GEMS: Gibbs Energy Minimization Software for Geochemical Modeling

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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.

GEM-Selekotor 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-Selekotor 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.

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
Process Simulators in GEM-Selektor

Titration-, Reaction-Extent and Path Diagrams

- 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

GtDemo:
Data samplers (for any data in project database)
Database Mode of GEM-Selektor

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

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

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

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.
Default ThermoDynamic Databases

New modeling projects can easily be created using default TDBs.

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

logK 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

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


- 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.

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**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](http://gems.web.psi.ch)  (>3000 downloads to date)
Our goal: To make GEMS the software of choice!

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