MINES thermodynamic database and GEMS tutorial resources

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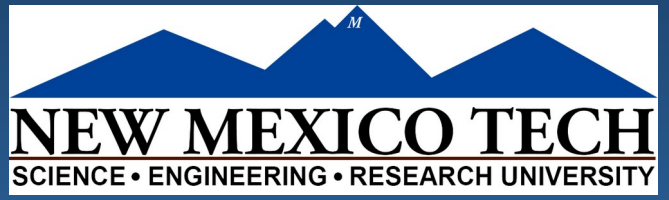
***Collaborators**:*

Nicole Hurtig (NMT), Ruiguang Pan (Indiana U.), Dan Miron (PSI), Dmitrii Kulik (PSI)



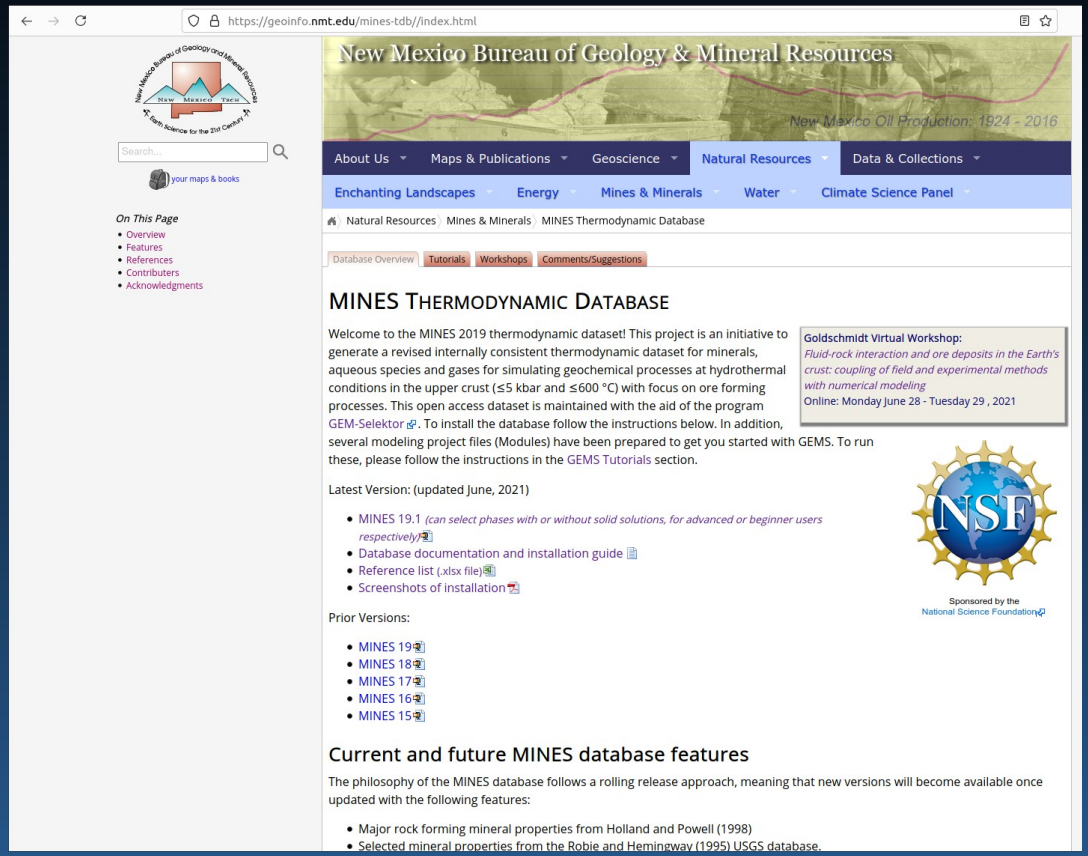
MINES thermodynamic database

Goals of the project

- **Internally consistent** dataset covering fluid-rock equilibria at hydrothermal conditions (≤5 kbar and ≤600 °C)
- Test and improve thermodynamic predictions by combining **experimental, theoretical,** and **natural** observations
- Facilitate use of GEMS and other codes to **simulate fluid-rock interaction and ore-forming processes**
- **Community effort**
  - Open access and rolling-release
  - Collaborators and direct contributors: Nicole Hurtig (NMT, USA), Ruiguang Pan (Indiana U.) and GEMS developer team: Dan Miron and Dmitrii Kulik (PSI, Switzerland)
  - Collaborations with students and diverse research groups and projects

MINES thermodynamic database

https://geoinfo.nmt.edu/mines-tdb



News...

- Version MINES2023 just released for the workshop! citable doi number = dynamic database!
- Currently tailored for use with GEMS/GEMSFITS
- Working on human readable .csv file and query page to generate custom download tables
- New JSON format to export to ThermoFun and generate reaction logK for other modeling programs (PHREEQC, etc.)

Gysi, A.P., Hurtig, N.C., Pan, R., Miron, G.D., and Kulik, D.A., 2023, MINES thermodynamic database, New Mexico Bureau of Geology and Mineral Resources, https://doi.org/10.58799/mines-tdb

Current status: MINES23

Basic framework

- Rock-forming minerals: 122 minerals from H&P98 database + non-silicate minerals from R&H95
- Aqueous species from SUPCRT92 implemented in GEMS
- Ternary non-ideal feldspar solid solution (built-in)
- Ideal multicomponent-multisite solid solutions:

  chlorite, actinolite, epidote, garnet, olivine, clinopyroxene, apatite, monazite, xenotime, biotite, celadonite, talc, montmorillonite, smectites (dio/trioctahedral), chabazite, heulandite

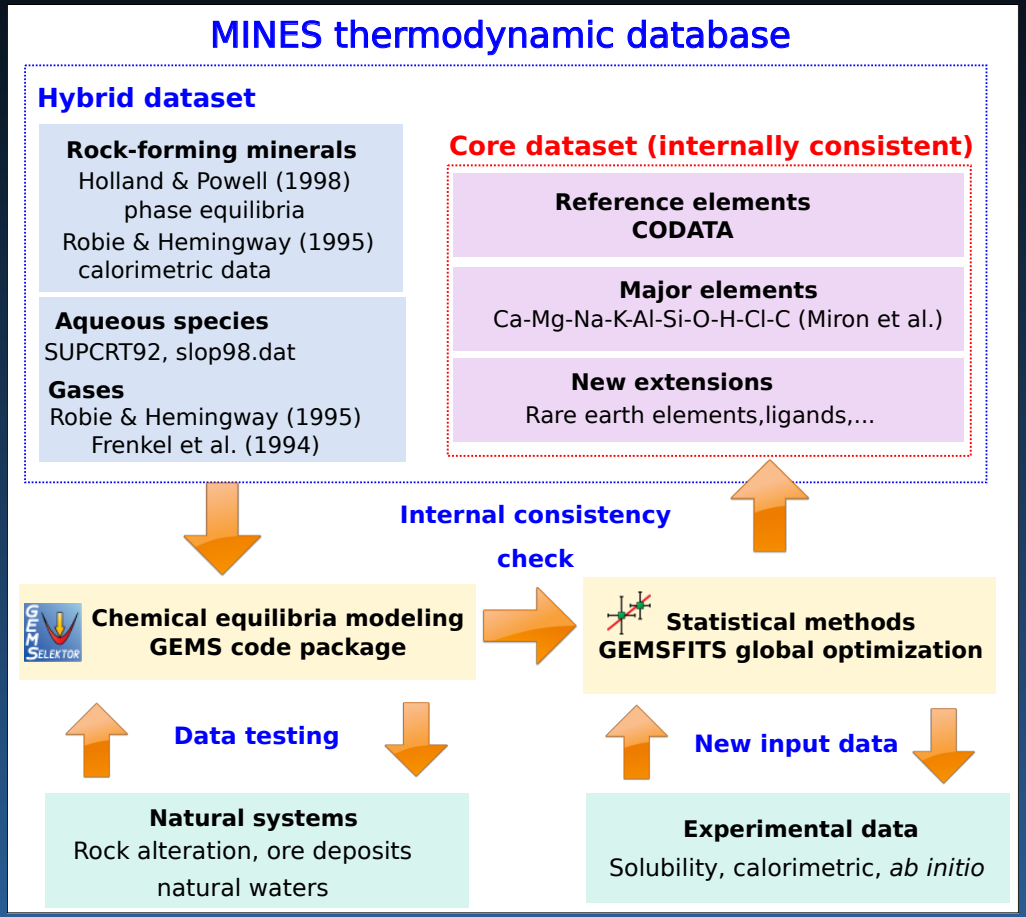
Statistical/optimization methods (GEMSFITS, internal consistency)

- Major cations: Na-, K-, Al-, Si-bearing species, + Ca-, Mg-, CO_2-bearing species (*Miron et al. 2016, 2017*)

Experimental data & Natural systems

- Zeolites (14 end members) and phyllosilicates (16 end members), solid solutions from *Gysi and Stefánsson (2011)*
- Experimental REE phosphate solubility experiments from our Ore Deposits and Critical Minerals Research Lab (Gysi et al. 2015, 2018; Van Hoozen et al., 2020; Gysi and Harlov, 2021)
- REE aqueous complexes (Migdisov et al. 2009; 2016), base and precious metals (Akinfiev and Zotov, 2001, 2010, 2014; Liu and McPhail, 2005; Brugger et al., 2007; Mei et al., 2015; Stefansson and Seward, 2003, etc...)

Conceptual model of MINES thermodynamic database updates and maintenance



upcoming MINES23.1

Internally consistent thermodynamic dataset for rare earth elements (REE) in REE-P-F-Cl-S-O-H system (Pan et al. submitted)

- Optimization and re-evaluation of experimental and thermodynamic data for REE using GEMSFITS

  → dG @25 °C optimized, and keep HKF EoS parameters for T dependence

  → REE3+ and REE hydroxyl complex update, and keep internal consistency to other species (chloride, fluoride, and sulfate complexes)

  1) Hydrothermal REE phosphate solubility experiments 100 – 250 °C: Gysi et al. (2015), Chem Geol; Gysi et al. (2018), GCA; Van Hoozen et al. (2020), GCA; Gysi and Harlov (2021), Chem Geol

  2) Aqueous REE fluoride, sulfate, and chloride complexes (summarized Migdisov et al., 2016)

Tellurium species (Hurtig et al. submitted)

- **Aqueous species**: 11 Te oxide and hydroxide aqueous species with oxidation states of Te(+2), Te(+4) and Te(+6)
- **Minerals**: tellurite, calaverite, hessite, weissite, vulcanite, frohbergite, altaite, tellurium and Zn-telluride

upcoming MINES23.x and ThermoExp_ODCM

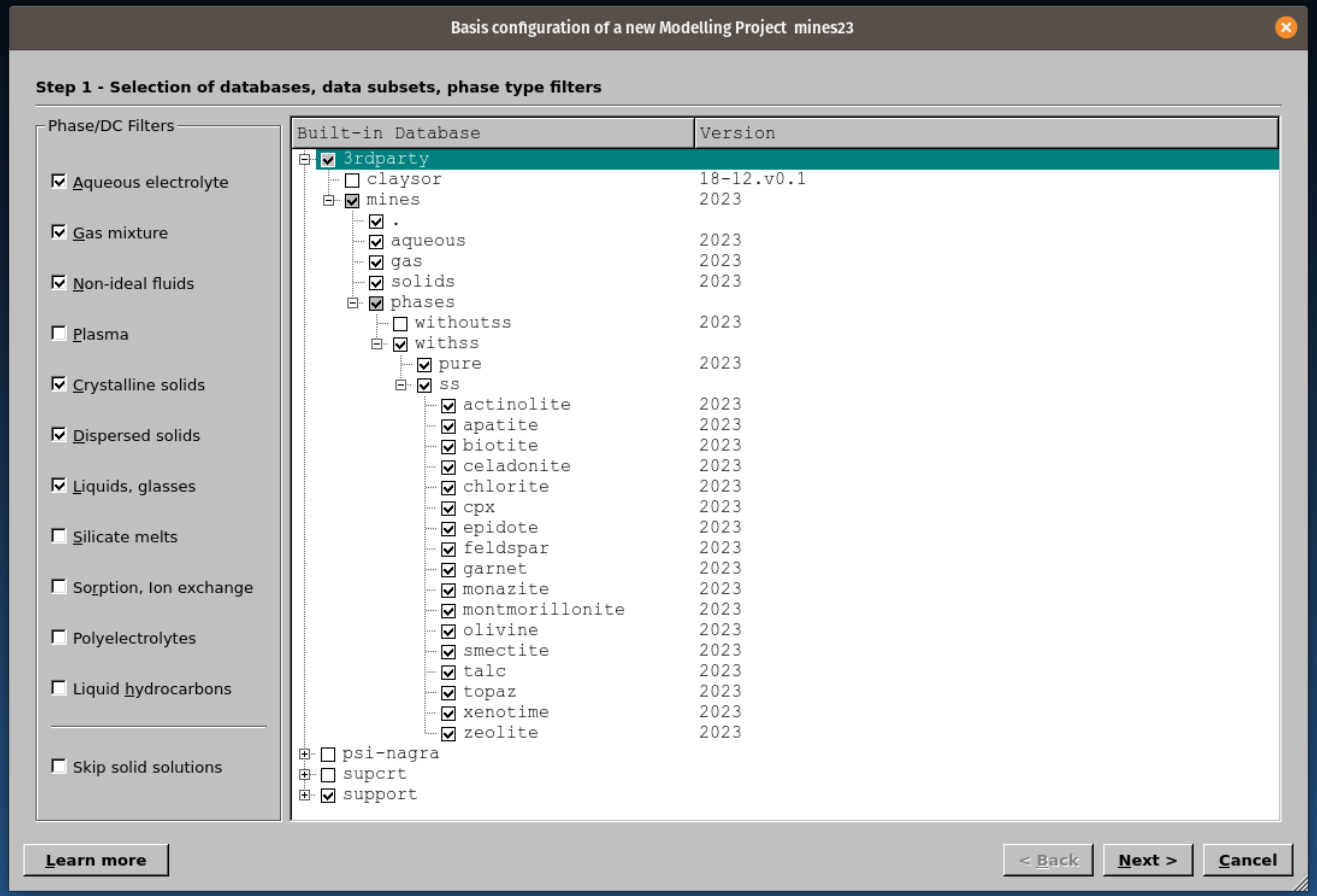
Experimental database (ThermoExp_ODCM) from Ore Deposits and Critical Minerals Lab at NMT

- New experimental database in several file formats (e.g. csv, JSON, etc.) to allow queries/search, easy live updates, and open access with citable source
- Working on addition of new hydrothermal solubility, calorimetry, spectroscopic, and UV-Vis experimental data including dG and dH measured as a function of T and supercritical conditions
- Compilation of existing thermodynamic properties for minerals and aqueous species
- Compatibility with ThermoEcos (https://thermohub.org/)

  → dG @T °C optimized, and develop different EoS parameters for T dependence

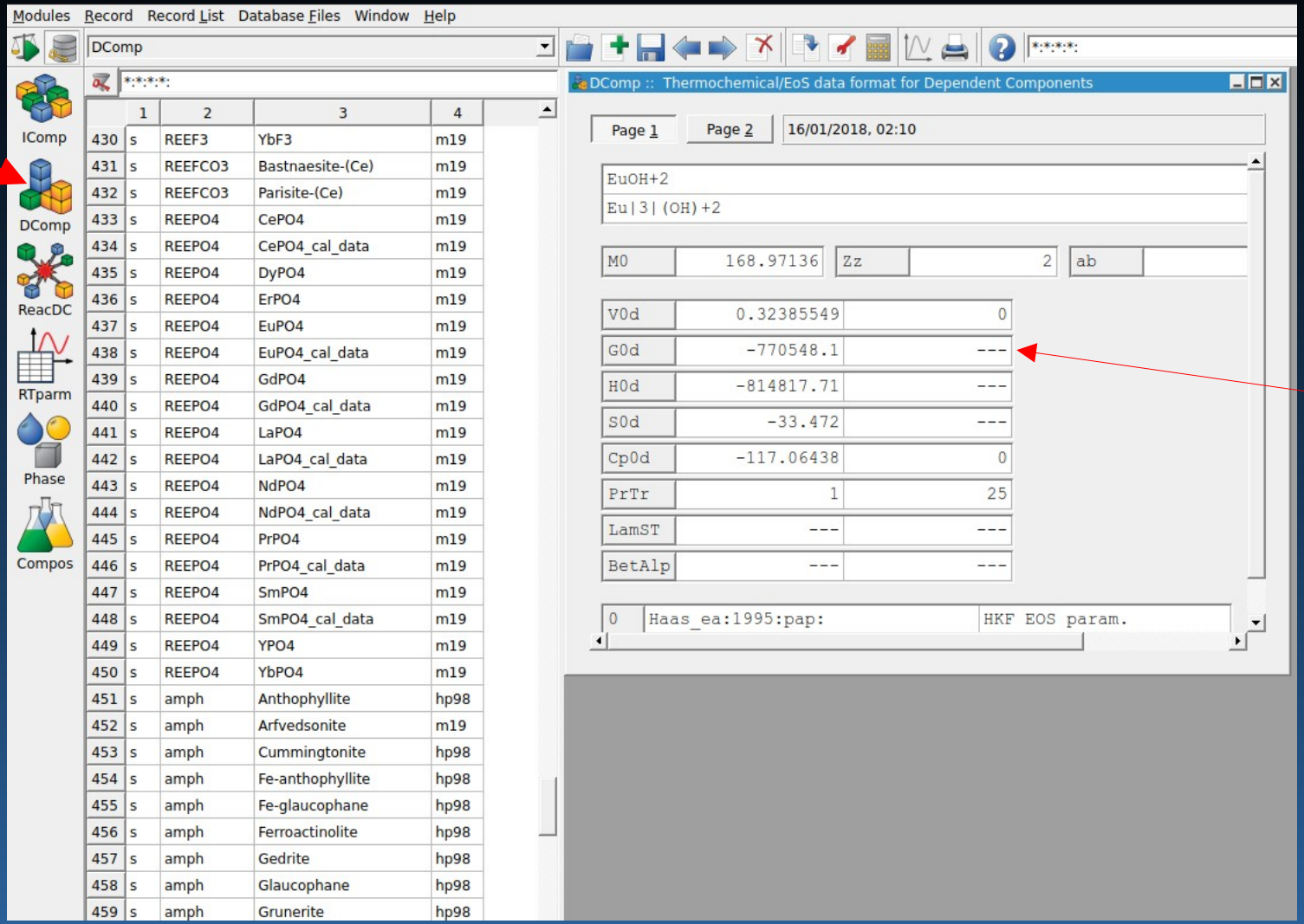
  → Feed MINES and other thermodynamic database allowing for future internally consistent optimizations and updates
- Impetus for other research groups to generate experimental databases that can be optimized

Selection of MINES when building a project in GEMS



- Extract MINES23-DB.Default.zip to your Download folder
- Copy the containing data to Gems3-app/Resources/DB.default folder
- More infos on the tutorial gitbook
- In this window you can select what phases to include (beginners please choose only without ss)

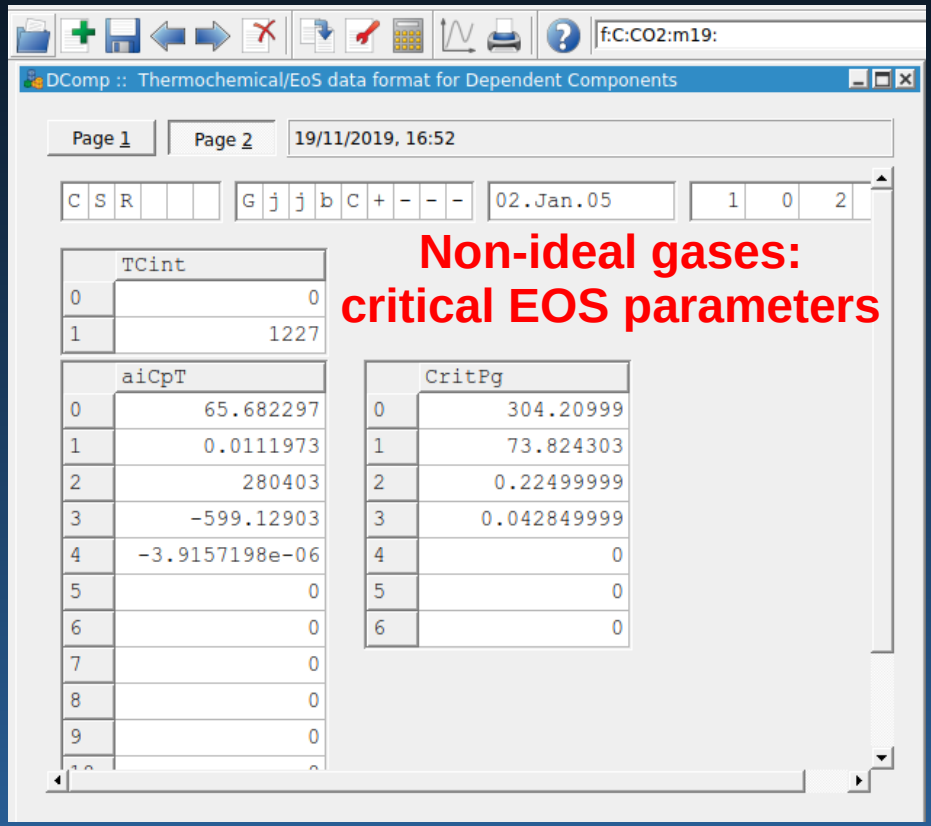
GEMS thermodynamic database mode (DComp)

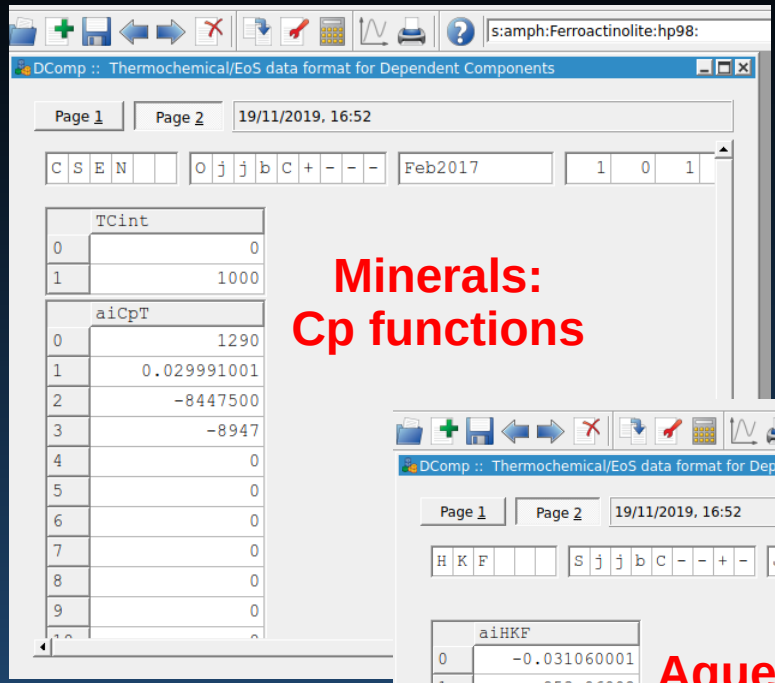


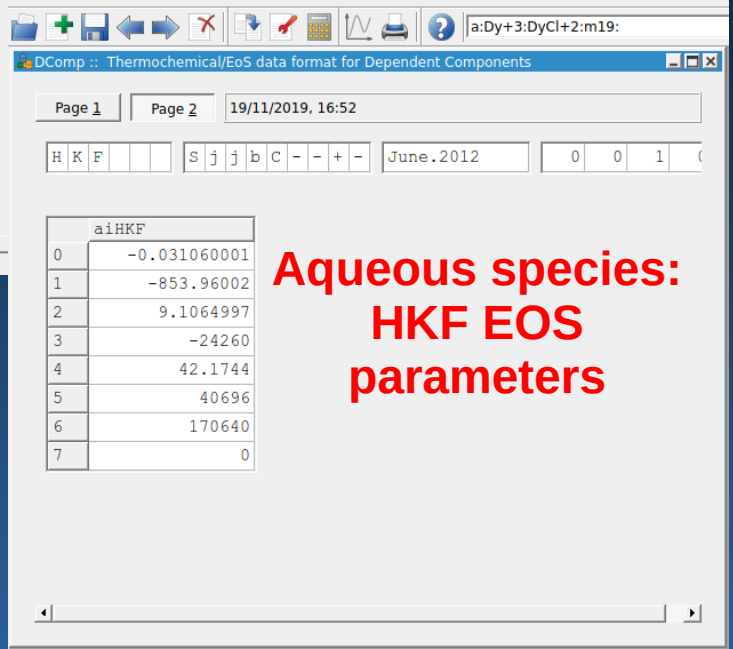
	1	2	3	4
430	s	REEF3	YbF3	m19
431	s	REEFCO3	Bastnaesite-(Ce)	m19
432	s	REEFCO3	Parisite-(Ce)	m19
433	s	REEPO4	CePO4	m19
434	s	REEPO4	CePO4_cal_data	m19
435	s	REEPO4	DyPO4	m19
436	s	REEPO4	ErPO4	m19
437	s	REEPO4	EuPO4	m19
438	s	REEPO4	EuPO4_cal_data	m19
439	s	REEPO4	GdPO4	m19
440	s	REEPO4	GdPO4_cal_data	m19
441	s	REEPO4	LaPO4	m19
442	s	REEPO4	LaPO4_cal_data	m19
443	s	REEPO4	NdPO4	m19
444	s	REEPO4	NdPO4_cal_data	m19
445	s	REEPO4	PrPO4	m19
446	s	REEPO4	PrPO4_cal_data	m19
447	s	REEPO4	SmPO4	m19
448	s	REEPO4	SmPO4_cal_data	m19
449	s	REEPO4	YPO4	m19
450	s	REEPO4	YbPO4	m19
451	s	amph	Anthophyllite	hp98
452	s	amph	Arfvedsonite	m19
453	s	amph	Cummingtonite	hp98
454	s	amph	Fe-anthophyllite	hp98
455	s	amph	Fe-glaucophane	hp98
456	s	amph	Ferroactinolite	hp98
457	s	amph	Gedrite	hp98
458	s	amph	Glaucophane	hp98
459	s	amph	Grunerite	hp98

Standard thermodynamic properties (G, H, S, and V)

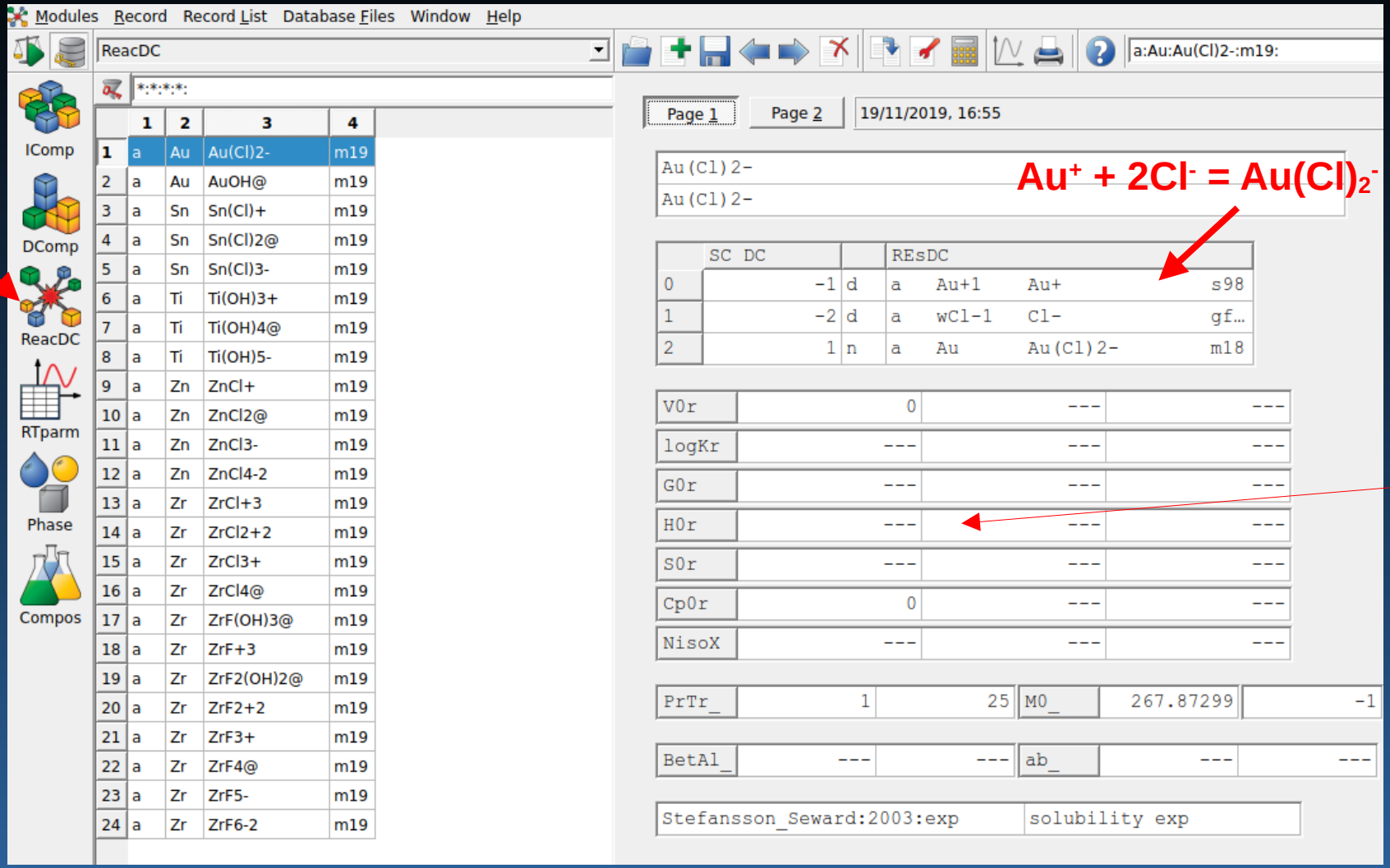
GEMS thermodynamic database mode (DComp)



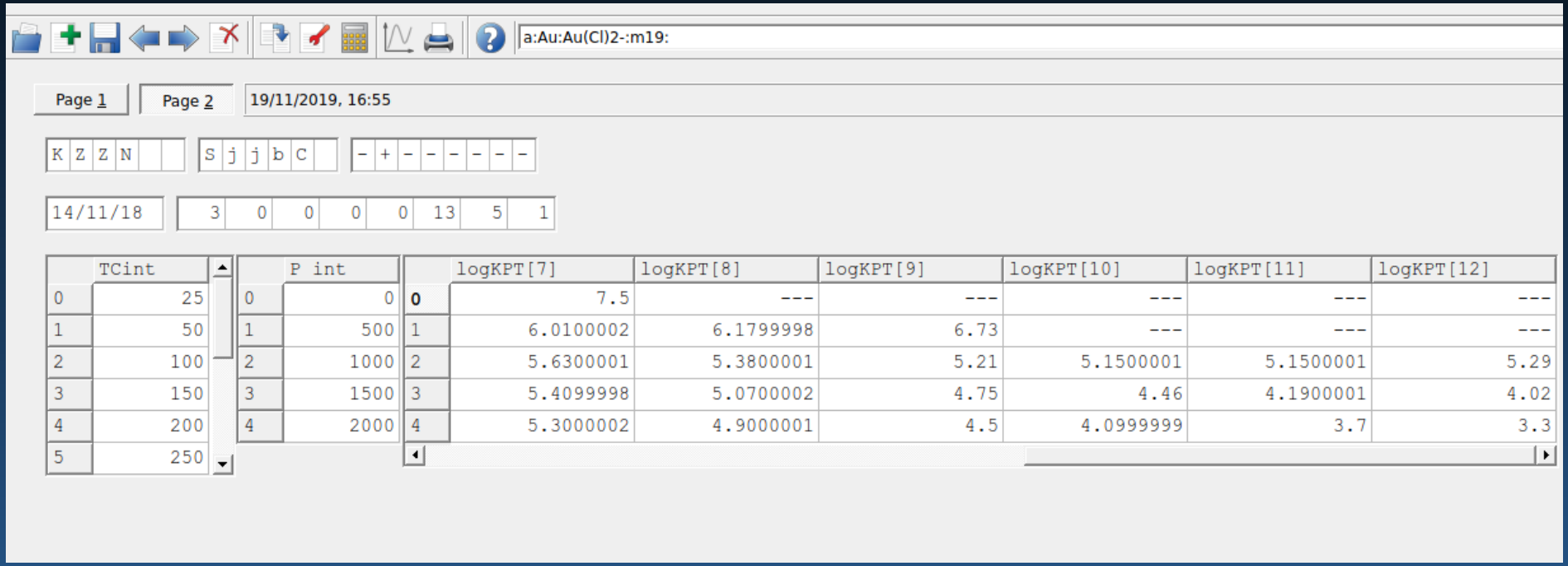




GEMS thermodynamic database mode (ReacDC)



Equilibrium constants (logK) as a function of pressure and temperature

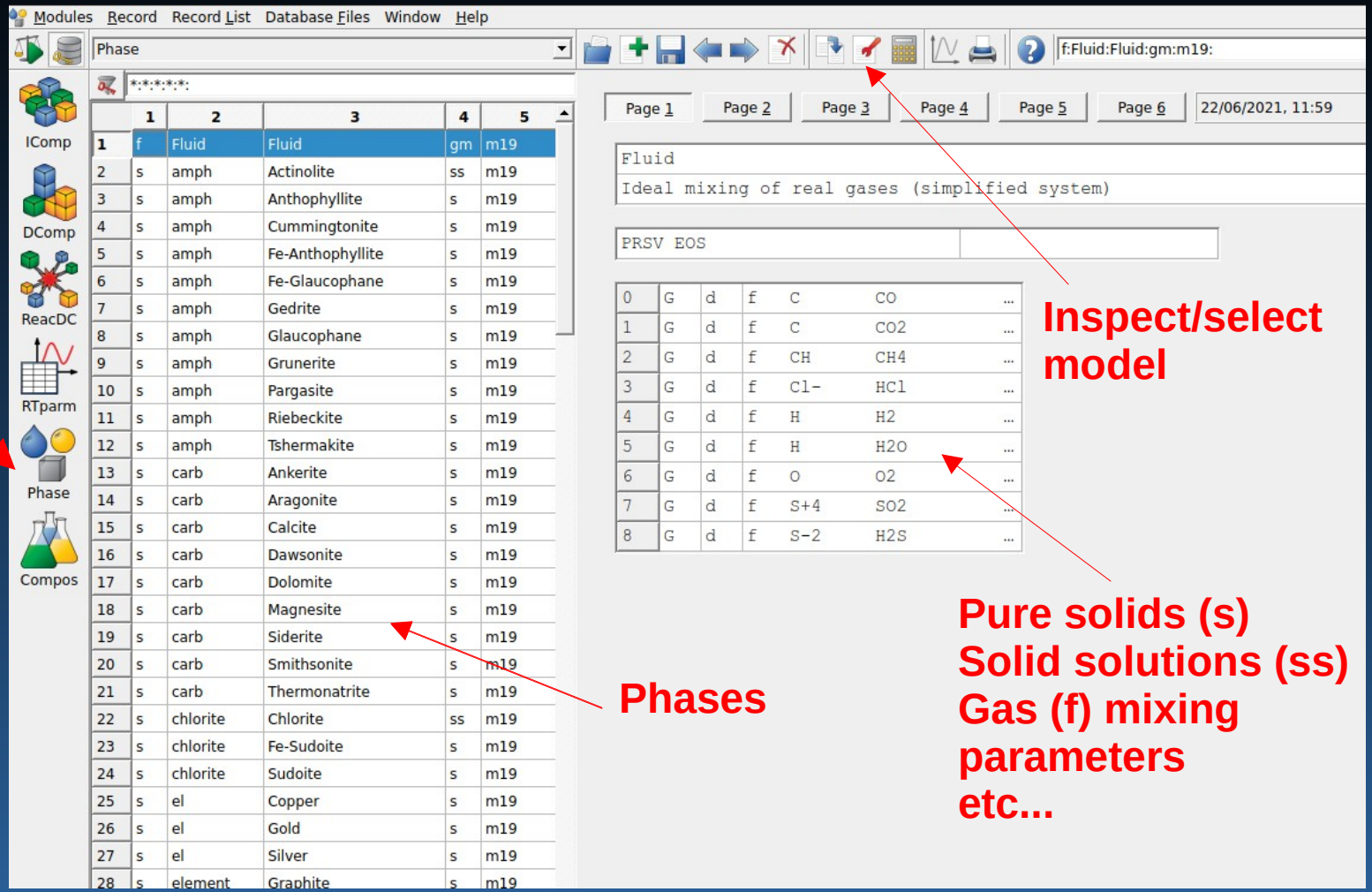


	TCint
0	25
1	50
2	100
3	150
4	200
5	250

	P int
0	0
1	500
2	1000
3	1500
4	2000

	logKPT[7]	logKPT[8]	logKPT[9]	logKPT[10]	logKPT[11]	logKPT[12]
0	7.5	---	---	---	---	---
1	6.0100002	6.1799998	6.73	---	---	---
2	5.6300001	5.3800001	5.21	5.1500001	5.1500001	5.29
3	5.4099998	5.0700002	4.75	4.46	4.1900001	4.02
4	5.3000002	4.9000001	4.5	4.0999999	3.7	3.3

GEMS thermodynamic database mode (Phase)

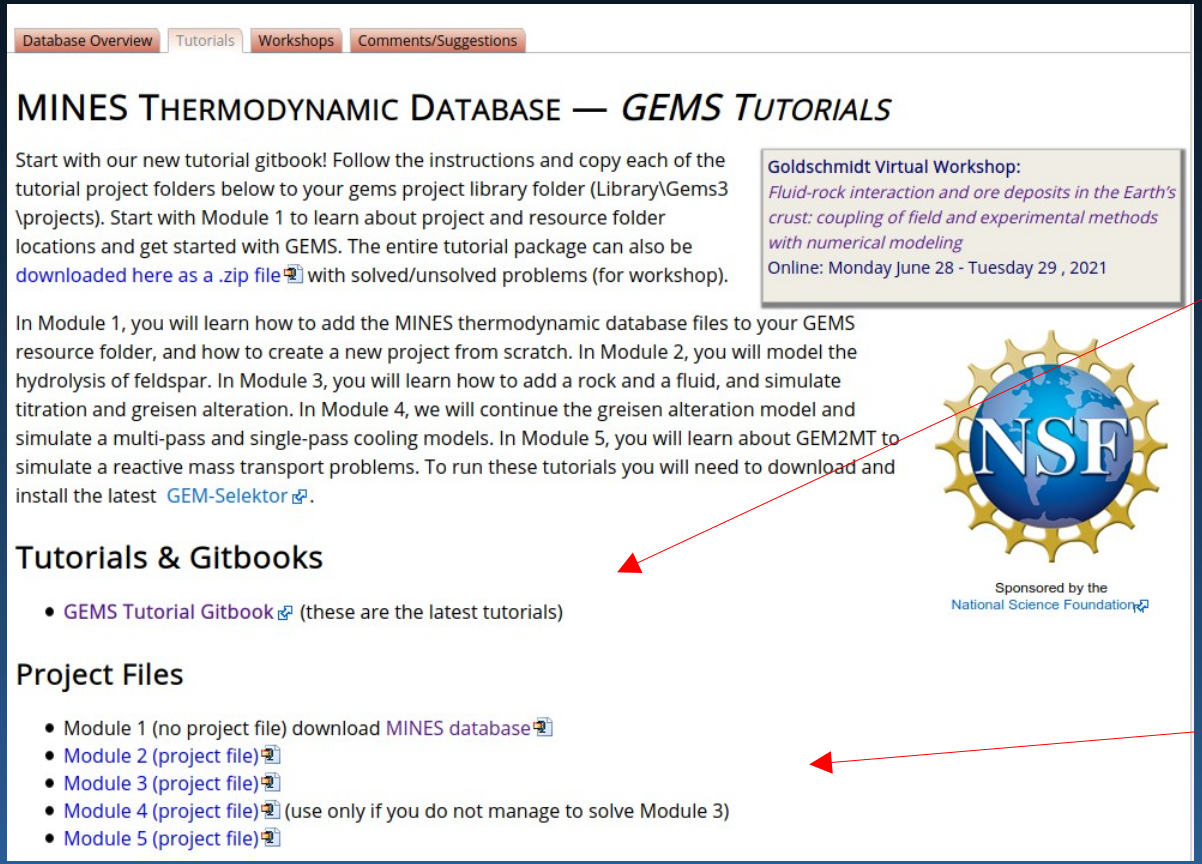


	1	2	3	4	5
1	f	Fluid	Fluid	gm	m19
2	s	amph	Actinolite	ss	m19
3	s	amph	Anthophyllite	s	m19
4	s	amph	Cummingtonite	s	m19
5	s	amph	Fe-Anthophyllite	s	m19
6	s	amph	Fe-Glaucophane	s	m19
7	s	amph	Gedrite	s	m19
8	s	amph	Glaucophane	s	m19
9	s	amph	Grunerite	s	m19
10	s	amph	Pargasite	s	m19
11	s	amph	Riebeckite	s	m19
12	s	amph	Tshermakite	s	m19
13	s	carb	Ankerite	s	m19
14	s	carb	Aragonite	s	m19
15	s	carb	Calcite	s	m19
16	s	carb	Dawsonite	s	m19
17	s	carb	Dolomite	s	m19
18	s	carb	Magnesite	s	m19
19	s	carb	Siderite	s	m19
20	s	carb	Smithsonite	s	m19
21	s	carb	Thermonatrite	s	m19
22	s	chlorite	Chlorite	ss	m19
23	s	chlorite	Fe-Sudoite	s	m19
24	s	chlorite	Sudoite	s	m19
25	s	el	Copper	s	m19
26	s	el	Gold	s	m19
27	s	el	Silver	s	m19
28	s	element	Graphite	s	m19

0	G	d	f	C	CO	...
1	G	d	f	C	CO2	...
2	G	d	f	CH	CH4	...
3	G	d	f	Cl-	HCl	...
4	G	d	f	H	H2	...
5	G	d	f	H	H2O	...
6	G	d	f	O	O2	...
7	G	d	f	S+4	SO2	...
8	G	d	f	S-2	H2S	...

Tutorial resources

https://geoinfo.nmt.edu/mines-tdb/tutorials
https://apgysi.github.io/gems-mines-tutorial/



Database Overview | Tutorials | Workshops | Comments/Suggestions

MINES THERMODYNAMIC DATABASE — *GEMS TUTORIALS*

Start with our new tutorial gitbook! Follow the instructions and copy each of the tutorial project folders below to your gems project library folder (Library\Gems3\projects). Start with Module 1 to learn about project and resource folder locations and get started with GEMS. The entire tutorial package can also be downloaded here as a .zip file with solved/unsolved problems (for workshop).

Goldschmidt Virtual Workshop:
Fluid-rock interaction and ore deposits in the Earth's crust: coupling of field and experimental methods with numerical modeling
Online: Monday June 28 - Tuesday 29 , 2021

In Module 1, you will learn how to add the MINES thermodynamic database files to your GEMS resource folder, and how to create a new project from scratch. In Module 2, you will model the hydrolysis of feldspar. In Module 3, you will learn how to add a rock and a fluid, and simulate titration and greisen alteration. In Module 4, we will continue the greisen alteration model and simulate a multi-pass and single-pass cooling models. In Module 5, you will learn about GEM2MT to simulate a reactive mass transport problems. To run these tutorials you will need to download and install the latest GEM-Selektor.

NSF

Sponsored by the National Science Foundation

Tutorials & Gitbooks

- GEMS Tutorial Gitbook (these are the latest tutorials)

Project Files

- Module 1 (no project file) download MINES database
- Module 2 (project file)
- Module 3 (project file)
- Module 4 (project file) (use only if you do not manage to solve Module 3)
- Module 5 (project file)

- **Here you can access the free gitbook tutorials with a step by step guide**
- **How to install the MINES database and model with GEMS**

Here you can download the module project files, extract and copy the folder into your GEMS Library/Gems3/projects folder

Tutorial resources

https://apgysi.github.io/gems-mines-tutorial/

A tutorial for geochemical modeling of fluid-rock interaction using GEM-Selektor and the MINES thermodynamic database

Alexander Gysi, New Mexico Tech, USA

2021-04-07

Prerequisites

GEM-Selektor (GEMS), is a numerical modeling program with a graphical user interface based on Gibbs energy minimization and permits calculating and solving fluid-rock interaction problems of interest in geochemistry.

- Installation instructions for GEMS and more information about this modeling program can be found on the GEMS team webpage: http://gems.web.psi.ch/GEMS3/techinfo.html.
- Information about the MINES database and project files for the tutorials can be found under https://geoinfo.nmt.edu/mines-tdb

Collaborators: Dmitrii Kulik (Paul Scherrer Institute), Dan Miron (Paul Scherrer Institute), and Nicole Hurtig (New Mexico Tech)

- **Module 1**: adding MINES thermodynamic database and first project
- **Module 2**: feldspar reaction path
- **Module 3**: greisenization, adding rock/fluid, titration model
- **Module 4**: greisenization single flow-through reactor, single/multipass
- **Module 5**: gem2mt, 1-D reactive mass transport
- **Module 6**: generating pH-activity diagrams

Thank you!
Questions/comments?

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Collaborators:

- Nicole Hurtig (NMT), Ruiguang Pan (Indiana U.), Dan Miron (PSI), Dmitrii Kulik (PSI)

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