

Wir schaffen Wissen – heute für morgen

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**Reactive transport with OGS-GEMS:
GEM-Selektor v.3 for dummies**

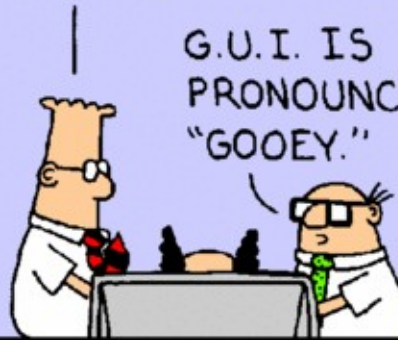
OKAY, JUST SHOW ME
HOW TO PROGRAM SO
I CAN HELP OUT ON
YOUR PROJECT.



S. Adams E-mail: SCOTTADAMS@AOL.COM

YOU'RE GOING TO BUILD
A "G.U.I." USING OBJECT-
ORIENTED DEVELOP-
MENT TOOLS...

G.U.I. IS
PRONOUNCED
"GOOEY."



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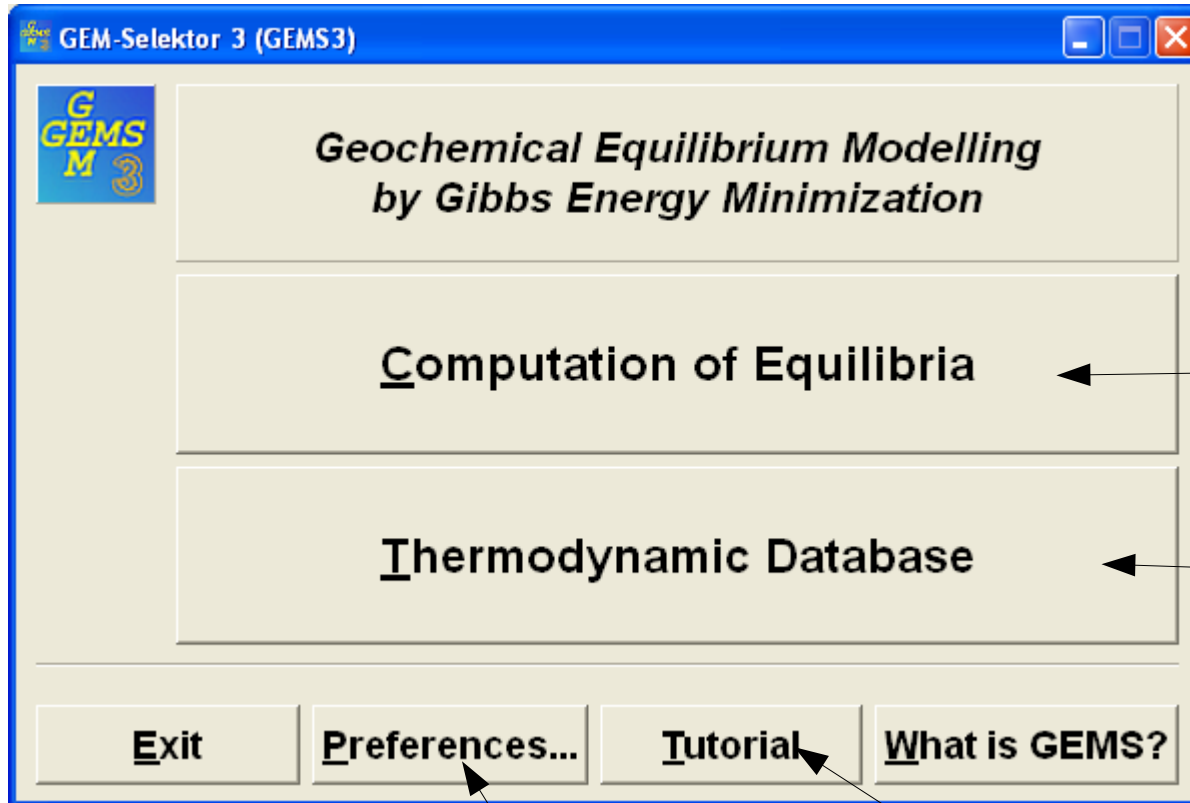
I USED MY
GUN OBJECT
TO BLAST
THE BUG
OBJECT IN
THE HALL
OBJECT!!

NOTICE
HOW
GOOEY IT
IS.



GEM-Selektor v3. for dummies

After starting of GEMS we see:



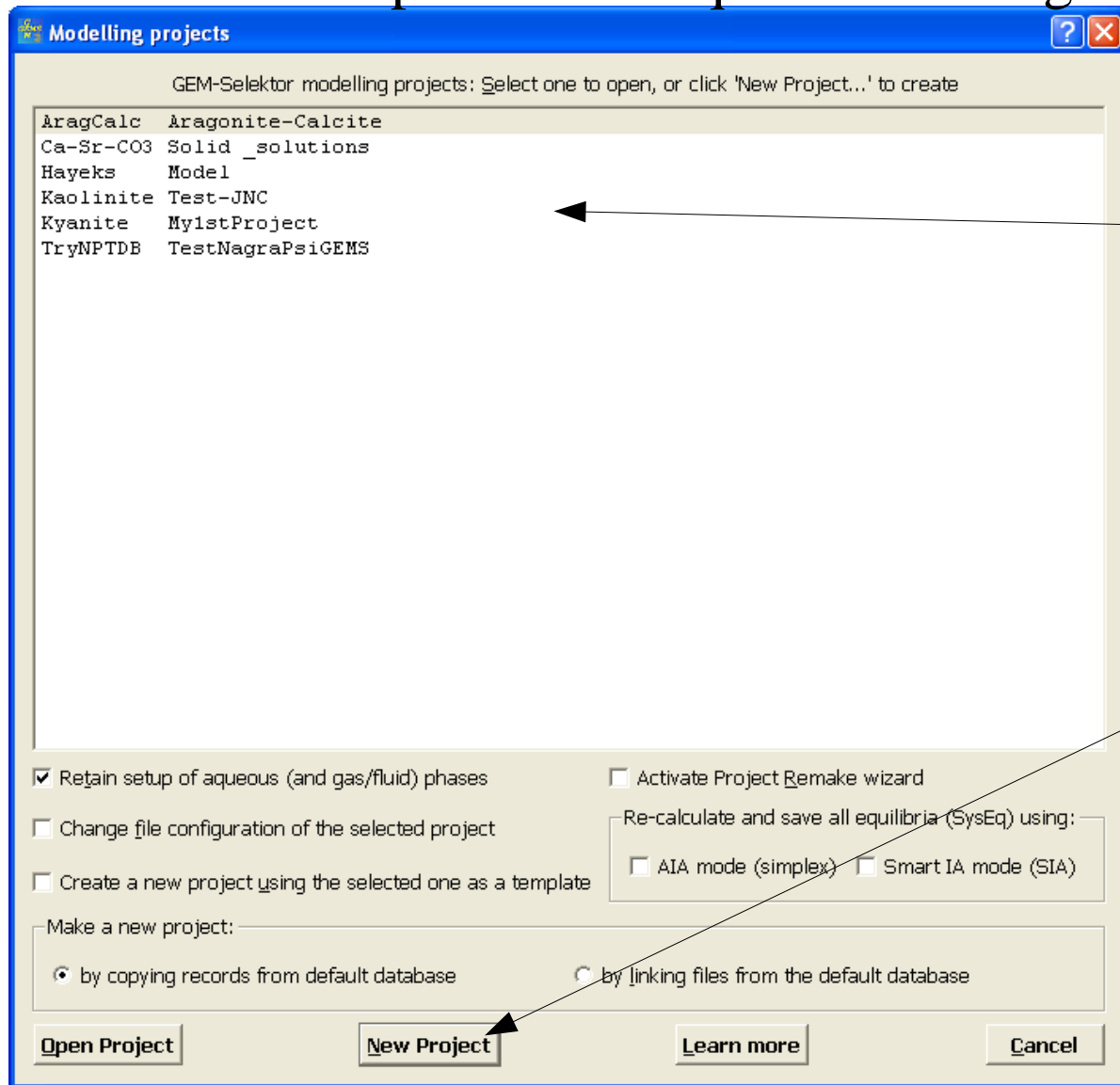
Open old projects
or create new ones.

Edit the general
thermodynamic
database.

Here we find/set the
path to the projects.

Unfortunately not all
tutorials are up to date.

Choose “computation of equilibria” and get:



Existing example
and old projects.

New projects start
here:

First we have to name the new project!

Project: Enter a new record key, please

MyWork:My1stProject

MyWork

Modelling project name

My1stProject

Comment to project definition

Ok Reset From List Help Cancel

1. Choose a new name for the project
2. Add a comment/short description so you have a chance after 10 years to identify the topic of the project.

Do not edit...will be updated automatically.

Selection of Independent Components into Modelling Project CalDol

Select chemical elements (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	Co Ni
4a	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh Pd
5a	Ag	Cd	In	Sn	Sb	Te	I	Xe	
6	Cs	Ba	REE	Hf	Ta	W	Re	Os	Ir Pt
6a	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
7	Fr	Ra	ACT						e(Zz)

☐ Isotopes

La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf		Yb	Lu

Other

Nit

...

...

...

...

...

...

...

...

...

...

Vol

Set filters Phases-> ☒ Gas ☒ Aqueous ☒ Solids ☐ Solutions ☐ Sorption
 Dataset: ☒ Kernel (NagraPSI) ☐ Complem.(SUPCRT) ☐ Supplem. ☐ Specific

Learn more

Cancel

Ok

This is the place where you choose the database and the independent component.

For the calcite-dolomite example we need:

Calcite CaCO_3

Dolomite $\text{CaMg}(\text{CO}_3)_2$

Quartz SiO_2 (the inert material of the porous medium)

Water (H_2O)

MgCl_2 (solution injected into the column)

For the calcite – dolomite example choose:

H, O, Ca, C, Mg, Cl & Si

Selection of Independent Components into Modelling Project CalDol

Select chemical elements (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	Co Ni
4a	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh Pd
5a	Ag	Cd	In	Sn	Sb	Te	I	Xe	
6	Cs	Ba	REE	Hf	Ta	W	Re	Os	Ir Pt
6a	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
7	Fr	Ra	ACT						
<input type="checkbox"/> Isotopes									
	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb Dy Ho Er Tm
	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk Cf Yb Lu

Other

Nit

...

...

...

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...

Vol

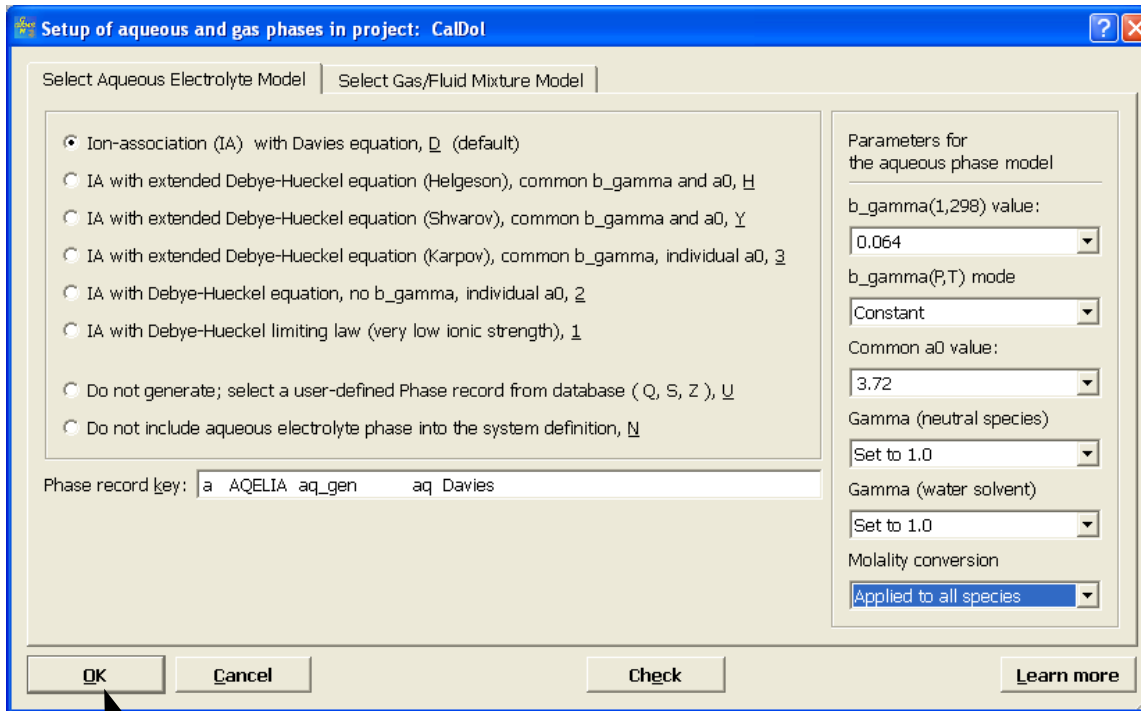
Set filters Phases-> ☒ Gas ☒ Aqueous ☒ Solids ☐ Solutions ☐ Sorption
 Dataset: ☒ Kernel (NagraPSI) ☐ Complem.(SUPCRT) ☐ Supplem. ☐ Specific

Learn more **Cancel** **Ok**

Proceed to create

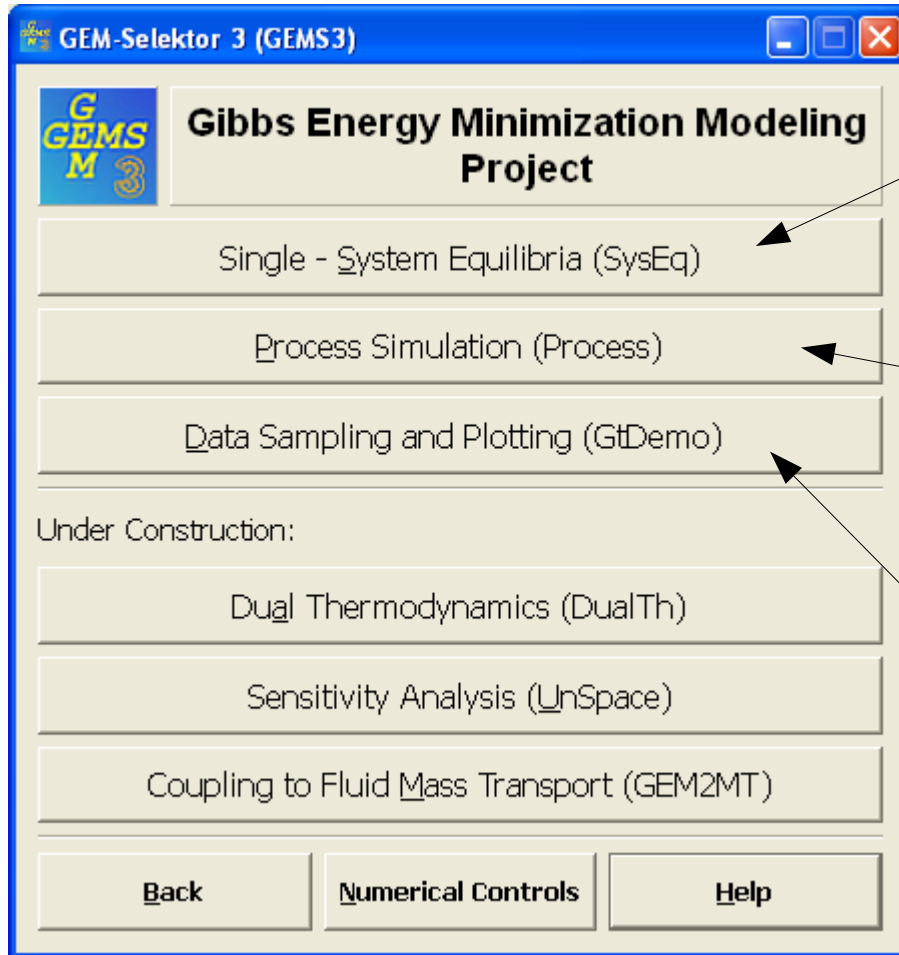
For the calcite – dolomite example choose:
H, O, Ca, C, Mg, Cl & Si

For relatively dilute solutions (no brine, ionic strength <0.3) at ambient temperatures and pressures we can use the default settings for activity and fluid/gas models.



Default settings are ok for the calcite-dolomite system.

We get the main project menu:



Interactive setup/calculation of our system(s).

Process simulator (scripting language) for batch calculations (e.g. titration).

Some plotting utilities...

We choose the SysEq entry.

Next the first actual record for our project has to be defined. A record represents a specific composition at a defined temperature and pressure. A project might contain many different records.

Do not change, is updated automatically.

SysEq: Please, enter a new record key:

CalDol:G:MySystem:0:0:1:25:0:

CalDol Modelling project name

G Thermodynamic potential to minimize {G GV}

MySystem Name of chemical system definition (CSD)

0 Variant number for bulk composition <integer>

0 Volume of the system (L) or 0 (no volume constraint)

1 Pressure in bar or 0 for Psat (H2O)

25 Temperature (deg. C)

0 Variant number for CSD constraints

Ok Reset From List Help Cancel

(parent) project

Do not change

Choose a meaningful name

Possible to change

The first screen of the new Chemical System Definition Wizard

GEM-Selektor System Setup: CalDol:G:Column:0:0:1:25:0:

Step 1 - Configuration of Chemical System Definition

Chemical system definition (CSD) contains the 'recipe' to set bulk elemental composition, the lists of phases and their components to be considered in the calculation of equilibrium states, and optional metastability constraints and/or parameters of surfaces and surface species.

This information is kept in the GEMS project data base in a SysEq record and may change from one such record to another. In addition, SysEq records keep the calculated primal and dual GEM solution, as well as the activity coefficients.

In this wizard, it is possible to (re)configure some optional CSD features (in most cases, e.g. by 'cloning' SysEq records, this is not necessary). It is recommended to fill out System name and Comment fields - this will help identify this CSD and recipe in the future.

CSD name:

Comment:

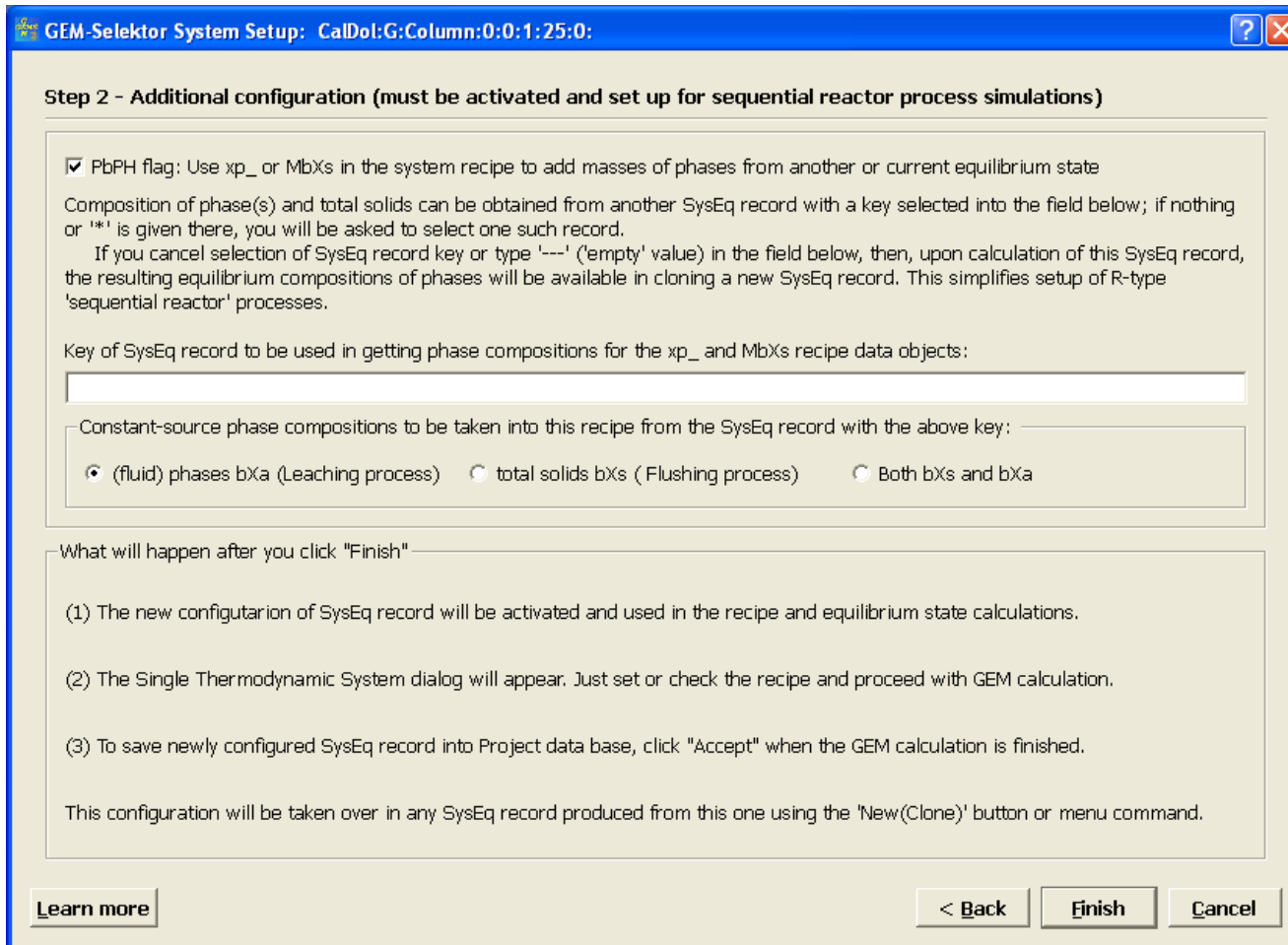
CSD optional settings

<input checked="" type="checkbox"/> Keep specific surface areas for phases (mandatory for sorption)	<input type="checkbox"/> Keep additional parameters for surface types (reserved)
<input checked="" type="checkbox"/> Keep specific surface energies for solid-aqueous (-gas) interfaces	<input type="checkbox"/> Keep uncertainties of bulk composition (vector b) elements
<input type="checkbox"/> Use electrostatic sorption models (DLM,CCM,TLM,BSM,...)	<input type="checkbox"/> Keep Pparc_ (partial pressures) of Dependent Components
<input type="checkbox"/> Keep area fractions and SCM codes for surface types	<input type="checkbox"/> Keep low/upp restrictions for amounts of phases (reserved)
<input type="checkbox"/> Keep size parameters r0, h0 of solid particles (pores), reserved	<input type="checkbox"/> Set a constraint on total volume V of the system (reserved)
<input type="checkbox"/> Keep diel.constant and el.conductivity of solid phases (reserved)	<input checked="" type="checkbox"/> Use electroneutrality equation (PE) in GEM calculations

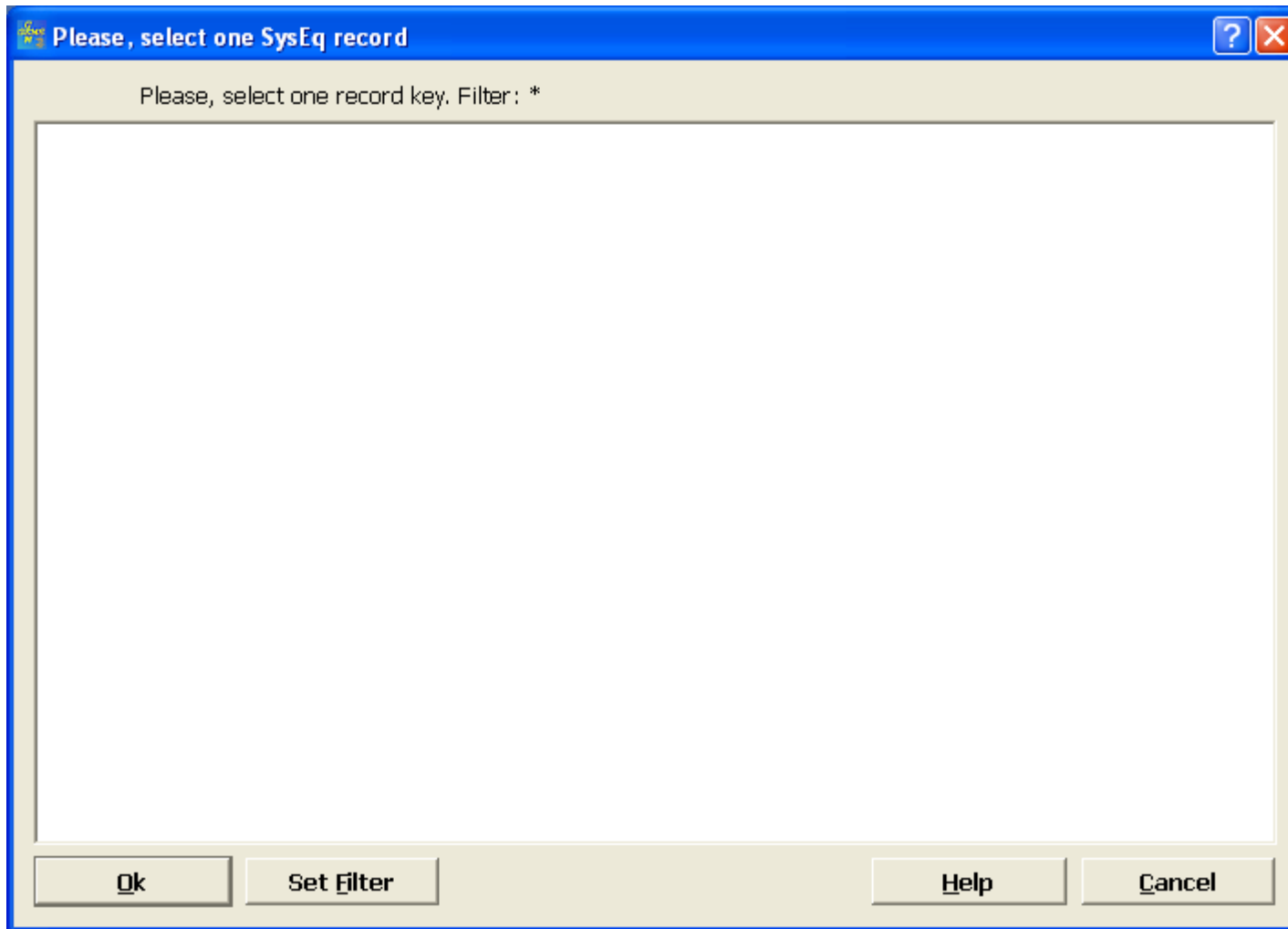
[Learn more](#)

For our example only name and comment should be inserted.

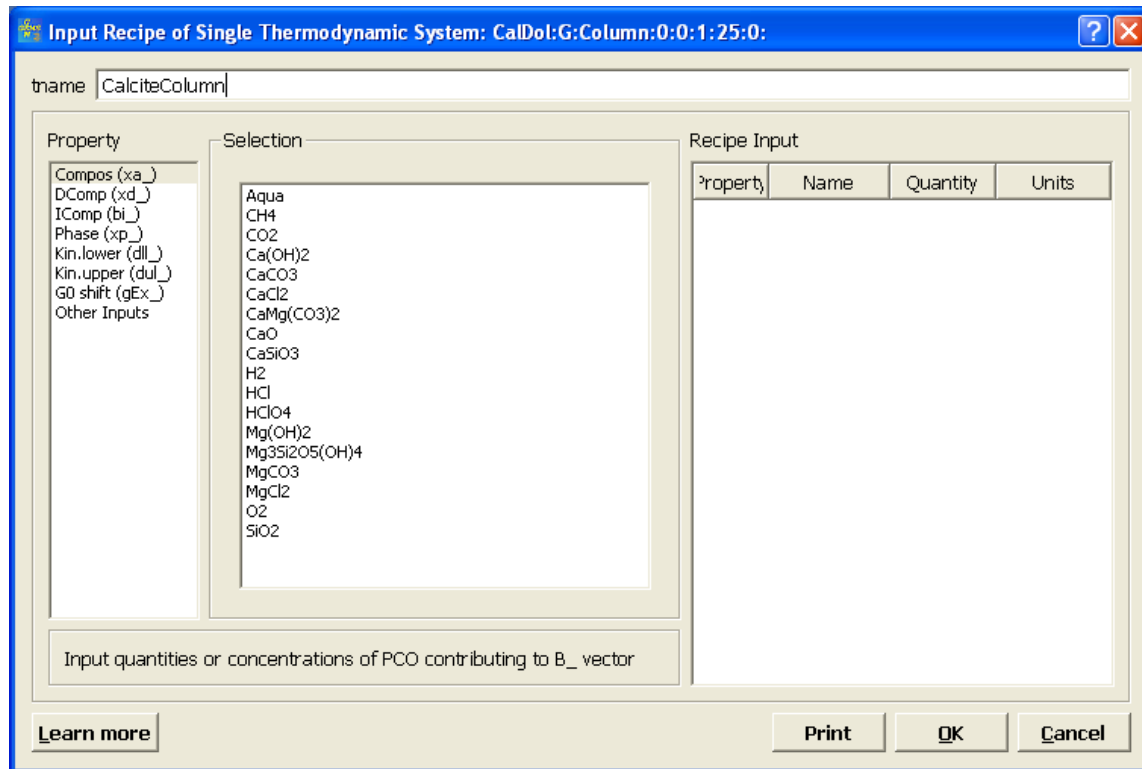
Read the lower part of the screen and press finish. No changes required for our specific setup.



We did not define any SysLq records, therefore the screen is empty. Just click ok.



This is the new unified Thermodynamic System Dialog.
Everything we need to actually set up (mix) our initial system!



The input can be done by

- Predefined mixtures:
Compos
- Dependent components
(aqueous species, solids
= minerals): DComp
- Independent
components: Icomp
- Phases

We may also control the amounts of dependent components and
adjust G0 values (equivalent to change $\log(k)$)

We start simple, just mix 1000 g of water, 40 g of calcite, 1000 g of quartz and 10 g of MgCl.

Input Recipe of Single Thermodynamic System: CalDol:G:Column: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
- CaCl2
- CaMg(CO3)2
- CaO
- CaSiO3
- H2
- HCl
- HClO4
- Mg(OH)2
- Mg3Si2O5(OH)4
- MgCO3
- MgCl2
- O2
- SiO2

Recipe Input

	Property	Name	Quantity	Units
1	xa_	Aqua	1000	g
2	xa_	CaCO3	40	g
3	xa_	MgCl2	10	g
4	xa_	SiO2	1000	g

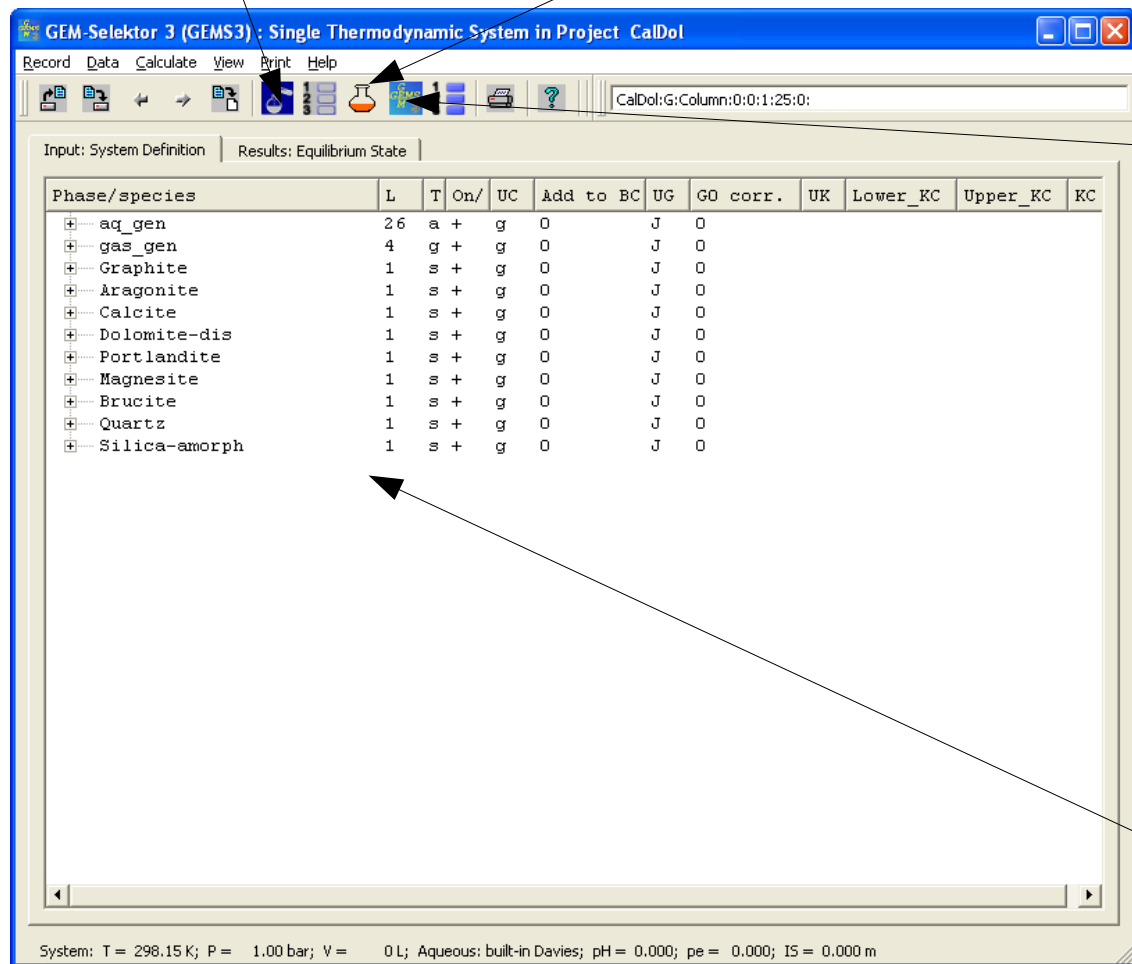
Input quantities or concentrations of PCO contributing to B_ vector

Learn more Print OK Cancel

Finally: The main project calculation menu

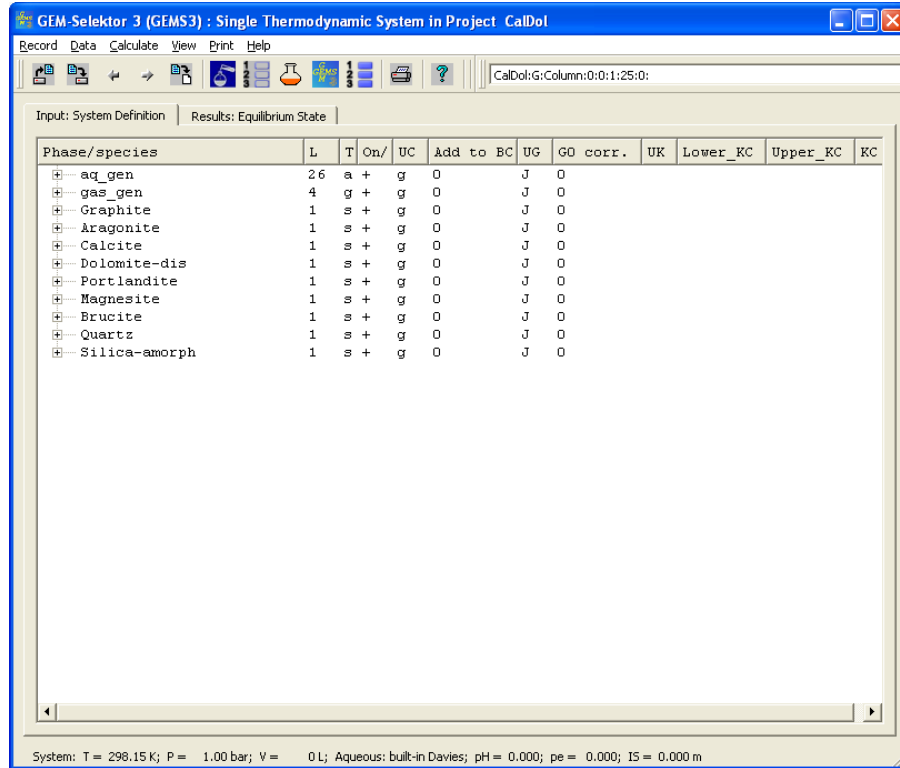
Recipe wizard

The “check if input composition is ok” button



The calculation button

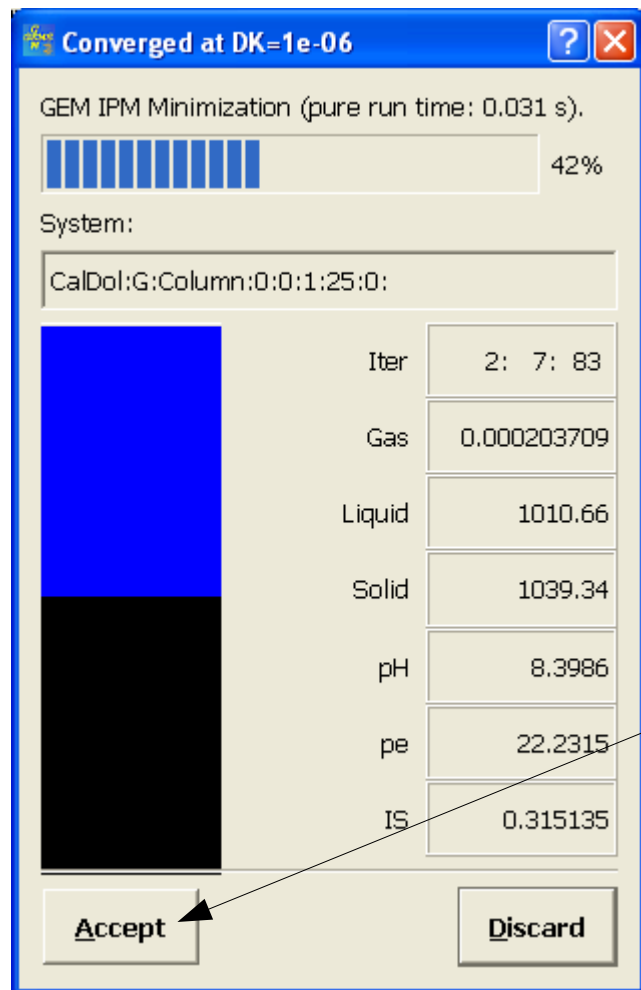
All the available phases for our project setup (depends on database)



For calculation:

1) press the “check”
button (bottle) → if no
additional dialog appears,
everything is ok

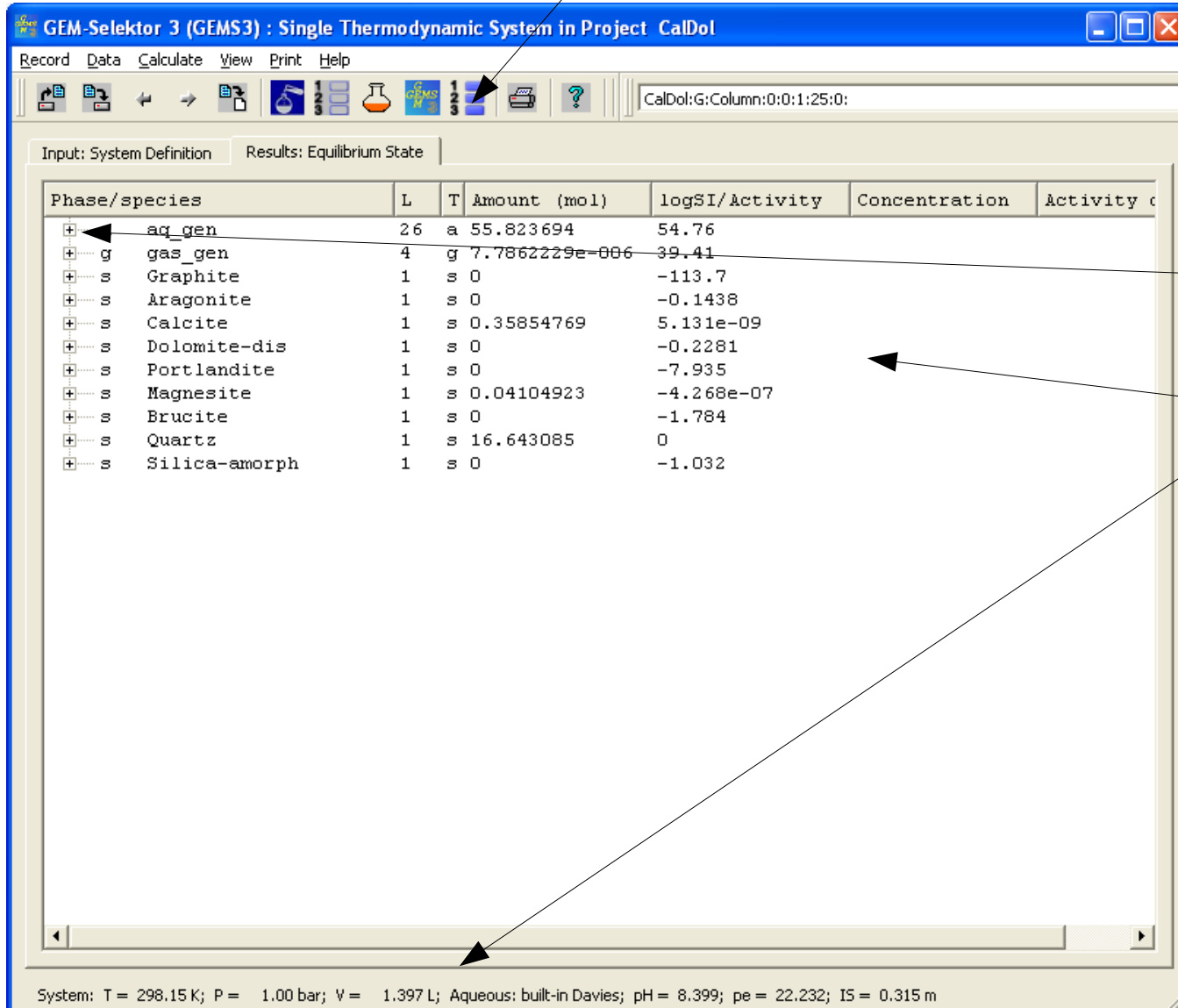
2) press the calculate
button (gems symbol)



If everything went well you get the following screen with some initial information.

Press accept to continue.

More detailed results are here



Expand
phases to
examine
content.

results

Now we start to tune our system to the desired state.

1) Phase and component selection

In our system the quartz should be an inert material which is a placeholder for the porous rock. We therefore switch off all solid mineral phases except quartz and components in the liquid (gas) phase that contain Si. Then only quartz contains Si and cannot transform/dissolve.

GEM-Selektor 3 (GEMS3) : Single Thermodynamic System in Project CalDol

Record Data Calculate View Print Help

CalDol:G:Column:0:0:1:25:0:

Input: System Definition Results: Equilibrium State

Phase/species	L	T	On/	UC	Add to BC	UG	GO corr.	UK	Lower_KC	Upper_KC	I
aq_gen	26	a +	g	0		J	0				
Ca(CO3)0		S +	M	0		J	0	M	0	1e+006	I
Ca(HCO3) +		S +	M	0		J	0	M	0	1e+006	I
Ca+2		S +	M	0		J	0	M	0	1e+006	I
CaOH+		S +	M	0		J	0	M	0	1e+006	I
Ca(HSiO3) +		S -	M	0		J	0	M	0	1e+006	I
CaSiO30		S +	M	0		J	0	M	0	1e+006	I
Mg(CO3)0		S +	M	0		J	0	M	0	1e+006	I
Mg(HCO3) +		S +	M	0		J	0	M	0	1e+006	I
Mg+2		S +	M	0		J	0	M	0	1e+006	I
MgOH+		S +	M	0		J	0	M	0	1e+006	I
Mg(HSiO3) +		S -	M	0		J	0	M	0	1e+006	I
MgSiO30		S -	M	0		J	0	M	0	1e+006	I
HSiO3-		S -	M	0		J	0	M	0	1e+006	I
SiO20		S -	M	0		J	0	M	0	1e+006	I
SiO3-2		S -	M	0		J	0	M	0	1e+006	I
CO20		S +	M	0		J	0	M	0	1e+006	I
CO3-2		S +	M	0		J	0	M	0	1e+006	I
HCO3-		S +	M	0		J	0	M	0	1e+006	I
CH40		S +	M	0		J	0	M	0	1e+006	I
ClO4-		S +	M	0		J	0	M	0	1e+006	I
Cl-		S +	M	0		J	0	M	0	1e+006	I
H20		S +	M	0		J	0	M	0	1e+006	I
O20		S +	M	0		J	0	M	0	1e+006	I
OH-		S +	M	0		J	0	M	0	1e+006	I
H+		T +	M	0		J	0	M	0	1e+006	I
H2O0		W +	M	0		J	0	M	0	1e+006	I
gas_gen	4	g +	g	0		J	0				
Graphite	1	s +	g	0		J	0				
Aragonite	1	s +	g	0		J	0				

Choose input definition

Here the components and phases are switched off: double-click

GEM-Selektor 3 (GEMS3) : Single Thermodynamic System in Project CalDol

Record Data Calculate View Print Help

CalDol:G:Column:0:0:1:25:0:

Input: System Definition Results: Equilibrium State

Phase/species	L	T	Amount (mol)	logSI/Activity	Concentration	Activity coeff.
a aq_gen	19	a	55.823517	0		
Ca(CO ₃) ₀	S		5.549629e-006	5.54955e-06	5.5496334e-006	0.999984
Ca(HCO ₃) ₊	S		3.4232304e-006	2.50562e-06	3.4232331e-006	0.73194657
Ca+2	S		0.02892492	0.00830254	0.028924943	0.28703732
CaOH+	S		6.7327033e-007	4.92798e-07	6.7327086e-007	0.73194657
Mg(CO ₃) ₀	S		8.3139204e-006	8.31379e-06	8.313927e-006	0.999984
Mg(HCO ₃) ₊	S		8.2614126e-006	6.04692e-06	8.2614191e-006	0.73194657
Mg+2	S		0.076099401	0.0218434	0.076099461	0.28703732
MgOH+	S		3.8755912e-005	2.83673e-05	3.8755943e-005	0.73194657
CO ₂ ₀	S		1.4882358e-007	1.48821e-07	1.488237e-007	0.999984
CO ₃ -2	S		1.3895857e-006	3.98863e-07	1.389586e-006	0.28703732
HCO ₃ -	S		3.2329006e-005	2.36631e-05	3.2329032e-005	0.73194657
CH ₄ ₀	S		0	6.62842e-137	0	1
ClO ₄ -	S		0	2.06678e-38	0	1
Cl-	S		0.21005977	0.153753	0.21005993	0.73194657
H ₂ ₀	S		0	1.51672e-41	0	1
O ₂ ₀	S		2.7278736e-011	2.72783e-11	2.7278758e-011	0.999984
OH-	S		4.8859143e-006	3.57623e-06	4.8859182e-006	0.73194657
H+	T		3.8004303e-009	2.78171e-09	3.8004333e-009	0.73194657
H ₂ O ₀	W		55.508329	0.994322	0.99435385	0.99996794
g gas_gen	4	g	0	-5.358		
s Graphite	1	s	0	-66.77		
s Aragonite	1	s	0	-0.1438		
s Calcite	1	s	0.34184259	1.043e-08		
Cal	O		0.34184259	1	1	1
s Dolomite-dis	1	s	0.028875151	1.26e-07		
s Portlandite	1	s	0	-7.774		
s Brucite	1	s	0	-1.394		
s Quartz	1	s	16.643283	0		

System: T = 298.15 K; P = 1.00 bar; V = 1.396 L; Aqueous: built-in Davies; pH = 8.556; pe = 10.301; IS = 0.315 m

After
“check”
and
“calculate”
we get the
results.

Concentration
of dissolved
species

Mole amount
of minerals

We may check the detailed results:

EqDemo :: CalDol:G:Column:0:0:1:25:0:

Help

EqIC EqPh EqDC EqSurf EqGen CalDol:G:Column:0:0:1:25:0: 28/09/2011, 14:33

CalciteColumn
This is the initial rock composition in the column.

	ICnam	b	Cb	u	lgm t	m t	ICnam
0	C ...	0.3996523	4.7361917e-015	-153.74561	-4.2260991	5.9415655e-005	C ...
1	Ca ...	0.3996523	7.7600679e-015	-275.22018	-1.5385827	0.028934589	Ca ...
2	Cl ...	0.21005977	-4.8576325e-017	-31.115257	-0.67765678	0.21005993	Cl ...
3	H ...	111.01675	9.8613826e-011	-43.41884	-4.0538789	8.8332617e-005	H ...
4	Mg ...	0.10502988	-6.0720406e-017	-234.39558	-1.1183028	0.076154793	Mg ...
5	O ...	89.993895	5.1172244e-012	-8.8453618	-3.6528392	0.00022241333	O ...
6	Si ...	16.643283	5.1731843e-012	-327.12692	0	0	Si ...
7	Zz ...	0	-7.6207033e-016	23.718641	0	-2.028847e-016	Zz ...

Why this?

Composition
in terms of
independent
components

Total dissolved
independent
components

Phase results



EqDemo :: CalDol:G:Column:0:0:1:25:0:

Help



EqIC EqPh EqDC EqSurf EqGen CalDol:G:Column:0:0:1:25:0:

28/09/2011, 14:33

CalciteColumn

This is the initial rock composition in the column.

	PHnam	Xa	Fa	phVol	phM
0	a aq_gen	55.823517	0	1004.3813	1010.4614
1	g gas_gen	0	-5.3575235	0	0
2	s Graphite	0	-66.770868	0	0
3	s Aragonite	0	-0.14383215	0	0
4	s Calcite	0.34184259	1.0428561e-008	12.625614	34.213999
5	s Dolomite-dis	0.028875151	1.2600815e-007	1.859271	5.3246067
6	s Portlandite	0	-7.7737315	0	0
7	s Brucite	0	-1.3937854	0	0
8	s Quartz	16.643283	0	377.6028	1000

Phase
volumes and
masses

pmXs 1039.5386

	C	Ca	Cl	H	Mg	O	Si	Zz
	0.39959289	0.37071774	0	0	0.028875151	34.485344	16.643283	
0	5.9415608e-005	0.028934566	0.21005977	111.01675	0.076154732	55.508552	0	-1.
1	0	0	0	0	0	0	0	0

	PHnam	L1	Aalp	Sigw	Sigg	Yof
0	a aq_gen	19	0	0	0	0
1	g gas_gen	4	0	0	0	0
2	s Graphite	1	0	0	0	0
3	s Aragonite	1	0	0	0	0
4	s Calcite	1	0	0	0	0

General system properties



Help



EqIC

EqPh

EqDC

EqSurf

EqGen

CalDol:G:Column:0:0:1:25:0:

28/09/2011, 14:33

CalciteColumn

This is the initial rock composition in the column.

GX	-11263.305	Mbx	2.05	mXs	1039.5386
----	------------	-----	------	-----	-----------

PG		TC		TK		Vx		IS	
0	1	0	25	0	298.15	0	0	pH	8.5556875
1	1	1	25	1	298.15	1	1396.469	pe	10.300875
								Eh	0.60816731

0	1	0	0	1	1	2	0	2	0	68	134	68	30	23	18	4	0	0
---	---	---	---	---	---	---	---	---	---	----	-----	----	----	----	----	---	---	---

	lgFug	lgPpG	Gfug	Gases
0	-5.3595811	-5.3595811	4.3693707e-006	CO2
1	-133.3221	-133.3221	0	CH4
2	-37.713125	-37.713125	0	H2
3	-7.6829836	-7.6829836	2.0749915e-008	O2

Total mass & volume

pH, redox, IS

Log partial gas pressures

Now we would like to make our system even more realistic (adjust the amount in the input wizard):

- 1) Reduce the amount of MgCl_2 as much as possible (set to $1.0\text{e-}8$ mol) → do not remove it completely as the gems solver can not deal with the case of zero amounts of independent components (same as in LMA)
- 2) Overall liquid phase volume should be 1 liter = 1000 ccm
- 3) Calcite should be $2.075\text{e-}4$ mol per liter liquid (after equilibration)
- 4) Porosity (volumetric “water” = liquid phase content) 0.32
→ achieve this by adjusting the amount of quartz

GEM-Selektor 3 (GEMS3) : Single Thermodynamic System in Project CalDol

Record Data Calculate View Print Help

Create...
New(Clone)...
Display F6
Remake...
Save
Save As...
Delete
Close F10

CalDol:G:Boundary:0:0:1:25:0:

Results: Equilibrium State

	L	T	Amount (mol)	logSI/Activity	Concentration	Activity coeff.
	19	a	55.823517	0		
en	4	g	0	-5.358		
te	1	s	0	-66.77		
ite	1	s	0	-0.1438		
te	1	s	0.34184259	1.043e-08		
te-dis	1	s	0.028875151	1.26e-07		
Portlandite	1	s	0	-7.774		
Brucite	1	s	0	-1.394		
Quartz	1	s	16.643283	0		

Create (clone) a new record from the existing one.

SysEq: Please, enter a new record key:

CalDol:G:Column:0:0:1:25:0:

CalDol Modelling project name

G Thermodynamic potential to minimize {G GV}

Boundary Name of chemical system definition (CSD)

0 Variant number for bulk composition <integer>

0 Volume of the system (L) or 0 (no volume constraint)

1 Pressure in bar or 0 for Psat (H2O)

25 Temperature (deg. C)

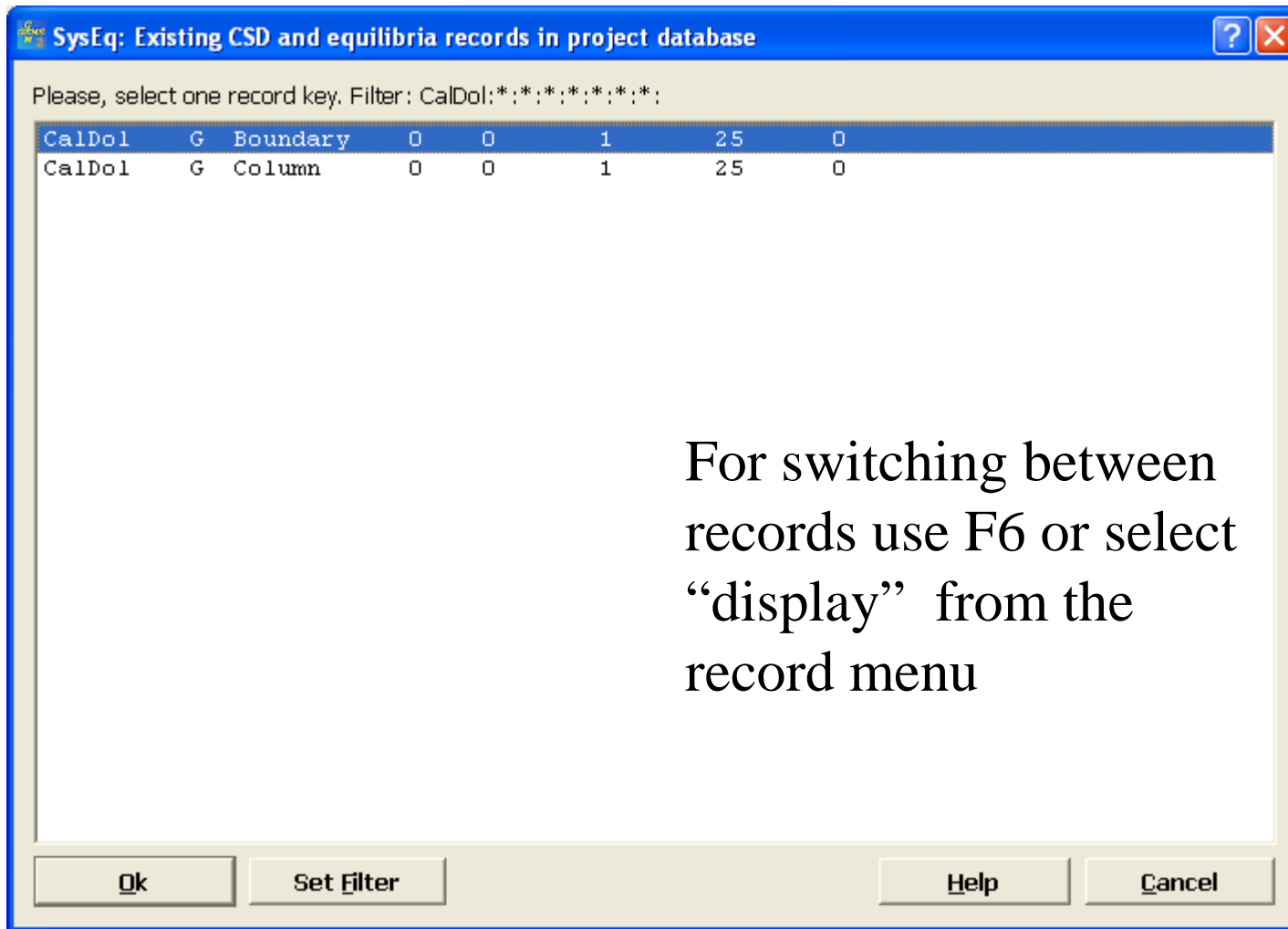
0 Variant number for CSD constraints

Ok Reset From List Help Cancel

Change the name

Now we would like define the injection solution
(adjust the amount in the input wizard):

- 1) Reduce the amount of calcite as much as possible (set to $1.0\text{e-}8$ mol) → do not remove it completely as the gems solver can not deal with the case of zero amounts of independent components (same as in LMA)
- 2) Overall liquid phase volume should be 1 liter = 1000 ccm
- 3) MgCl_2 should be $1.0\text{e-}3$ mol per liter liquid (after equilibration)
- 4) Porosity (volumetric “water” = liquid phase content) 0.32
→ achieve this by adjusting the amount of quartz



For switching between records use F6 or select “display” from the record menu

GEM-Selektor 3 (GEMS3) : Single Thermodynamic System in Project CalDol

Record Data Calculate View Print Help

Thermodynamic data at T,P...
Detailed bulk composition...

Input Write GEMIPM2K files
Read GEMIPM2K DBR file...

Equilibrium State

CalDol:G:Boundary:0:0:1:25:0:

Phase	L	T	Amount (mol)	logSI/Activity	Concentration	Activity coeff.
+ a aq_gen	19	a	55.823517	0		
+ g gas_gen	4	g	0	-5.358		
+ s Graphite	1	s	0	-66.77		
+ s Aragonite	1	s	0	-0.1438		
+ s Calcite	1	s	0.34184259	1.043e-08		
+ s Dolomite-dis	1	s	0.028875151	1.26e-07		
+ s Portlandite	1	s	0	-7.774		
+ s Brucite	1	s	0	-1.394		
+ s Quartz	1	s	16.643283	0		

Export the record for use with OGS-GEMS

Pitfalls when setting up systems with GEMS:

Units!

→ concentrations: mol/(kg H₂O) vs. mol/l vs. mol/m³

When exporting systems for OGS-GEMS make sure, that all records which are used in the same model have identical phase/component setup (same phases and components are switched on/off).

Problems with convergence of GEMS? Set the REDOX by adding tiny amounts of O₂ (oxidizing) or H₂ (reducing).

Thanks to Dimitrii Kulik for the excellent work on improving GEMS-PSI and to Haibing Shao and the OGS-community for the OGS-GEMS coupling.

