PAUL SCHERRER INSTITUT

PSI

Wir schaffen Wissen – heute für morgen

Paul Scherrer Institut

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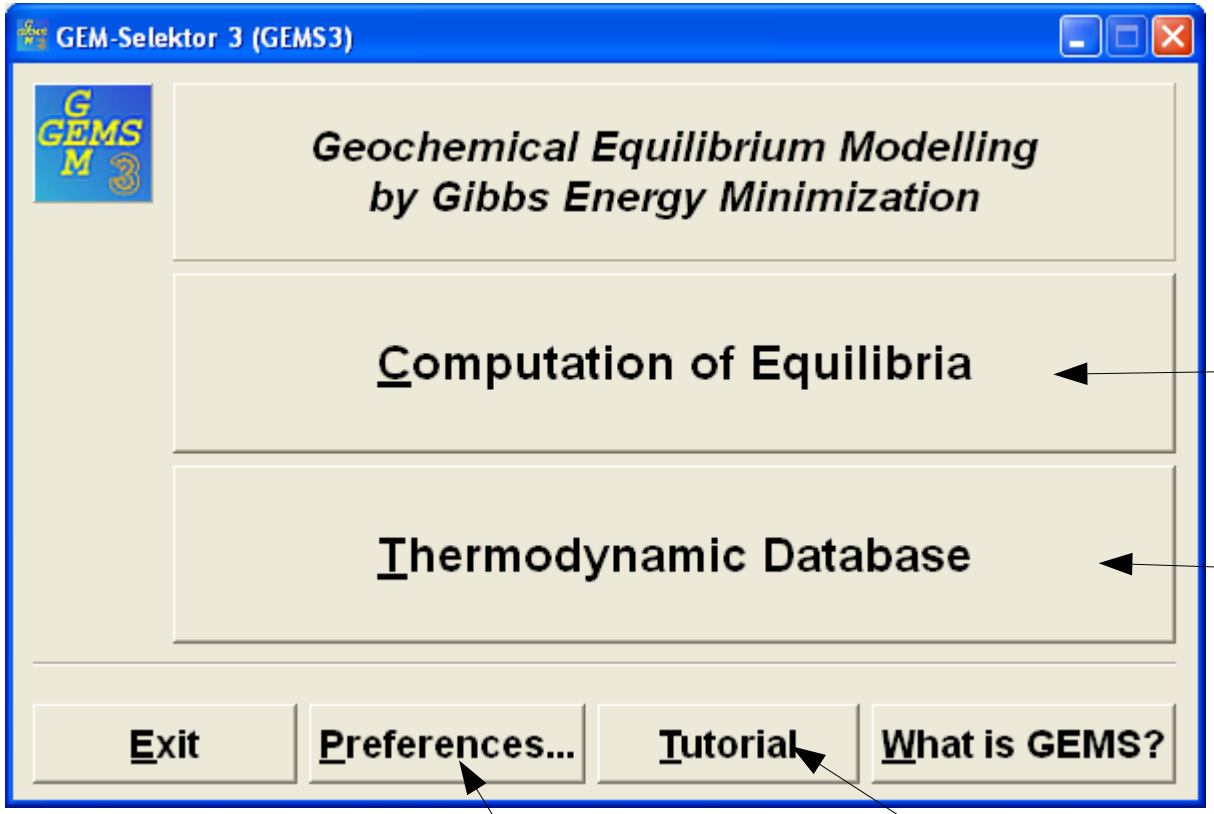
Reactive transport with OGS-GEMS: GEM-Selektor v.3 for dummies


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 DEVELOPMENT TOOLS...
G.U.I. IS PRONOUNCED "GOOEY."
I USED MY GUN OBJECT TO BLAST THE BUG OBJECT IN THE HALL OBJECT!!
NOTICE HOW GOOEY IT IS.
10/11 © 1995 United Feature Syndicate, Inc.(NYC)

GEM-Selektor v3. for dummies

After starting of GEMS we see:



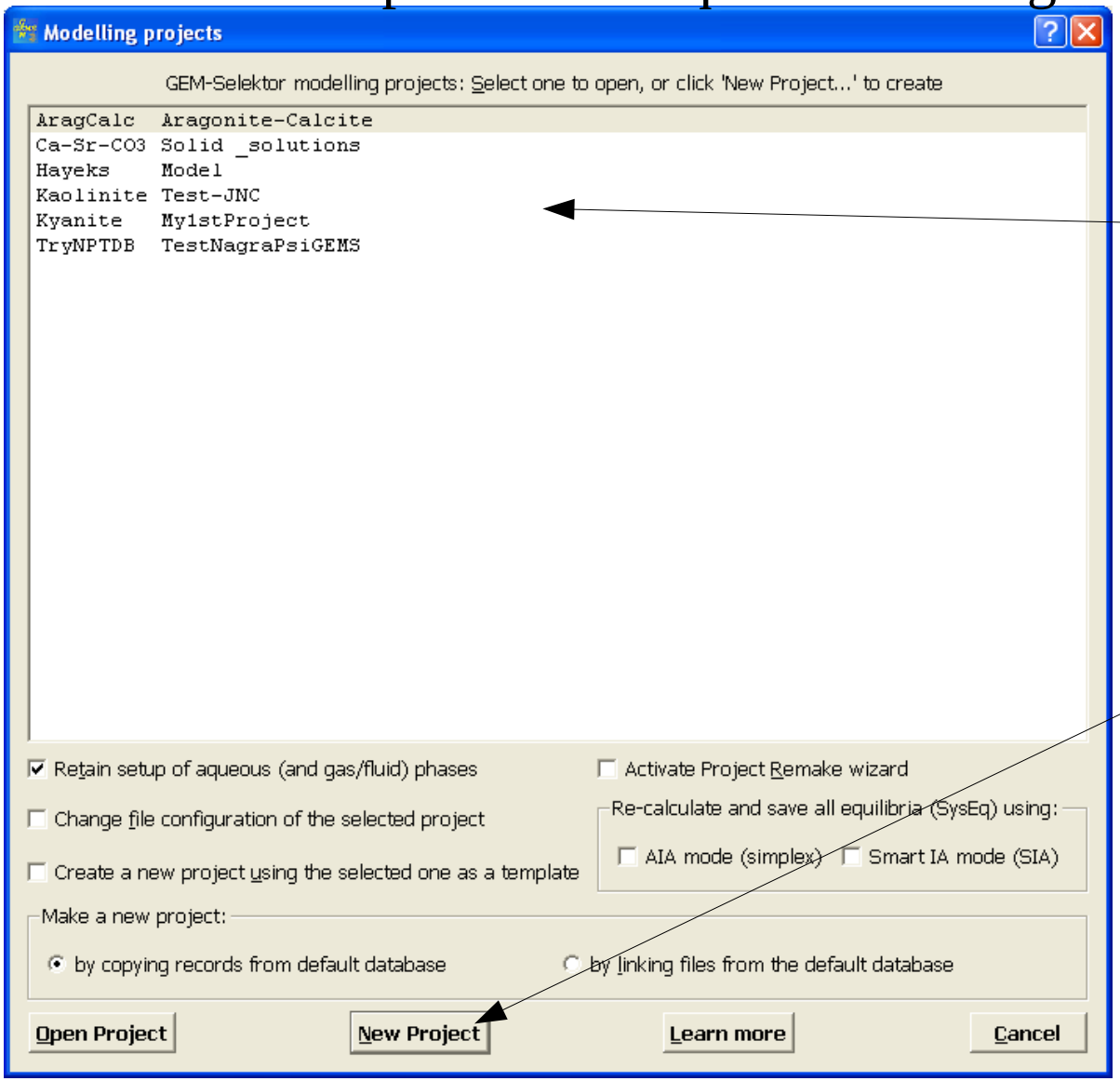
Open old projects or create new ones.

Edit the general thermodynamic database.

Here we find/set the path to the projects.

Unfortunately not all tutorials are up to date.

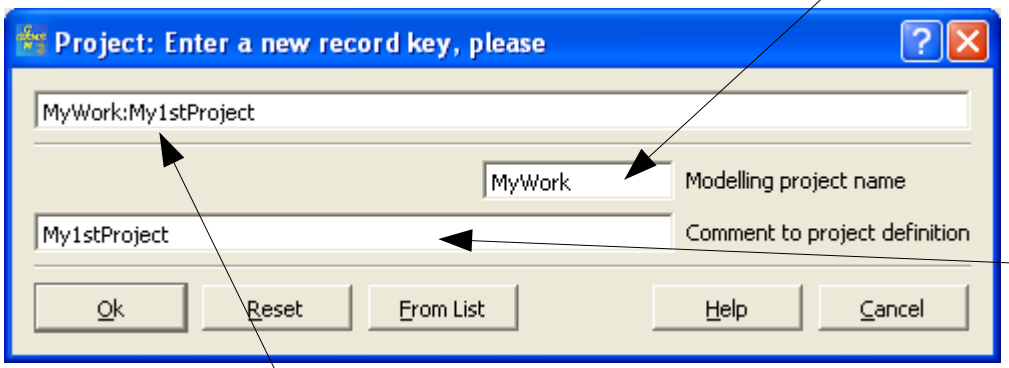
Choose “computation of equilibria” and get:



Existing example and old projects.

New projects start here:

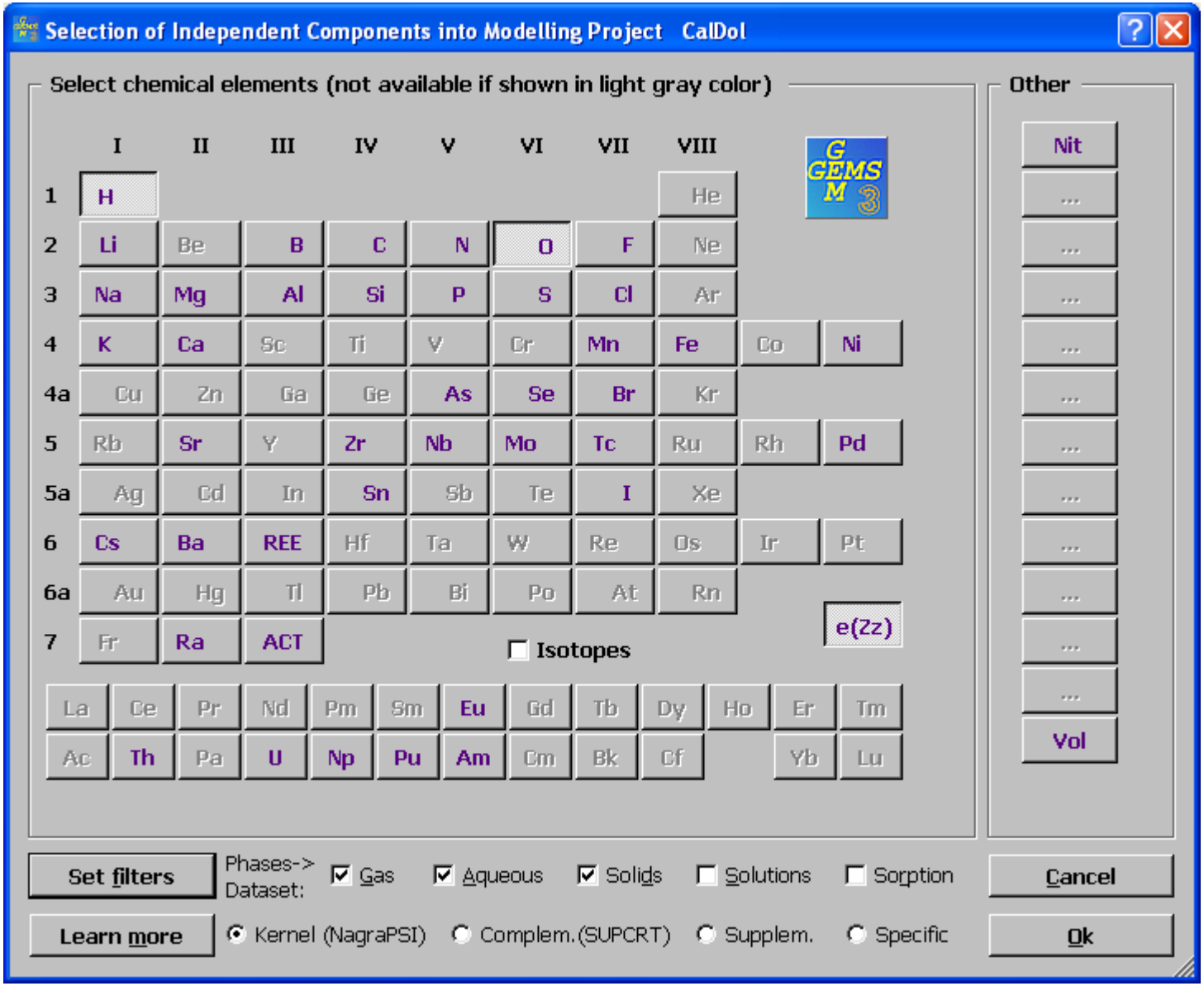
First we have to name the new project!



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.



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

For the calcite-dolomite example we need:

Calcite $CaCO_3$

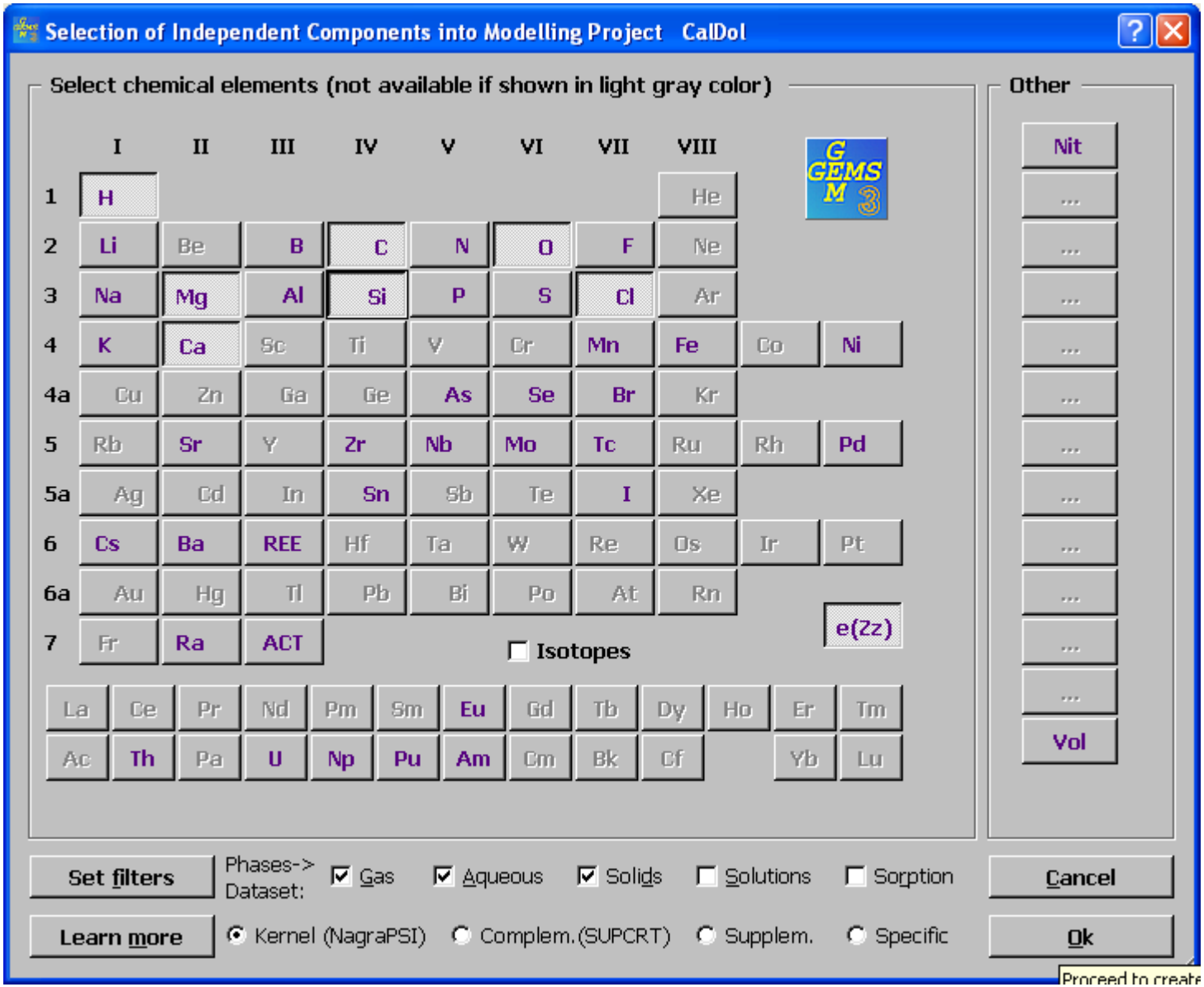
Dolomite $CaMg(CO_3)_2$

Quartz SiO_2 (the inert material of the porous medium)

Water (H_2O)

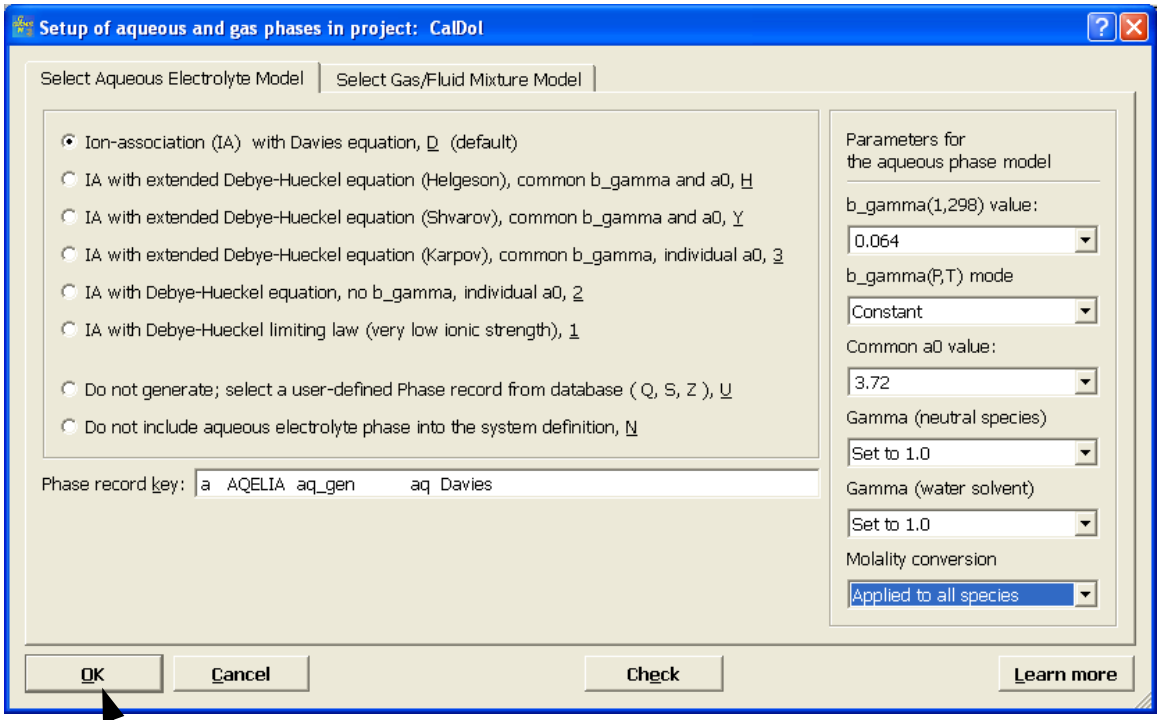
$MgCl_2$ (solution injected into the column)

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



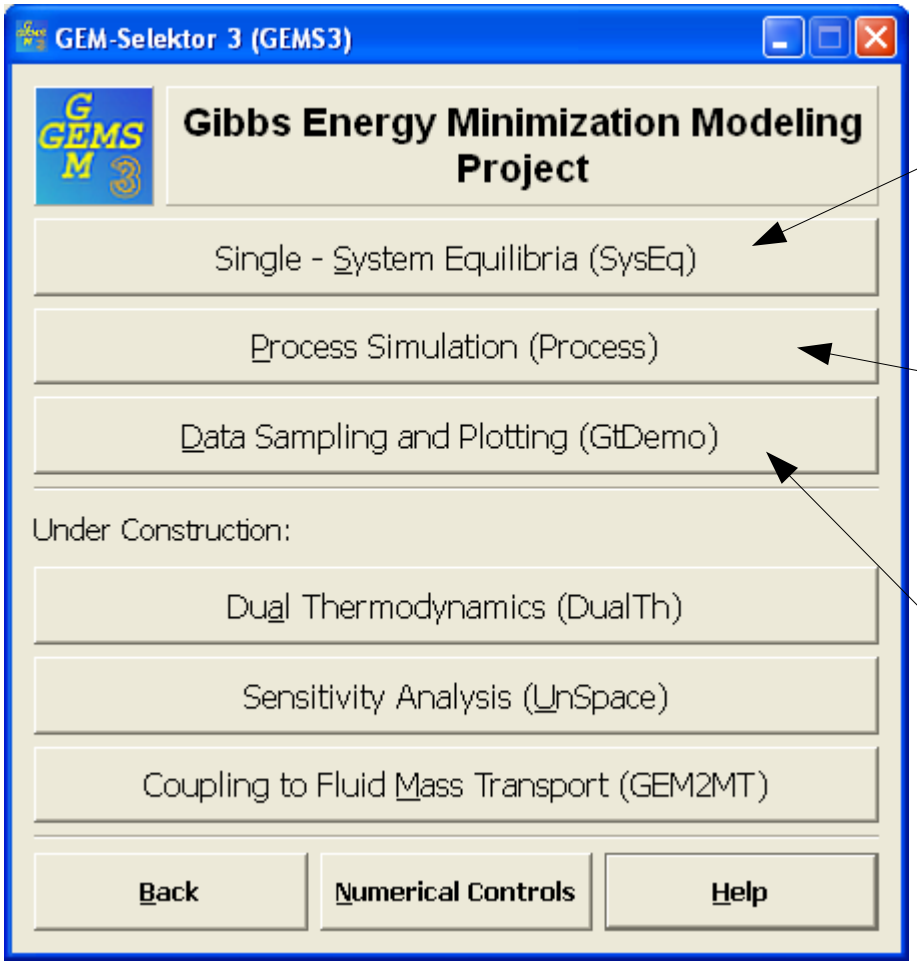
For the calcite – dolomite example choose: H, O, Ca, C, Mg, Cl & Si

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 out system(s).

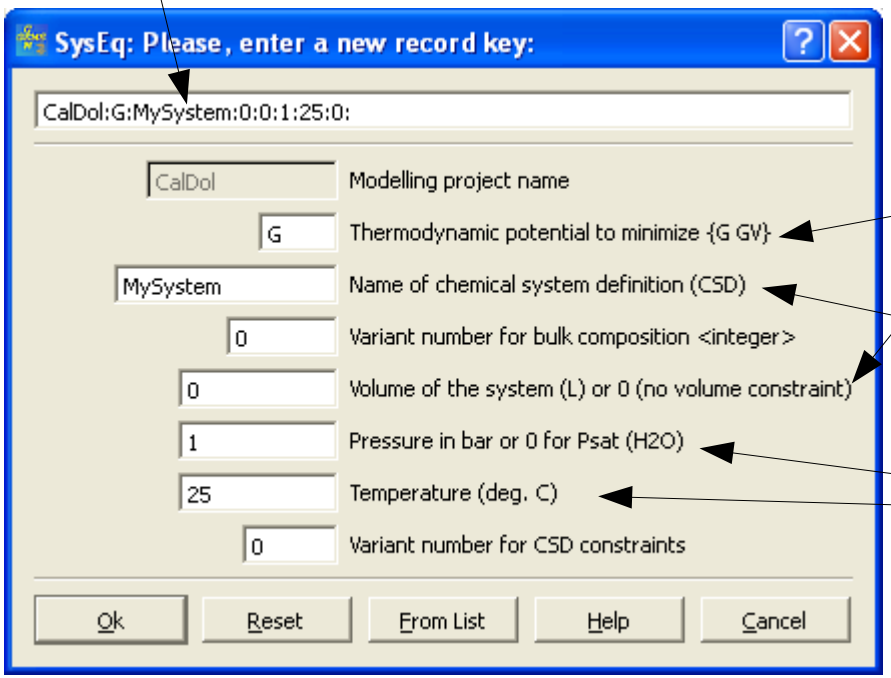
Process simulator (scripting language) for batch calculations (e.g. titration).

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.



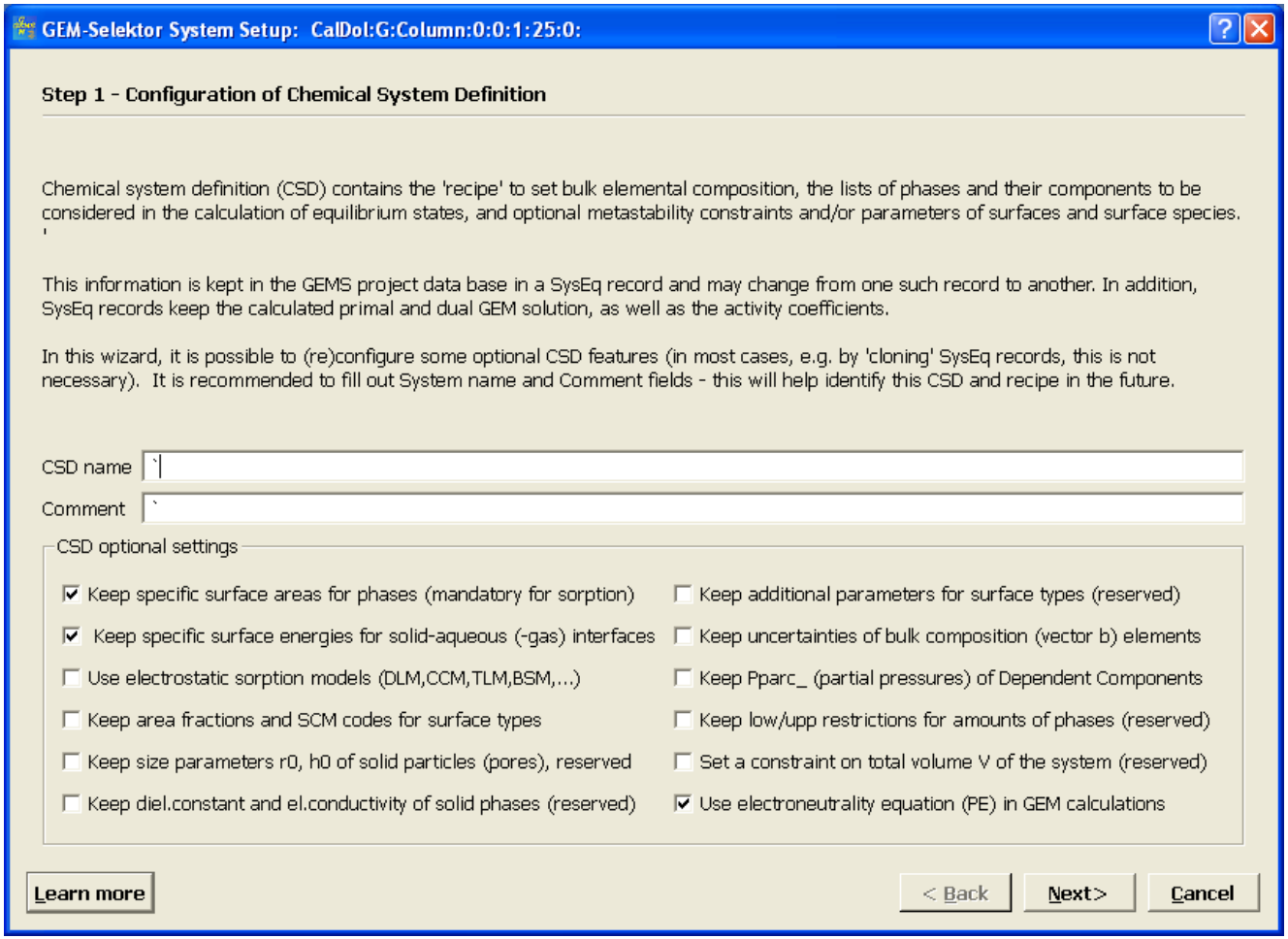
(parent) project

Do not change

Choose a meaningful name

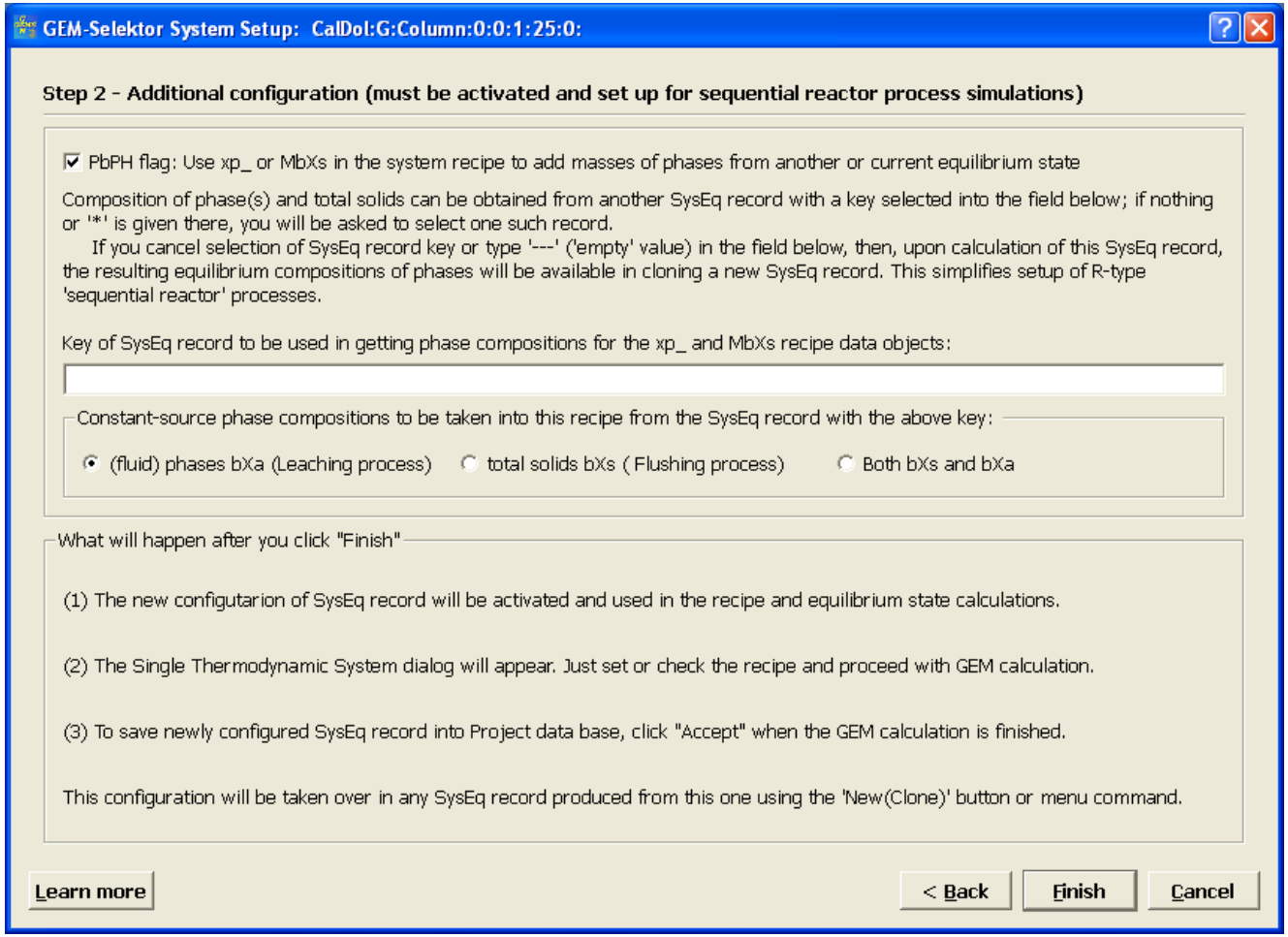
Possible to change

The first screen of the new Chemical System Definition Wizard

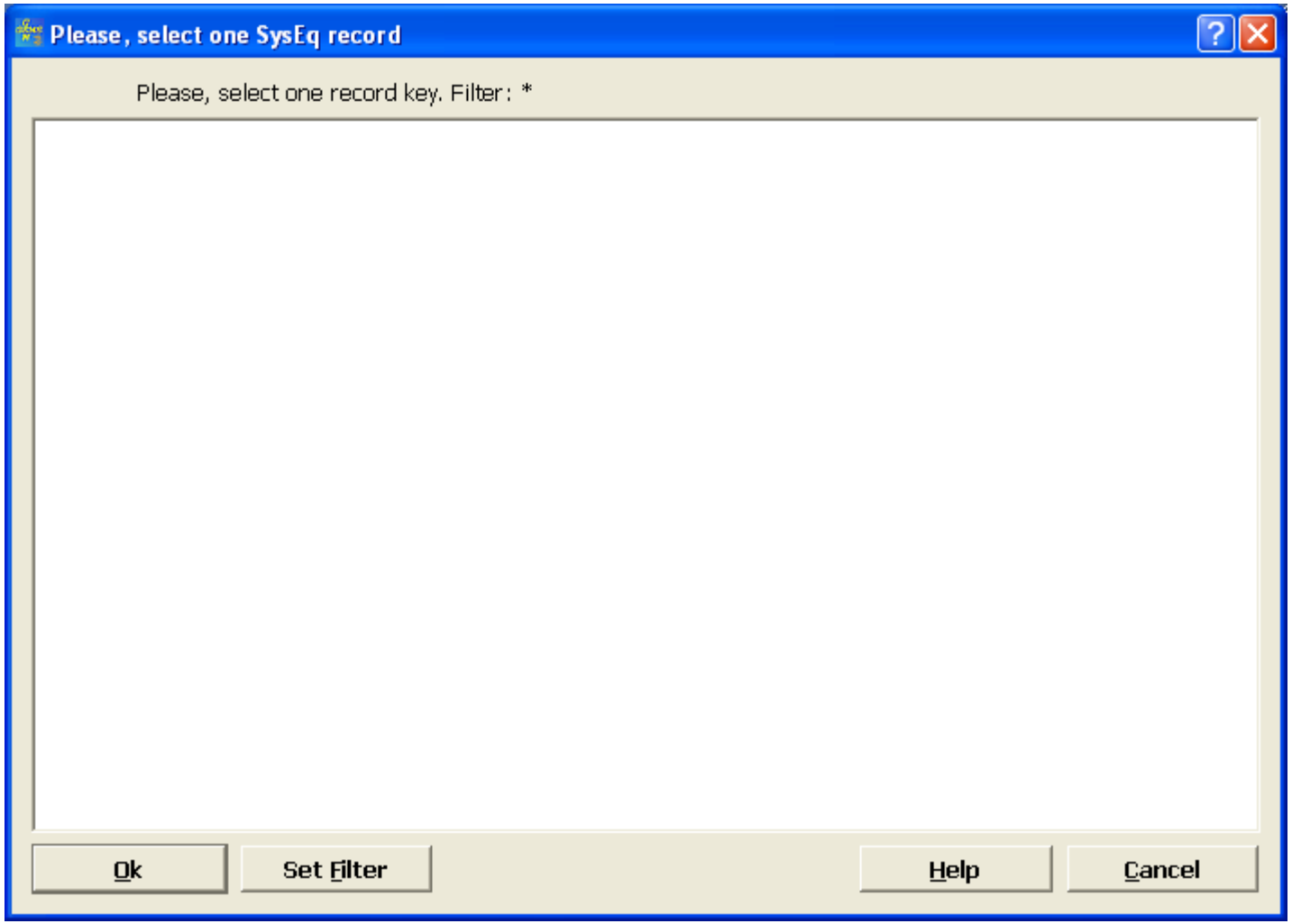


For our example only name and comment should be inserted.

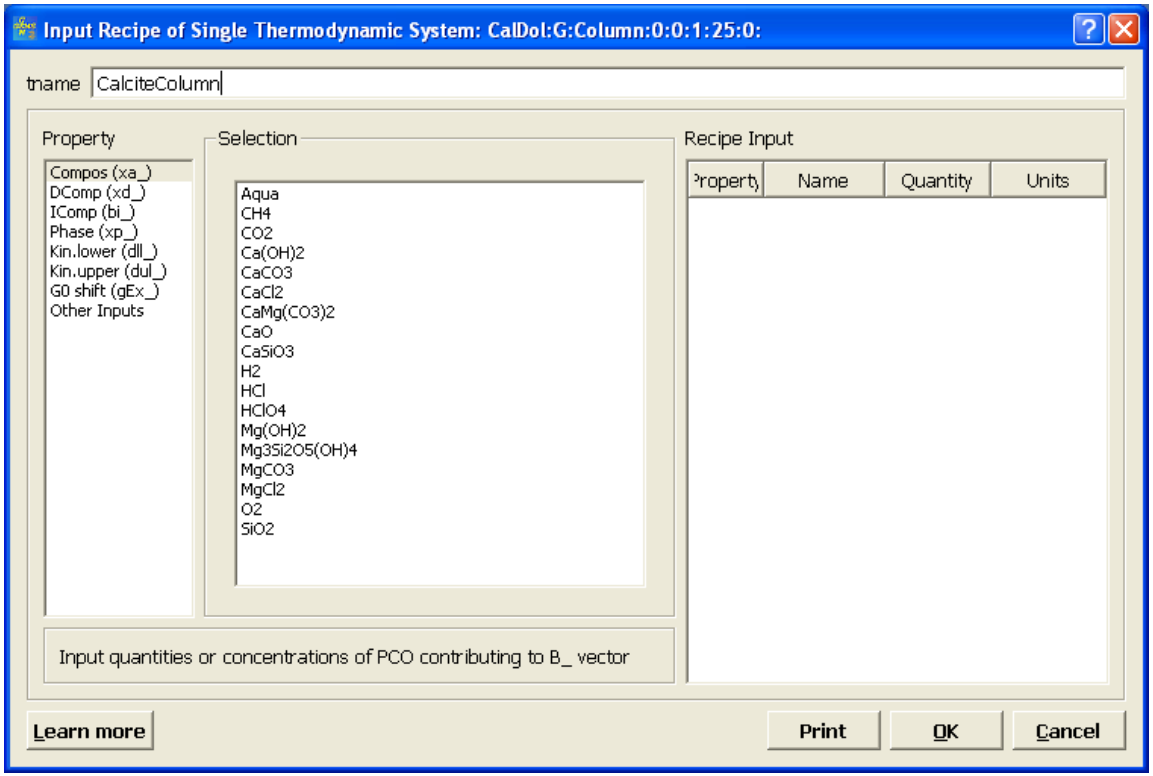
Read the lower part of the screen and press finish. No changes required for our specific setup.



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



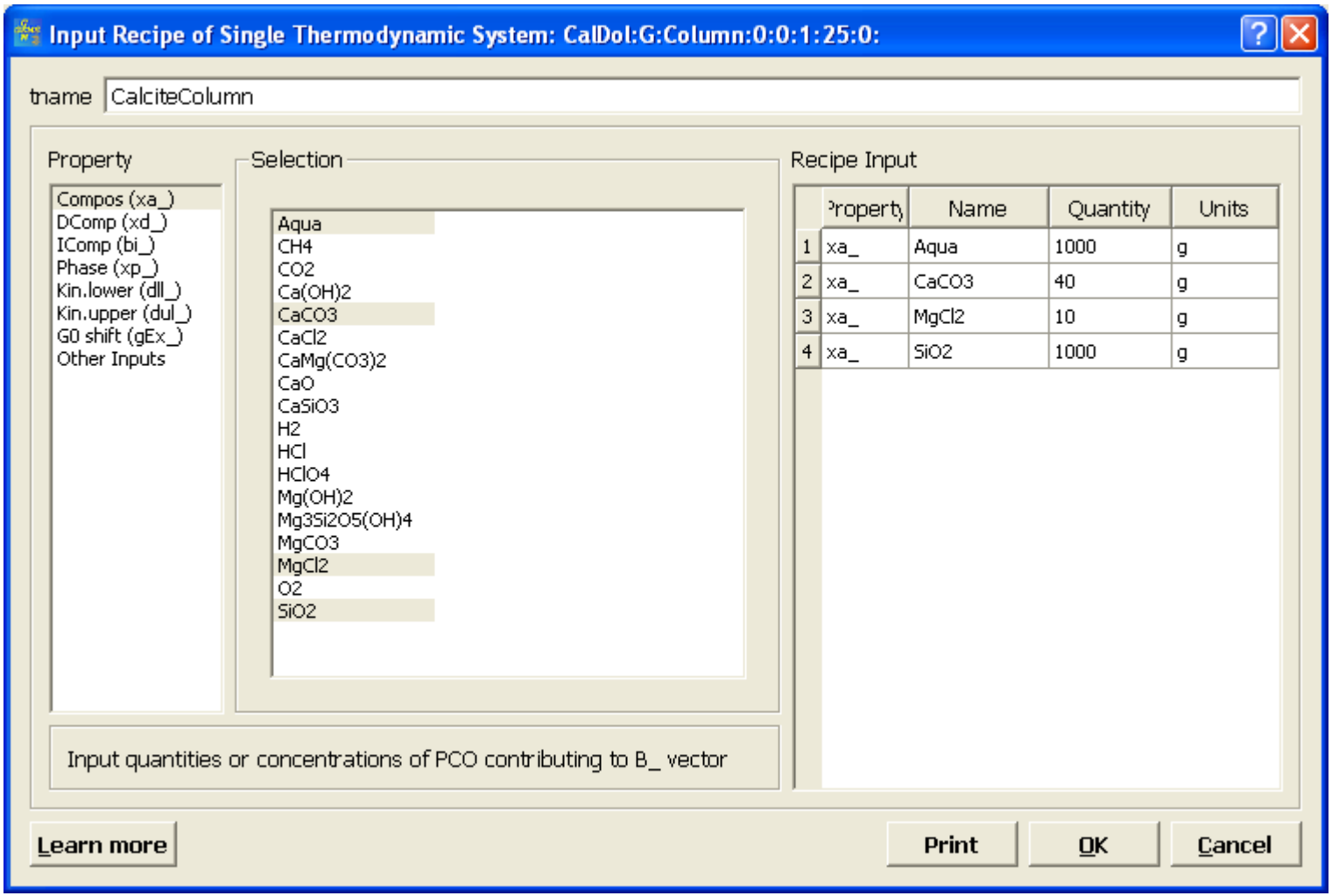
This is the new unified Thermodynamic System Dialog.
Everything we need to actually set up (mix) our initial system!



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))

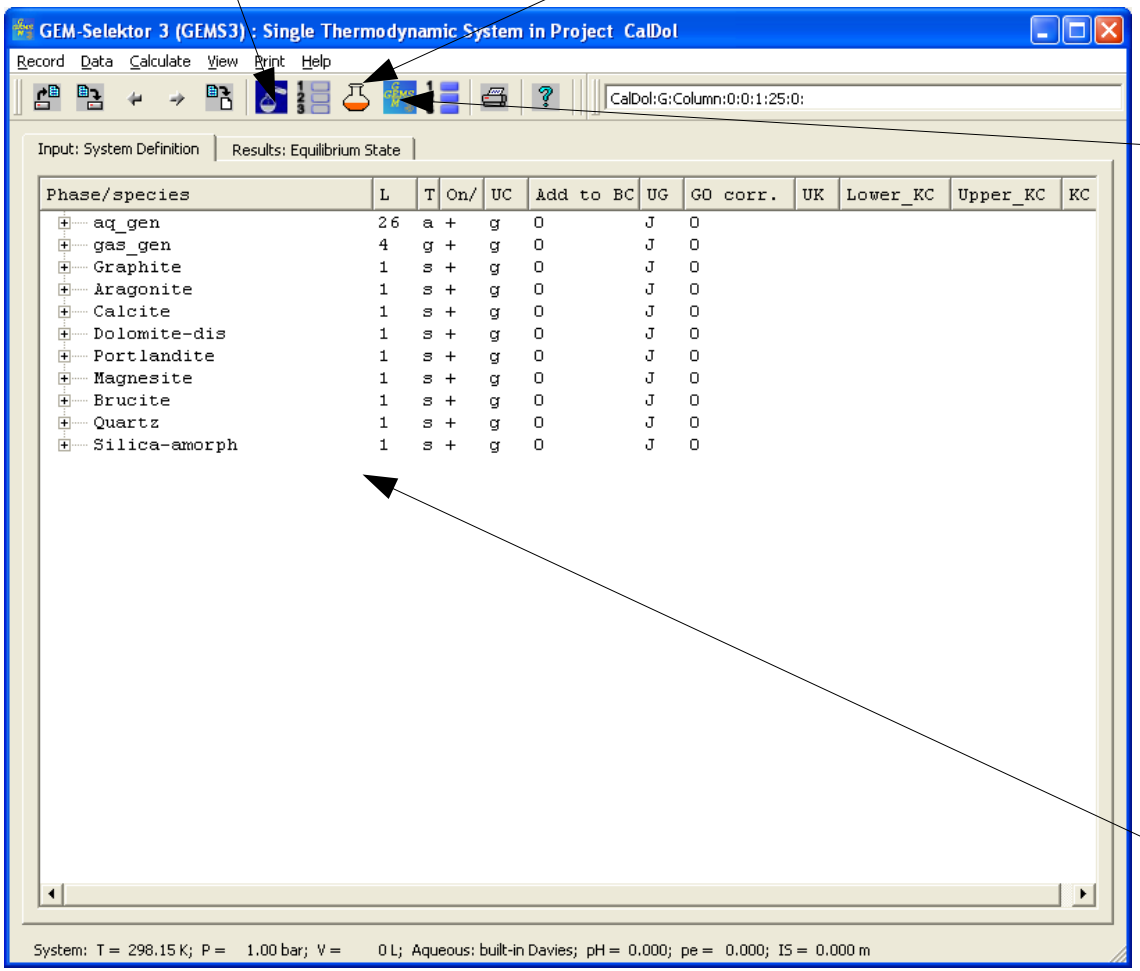
We start simple, just mix 1000 g of water, 40 g of calcite, 1000 g of quartz and 10 g of MgCl.



Finally: The main project calculation menu

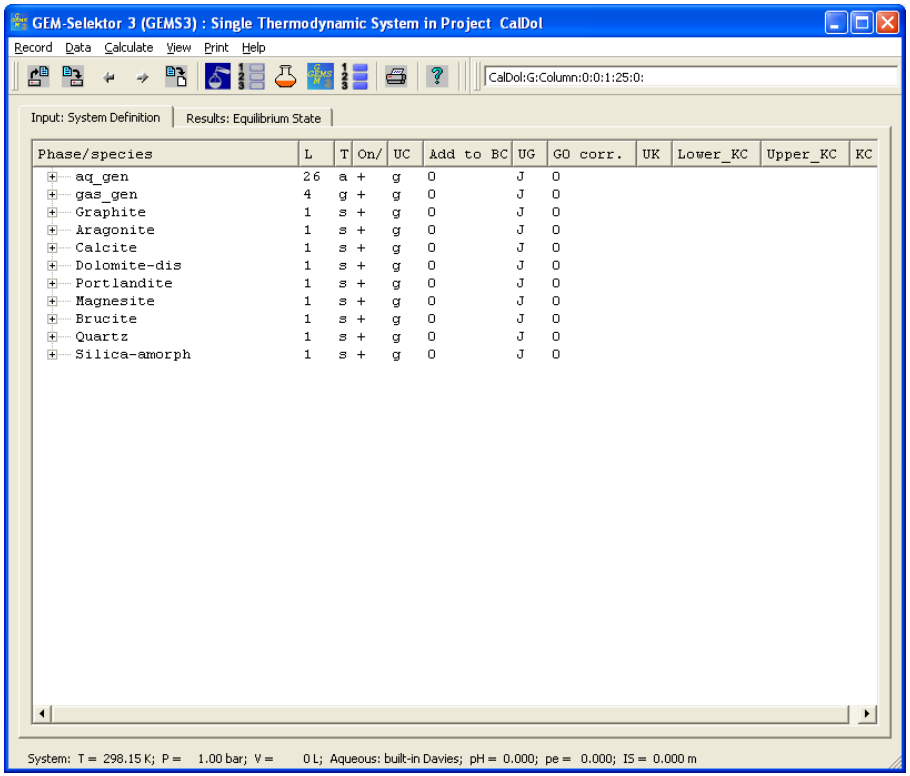
Recipe wizard

The “check if input composition is ok” button



The calculation button

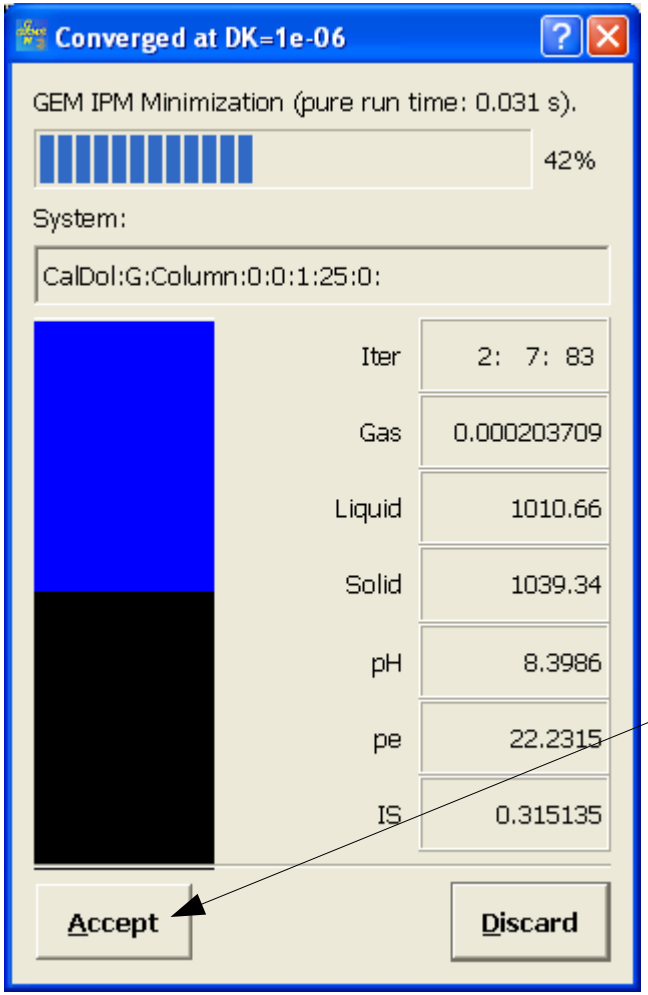
All the available phases for our project setup (depends on database)



For calculation:

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

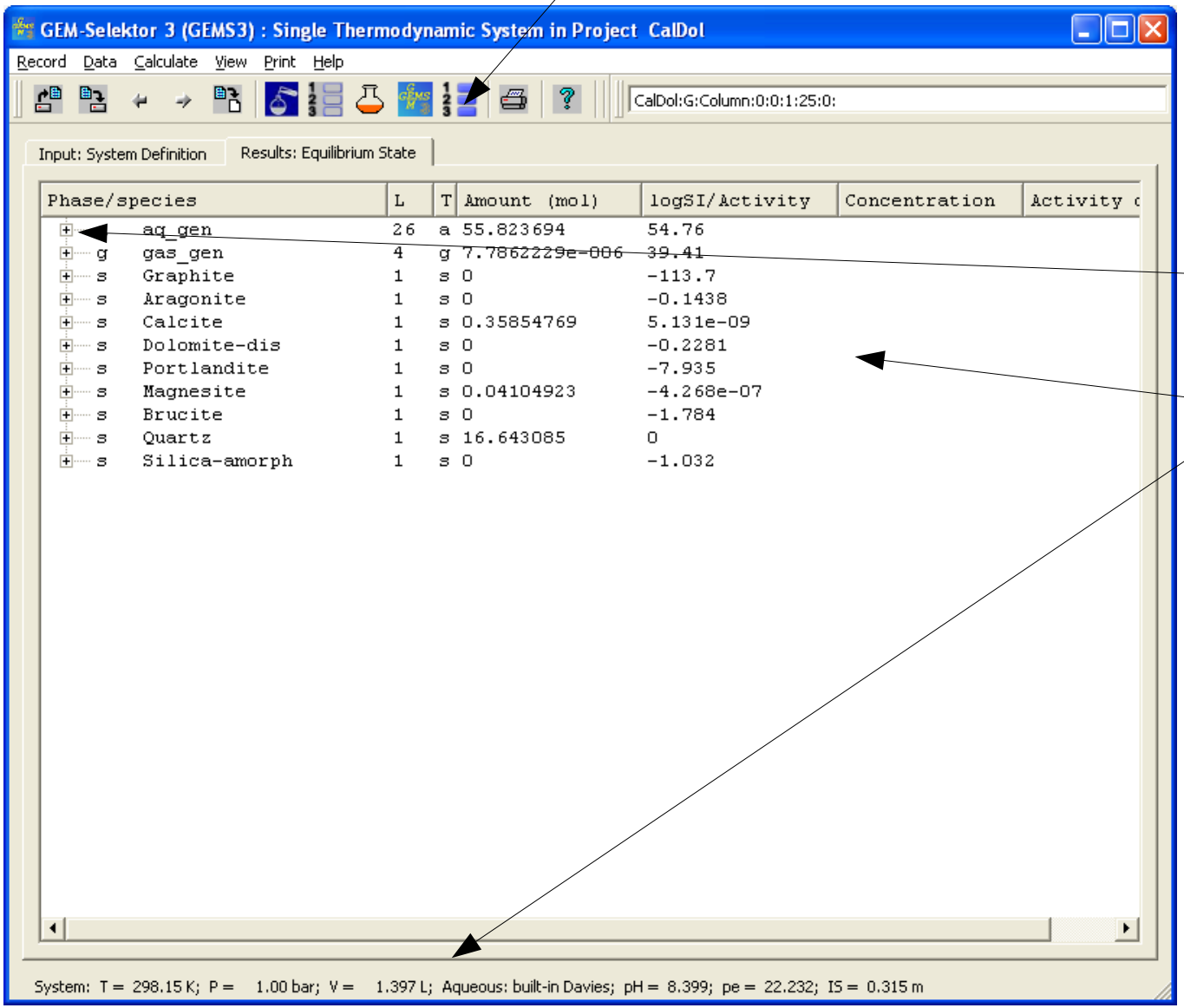
2) press the calculate button (gems symbol)



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

Press accept to continue.

More detailed results are here

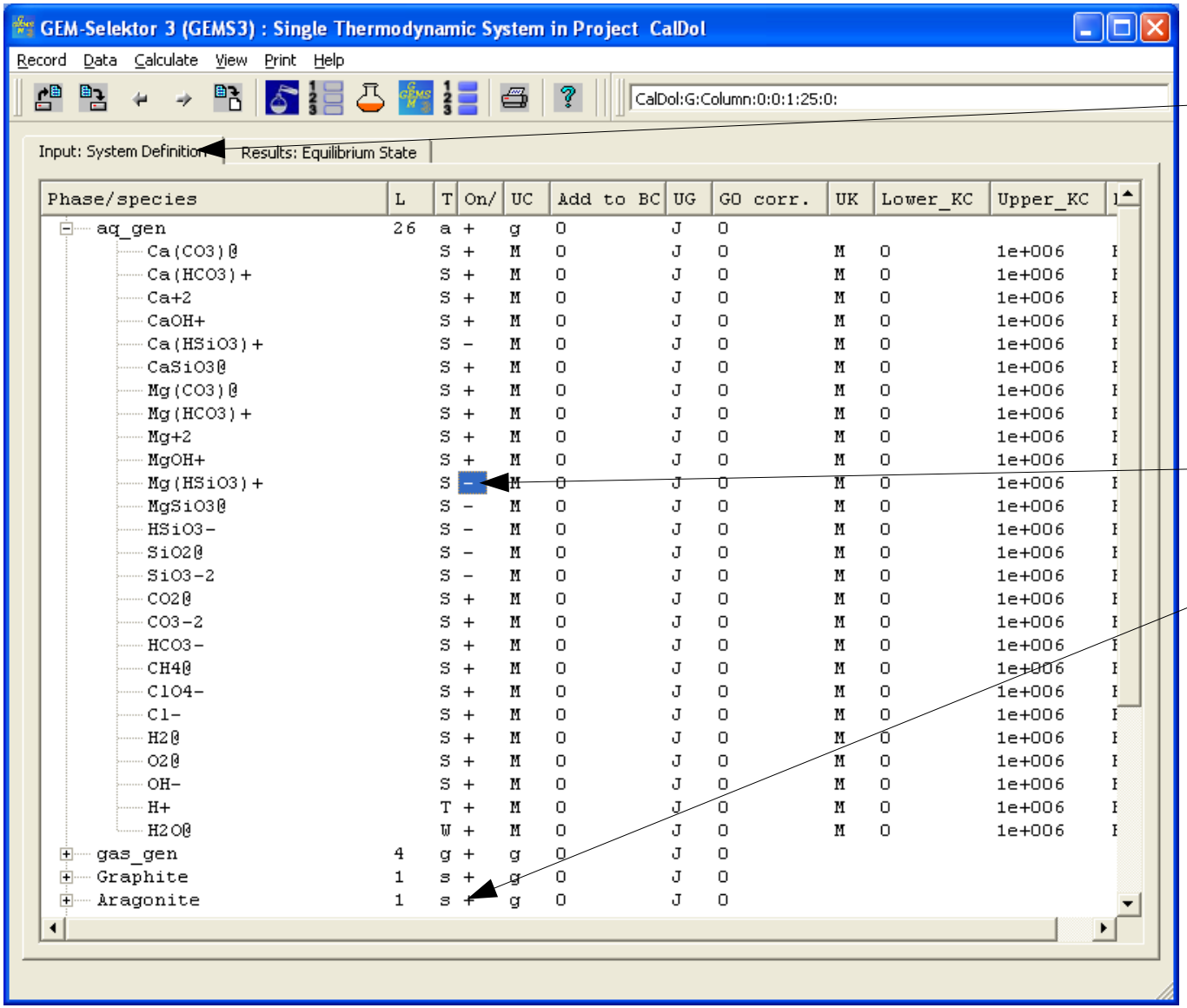


Expand phases to examine content.

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.



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(CO3)@		S	5.549629e-006	5.54955e-06	5.5496334e-006	0.999984
Ca(HCO3)+		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(CO3)@		S	8.3139204e-006	8.31379e-06	8.313927e-006	0.999984
Mg(HCO3)+		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
CO2@		S	1.4882358e-007	1.48821e-07	1.488237e-007	0.999984
CO3-2		S	1.3895857e-006	3.98863e-07	1.3895868e-006	0.28703732
HCO3-		S	3.2329006e-005	2.36631e-05	3.2329032e-005	0.73194657
CH4@		S	0	6.62842e-137	0	1
ClO4-		S	0	2.06678e-38	0	1
Cl-		S	0.21005977	0.153753	0.21005993	0.73194657
H2@		S	0	1.51672e-41	0	1
O2@		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
H2O@		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		

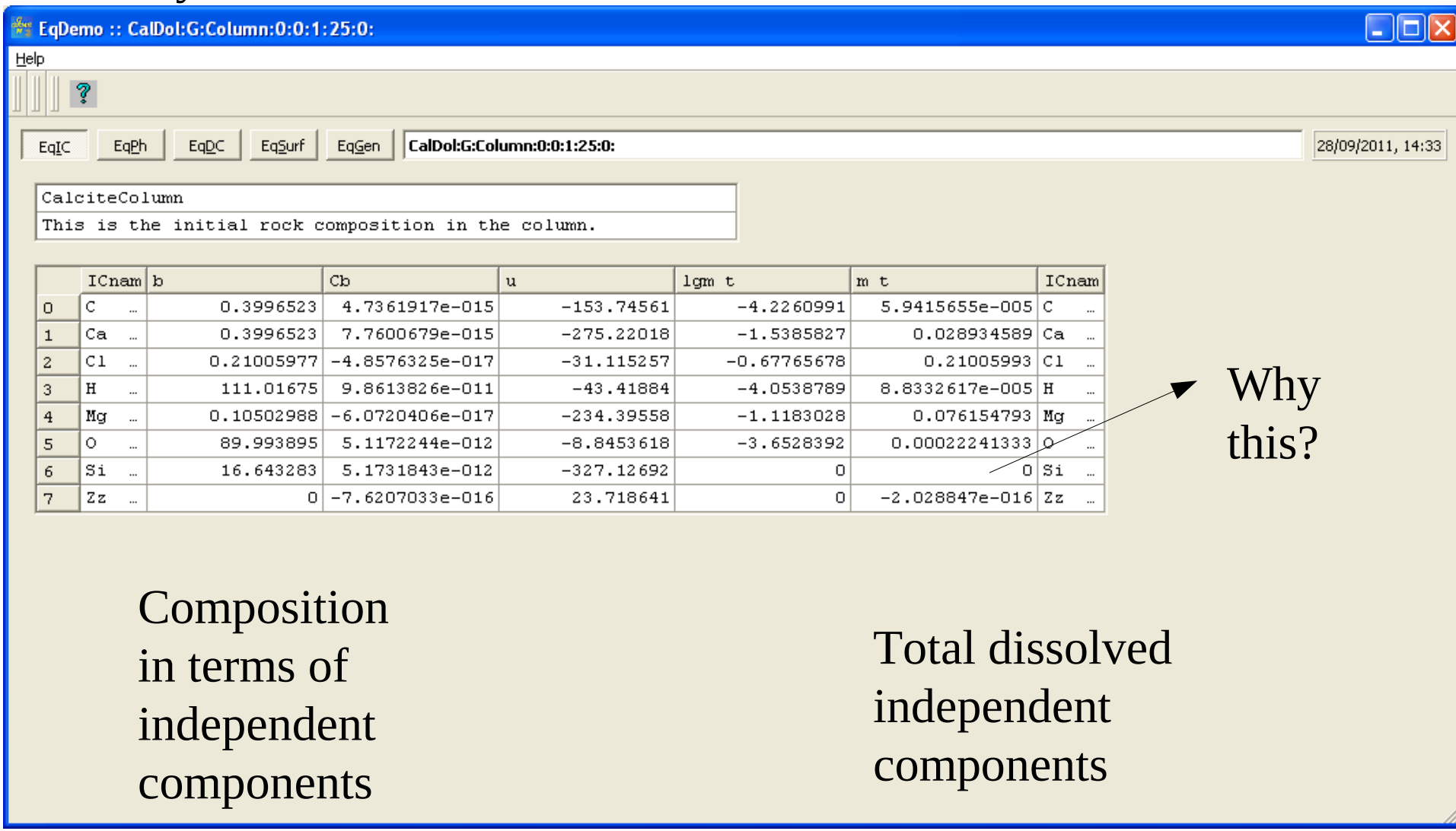
System: T = 298.15 K; P = 1.00 bar; V = 1.396 L; Aqueous: built-in Davies; pH = 8.556; pe = 10.301; IS = 0.315 m

After "check" and "calculate" we get the results.

Concentration of dissolved species

Mole amount of minerals

We may check the detailed results:



	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

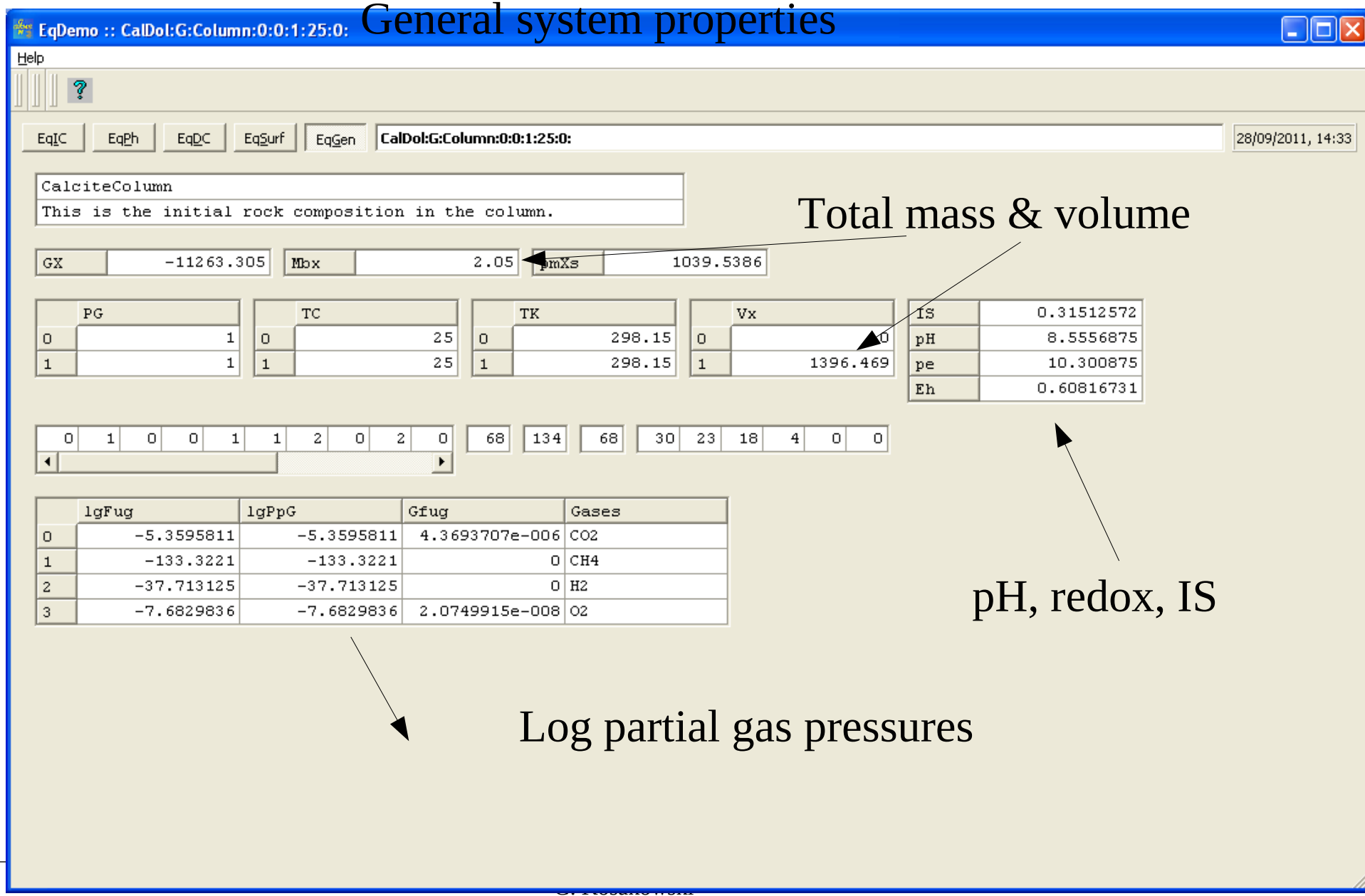
pmXs	1039.5386

	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	-1.7
1	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

Phase volumes and masses

General system properties



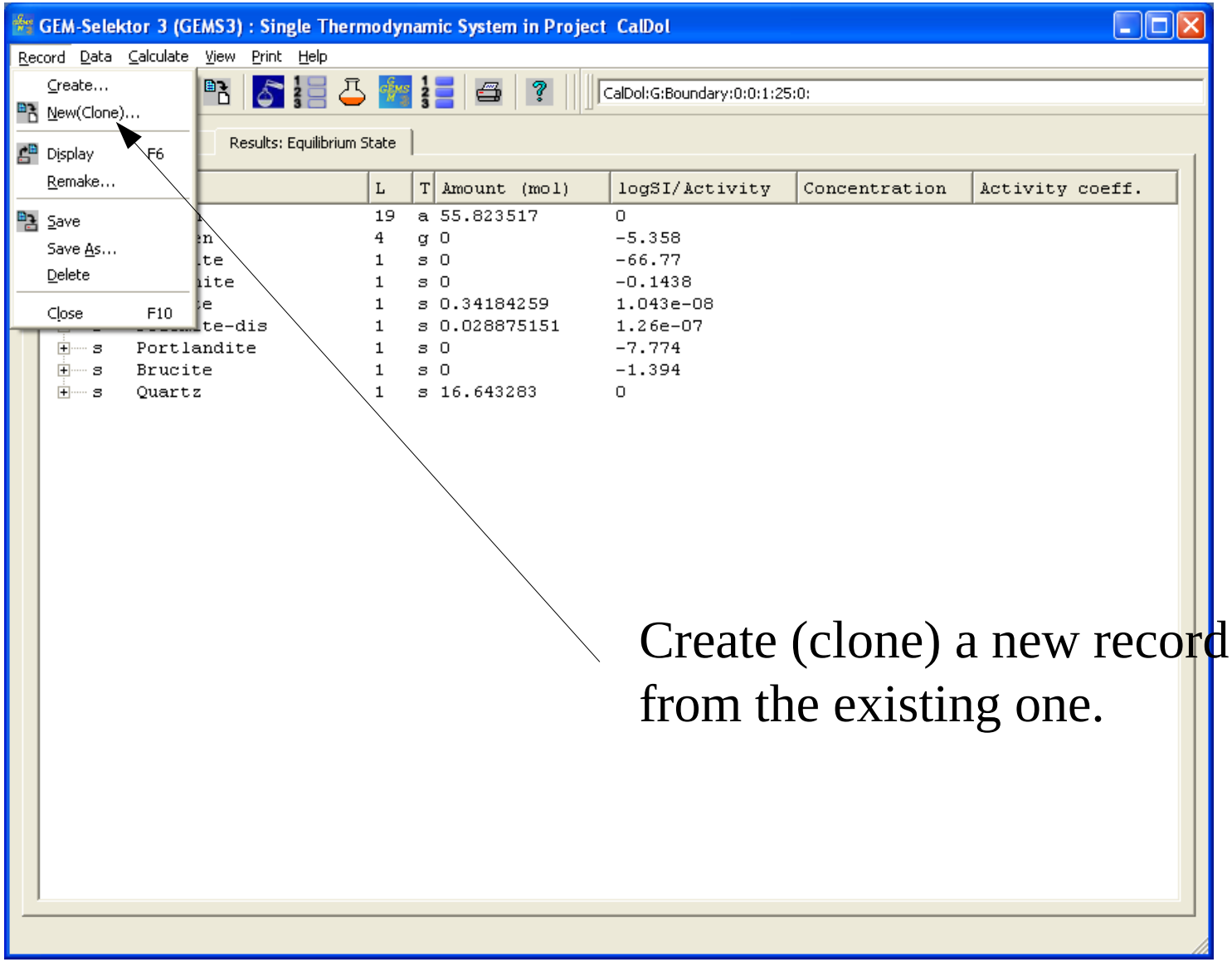
Total mass & volume

pH, redox, IS

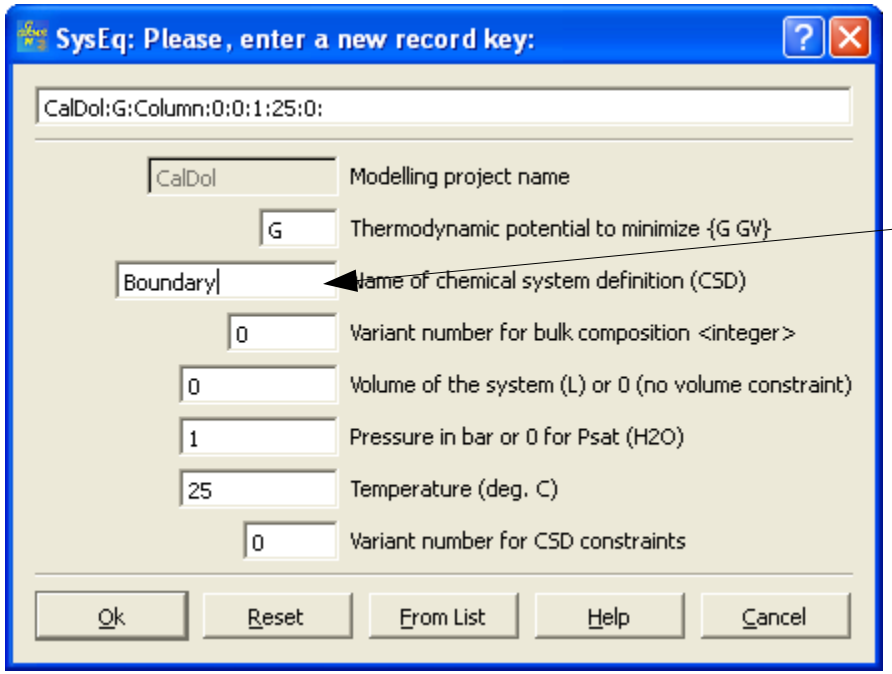
Log partial gas pressures

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

1) Reduce the amount of MgCl2 as much as possible (set to 1.0e-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 2.075e-4 mol per liter liquid (after equilibration)
4) Porosity (volumetric “water” = liquid phase content) 0.32 → achieve this by adjusting the amount of quartz



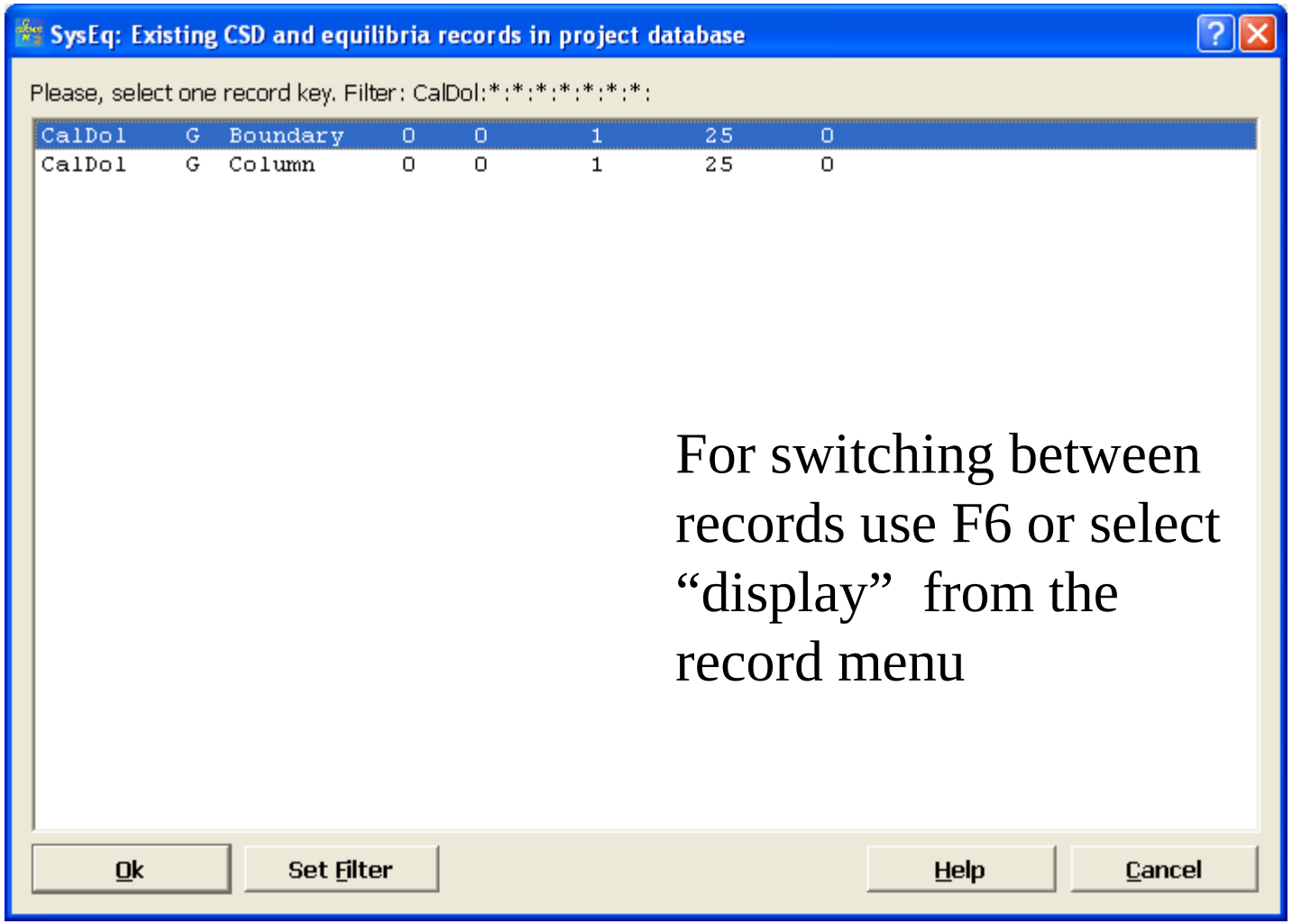
Create (clone) a new record from the existing one.



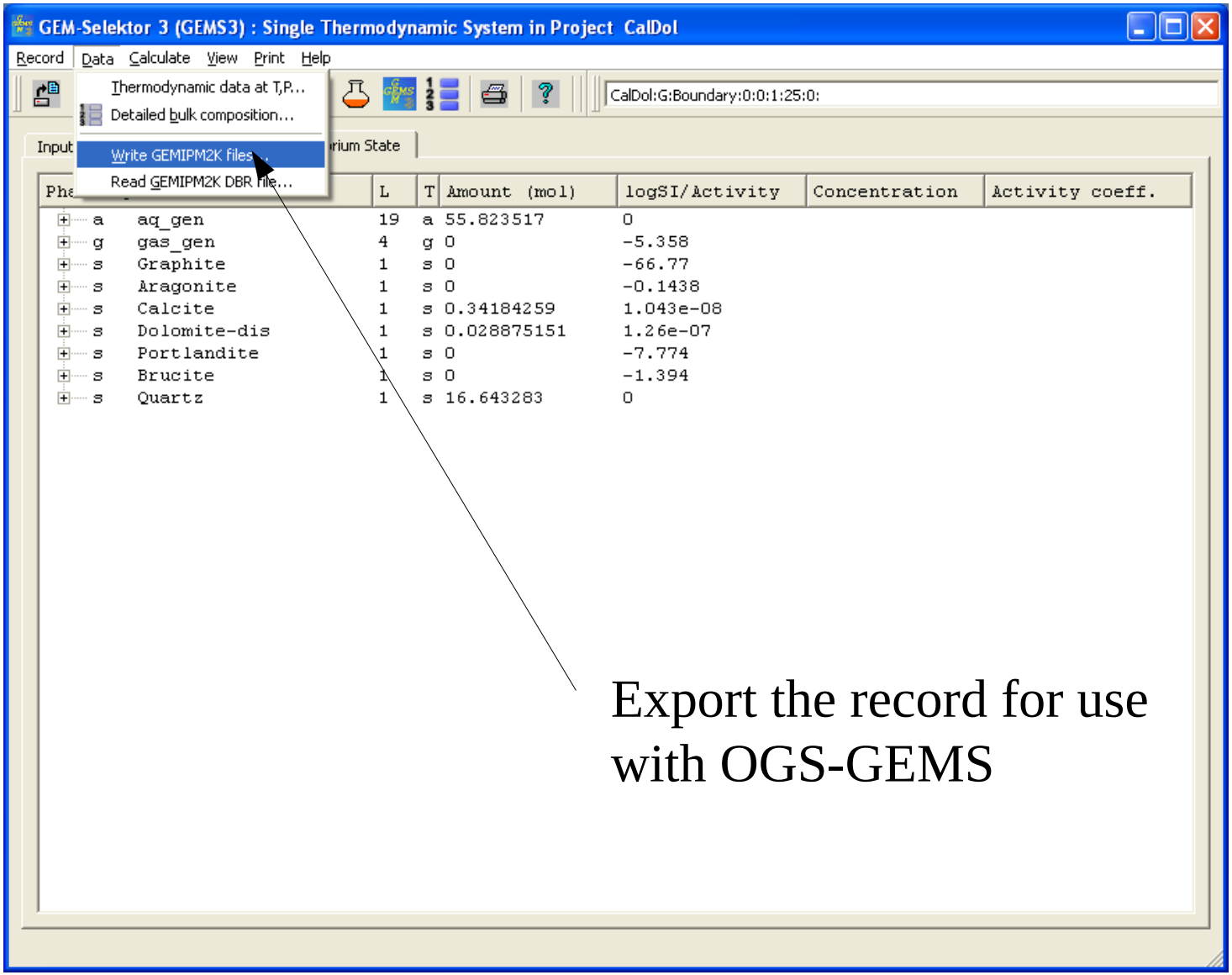
Change the name

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 1.0e-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) MgCl2 should be 1.0e-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



Export the record for use with OGS-GEMS

Pitfalls when setting put systems with GEMS:

Units!

→ concentrations: mol/(kg H_2O) vs. mol/l vs. mol/m^3

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.