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GEMS SELEKTOR

GEMS: Gibbs Energy Minimization Software for Geochemical Modeling

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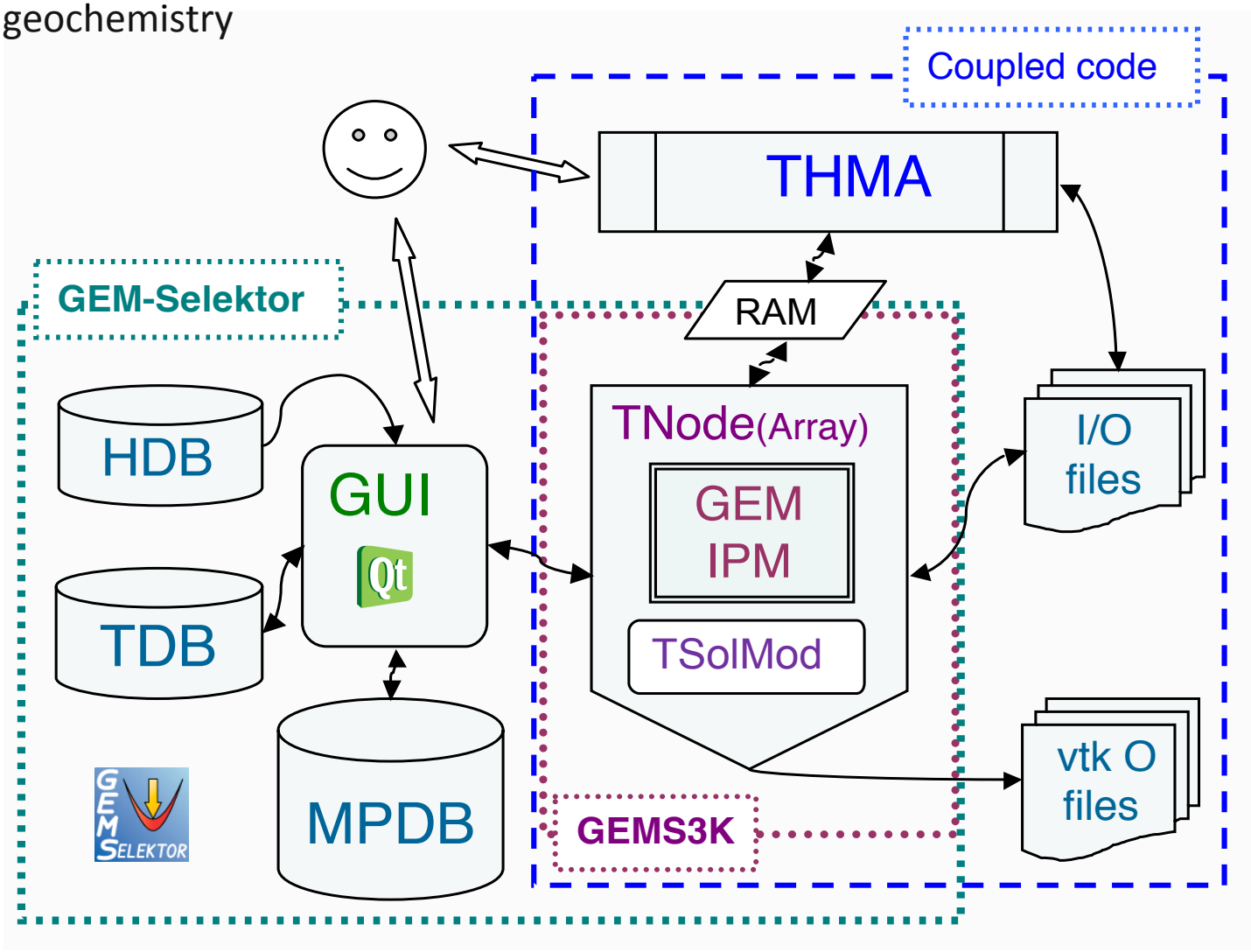
Motivation and Introduction

Geochemical thermodynamic modeling is relevant in geochemistry

To be efficient, it needs advanced software!

We offer **GEMS** - a software collection for modeling (geo) chemical processes in systems with:

- non-ideal fluids;
- condensed solutions;
- aqueous electrolytes;
- adsorption, ion exchange;
- many pure condensed phases;
- metastable species/phases.



From Kulik *et al.* (2013) *Comput. Geosci.* **17**, 1-24.

GEM-Selektor Code Package – Main Part of GEMS

GEM-Selektor v.3 can:

- perform forward- or inverse modeling tasks;
- plot or export the results;
- create GEMS3K input files per mouse-click.

The usage is organized in *modeling projects,* each keeping the input and the results for a given research application. Any project can be shared with others.

GEM-Selektor GUI integrates:

- GEMS3K solver of chemical equilibria;
- codes for calculating thermodynamic data at *T,P*;
- built-in script interpreter;
- database management system;
- graphic presentation dialogs;
- context-driven help browser;
- extensive help database and default TDBs.

Installers for PC (Windows XP, 7, 8; Linux; Mac OS X)

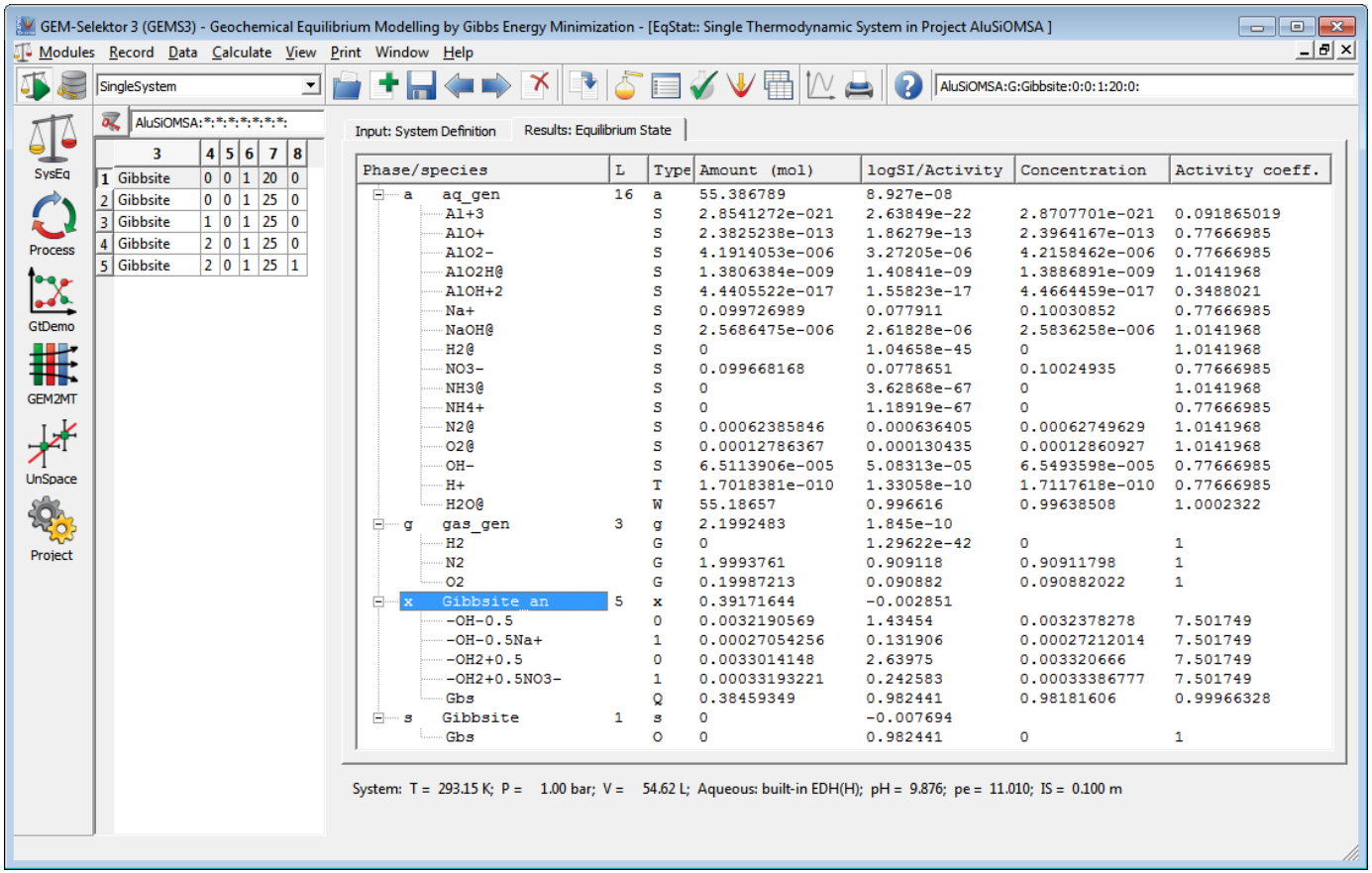
- Default TDBs
- Modular
- Interactive
- User-friendly
- HQ plots
- User scripts
- Runtime help
- Coded in C ++
- Built on Qt5

(www.qt -project.org)

Equilibria Calculation Mode

To set up and compute single equilibrium states, sequential processes, diagrams, or reactive transport simulations.

Single System Speciation Dialog



	3	4	5	6	7	8
1	Gibbsite	0	0	1	20	0
2	Gibbsite	0	0	1	25	0
3	Gibbsite	1	0	1	25	0
4	Gibbsite	2	0	1	25	0
5	Gibbsite	2	0	1	25	1

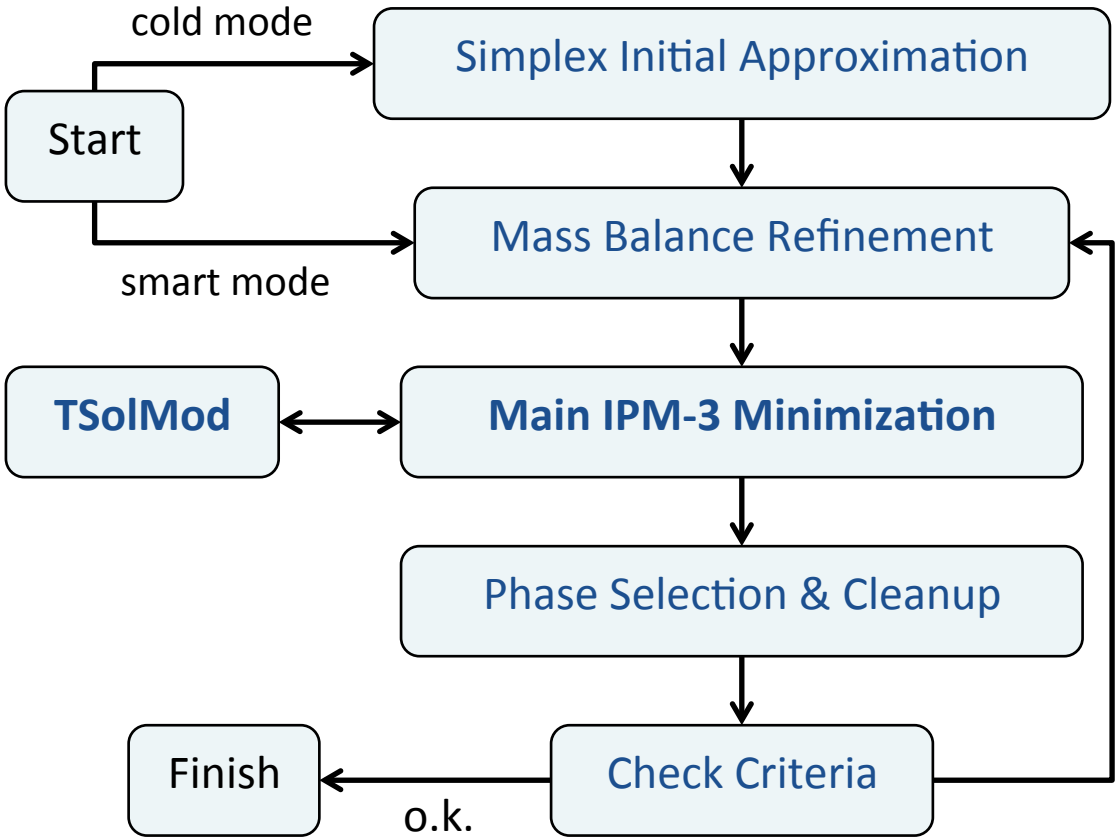
Phase/species	L	Type	Amount (mol)	logSI/Activity	Concentration	Activity coeff.
a aq_gen	16	a	55.386789	8.927e-08		
Al+3		S	2.8541272e-021	2.63849e-22	2.8707701e-021	0.091865019
AlO+		S	2.3825238e-013	1.86279e-13	2.3964167e-013	0.77666985
AlO2-		S	4.1914053e-006	3.27205e-06	4.2158462e-006	0.77666985
AlO2H@		S	1.3806384e-009	1.40841e-09	1.3886891e-009	1.0141968
AlOH+2		S	4.4405522e-017	1.55823e-17	4.4664459e-017	0.3488021
Na+		S	0.099726989	0.077911	0.10030852	0.77666985
NaOH@		S	2.5686475e-006	2.61828e-06	2.5836258e-006	1.0141968
H2@		S	0	1.04658e-45	0	1.0141968
NO3-		S	0.099668168	0.0778651	0.10024935	0.77666985
NH3@		S	0	3.62868e-67	0	1.0141968
NH4+		S	0	1.18919e-67	0	0.77666985
N2@		S	0.00062385846	0.000636405	0.00062749629	1.0141968
O2@		S	0.00012786367	0.000130435	0.00012860927	1.0141968
OH-		S	6.5113906e-005	5.08313e-05	6.5493598e-005	0.77666985
H+		T	1.7018381e-010	1.33058e-10	1.7117618e-010	0.77666985
H2O@		W	55.18657	0.996616	0.99638508	1.0002322
g gas_gen	3	g	2.1992483	1.845e-10		
H2		G	0	1.29622e-42	0	1
N2		G	1.9993761	0.909118	0.90911798	1
O2		G	0.19987213	0.090882	0.090882022	1
x Gibbsite_an	5	x	0.39171644	-0.002851		
-OH-0.5		0	0.0032190569	1.43454	0.0032378278	7.501749
-OH-0.5Na+		1	0.00027054256	0.131906	0.00027212014	7.501749
-OH2+0.5		0	0.0033014148	2.63975	0.003320666	7.501749
-OH2+0.5NO3-		1	0.00033193221	0.242583	0.00033386777	7.501749
Gbs		Q	0.38459349	0.982441	0.98181606	0.99966328
s Gibbsite	1	s	0	-0.007694		
Gbs		O	0	0.982441	0	1

Recipe Wizard: Easy setup of system bulk chemical composition from Predefined Composition Objects (PCO), stoichiometries of species, phases; amounts of elements

GEMS3K Speciation Solver (for Coupled Codes)

Solves for equilibria in complex geochemical systems with many highly non-ideal solutions (includes the TSolMod library of models of mixing in phases)

- Yields speciation and activities in all phases
- Chemical potentials
- Phase stability indexes
- Selects stable phases
- Refines mass balance
- Keeps metastable phases
- Is robust (with cold start)
- Is fast (with smart start)



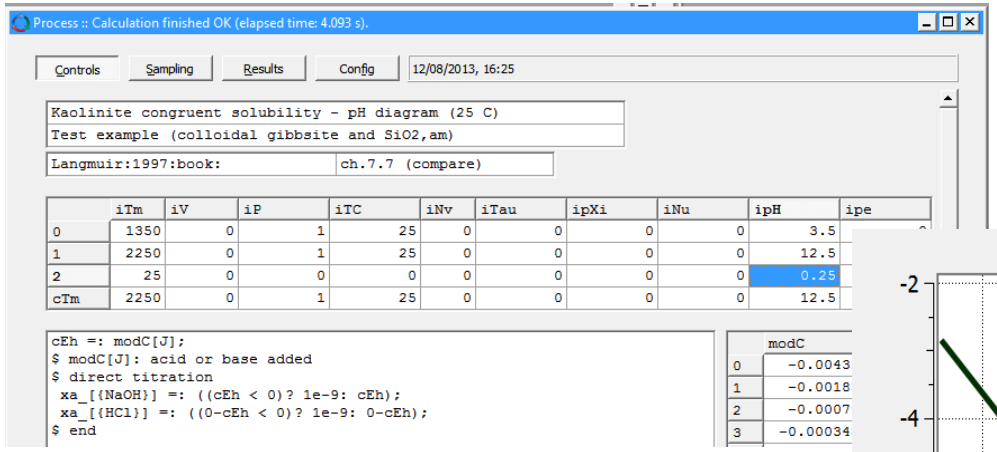
Written in C/C++, open-source, portable, runs on parallel systems; is fit for RMT codes.

Fast GEM IPM-3 convex programming algorithm

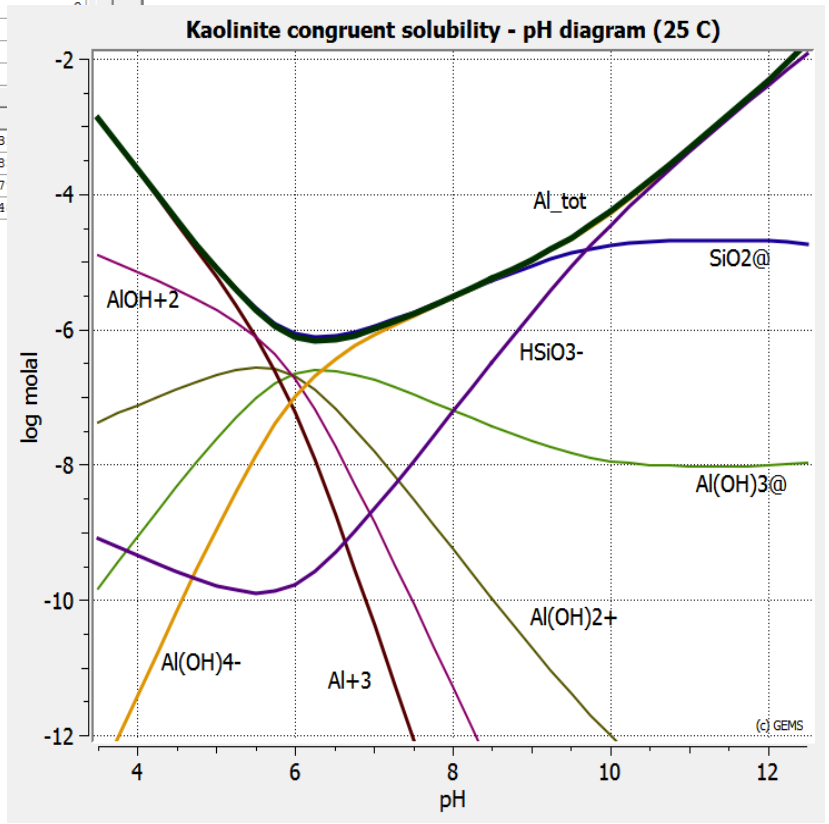
[Karpov *et al.* (2001) *Geochem. Internat.* **39**, 1108-1119]
[Kulik *et al.* (2013) *Comput. Geosci.* **17**, 1-24]

Process Simulators in GEM-Selektor

Titration-, Reaction-Extent and Path Diagrams



GtDemo:
Data samplers
(for any data in
project database)



- Forward and inverse titrations
- Easy flow-through simulations
- User-defined process-control and data-sampling scripts
- Process remake wizards generating simple scripts for various scenarios
- Tabulation, copy-paste of results
- Plotting over the experimental data
- Saves bitmap or HQ vector plots

Database Mode of GEM-Selektor

To add or manage data records for: elements; compounds; phases; compositions; systems; processes; tabulators; projects; bib.references; etc.

DComp: Thermochemical/EoS data record format for the Dependent Components (DC, compounds, species)

ReacDC: Reaction-based DC data record format. Can refer to DComp or other ReacDC records (up to 6 levels of recursion).

Gets standard-state properties of 'new' DC from properties of the reaction and that of other DCs. Various *T* extrapolations of the properties of 'new' DC.

IComp: Core data for elements or Independent Components (IC)

RTParm: Tabulates and plots *T,P* trends for one Dcomp or ReacDC

ReacDC :: Reaction-defined data format for Dependent Components (species)

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UO2(CO3)2-2 aqueous complex
U|6|O2(CO3)2-2

	SC DC		REsDC			
0	-1	d	a	U+6	UO2+2	anp
1	-2	d	a	wC+4	CO3-2	bnp
2	1	n	a	U+6	UO2(CO3)2-2	cnu

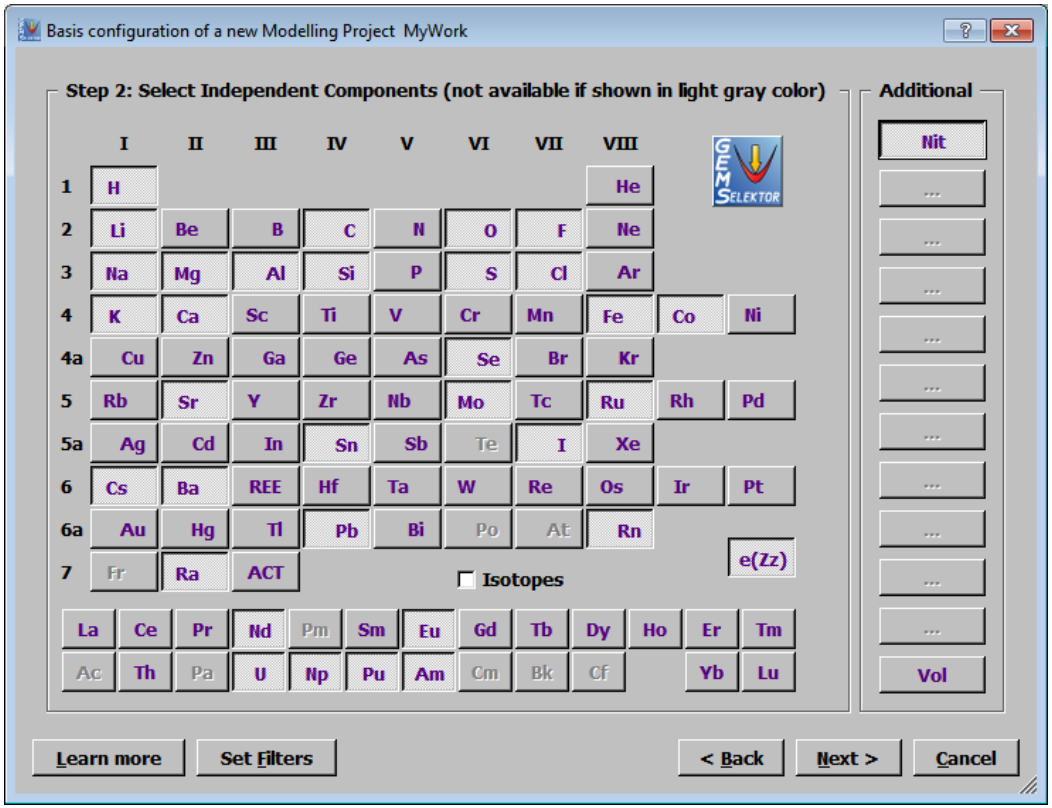
V0r	0.681667	0	---
logKr	4.0738028e+016	16.61	0.09
G0r	-94810.578	-2103387.6	---
H0r	18500	-2351221	---
S0r	380.046	181.724	---
Cp0r	0	-540.595	---
NisoX	---	---	---

PrTr	1	25	M0	390.046	-2
BetAl	---	---	ab	4	---

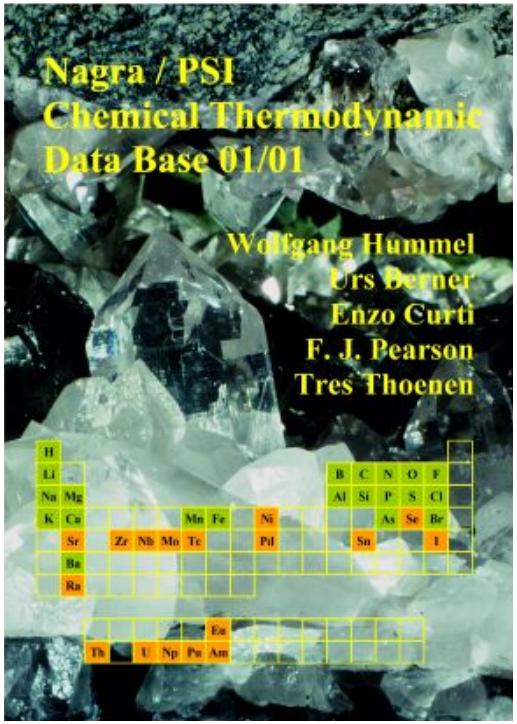
JULY_GEMS:2009:dat: | logK, dHr

Default ThermoDynamic Databases

New modeling projects can easily be created using default TDBs.



PSI/Nagra 12/07 TDB
[Thoenen ea, this conference]



log*K* at 1 bar 25 C , enhanced with *T,P* corrections from SUPCRT

3rd-party: Cemdata'07

www.empa.ch/cemdata

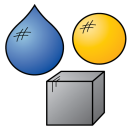
3rd-party: HERACLES

www.psi.ch/heracles/heracles

Complementary: SUPCRT (Slop98)

www.asu.edu/geopig

Phase Definitions: Connections to Chemistry



Realistic models of phases for realistic systems!

- Aqueous electrolyte (ion-association or SIT)
- Gas (fluid) mixture; plasma
- Solid solutions, liquid solutions, melts
- Sorption (+ surface species), ion exchange
- Non-ideal mixing in solution phases
- Models of mixing: built-in, or user scripts
- Pure condensed phases
- Particulate/porous phases
- Phases are constructed from DCs
- Ideal gas mixture and ion-association aqueous phase are automatically assembled when opening the modeling project

a:SIT_1:aq_sit:aq:nagra-psi_:

Phase :: Definition of thermodynamic phase

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Ph ncp	4	2	Ph npx	2	Ph nsi	0

	ipxT	ipxT	ph cf[0]	ph cf[1]
0	2	14	0.09	0
1	14	4	0.04	0
2	5	0	0.89	0
3	1	3	0.91	0

0	a	Ca	Ca+2	...
1	a	Ca	CaOH+	...
2	a	K	K+	...
3	a	K	KOH@	...
4	a	Na	Na+	...
5	a	Na	NaOH@	...
6	a	wCl+7	ClO4-	...
7	a	wCl-1	Cl-	...
8	a	wH0	H2@	...
9	a	wN+5	NO3-	...
10	a	wN-3	NH3@	...
11	a	wN-3	NH4+	...
12	a	wN0	N2@	...
13	a	wO0	O2@	...
14	a	wX	OH-	...
15	a	w_	H+	...
16	a	w_	H2O@	...

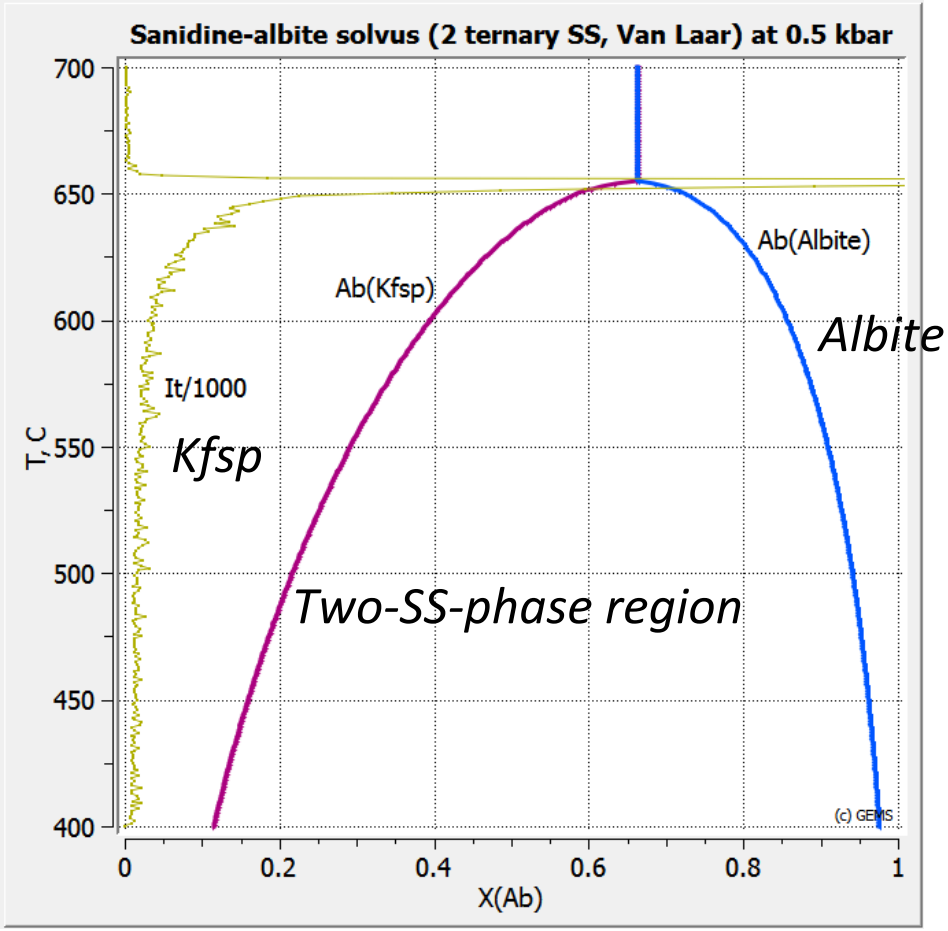
Compos: Predefined Composition Object (PCO) records (e.g., rock, fluid) to simplify Chemical System Definitions (CSD), as well as Process simulation control scripts.

TSolMod library: Models of Mixing in Phases

Provides >25 built-in non-ideal fluid, gas, liquid, and solid solution models. Connects GEMS to a wide range of geochemical, petrological, material science, and chemical engineering applications [Wagner *et al.* (2012) *Can. Mineral.* **50**, 1173-1195]

- Open C++ design for easy extension with new activity or EoS models.
- Generic and flexible interaction parameter exchange protocol.
- Efficient parameter transfer from Phase records to GEMS3K solver code via the IPM I/O file.
- Multi-site (sublattice) solid solutions can be processed.

Always under extension (now with integral phase properties; specific solid solution models for rock-forming minerals).



System: Aq phase + 2 ternary SS

On-going and Future Development

TKinMet library: Kinetic rate laws of mineral-aqueous reactions.

TSorpMod library: Sorption models with linked phase metastability.

GEMSFIT: Generic parameter-fitting code coupled with GEMS3K.

GEMSPHAD: Phase diagram plotting engine coupled to the GEMS4K code with the even faster and numerically more robust GEM IPM-4 algorithm.

Licenses and Availability

- GEM-Selektor v.3 package can be downloaded free of charge and used “as is” in the public interest and for the advancement of science.
- GEMS3K standalone code (including the TSolMod library) is available open-source under the **LGPL v.3** license in order to promote its use in coupled reactive transport codes, also on high-performance computers.

Get GEMS from **http://gems.web.psi.ch** (>3000 downloads to date)

Our goal: To make GEMS the software of choice!

Acknowledgments: Nagra, Wettingen; SNSF; CCES; ETHIIRA for partial financial support. Thanks to Gillian Grün for designing the GEMS logo and icons used in GEMS GUI.