*Earth and Space Science*

Supporting Information for

**pyUserCalc: A revised Jupyter notebook calculator for uranium-series disequilibria in basalts**

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**Additional Supporting Information (Files uploaded separately)**

Caption for Data Set S1

**Introduction**

The provided file is a compressed directory containing the following files:

- README.md
- pyUserCalc_manuscript.ipynb
- pyUserCalc-v3.1.ipynb
- twolayermodel.ipynb
- UserCalc.py

as well as a "data" directory containing three sample data files:

- sample.csv
- simple_sample.csv
- sample_twolayer_model.csv

This file directory can be used to access and run the pyUserCalc code described in the manuscript using a standard Python distribution and Jupyter browser environment.

**Data Set S1.** The provided file is a compressed directory that contains Python and Jupyter notebook code files. The directory, once uncompressed, can be used to access and run the model code described in the manuscript using a standard Python distribution (such as Anaconda) and Jupyter browser environment, like JupyterLab or Jupyter Notebook. The *README.md* text file explains what code is in the directory. The directory file *pyUserCalc_manuscript.ipynb* is a Jupyter notebook version of the full manuscript, where the reader can actively run and test the embedded Python code cells. The file *pyUserCalc-v3.1.ipynb* is a Jupyter notebook containing the fully functional code for production work with the model. *twolayermodel.ipynb* is a Jupyter notebook tool for producing two-layer mantle input data files. *UserCalc.py* is a Python file containing the UserCalc driver and model classes, as well as some convenient visualization methods that can be imported using either of the notebook files. The "data" directory contains the sample data files, *sample.csv* and *simple_sample.csv*, which are used for example calculations in the two notebook files and also provide a useful template for other data input files, as well as the output from the two layer calculator, *sample_twolayer_model.csv*.

The supporting directory is also provided in a public Git repository (https://gitlab.com/ENKI-portal/pyUsercalc); if preferred, readers can request a free ENKI GitLab account and access and run these code files online using the ENKI JupyterLab browser environment. To do this, the reader should 1) register for a GitLab account (https://gitlab.com/ENKI-portal), log into the ENKI cloud server (https://server.enki-portal.org/hub/login), close the welcome screen, open a Terminal window and type "git clone https://gitlab.com/ENKI-portal/pyUsercalc.git" to clone the repository, and then open the desired notebook files in the pyUserCalc directory.

Alternately, the manuscript notebook is provided for direct access using a binder container (https://mybinder.org/v2/gl/ENKI-portal%2FpyUsercalc/master?filepath=pyUserCalc_manuscript.ipynb).