pypsbuilder

not that simplistic THERMOCALC front-end
for constructing pseudosections

Ondrej Lexa

Institute of Petrology and Structural Geology
Faculty of Science
Charles University

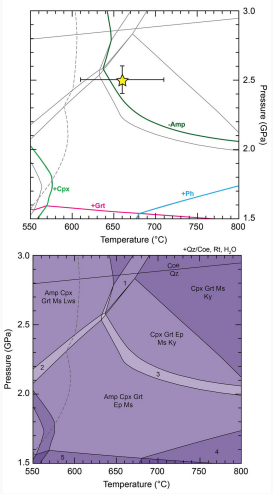
February 11, 2025

Motivation

How to study metamorphic rocks?

Metamorphic petrology examines the mineralogical and textural transformations that occur in rocks due to changes in **pressure** and **temperature** within the Earth's crust.

- **Conventional thermobarometry** analyzes the minerals within a rock to retroactively determine the conditions under which they formed.
- Alternatively, **phase equilibrium modeling** utilizes a rock's bulk composition to predict which minerals will be stable under given conditions.



How phase equilibrium modeling helps?

- **Predicts mineral stability and composition**: Phase equilibrium modeling determines which minerals are stable under specific pressure-temperature (P-T) conditions, helping to reconstruct the metamorphic history of a rock. It provides insights into how mineral compositions change with metamorphism, helping to track element redistribution and reactions over time
- **Traces P-T paths**: By modeling mineral assemblages across different conditions, geologists can infer the pressure-temperature path a rock has experienced, revealing its tectonic evolution.
- **Links to geodynamics**: Understanding mineral stability under different conditions helps relate metamorphic processes to larger-scale geological events, such as subduction, collision, and exhumation.

P-T pseudosections in metamorphic petrology

P-T pseudosections are powerful tools for understanding metamorphic processes. Their key advantages include:

- Unlike traditional phase diagrams, pseudosections are calculated for a **specific rock's bulk composition**.
- They define the stable mineral assemblages over a range of pressure-temperature (P-T) conditions, helping to reconstruct metamorphic histories accurately.
- By comparing observed mineral assemblages with modeled pseudosections, geologists can infer the **P-T evolution of a rock**, revealing burial, heating, and exhumation processes.
- Pseudosections predict not just which minerals are stable but also their **modal abundances and compositions**.

Available tools for pseudosection modeling

- **Perple_X** and **Theriak-Domino** rely on Gibbs free energy minimization, making them ideal for finding stable assemblages and phase diagrams. Perple_X is particularly suited for more complex systems, while Theriak-Domino produces aesthetically pleasing diagrams.
- **MAGEMin** is latest Gibbs energy minimization solver. Primarily developed to predict phase equilibrium in magmatic systems, but other databases are available.
- **THERMOCALC** differs in that it uses an algorithm to solve non-linear thermodynamic equations rather than automatically finding the equilibrium assemblage. It solves statements of equality of chemical potential among the end-members of the phases, supplemented where necessary by mass-balance or direct constraints on compositional variables. It offers great flexibility but **requires more manual effort and expertise**.

What should I choose?

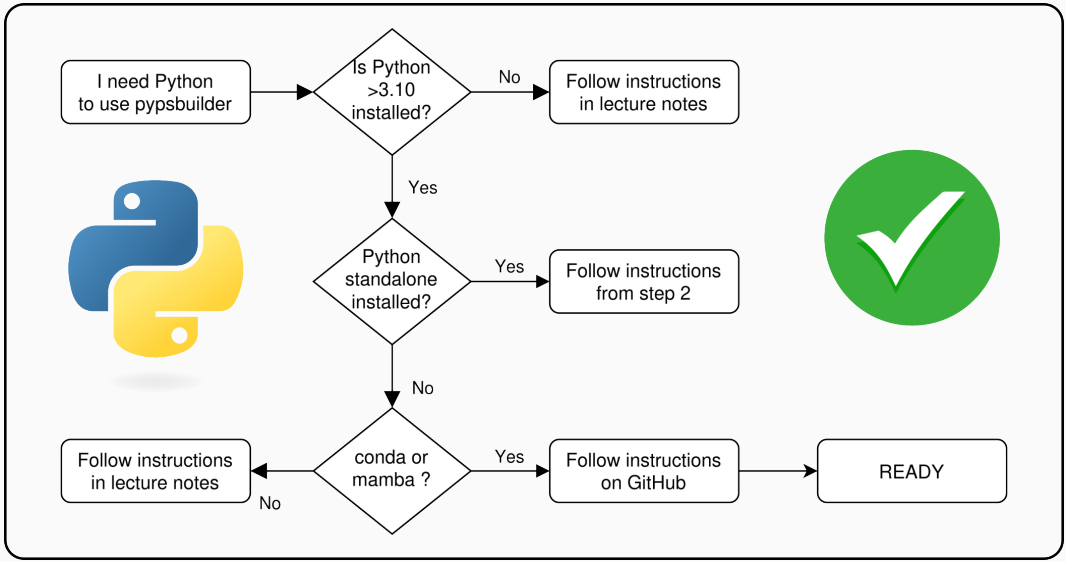
"Ease may be quick, but depth comes with effort."

pypsbuilder - THERMOCALC frontend

pypsbuilder is developed with the idea to make this tedious process much easier and more enjoyable while keeping the concept to force users to understand the **Phase Rule**, **Schreinemaker's analysis**, and how variance changes across field boundaries.

- setup Python environment
- setup THERMOCALC project folder
- running pseudosection builder
- using pseudosection explorer

Correct Python installation



Install Python

- Download Python
  - Go to the official Python website: https://www.python.org/downloads
  - Click Download Python (version 3.12 recommended, latest should be OK as well)
- Install Python
  - Open the downloaded file and start the installation.
  - Important: Check the box "**Add Python to PATH**" before clicking **Install Now**.
  - Follow the prompts to complete the installation.
- Verify Installation
  - Open Command Prompt (Windows) or Terminal (Mac/Linux).
  - Type

```
python --version
```

  - If Python is installed correctly, it will display the version (e.g., Python 3.12.x).

Create a Virtual Environment

- Open Terminal or Command Prompt
- Navigate to Your Project Folder (Optional)

```
cd path/to/your/project
```

- Create a Virtual Environment

```
python -m venv .venv
```

  - this creates a virtual environment named `.venv` in your project directory.

Create a Virtual Environment

- Activate the Virtual Environment
  - Windows (Command Prompt):

```
.venv\Scripts\activate
```

  - Windows (PowerShell): *See notes on GitHub in case of execution policy error*

```
.venv\Scripts\Activate.ps1
```

  - Mac/Linux:

```
source .venv/bin/activate
```

- Verify Installation
  - Open Command Prompt (Windows) or Terminal (Mac/Linux).
  - Type

```
python --version
```

  - It should show the Python version inside the virtual environment.

Install pypsbuilder in the virtual environment

- Once activated, you can install pypsbuilder inside the environment:

```
pip install pypsbuilder[pyqt6,jupyter]
```

This will install all required software to run pypsbuilder in virual environment.

For more details check Python venv webpage.

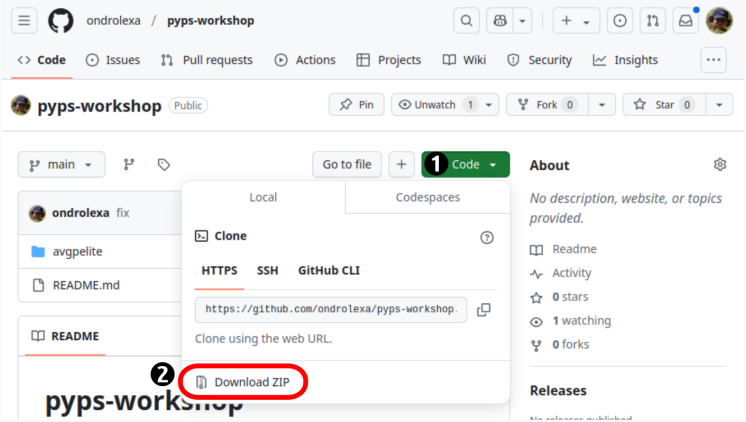
THERMOCALC project folder

Before any calculations, we need to prepare project folder with following files:

- `tc350beta.exe`[Win], `tc350beta`[Linux/MacOS] - THERMOCALC executable
- `tc-ds<version>.txt` - end-member thermodynamic dataset 6.2 (Holland & Powell, 2011)
- `tc-<system>.txt` - HPx-eos activity–composition models
- `tc-<project>.txt` - script file
- `tc-prefs.txt` - preferences file

THERMOCALC project folder

We will start with tutorial project `avgpelite`. You can download related files from GitHub repository https://github.com/ondrolexa/pyps-workshop.



Preference file `tcprefs.txt`

In the preference file you provide calculation mode (1=pseudosections), what dataset you're using (`tc-ds62.txt`) and what is the name of the project. It refers to the name of the scriptfile (`tc-avgpelite.txt`).

```
setpagewidth 700
dataset 62
calcmode 1
scriptfile avgpelite
*
```

Script file `tc-avgpelite.txt`

The scriptfile contains most important information controlling THERMOCALC calculations.

- `axfile`
- `inexcess`, `omit`
- `diagramPT`
- pypsbuilder tags - used by pypsbuilder to manipulate the scriptfile. Tags are ignored by THERMOCALC.

```
axfile mp50MnNCKFMASHTO

inexcess H2O
omit sp0 sp1 Ni NiO opx ab plc pl
   ksp abh ilm hemm ilm0 ksp0 mt0
   mt1 heme hem

diagramPT 5.9 13.1 540 710
```

PSBCALC tags

Enclose the calculation scripts. At the beginning, it has to contain scripts not producing errors. Later, it is fully controlled by pypsbuilder.

```
%{PSBCALC-BEGIN}
calcP 5.9 13.1
calcT 540 710 3.4
calctatp no
with ru g bi pl4tr st q mu
zeromodeisopleth st
%{PSBCALC-END}
```

PSBBULK tags

Enclose the definition of bulk-rock composition. Note that H2O needs to be provided even if in excess.

```
%{PSBBULK-BEGIN}
bulk H2O SiO2 Al2O3 CaO MgO FeO K2O Na2O TiO2 MnO O
bulk 35.0 71.13 11.61 1.39 4.65 5.78 2.68 1.99 0.67 0.10 0.01
%{PSBBULK-END}
```

PSBGUESS tags

It must be placed before the default starting guesses provided in the downloaded set. It is used by pypsbuilder to tune starting guesses.

```
%{PSBGUESS-BEGIN}
%{PSBGUESS-END}

% ------------------------------------------------------------
% Starting guesses in MnNCKFMASHTO (over-ridden by any above)
```


WE ARE READY...
I THINK WE'RE READY...NO! WE ARE READY!

Starting situation – ky-st fields

The most critical part is to start your calculations with a correctly selected stable assemblage. There are plenty of ways to get it. Check already published pseudosection with similar composition, use Perple_X or MAGEMin, use dogmin, etc.