

# MINES thermodynamic database and GEMS tutorial resources

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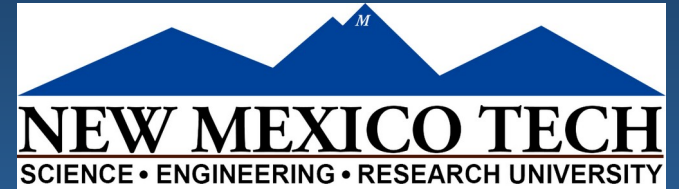
*New Mexico Bureau of Geology and Mineral Resources*

*Earth & Environmental Science Department*

*New Mexico Institute of Mining and Technology*

## **Collaborators:**

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



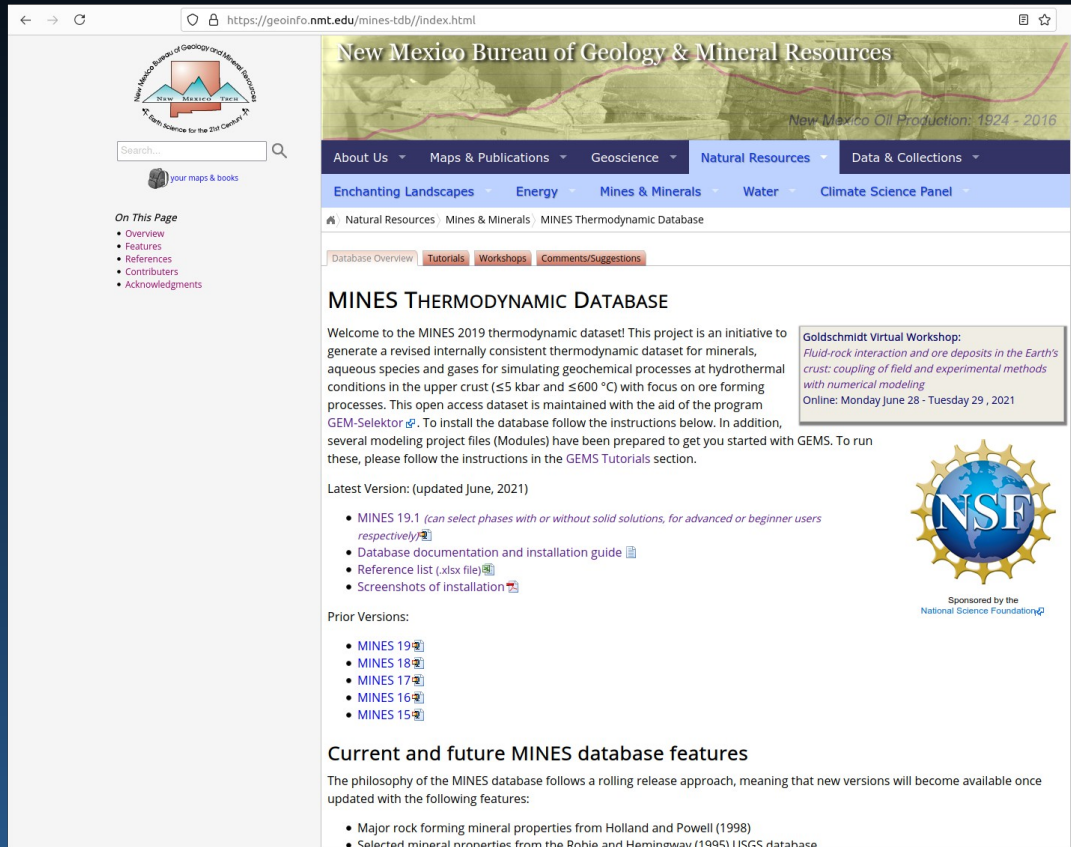
# MINES thermodynamic database

## Goals of the project

- **Internally consistent** dataset covering fluid-rock equilibria at hydrothermal conditions ( $\leq 5$  kbar and  $\leq 600$  °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>



New Mexico Bureau of Geology & Mineral Resources

Search...

your maps & books

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Natural Resources | Mines & Minerals | MINES Thermodynamic Database

Database Overview | Tutorials | Workshops | Comments/Suggestions

## MINES THERMODYNAMIC DATABASE

Welcome to the MINES 2019 thermodynamic dataset! This project is an initiative to generate a revised internally consistent thermodynamic dataset for minerals, aqueous species and gases for simulating geochemical processes at hydrothermal conditions in the upper crust ( $\leq 5$  kbar and  $\leq 600$  °C) with focus on ore forming processes. This open access dataset is maintained with the aid of the program GEM-Selektor. To install the database follow the instructions below. In addition, several modeling project files (Modules) have been prepared to get you started with GEMS. To run these, please follow the instructions in the GEMS Tutorials section.

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

Latest Version: (updated June, 2021)

- MINES 19.1 (can select phases with or without solid solutions, for advanced or beginner users respectively)
- Database documentation and installation guide
- Reference list (xlsx file)
- Screenshots of installation

Prior Versions:

- MINES 19
- MINES 18
- MINES 17
- MINES 16
- MINES 15

### Current and future MINES database features

The philosophy of the MINES database follows a rolling release approach, meaning that new versions will become available once updated with the following features:

- Major rock forming mineral properties from Holland and Powell (1998)
- Selected mineral properties from the Robie and Hemingway (1995) USGS database.

## 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

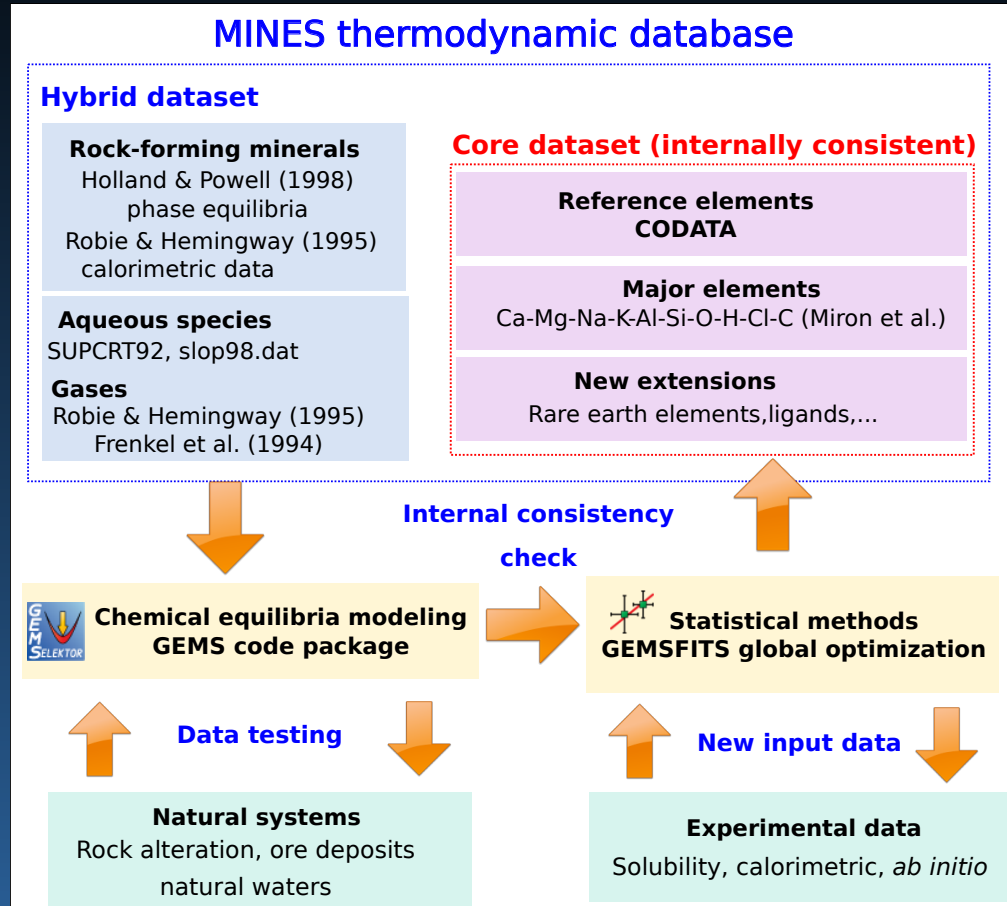
## Statistical/optimization methods (GEMSFITS, internal consistency)

- Major cations: Na-, K-, Al-, Si-bearing species, + Ca-, Mg-, CO<sub>2</sub>-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 (*Akinfiyev 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
  - REE<sup>3+</sup> 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

Basis configuration of a new Modelling Project mines23

Step 1 - Selection of databases, data subsets, phase type filters

Phase/DC Filters

- Aqueous electrolyte
- Gas mixture
- Non-ideal fluids
- Plasma
- Crystalline solids
- Dispersed solids
- Liquids, glasses
- Silicate melts
- Sorption, Ion exchange
- Polyelectrolytes
- Liquid hydrocarbons
- Skip solid solutions

| Built-in Database                                   | Version    |
|---|------------|
| <input checked="" type="checkbox"/> 3rdparty        |            |
| <input type="checkbox"/> claysor                    | 18-12.v0.1 |
| <input checked="" type="checkbox"/> mines           | 2023       |
| <input checked="" type="checkbox"/> .               |            |
| <input checked="" type="checkbox"/> aqueous         | 2023       |
| <input checked="" type="checkbox"/> gas             | 2023       |
| <input checked="" type="checkbox"/> solids          | 2023       |
| <input checked="" type="checkbox"/> phases          |            |
| <input type="checkbox"/> withoutss                  | 2023       |
| <input checked="" type="checkbox"/> withss          |            |
| <input checked="" type="checkbox"/> pure            | 2023       |
| <input checked="" type="checkbox"/> ss              |            |
| <input checked="" type="checkbox"/> actinolite      | 2023       |
| <input checked="" type="checkbox"/> apatite         | 2023       |
| <input checked="" type="checkbox"/> biotite         | 2023       |
| <input checked="" type="checkbox"/> celadonite      | 2023       |
| <input checked="" type="checkbox"/> chlorite        | 2023       |
| <input checked="" type="checkbox"/> cpx             | 2023       |
| <input checked="" type="checkbox"/> epidote         | 2023       |
| <input checked="" type="checkbox"/> feldspar        | 2023       |
| <input checked="" type="checkbox"/> garnet          | 2023       |
| <input checked="" type="checkbox"/> monazite        | 2023       |
| <input checked="" type="checkbox"/> montmorillonite | 2023       |
| <input checked="" type="checkbox"/> olivine         | 2023       |
| <input checked="" type="checkbox"/> smectite        | 2023       |
| <input checked="" type="checkbox"/> talc            | 2023       |
| <input checked="" type="checkbox"/> topaz           | 2023       |
| <input checked="" type="checkbox"/> xenotime        | 2023       |
| <input checked="" type="checkbox"/> zeolite         | 2023       |
| <input type="checkbox"/> psi-nagra                  |            |
| <input type="checkbox"/> supcrt                     |            |
| <input checked="" type="checkbox"/> support         |            |

[Learn more](#)    < Back    Next >    Cancel

- 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)

The screenshot shows the GEMS software interface in DComp mode. The left sidebar contains icons for IComp, DComp (highlighted with a red arrow), ReacDC, RTparm, Phase, and Compos. The main window displays a table of components and their properties.

|     | 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 |

The right window shows thermochemical data for dependent components. The title is "DComp :: Thermochemical/EoS data format for Dependent Components". The page is "Page 1" of "Page 2" and the date is "16/01/2018, 02:10". The component is "EuOH+2" with the formula "Eu | 3 | (OH) + 2". The properties are:

|        |            |    |     |    |
|--------|------------|----|-----|----|
| M0     | 168.97136  | Zz | 2   | ab |
| V0d    | 0.32385549 |    | 0   |    |
| G0d    | -770548.1  |    | --- |    |
| H0d    | -814817.71 |    | --- |    |
| S0d    | -33.472    |    | --- |    |
| Cp0d   | -117.06438 |    | 0   |    |
| PrTr   | 1          |    | 25  |    |
| LamST  | ---        |    | --- |    |
| BetAlp | ---        |    | --- |    |

The bottom of the right window shows the source "0 Haas\_ea:1995:pap:" and the EOS parameter "HKF EOS param.".

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

# GEMS thermodynamic database mode (DComp)

DComp :: Thermochemical/EoS data format for Dependent Components

Page 1 Page 2 19/11/2019, 16:52

C S R G j j b C + - - - 02.Jan.05 1 0 2

**Non-ideal gases:  
critical EOS parameters**

| TCint |      |
|-------|------|
| 0     | 0    |
| 1     | 1227 |

| aiCpT |                |
|-------|----------------|
| 0     | 65.682297      |
| 1     | 0.0111973      |
| 2     | 280403         |
| 3     | -599.12903     |
| 4     | -3.9157198e-06 |
| 5     | 0              |
| 6     | 0              |
| 7     | 0              |
| 8     | 0              |
| 9     | 0              |

| CritPg |             |
|--------|-------------|
| 0      | 304.20999   |
| 1      | 73.824303   |
| 2      | 0.22499999  |
| 3      | 0.042849999 |
| 4      | 0           |
| 5      | 0           |
| 6      | 0           |

s:\amph:Ferroactinolite:hp98:

DComp :: Thermochemical/EoS data format for Dependent Components

Page 1 Page 2 19/11/2019, 16:52

C S E N O j j b C + - - - Feb2017 1 0 1

**Minerals:  
Cp functions**

| TCint |      |
|-------|------|
| 0     | 0    |
| 1     | 1000 |

| aiCpT |             |
|-------|-------------|
| 0     | 1290        |
| 1     | 0.029991001 |
| 2     | -8447500    |
| 3     | -8947       |
| 4     | 0           |
| 5     | 0           |
| 6     | 0           |
| 7     | 0           |
| 8     | 0           |
| 9     | 0           |

a:Dy+3:DyCl+2:m19:

DComp :: Thermochemical/EoS data format for Dependent Components

Page 1 Page 2 19/11/2019, 16:52

H K F S j j b C - - + - June.2012 0 0 1

**Aqueous species:  
HKF EOS  
parameters**

| aiHKF |              |
|-------|--------------|
| 0     | -0.031060001 |
| 1     | -853.96002   |
| 2     | 9.1064997    |
| 3     | -24260       |
| 4     | 42.1744      |
| 5     | 40696        |
| 6     | 170640       |
| 7     | 0            |

# GEMS thermodynamic database mode (ReacDC)

Modules Record Record List Database Files Window Help

ReacDC

\*\*\*\*\*

|    | 1 | 2  | 3          | 4   |
|----|---|----|------------|-----|
| 1  | a | Au | Au(Cl)2-   | m19 |
| 2  | a | Au | AuOH@      | m19 |
| 3  | a | Sn | Sn(Cl)+    | m19 |
| 4  | a | Sn | Sn(Cl)2@   | m19 |
| 5  | a | Sn | Sn(Cl)3-   | m19 |
| 6  | a | Ti | Ti(OH)3+   | m19 |
| 7  | a | Ti | Ti(OH)4@   | m19 |
| 8  | a | Ti | Ti(OH)5-   | m19 |
| 9  | a | Zn | ZnCl+      | m19 |
| 10 | a | Zn | ZnCl2@     | m19 |
| 11 | a | Zn | ZnCl3-     | m19 |
| 12 | a | Zn | ZnCl4-2    | m19 |
| 13 | a | Zr | ZrCl+3     | m19 |
| 14 | a | Zr | ZrCl2+2    | m19 |
| 15 | a | Zr | ZrCl3+     | m19 |
| 16 | a | Zr | ZrCl4@     | m19 |
| 17 | a | Zr | ZrF(OH)3@  | m19 |
| 18 | a | Zr | ZrF+3      | m19 |
| 19 | a | Zr | ZrF2(OH)2@ | m19 |
| 20 | a | Zr | ZrF2+2     | m19 |
| 21 | a | Zr | ZrF3+      | m19 |
| 22 | a | Zr | ZrF4@      | m19 |
| 23 | a | Zr | ZrF5-      | m19 |
| 24 | a | Zr | ZrF6-2     | m19 |

Page 1 Page 2 19/11/2019, 16:55

Au(Cl) 2- Au<sup>+</sup> + 2Cl<sup>-</sup> = Au(Cl)<sub>2</sub><sup>-</sup>

Au(Cl) 2-

|   | SC | DC |   | REsDC              |
|---|----|----|---|--------------------|
| 0 |    | -1 | d | a Au+1 Au+ s98     |
| 1 |    | -2 | d | a wCl-1 Cl- gf...  |
| 2 |    | 1  | n | a Au Au(Cl) 2- m18 |

|       |     |     |     |
|-------|-----|-----|-----|
| V0r   | 0   | --- | --- |
| logKr | --- | --- | --- |
| G0r   | --- | --- | --- |
| H0r   | --- | --- | --- |
| S0r   | --- | --- | --- |
| Cp0r  | 0   | --- | --- |
| NisoX | --- | --- | --- |

|        |     |     |     |           |     |
|--------|-----|-----|-----|-----------|-----|
| PrTr_  | 1   | 25  | M0_ | 267.87299 | -1  |
| BetAl_ | --- | --- | ab_ | ---       | --- |

Stefansson\_Seward:2003:exp solubility exp

LogK and standard properties of reaction (G, H, S, V)



# GEMS thermodynamic database mode (Phase)

The screenshot displays the GEMS software interface in Phase mode. The left sidebar contains various icons for different modules, with the 'Phase' icon highlighted by a red arrow. The main window shows a list of phases, with the first row selected. The right panel provides details for the selected phase, including its name, description, and a table of components.

| 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  |

**Inspect/select model**

**Pure solids (s)  
Solid solutions (ss)  
Gas (f) mixing parameters  
etc...**

**Phases**

# Tutorial resources

<https://geoinfo.nmt.edu/mines-tdb/tutorials>

<https://apgyisi.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).

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](#).


### 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 \(project file\)](#)

**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



Sponsored by the  
National Science Foundation

- 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://apgyisi.github.io/gems-mines-tutorial/>

## 1 Create your first project in GEMS

- 1.1 Installing the MINES thermody...
- 1.2 Creating a new project from sc...
- 1.3 Your first fluid-rock equilibrium ...
- 1.4 Outcomes

## 2 Feldspar reaction path

- 2.1 Compute the chemical equilibri...
- 2.2 Compute a titration model (Pro...
- 2.3 Modify P-T of the feldspar reac...
- 2.4 Tweak and plot the results
- 2.5 Compute a cooling model (Pro...
- 2.6 Outcomes

## 3 Greisenization Part (I)

- 3.1 Create a custom rock and fluid
- 3.2 Add minerals and aqueous spe...
- 3.3 Titration of leucogranite to grei...
- 3.4 Outcomes

## 4 Greisenization Part (II)

- 4.1 Multi-pass (leaching) model
- 4.2 Modify P-T of the leaching model
- 4.3 Single-pass flushing and cooli...

## 5 GEM2MT reactive mass transport si...

- 5.1 "Sequential reactors chain" S ...
- 5.2 Flow-through reactors chain (F...
- 5.3 One-dimensional reactive tran...

## 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)

### Funding sources:

- NSF grant EAR-2032761 (1649656) and NSF CAREER EAR-2039674 (1845258)
- Office of Science, U.S. Department of Energy, Grant No. DE-SC0021106 and DE-SC0022269

