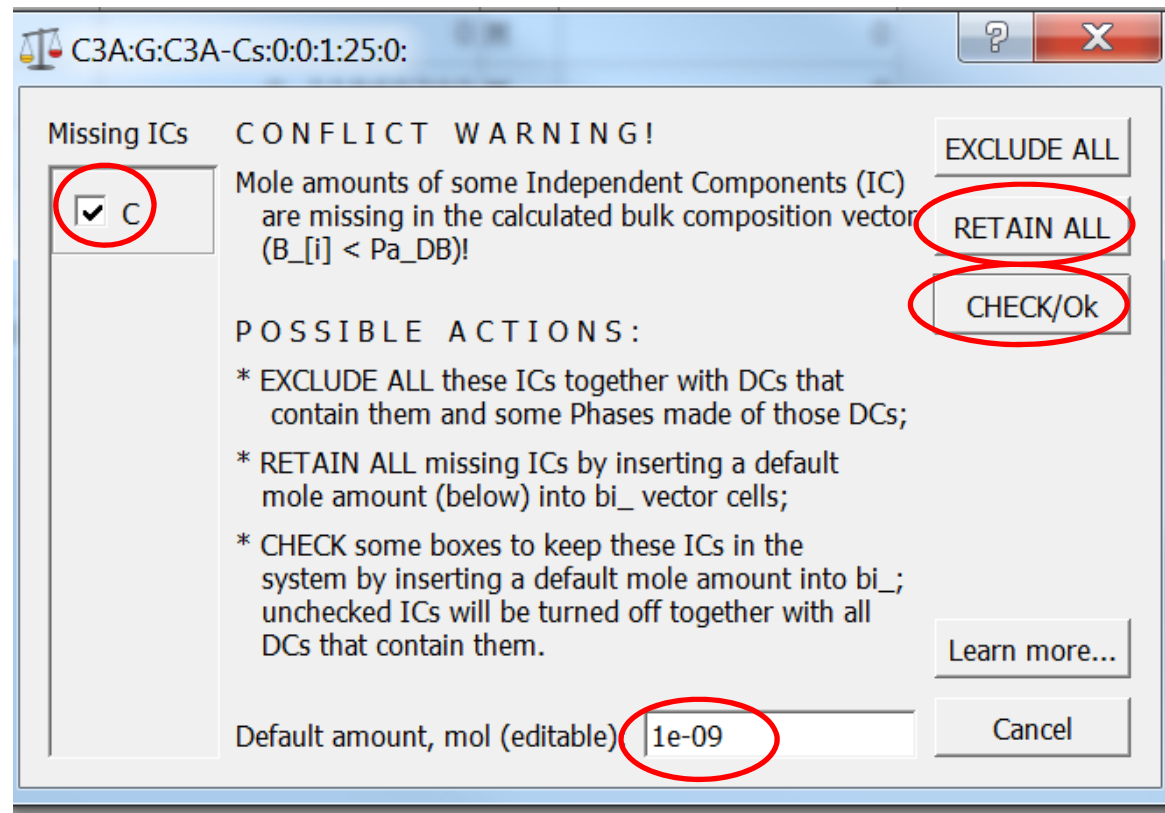
Hydration of $C_3A + CaO + CaSO_4$ – system creation (recipe)

Check system definition



we keep carbonate in this example

=> adds a very small amount of C (10^{-9} M), has a negligible effect



GEMS interface

2 equivalent input options

Recipe wizard (previous page)

Detailed input recipe

Brings you always back to this screen

The screenshot shows the GEM-Selektor 3 (GEMS3) software interface. The main window displays the 'Input: System Definition' tab, which contains a table of phases and species. The table has columns for 'Phase/species', 'L', 'T', 'On/UC', 'Add to BC', 'UG', 'G0', 'corr.', and 'UK'. The 'Phase/species' column lists various chemical species, including 'aq_gen', 'gas_gen', 'ettringite', 'SO4_OH_AFm', 'OH_SO4_AFm', 'SO4_CO3_AFt', 'CO3_SO4_AFt', 'Al(OH)3am', 'Al(OH)3mic', 'Gibbsite', 'Graphite', 'Mayenite', 'Aluminate', 'CA', 'CA2', 'C2AH75', 'C3AH6', 'C4AH11', 'C4AH13', and 'C4AH19'. The 'L' column indicates the number of moles of each species. The 'T' column indicates the phase type (a for aqueous, g for gas, s for solid). The 'On/UC' column indicates the oxidation state and charge. The 'Add to BC' column indicates the boundary conditions. The 'UG' column indicates the Gibbs energy of formation. The 'G0' column indicates the Gibbs energy of formation. The 'corr.' column indicates the correction factor. The 'UK' column indicates the unit factor.

Annotations on the screenshot include:

- A red circle around the 'SysEq' icon in the left sidebar, with an arrow pointing to it from the text 'Brings you always back to this screen'.
- Two red circles around the 'Recipe wizard' and 'Detailed input recipe' icons in the top toolbar, with arrows pointing to them from the text '2 equivalent input options'.
- A red box around the list of phases/species, with an arrow pointing to it from the text 'all main cement hydrates relevant to the system CaO-Al₂O₃-CaSO₄-CaCO₃-H₂O included'.
- A red box around the last four species (C4AH11, C4AH13, C4AH19), with an arrow pointing to it from the text 'AFm with different H₂O content'.

System: T = 298.15 K; P = 1.00 bar; V = 0 L; Aqueous: built-in Davies; pH = 0.000; pe = 0.000; IS =

Hydration of $C_3A + CaO + CaSO_4$ – system creation (input)

Input: System Definition | Results: Equilibrium State

Phase/species	L	T	On/UC	Add to BC	UG	G0 corr.	UK
ettringite	2	s	+	g	0	J	0
ettringite	2	s	+	M	0	J	0
ettringite30	2	s	+	M	0	J	0
SO4_OH_AfM	2	s	+	g	0	J	0
OH_SO4_AfM	2	s	+	g	0	J	0
SO4_CO3_AfT	2	s	+	g	0	J	0
tricarboalu03	2	s	+	g	0	J	0
ettringite03_ss	2	s	+	g	0	J	0
CO3_SO4_AfT	2	s	+	g	0	J	0
tricarboalu03	2	s	+	g	0	J	0
ettringite03_ss	2	s	+	g	0	J	0
Al(OH)3am	1	s	+	g	0	J	0
Al(OH)3mic	1	s	+	g	0	J	0
Gibbsite	1	s	+	g	0	J	0
Graphite	1	s	+	g	0	J	0
Mayenite	1	s	+	g	0	J	0
Aluminate	1	s	+	g	0	J	0
CA	1	s	+	g	0	J	0
CA2	1	s	+	g	0	J	0
C2AH75	1	s	+	g	0	J	0
C3AH6	1	s	+	g	0	J	0
C4AH11	1	s	+	g	0	J	0
C4AH13	1	s	+	g	0	J	0
C4AH19	1	s	+	g	0	J	0
CAH10	1	s	+	g	0	J	0
C4AsH105	1	s	+	g	0	J	0
C4AsH12	1	s	+	g	0	J	0
C4AsH14	1	s	+	g	0	J	0
C4AsH16	1	s	+	g	0	J	0
C4AsH9	1	s	+	g	0	J	0
C4AcH9	1	s	+	g	0	J	0
C4Ac0.5H105	1	s	+	g	0	J	0
C4Ac0.5H12	1	s	+	g	0	J	0
C4Ac0.5H9	1	s	+	g	0	J	0
C4AcH11	1	s	+	g	0	J	0

System: T = 298.15 K; P = 1.00 bar; V = 0 L; Aqueous: built-in Davies; pH = 0.000; pe = 0.000; IS =

On/off switch for phases

SO₄-AFt solid solution 30-32 H₂O

2 AFt solid solutions containing sulfate+carbonate

SO₄-AFt with less water (metaettringite; for low water content)

Monosulfate with different water content (relevant for low w/c)

I = ideal solid solution

Number of components
1: pure phase
≥ 2: solid solutions

J = junior end-member
M = major end-member of solid solution

Hydration of $C_3A + CaO + CaSO_4$ – system creation (recipe)

Experimental conditions: React 5 g C_3A , 2.52 g $CaSO_4$ and 2.5 g CaO with 50 g water (add 1 g O_2 to simulate gas phase)

Compos DComp Phase IComp Surfaces Config 30/01/2018, 15:19

C3A + CaSO4

Description of experiment

Masses	0	1	1	1	0	0
Volums	1	1	0	0	0	0

AC	CCvp		xa
0	+	Al(OH)3	MIN Aluminum-hydroxide... g 0
1	+	Al2O3	MIN Aluminum-oxide_1M_ g 0
2	+	Aqua	AQ 1_mole_H2O_ g 50
3	+	C12A7	MIN Mayenite_1M_ g 0
4	+	C3A	MIN Tricalcium_alumina... g 5
5	+	C4A3s	MIN Yeelimite_1M_ g 0
6	+	CA	MIN Calcium_aluminate_... g 0
7	+	CA2	MIN Calcium_dialuminat... g 0
8	+	CH4	GA Methane_1M_ g 0
9	+	CO2	GA Carbon-dioxide_1M_ g 0
10	+	Ca(OH)2	MIN Calcium-hydroxide_... g 0
11	+	CaCO3	MIN Calcium-carbonate_... g 0
12	+	CaO	MIN Calcium-oxide_1M_ g 2.5
13	+	CaSO4	MIN Calcium-sulfate_1M_ g 2.52
14	+	CaSO4_05H2O	MIN hemihydrate_1M_ g 0
15	+	Gypsum	MIN Ca-sulfate-2H2O-1M_ g 0
16	+	H2	GA Hydrogen_1M_ g 0
17	+	H2S	GA Hydrogen-sulfide_1... g 0

Detailed input recipe

Input generated before by the input wizard => 2 equivalent options to input data

Hydration of $C_3A + CaO + CaSO_4$ – system creation (recipe)

Experimental conditions: React 5 g C_3A , 2.52 g $CaSO_4$ and 2.5 g CaO with 50 g water (add 1 g O_2 to simulate gas phase)

Calculated during check

The screenshot shows a software interface with a toolbar at the top containing icons for file operations, navigation, and simulation. Below the toolbar are several tabs: 'Compos', 'DComp', 'Phase', 'IComp' (highlighted with a red box), 'Surfaces', and 'Config'. A date and time stamp '24/04/2019, 16:' is visible on the right. Below the tabs is a text area with 'Summary of input in mol' in red. At the bottom is a table with columns for IC, ICvp, B, and bi.

	IC	ICvp	B	bi
0	+	Al e Aluminum_	0.037010516 M	0
1	+	C e Carbon_	1e-009 M	1e-009
2	+	Ca e Calcium_	0.11860702 M	0
3	+	H h Hydrogen_	5.5508373 M	0
4	+	O o Oxygen_	3.0113217 M	
5	+	S e Sulfur_	0.018510003 M	
6	+	Zz z Electric_cha...	0 M	0

$Al/SO_3 = 2$
 $A/S = Al_2O_3/SO_3 = 1$

Hydration of $C_3A + CaO + CaSO_4$ – calculation of equilibrium

Experimental conditions: React 5 g C_3A , 2.52 g $CaSO_4$ and 2.5 g CaO with 50 g water (add 1 g O_2 to simulate gas phase)

Start calculation

The screenshot shows a software interface with a toolbar at the top. A red circle highlights a downward-pointing arrow icon in the toolbar, with an arrow pointing to a 'Running...' dialog box. The dialog box contains the text: 'GEM IPM calculation (run time: 0.19 s)', '0%', and 'System: C3A:G:C3A-Cs:0:0:1:25:0:'. Below this, another dialog box titled 'E06IPM: IPM Main Descent:' is open, displaying a yellow warning triangle and the message: 'IPM convergence criterion tolerance (Pa_DK) could not be reached (more than Pa_IIM iterations done);'. The 'OK' button in this dialog is circled in red. A red arrow points from the 'OK' button to a 'Project' icon (two interlocking gears) in a vertical sidebar on the left, which is also circled in red. The sidebar contains several icons labeled: Modul, SysEq, Process, GtDemo, GEM2MT, UnSpace, and Project. The background shows a table with columns for 'pH', 'pe', and 'IS', with values 12.4786, 8.29314, and 0.0528814 respectively. Other text in the background includes 'calcium_al', 'limite_1M', 'cium_alumi', 'cium_dialu', 'ane_1M_44', and 'GA Carbon-dioxid'.

Convergence problem can occur

- 1) Can be solved in «projects» by setting smoothing parameter to 0.01
- 2) Remove solid solution with only 1 solid

Convergence problem - workaround

GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [Project :: Numerical and Configuration ...]

Modules Record Window Help

Project C3A:*

1 C3A Course

PLists **Controls** Settings Config 26/03/2020, 13:16

Pa_SPP Tolerances and controls: GEMSGUI v.3.7.0 and GEMS3K v.3.7.0

Pa_DK	1e-005	Pa_IIM	7000	Pa_LLG	30000	Pa_AG	1	Pa_DGC	0.01
Pa_DHB	1e-013	Pa_DFY	1e-005	1e-005	1e-005	1e-005	1e-005	1e-005	1e-006
Pa_DB	1e-017	Pa_DS	1e-020	Pa_XMI	1e-013	1e-013	1e-033	1e-020	1e-005
Pa_EPS	1e-010	0.001	Pa_GAN	1	1000	0.001	Pa_DG	1000	
Pa_DPV	130	1	0	Pa_DF	0.01	0.01	Pa_DNS	12.05	
Pa_PE	1	Pa_PC	2	Pa_PRD	2	-5	1	Pa_DKI	1e-010

2. Coverage 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

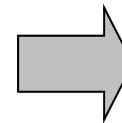
=> **0.01 works**

Do not touch the other values !!!

Hydration of $C_3A + CaO + CaSO_4$ – calculation of equilibrium

Experimental conditions: React 5 g C_3A , 2.52 g $CaSO_4$ and 2.5 g CaO with 50 g water (add 1 g O_2 to simulate gas phase)

Start calculation



Converged at DK=1e-... ? X

GEM IPM calculation (run time: 0.013 s)

100%

System:

C3A:G:C3A-Cs:0:0:1:25:0:

Iter	1: 8: 356
Gaseous	0.100025
Aqueous	44.9396
Liquid	0
Solid	15.0804
pH	12.4765
pe	8.29621
IS	0.0525917

Accept Dismiss

Hydration of $C_3A + CaO + CaSO_4$ – results

GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [EqStat: Single Thermodynamic System ...]

Modules Record Data Calculate View Print Window Help

SingleSystem

C3A:*.:.:.:.:.:.:.:

Input: System Definition Results: Equilibrium State

Phase/species	L	T	Amount (mol)	logSI/Activity	Concentrat
a	aq_gen	29	a	2.4932653	-8.615e-09
g	gas_gen	6	g	0.0031708121	-1.23e-09
s	ettringite	2	s	0.00091958053	1.187e-06
s	SO4_OH_AFm	2	s	0.008792363	-6.154e-08
s	OH_SO4_AFm	2	s	0.008792363	-6.154e-08
s	SO4_CO3_AfT	2	s	0	-0.03101
s	CO3_SO4_AfT	2	s	0	-0.03101
s	Al(OH)3am	1	s	0	-3.174
s	Al(OH)3mic	1	s	0	-2.264
s	Gibbsite	1	s	0	-1.811
s	Graphite	1	s	0	-84.68
s	Mayenite	1	s	0	-130.4
s	Aluminate	1	s	0	-36.48
s	CA	1	s	0	-11.04
s	CA2	1	s	0	-15.19
s	C2AH75	1	s	0	-2.469
s	C3AH6	1	s	0	-0.9693
s	C4AH11	1	s	0	-3.156
s	C4AH13	1	s	0	-1.422
s	C4AH19	1	s	0	-1.222
s	CAH10	1	s	0	-3.47
s	C4AsH105	1	s	0	-1.423
s	C4AsH12	1	s	0	-0.07732
s	C4AsH14	1	s	0	-0.05177

System: T = 298.15 K; P = 1.00 bar; V = 0.131 L; Aqueous: built-in EDH(H); pH = 12.477; pe = 8.296; IS = 0.053 m

Calculated single system

Calculations

Hydration of $C_3A + CaO + CaSO_4$ – results

GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [EqStat:: Single Thermodyn

Name of single system

2.5 mol aqueous phase
(water + dissolved ions)

0.0032 mol gaseous phase

Solid products:

0.0009 mol ettringite

0.0176 mol monosulfate

0.0418 mol portlandite

The screenshot shows the GEM-Selektor 3 software interface. The main window displays the results of a geochemical equilibrium calculation. The table below shows the phase/species, their amounts in moles, and their logS values. Red annotations highlight the 'C3A-Cs' phase in the input table and the 'SO4_OH_AFm' and 'OH_SO4_AFm' phases in the results table, which are identified as a solid solution between monosulfate (C_4AsH_{12}) and C_4AH_{13} .

Phase/species	L	T	Amount (mol)	logS
aq_gen	29	a	2.4932653	-8.6
gas_gen	6	g	0.0031708121	-1.2
ettringite	2	s	0.00091958053	1.18
SO4_OH_AFm	2	s	0.008792363	-6.1
OH_SO4_AFm	2	s	0.008792363	-6.1
SO4_CO3_AFT	2	s	0	-0.0
...
Al(OH)3am	1	s	0	-3.1
Al(OH)3hl12	1	s	0	-2.2
Gibbsite	1	s	0	-1.8
Graphite	1	s	0	-84.
Mayenite	1	s	0	-130
Aluminate	1	s	0	-36.
CA	1	s	0	-11.
CA2	1	s	0	-15.
C2AH75	1	s	0	-2.4
C3AH6	1	s	0	-0.9
C4AH11	1	s	0	-3.1
C4AH13	1	s	0	-1.4
C4AH19	1	s	0	-1.2
CAH10	1	s	0	-3.4
C4AsH105	1	s	0	-1.4
C4AsH12	1	s	0	-0.0
C4AsH14	1	s	0	-0.0

System: T = 298.15 K; P = 1.00 bar; V = 0.131 L; Aqueous: built-in EDH(H); pH =

Hydration of $C_3A + CaO + CaSO_4$ – results

Solid solutions

Phase/species	L	T	Amount (mol)	logSI/Activity	Concentration
a aq_gen	29	a	2.4932653	-8.615e-09	
g gas_gen	6	g	0.0031708121	-1.23e-09	
s ettringite	2	s	0.00091958053	1.187e-06	
ettringite		I	0.00073534039	0.79965	0.79964763
ettringite30		I	0.00018424014	0.200353	0.20035237
s SO4_OH_AFm	2	s	0.008792363	-6.154e-08	
C4AH13		J	0.00091690195	0.0378465	0.10428391
monosulphate12		M	0.007875461	0.836918	0.89571609
s OH_SO4_AFm	2	s	0.008792363	-6.154e-08	
C4AH13		M	0.00091690195	0.0378465	0.10428391
monosulphate12		J	0.007875461	0.836918	0.89571609
s SO4_CO3_Aft	2	s	0	-0.03101	
tricarboalu03		J	0	0.00244367	0
ettringite03_ss		M	0	0.929907	0
s CO3_SO4_Aft	2	s	0	-0.03101	
tricarboalu03		M	0	0.00244367	0
ettringite03_ss		J	0	0.929907	0
s Al(OH)3am	1	s	0	-3.174	
AlOHam		O	0	0.000669392	0

ideal solid solution:

80 mol-% ettringite-32H₂O
20 mol-% ettringite-30 H₂O

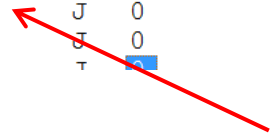
Non ideal solid solution:

10 mol-% C₄AH₁₃
90 mol-% C₄AsH₁₂

Incomplete solid solution (hardly any CO₃ endmember; normally not stable, can be deactivated:

Hydration of $C_3A + CaO + CaSO_4$ – system creation (recipe)

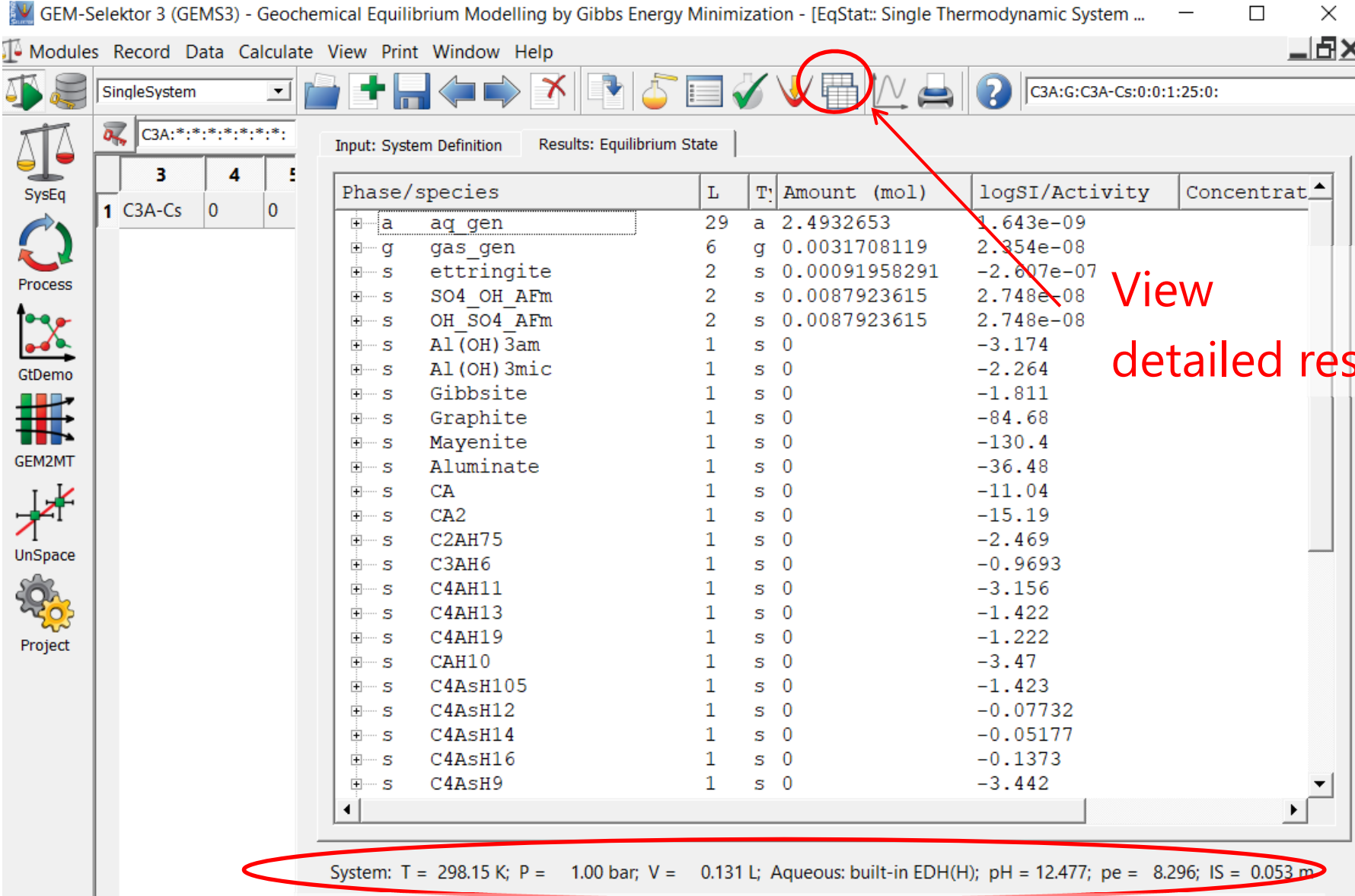
Input: System Definition		Results: Equilibrium State									
Phase/species	L	T	On/UC	Add to BC	UG	G0 corr.	UK	Lower_KC	Upper_KC	KC type	
ettringite	2	s +	g	0	J	0					
SO4_OH_AFm	2	s +	g	0	J	0					
OH_SO4_AFm	2	s +	g	0	J	0					
SO4_CO3_AFt	2	s -	g	0	J	0					
tricarboalu03		J -	M	0	J	0	M	0	1000000	B	
ettringite03_ss		M -	M	0	J	0	M	0	1000000	B	
CO3_SO4_AFt	2	s -	g	0	J	0					
tricarboalu03		M -	M	0	J	0	M	0	1000000	B	
ettringite03_ss		J -	M	0	J	0	M	0	1000000	B	
Al(OH)3am	1	s +	g	0	J	0					
Al(OH)3mic	1	s +	g	0	J	0					
Gibbsite	1	s +	g	0	J	0					
Graphite	1	s	g	0	J	0					



As we have very little carbonate in the system in the first calculation we may switch off the carbonate-sulfate AFt solid solutions

(In the input page)

Hydration of $C_3A + CaO + CaSO_4$ – results



GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [EqStat:: Single Thermodynamic System ...

Modules Record Data Calculate View Print Window Help

SingleSystem

C3A:*.:.:.:.:.:.:.:.:.:

Input: System Definition Results: Equilibrium State

Phase/species	L	T	Amount (mol)	logSI/Activity	Concentrat
a aq_gen	29	a	2.4932653	1.643e-09	
g gas_gen	6	g	0.0031708119	2.354e-08	
s ettringite	2	s	0.00091958291	-2.607e-07	
s SO4_OH_AFm	2	s	0.0087923615	2.748e-08	
s OH_SO4_AFm	2	s	0.0087923615	2.748e-08	
s Al(OH)3am	1	s	0	-3.174	
s Al(OH)3mic	1	s	0	-2.264	
s Gibbsite	1	s	0	-1.811	
s Graphite	1	s	0	-84.68	
s Mayenite	1	s	0	-130.4	
s Aluminate	1	s	0	-36.48	
s CA	1	s	0	-11.04	
s CA2	1	s	0	-15.19	
s C2AH75	1	s	0	-2.469	
s C3AH6	1	s	0	-0.9693	
s C4AH11	1	s	0	-3.156	
s C4AH13	1	s	0	-1.422	
s C4AH19	1	s	0	-1.222	
s CAH10	1	s	0	-3.47	
s C4AsH105	1	s	0	-1.423	
s C4AsH12	1	s	0	-0.07732	
s C4AsH14	1	s	0	-0.05177	
s C4AsH16	1	s	0	-0.1373	
s C4AsH9	1	s	0	-3.442	

System: T = 298.15 K; P = 1.00 bar; V = 0.131 L; Aqueous: built-in EDH(H); pH = 12.477; pe = 8.296; IS = 0.053 m

View detailed results

General information: pH, ionic strength, redox, ...

Hydration of $C_3A + CaO + CaSO_4$ – results

Detailed information about composition of aqueous, gaseous and solid phases

GEM-Selektor 3 (GEMS3) - Geochemical Equilibrium Modelling by Gibbs Energy Minimization - [EqDemo :: C3A:G:C3A-Cs:0:0:1:25:0:]

Modules Record Data Calculate View Print Window Help

EqDemo C3A:G:C3A-Cs:0:0:1:25:0:

EqIC **EqPh** EqDC EqSurf EqGen 26/03/2020, 13:36

Solid phases **total amount [mol]** **Volume [cm³]** **Mass [g]**

	PHnam	L1	Xa	Fa	phVol	phM
0	a aq_gen	29	2.4932653	1.6432721e-009	44.984034	44.939588
1	g gas_gen	6	0.0031708119	2.3535764e-008	78.603512	0.10002508
2	s ettringite	2	0.00091958291	-2.607211e-007	0.65031459	1.1475405
3	s SO4_OH_AFm	2	0.0087923615	2.7476736e-008	2.693842	5.4165243
4	s OH_SO4_AFm	2	0.0087923615	2.7476736e-008	2.693842	5.4165243
5	s Al(OH)3am	1	0	-3.1743193	0	0
6	s Al(OH)3mic	1	0	-2.2643225	0	0
7	s Gibbsite	1	0	-1.8111723	0	0
8	s Graphite	1	0	-84.68486	0	0
9	s Mayenite	1	0	-130.37467	0	0
10	s Aluminate	1	0	-36.481442	0	0
11	s CA	1	0	-11.042065	0	0
12	s CA2	1	0	-15.191921	0	0
13	s C2AH75	1	0	-2.4694892	0	0

m_{SO4-AFt} = 1.15 g

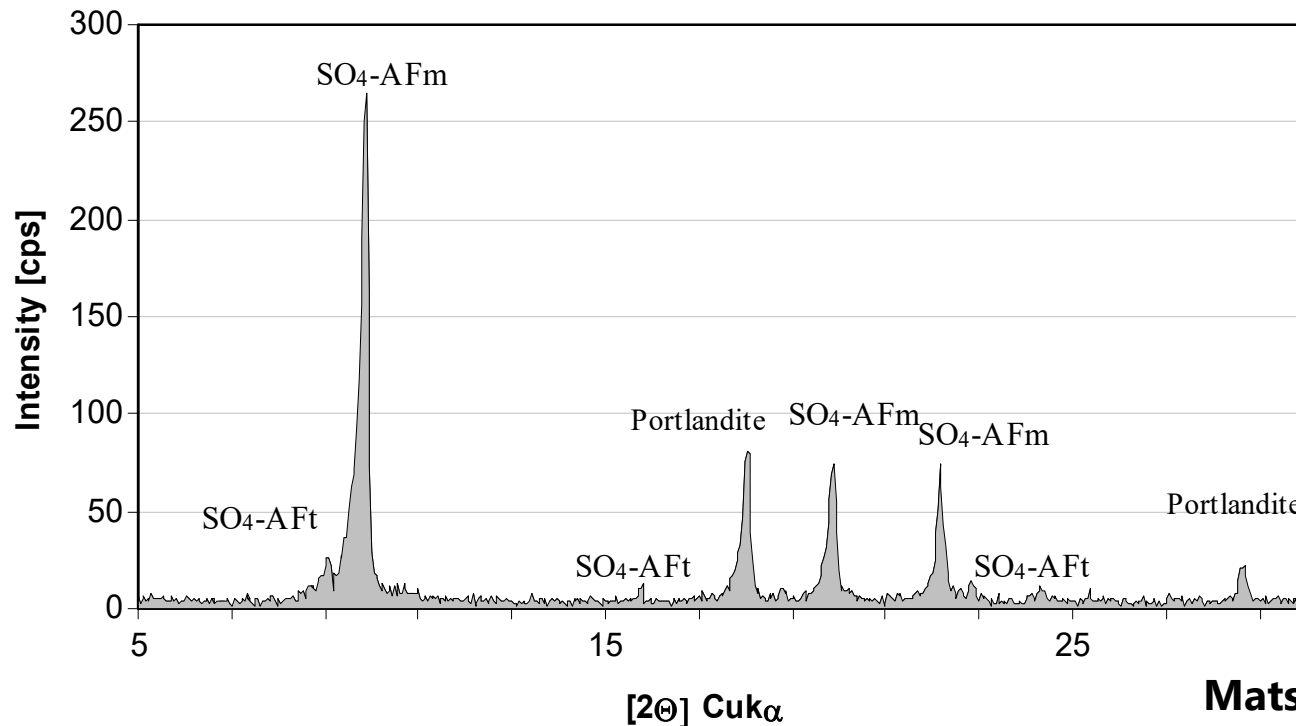
m_{SO4-AFm} = 10.83 g

m_{Portlandite} = 3.10 g

Hydration of $C_3A + CaO + CaSO_4$ – results

Comparison to experiments:

Hydration of C_3A at $SO_3/Al_2O_3 = 1$, cured 28 d at $25^\circ C$, solid phases by XRD



Matschei 2007

Qualitatively very good agreement between experimental and calculated results

Phase assemblage SO_4 -AFm - SO_4 -AFt - portlandite - aq. predicted and observed.

Quantification with help of GEMS possible.

Hydration of $C_3A + CaO + CaSO_4$ – results

Composition of aqueous phase

EqIC EqPh EqDC EqSurf EqGen 26/03/2020, 13:36

C3A + CaSO4

Output: total molalities in aqueous phase (mol/kg H₂O)

	ICnam	b	Cb	u	lqm t	m t	ICnam
0	Al ...	0.037010516	1.3578917e-017	-324.92795	-4.3723484	4.2427904e-005	Al ...
1	C ...	1e-009	-2.6864406e-026	-194.9941	-7.6519556	2.2286631e-008	C ...
2	Ca ...	0.11860702	-1.5518762e-017	-266.15404	-1.6910673	0.020367266	Ca ...
3	H ...	5.5508373	1.241501e-016	-47.83096	-1.390652	0.040676917	H ...
4	O ...	3.0113217	-9.3112574e-017	-0.016474237	-1.3631496	0.043336159	O ...
5	S ...	0.018510003		0	-275.13628	7.5706847e-006	S ...
6	Zz ...	0	2.0011687e-020	19.102731		0	Zz ...

total mol in system (input)

Log₁₀ of total molalities

Tutorial – single systems: hydration of C_3A

Hydration of C_3A ($Ca_3Al_2O_6$)^a

- 1) Simulation of reaction $C_3A + CaO + CaSO_4$ **Guided tutorial**
 - 2) Simulation of reaction $C_3A + CaO + CaCO_3$
 - 3) Simulation of reaction $C_3A + CaCO_3$
 - 4) Simulation of reaction $C_3A + C + CaSO_4 + CaCO_3$
- Individual work**

See Seligmann & Greening ICCI 1969 and various papers by Kuzel et al. (Kuzel & Pöllmann CCR 1991, Kuzel et. al CCR 1996) for experimental verification

Hydration of $C_3A + CaCO_3$

Experimental problem part 2:

Reaction of C_3A with CaO plus calcium carbonate

5 g C_3A + 1.86 g $CaCO_3$ + 2.5 g CaO + 50 g H_2O

+ 0.1 g O_2 (oxidizing conditions, CO_2 -free = no carbonation)

molar ratio $SO_3/Al_2O_3 = 0$, molar ratio $CO_2/Al_2O_3 = 1$

Experimental problem part 3:

Reaction of C_3A with calcium carbonate (no surplus of CaO)

5 g C_3A + 1.86 g $CaCO_3$ + 50 g H_2O

+ 0.1 g O_2 (oxidizing conditions, CO_2 -free = no carbonation)

molar ratio $SO_3/Al_2O_3 = 0$, molar ratio $CO_2/Al_2O_3 = 1$

Hydration of $C_3A + CaCO_3 + CaSO_4$

Experimental problem part 4:

Reaction of C_3A with CaO , calcium carbonate, calcium sulfate

5 g C_3A + + 1.86 g $CaCO_3$ + 2.52 g $CaSO_4$ + 2.5 g CaO
+ 50 g H_2O
+ 0.1 g O_2 (oxidizing conditions, CO_2 -free = no carbonation)

molar ratio $SO_3/Al_2O_3 = 1$, molar ratio $CO_2/Al_2O_3 = 1$



Hydration of C_3A + $CaCO_3$ and/or $CaSO_4$

Experimental problem part 2 - 4

Hints:

- Create new system for part 2
- Keep carbonate solid solutions switched on
- For part 3 + 4 it might be convenient to clone the system from part 2 (only if we keep S in the system)