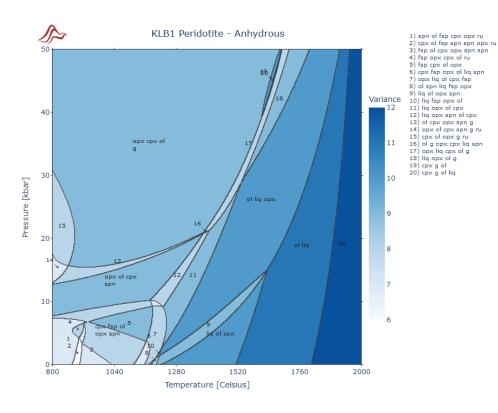
MAGEMinApp: introduction





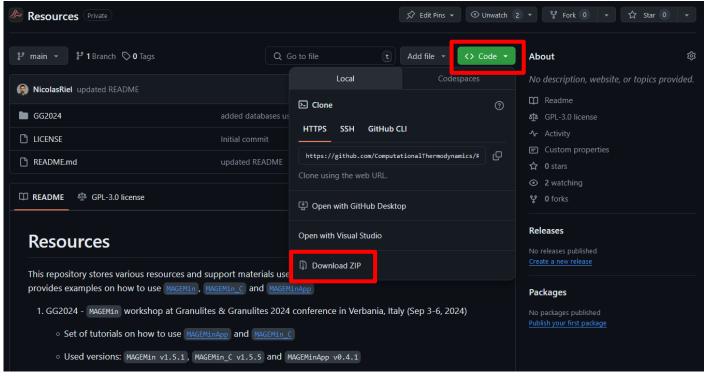


MAGEMin github: ComputationalThermodynamics

First, download the resources for the shortcourse from Github:



https://github.com/ComputationalThermodynamics/Resources



- The GG2024 folder includes:
- Bulk rock input file example
- Trace element input file
- Reference database used in MAGEMinApp
- The pdfs used in the short course
- MAGEMin_C Julia scripts used during the course

MAGEMinApp: launching the App in parallel

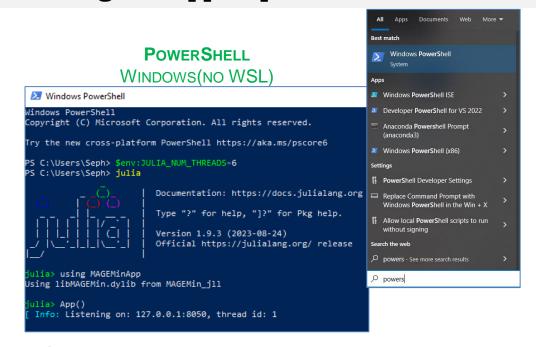
VISUAL STUDIO CODE MAC, LINUX AND WINDOWS(USING WSL)

```
o seph42@DESKTOP-2V82075:~$ julia -t 6

| Occumentation: https://docs.julialang.org
| For Pkg help.
| Occumentation: https://docs.julialang.org
| Occumen
```

julia –t 6 using MAGEMinApp App()

Favored way (better performances on Mac and Linux)



\$env:JULIA_NUM_THREADS=6
julia
using MAGEMinApp
App()

Arour

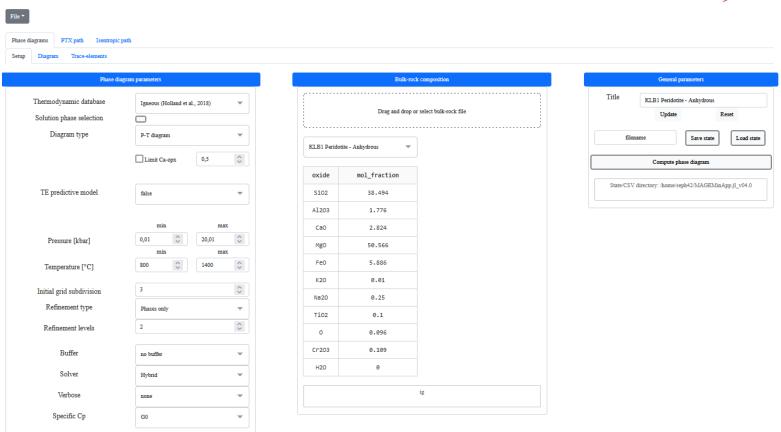
Around 2.5 times slower than using WSL

MAGEMinApp: interface (Phase diagrams)



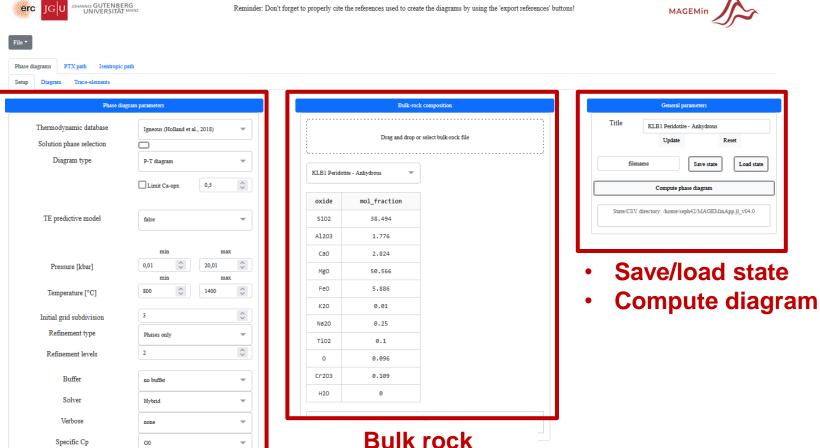
Reminder: Don't forget to properly cite the references used to create the diagrams by using the 'export references' buttons!





id=6a7eedce-5:5f5-4ca6-a394-d988df521e13, MAGEMimApp GUI v=0.4.0

MAGEMinApp: interface (Phase diagrams)

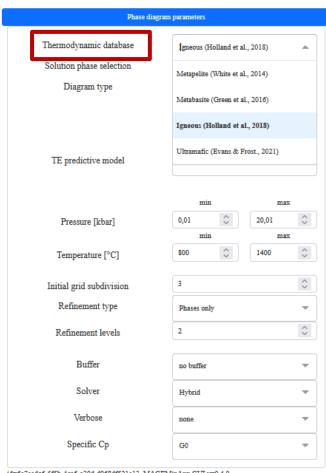


Grid properties

composition(s)

Load state

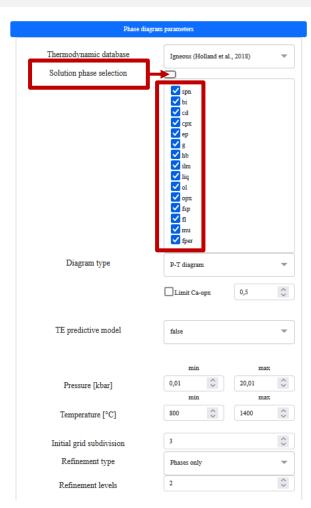
MAGEMinApp: Thermodynamic database



- Metapelite (White et al., 2024) **MnNCKFMASHTO**
- Metabasite (Green et al., 2016) **NCKFMASHTO**
- Igneous (Holland et al., 2018) **NCKFMASHTOC**r
- Ultramafic (Evans & Frost, 2021) **FMASOSH**
- Dry igneous alkaline (Weller et al., in review) NCKFMASHTOCr (upcoming)
- Mantle (Stixrude and Lithgow-Bertelloni, 2011) NCFMAS (upcoming)

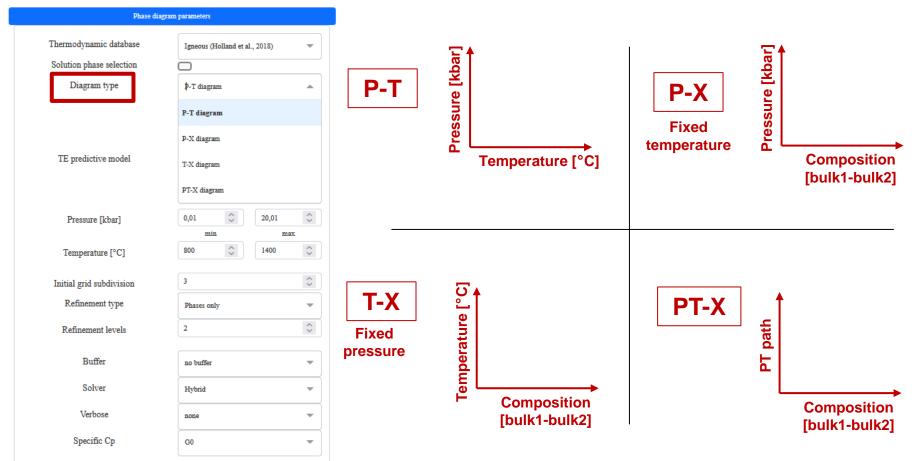
6

MAGEMinApp: solution phase selection



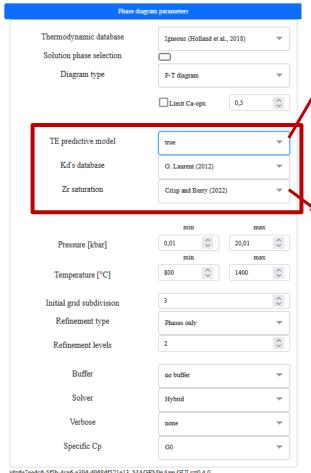
- Allow to deactivate solution phase models
- Note that solution phase models from different dataset cannot be mixed (yet)

MAGEMinApp: diagram types



8

MAGEMinApp: Trace element predictive model

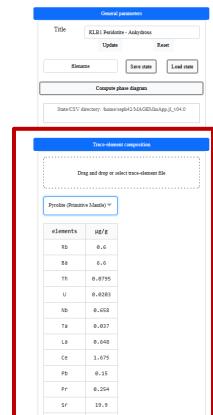


Activate trace-element partitioning at supra-solidus conditions

Displays trace element bulk panel on the right

Gives the option to select among 3 zirconium saturation models

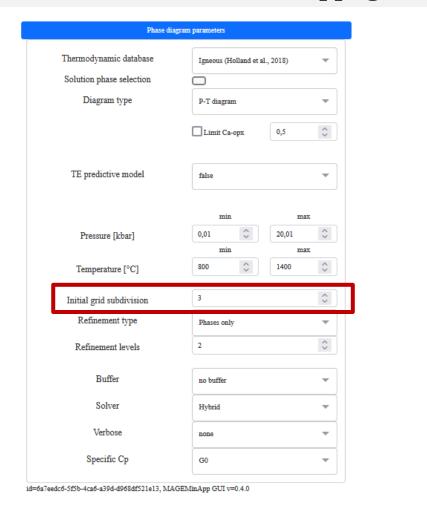


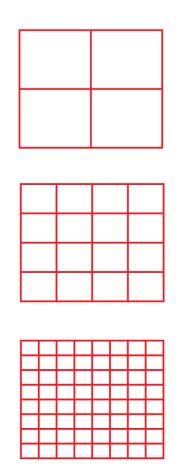


Nd

1.25

MAGEMinApp: grid subdivision and refinement





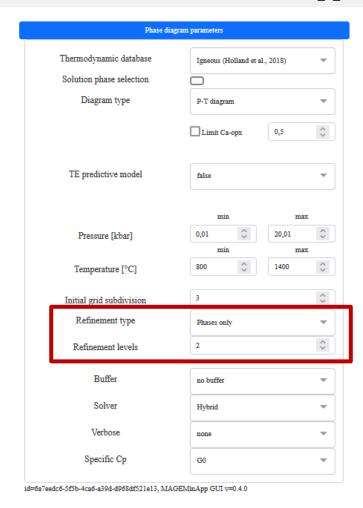
1 initial grid subdivision

2 initial grid subdivisions

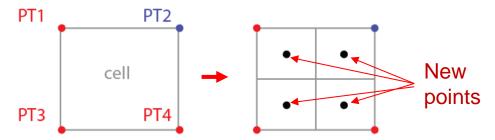
3 initial grid subdivisions

10

MAGEMinApp: grid subdivision and refinement

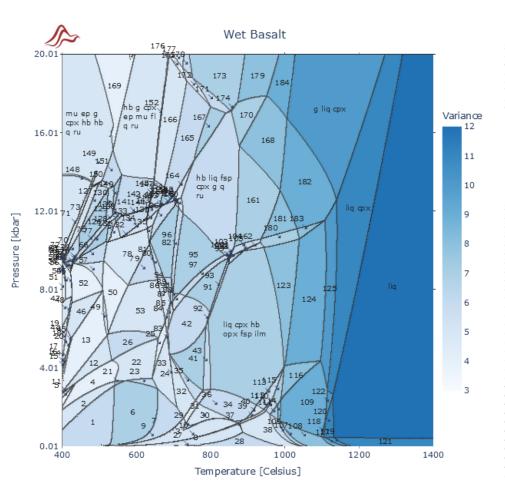


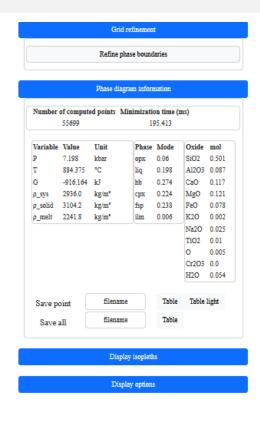
- Phase only refines (split) cells when a phase change is recorded in one of the four corners
- Dominant end-member
 refines (split) cells when the dominant
 end-member of any solution phase
 model changes in one of the four
 corners



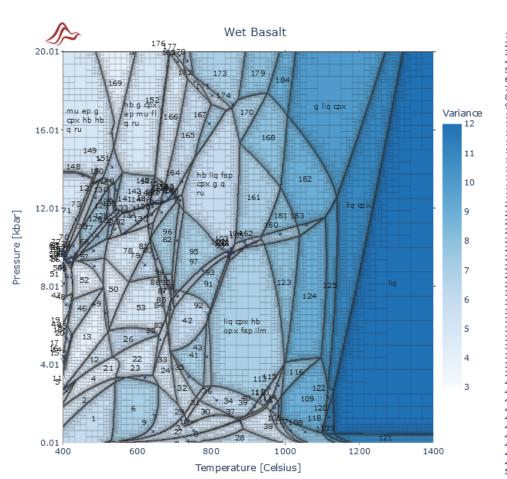
Refinement levels
 Number of successive grid refinements

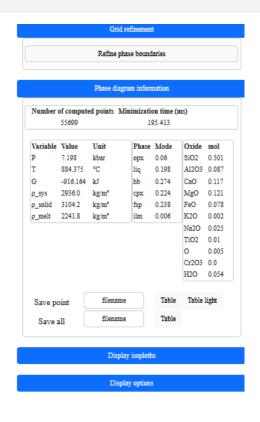
MAGEMinApp: grid refinement



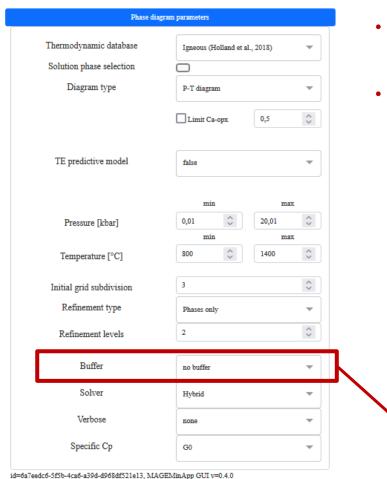


MAGEMinApp: grid refinement





MAGEMinApp: buffers

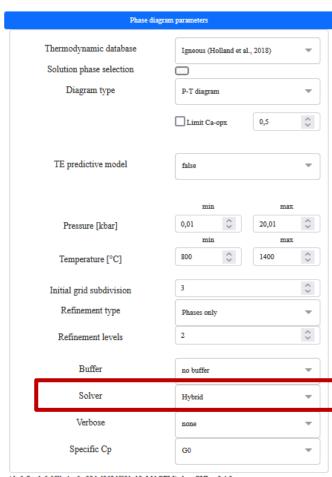


- Oxygen buffers
 QFM, MW, QIF, CCO, HM, NNO
- Fix activity
 H2O, O2, SiO2, FeO, MgO, Al2O3, TiO2



- Selecting a buffer displays the option to apply a shift in the RTlog scale
- e.g., +2 QFM
- Allow to provide the activity value in case activity is selected

MAGEMinApp: solvers

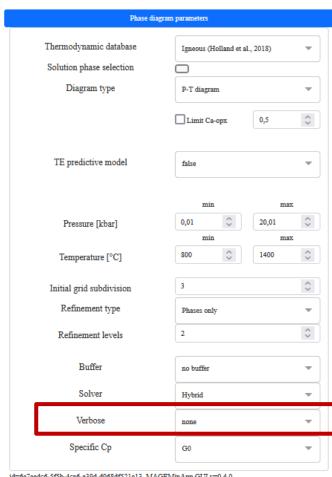


Default MAGEMin solver to perform stable phase equilibria calculation

No need to be changed in normal use

15

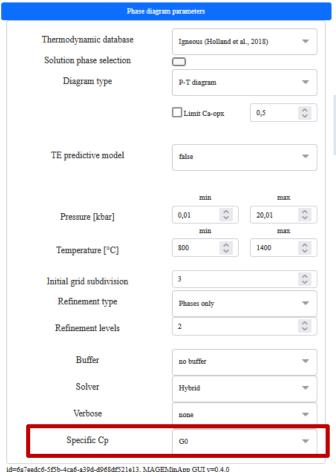
MAGEMinApp: solvers



Displays details of the calculation(s) in the Julia terminal

mostly used for debugging

MAGEMinApp: Specific heat capacity



Method to compute specific heat capacity

$$Cp = -T \frac{\Delta^2 G}{\Delta T^2} = -T \frac{G^{(T+\delta T)} + G^{(T-\delta T)} - 2G^{(T)}}{\delta T^2}$$

where Cp is the specific heat capacity, T is the temperature

Can be computed using

- 1. phase aggregate

Without reactions

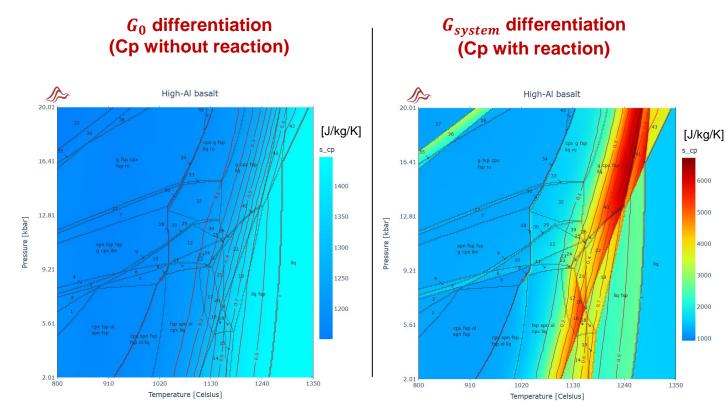
- 2. phase assemblage
- (G_{system})

With reactions

Note that when **G**_system is selected, solver must be set to legacy

higher accuracy at suprasolidus conditions is needed to compute Gibbs second derivative

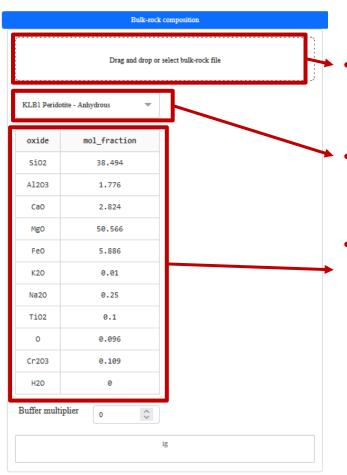
Specific heat capacity: what difference does it make?



- Cheap to compute
- Ignores latent heat

- More expensive to compute
- Correct heat budget
- To be chosen for geodynamic coupling

MAGEMinApp: bulk rock composition



Load custom bulk rock composition(s)

Select predefined bulk rock composition for testing

Bulk rock composition displayed in mol%
note that only the oxides taken into account in the
database are displayed

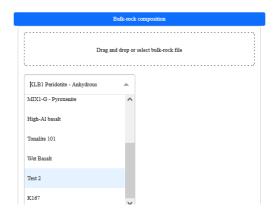
MAGEMinApp: bulk rock input file format

Example of input file provided in:

https://github.com/ComputationalThermodynamics/Resources/GG2024/bulkrock_composition_input_files/

```
# HEADER
title; comments; db; sysUnit; oxide; frac; frac2
#BUIK-ROCK-COMPOSITION
Test-2; Moo-et-al., 2000; ig; mol; [Sio2, Al203, Cao, Mgo, Feo, K2O, Na20, Tio2, O, Cr203, H20]; [48.97, 11.76, 13.87, 4.21, 8.97, 1.66, 10.66, 1.36, 1.66, 0.01, 5.0];
K167; Moo-et-al., 2000; ig; mol; [Sio2, Al203, Cao, Mgo, Feo, K20, Na20, Tio2, O, Cr203, H20]; [50.3162, 8.0778, 11.6616, 11.3262, 9.1893, 0.4312, 2.4051, 2.271, 4.312, 0.0096, 0.0];
Test-3; Coin-& Kwak, 1984; mb; wt; [Sio2, Al203, Cao, Mgo, Feo3, K20, Na20, Tio2, Feo, H20]; [55.12, 12.76, 4.32, 5.21, 2.45, 1.66, 10.66, 1.36, 1.66, 2.0];
Simon; Shorn-Simon, 2023; mb; mol; [Sio2, Al203, Cao, Mgo, Feo, K20, Na20, Tio2, O, H20]; [61.8, 8.57, 9.26, 5.05, 7.27, 0.21, 3.43, 1.25, 0.73, 2.85];
```

 Note that either [..., Fe2O3, FeO,...] or [..., FeO, O, ...] must me provided for the database accounting for O



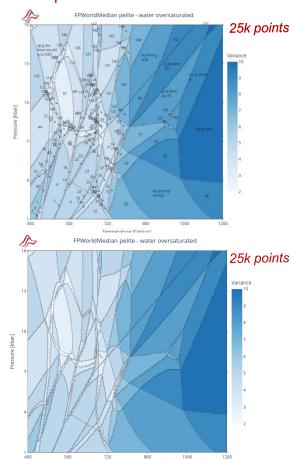
Once loaded, the bulk-rock composition appear in the dropdown menu

Note that the bulk are attached to a database, this is why only Test 2 and K167 appear in the dropdown menu

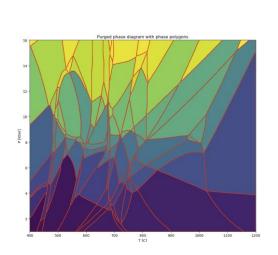
MAGEMinApp: upcoming

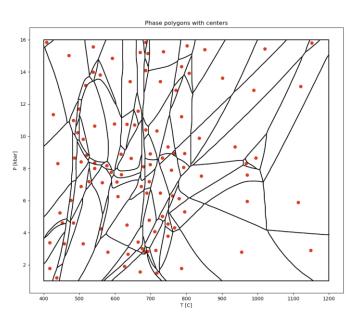
Improved reaction line extraction and field center finder

With Anton Popov (JGU Mainz)



Temperature [Celsius]





 \rightarrow vectorized reaction lines and accurate labelling of non convex fields!

Julia interface: MAGEMin_C



https://github.com/ComputationalThermodynamics/MAGEMin_C



Install MAGEMin_C

```
single point minimization(P, T, data, X=X, Xoxides=Xoxides, sys in=sys in
                                                                                                                                            : 10.0
                                                                                                                                                     [kbar]
julia> using MAGEMin C
                                                                                                                                            : 1100.0
                                                                                                                                                     [Celsius]
                                                                                                                                  Stable phase | Fraction (mol fraction)
julia> data
                = Initialize MAGEMin("ig", verbose=false);
                                                                                                                                             0.75136
julia> P,T
                = 10.0, 1100.0
julia> Xoxides = ["SiO2"; "Al2O3"; "CaO"; "MgO"; "FeO"; "Fe2O3"; "K2O"; "Na2O"; "TiO2"; "Cr2O3"; "H2O"]
                                                                                                                                  Stable phase | Fraction (wt fraction)
julia> X
                 = [48.43; 15.19; 11.57; 10.13; 6.65; 1.64; 0.59; 1.87; 0.68; 0.0; 3.0];
                                                                                                                                             0.22897
julia> sys in = "wt"
                                                                                                                                  Stable phase | Fraction (vol fraction)
                                                                                                                                             0.77373
julia> out
                 = single point minimization(P, T, data, X=X, Xoxides=Xoxides, sys in=sys in)
                                                                                                                                             0.19218
                                                                                                                               Gibbs free energy: -916.874646 (45 iterations; 81.05 ms)
                                                                                                                               Oxygen fugacity
                                                                                                                                                 : -7.68808396800797
                                                                                                                                                 : 1.2159893622277753
```

```
out. `+ tab`
```

julia> out.												
G_system	Gamma	MAGEMin_ver	M_sys	PP_vec	P_kbar	SS_vec	T_C	V	Vp	Vp_S	Vs	Vs_S
X	aA1203	aFe0	aH20	aMg0	aSiO2	aTiO2	alpha	bulk	bulkMod	bulkModulus_M	bulkModulus_S	bulk_F
bulk_F_wt	bulk_M	bulk_M_wt	bulk_S	bulk_S_wt	bulk_res_norm	bulk_wt	ср	dQFM	dataset	enthalpy	entropy	f02
frac_F	frac_F_wt	frac_M	frac_M_wt	frac_S	frac_S_wt	iter	mSS_vec	n_PP	n_SS	n_mSS	oxides	ph
ph_frac	ph_frac_vol	ph_frac_wt	ph_id	ph_type	rho	rho_F	rho_M	rho_S	s_cp	shearMod	shearModulus_S	status
time ms												