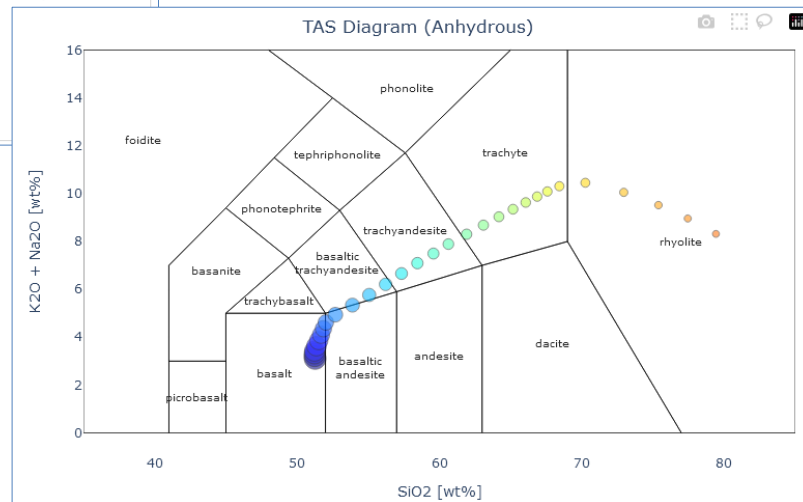
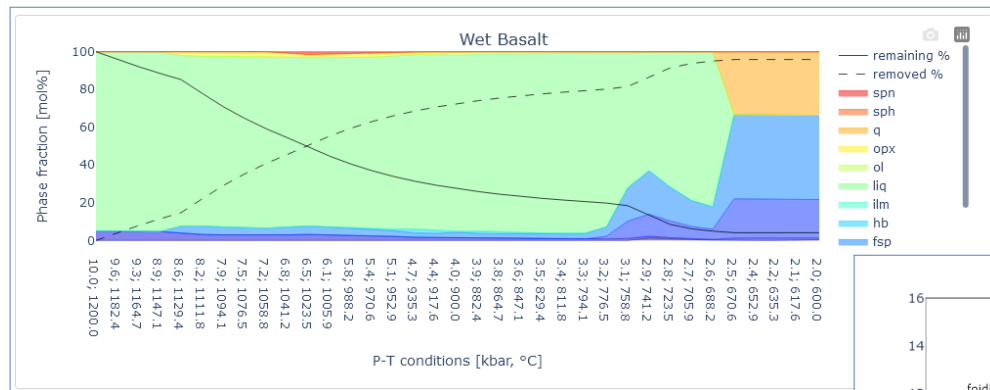


# MAGEMinApp: PTX paths



# MAGEMinApp: PTX paths interface

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

MAGEMin

File

Phase diagrams **PTX path** Isentropic path

Setup **Diagram** Trace-elements

Phase diagram parameters

Thermodynamic database Igneous (Holland et al., 2018)

Solution phase selection

Diagram type P-T diagram

H<sub>2</sub>O-saturated at solidus false

Limit Ca-opt 0.5

TE predictive model false

Pressure [kbar] 0.01 20.01

Temperature [°C] 800 1400

Initial grid subdivision 3

Refinement type Phases only

Refinement levels 2

Buffer no buffer

Solver Hybrid

Verbose none

Specific Cp 00

Bulk-rock composition

Drag and drop or select bulk-rock file

KLB1 Peridotite - Anhydrous

oxide	mol_fraction
SiO <sub>2</sub>	38.494
Al <sub>2</sub> O <sub>3</sub>	1.776
CaO	2.304
MgO	50.566
FeO	5.886
K <sub>2</sub> O	0.01
Na <sub>2</sub> O	0.25
TiO <sub>2</sub>	0.1
O	0.096
Cr <sub>2</sub> O <sub>3</sub>	0.109
H <sub>2</sub> O	0

General parameters

Title KLB1 Peridotite - Anhydrous

Update Reset

filename Save state Load state

File

Phase diagrams **PTX path** Isentropic path

Setup **Diagram** Trace-elements

Phase diagram parameters

Thermodynamic database Igneous (Holland et al., 2018)

Solution phase selection

# MAGEMinApp: PTX path, path definition (batch melting)

- The database/bulk-rock interface of the PTX paths tab is overall similar to the one of the phase diagrams

Configuration

Thermodynamic database: Igneous (Holland et al., ...)

Solution phase selection: ☐

Limit Ca-opx: ☐ 0.5

Buffer: no buffer

Solver: Hybrid

Verbose: none

Bulk-rock composition

Drag and drop or select bulk-rock file

KLB1 Peridotite - Anhydrous

oxide	mol_fraction
SiO2	38.494
Al2O3	1.776
CaO	2.824
MgO	50.566
FeO	5.886
K2O	0.01
Na2O	0.25
TiO2	0.1
O	0.096
Cr2O3	0.109
H2O	0

Igneous (Holland et al., 2018)

- Keep the default value for the database and the predefined bulk-rock (KLB-1 Peridotite)
  - Click on find solidus and find liquidus to get the temperature range and modify the P-T points accordingly
- Note that the defined path is previewed in the central panel

Path definition

Pressure [kbar]: 10

Tolerance [K]: 0.01

Find solidus: 1183.112144470214

Pressure [kbar]: 10

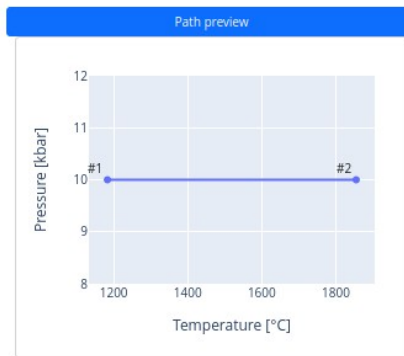
Tolerance [K]: 0.01

Find liquidus: 1855.734252929687

Define P-T points

	P [kbar]	T [°C]
×	10	1183
×	10	1855

Add new point



Path options

Resolution: 32

P-T-X Mode: Equilibrium

Assimilation: false

Compute path

Save path: filename Table csv file

Export references: filename bibtex file

Display options

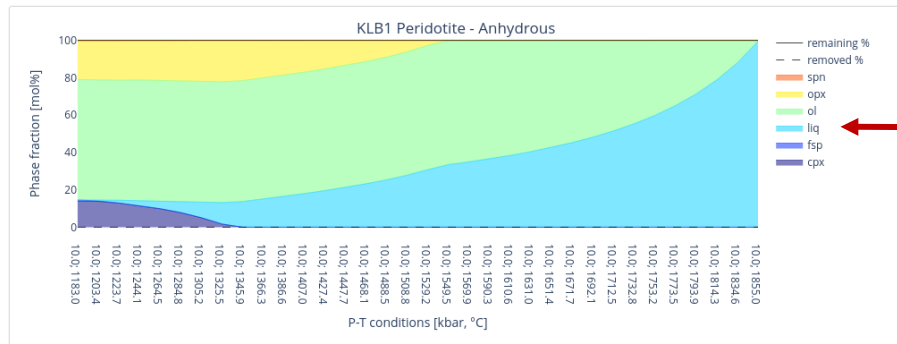
System unit: mol%

Database and bulk-rock selection panel

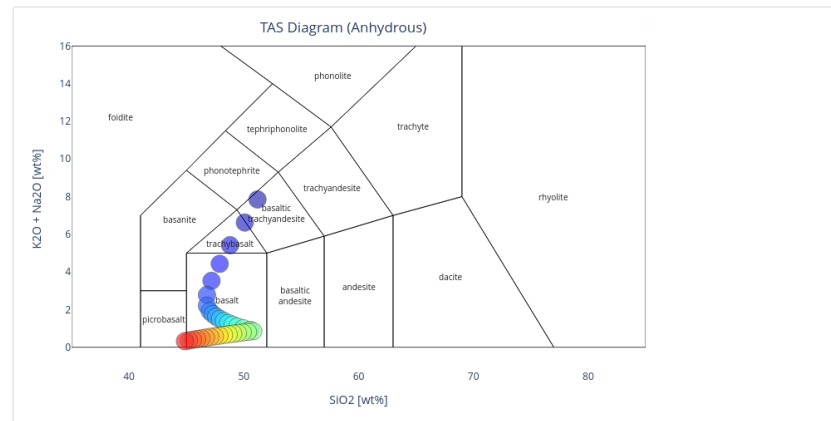
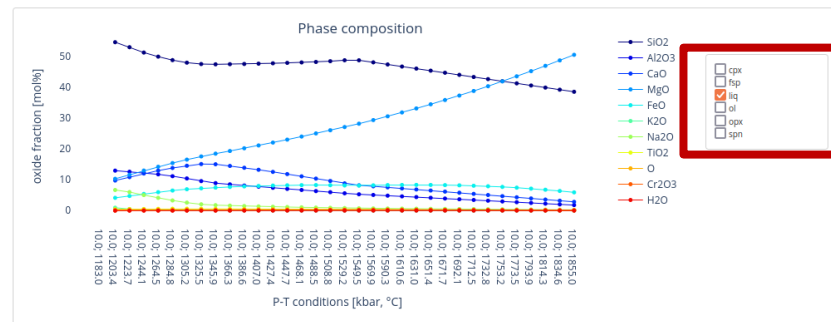
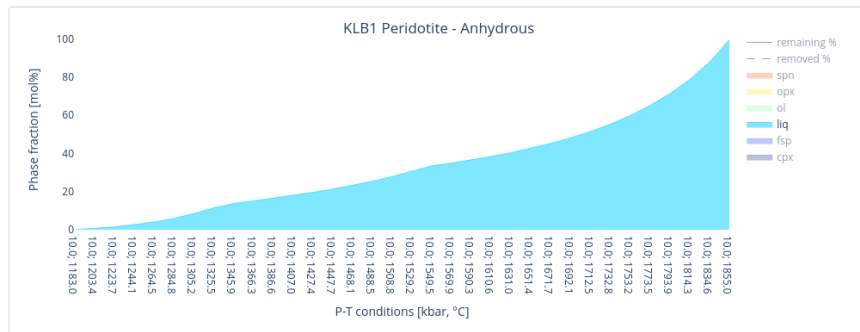
- Finally on the right panel set the resolution to 32 (number of intermediate PT calculations between P-T points)
- Then compute path!

# MAGEMinApp: PTX path, path visualization (batch melting)

- The result of the PTX path should look like this...



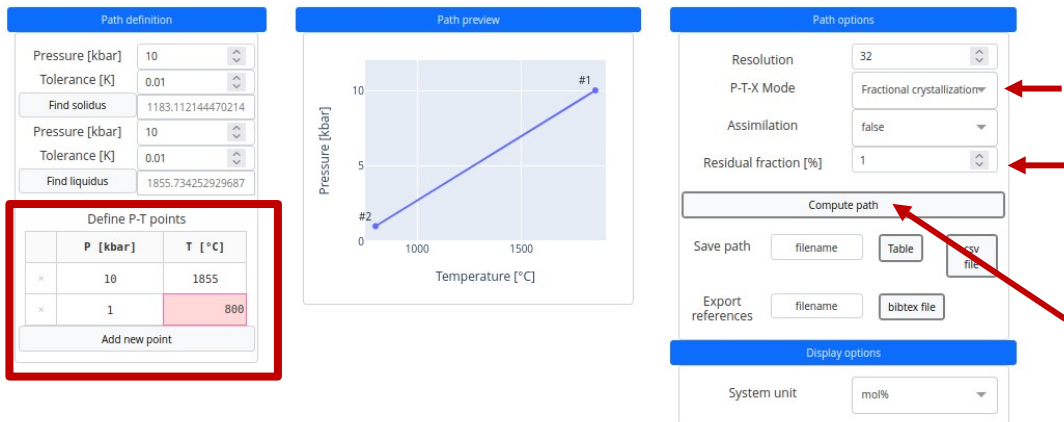
- The plot can be saved by clicking on the camera in the top right corner
- Double clicking on the label of one phase will isolate it:



- Composition profile can be displayed by selecting given solution phase models
- If "liq" is selected, a TAS diagram showing the melt composition evolution will be displayed

# MAGEMinApp: PTX path, fractional crystallization

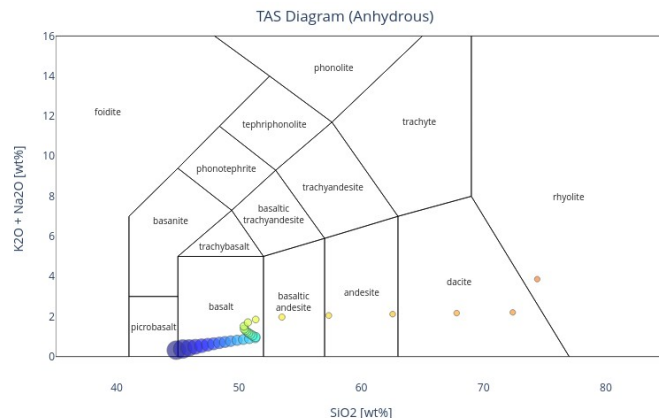
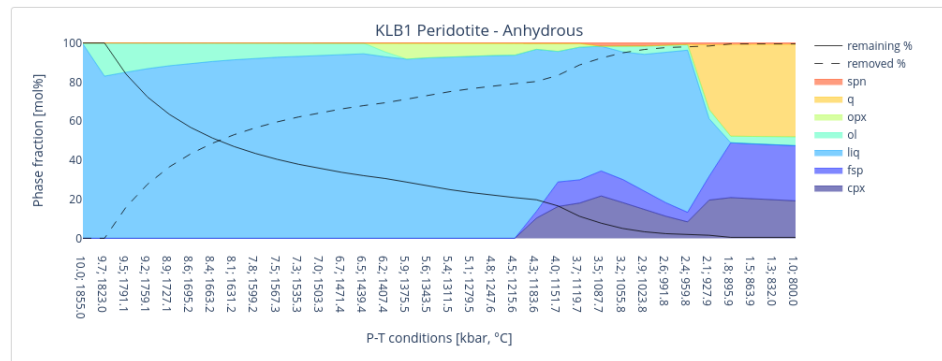
- First let's change the PT path as:



Select fractional crystallization

Choose residual fraction to be 1%  
(fraction of residual solid transported with the melt)

Compute path



Note that in the TAS diagram for "liq" composition, the size of the circles scales with the fraction of melt

# MAGEMinApp: PTX path, fractional melting

- Change database to “Metabasite”, select “aug” (Augite) and choose “Nature amphibolite...” bulk-rock composition from the list  
(you can also load your own bulk if you prefer)

**Configuration**

Thermodynamic database  
Solution phase selection

Metabasite (Green et al.)  
☐

clinopyroxene

Omph ☒ Aug

Buffer

no buffer

Solver

Hybrid

Verbose

none

**Bulk-rock composition**

Drag and drop or select bulk-rock file

Natural amphibolites amr.

oxide	mol_fraction
SiO2	51.08
Al2O3	9.68
CaO	13.26
MgO	11.21
FeO	11.66
K2O	0.16
Na2O	0.79
TiO2	1.37
O	0.8
H2O	20

Metabasite (Green et al., 2016)

**Path definition**

Pressure [kbar]

10

Tolerance [K]

0.01

Find solidus

746.8866348266602

Pressure [kbar]

10

Tolerance [K]

0.01

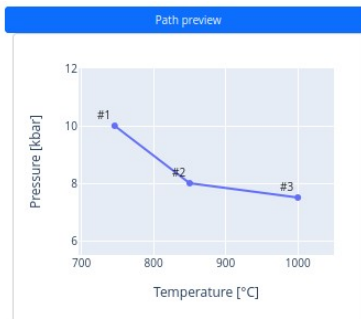
Find liquidus

1855.734252929687

**Define P-T points**

	P [kbar]	T [°C]
×	10	746
×	8	850
×	7.5	1000

Add new point



**Path options**

Resolution

32

P-T-X Mode

Fractional melting

Assimilation

false

Connectivity threshold [%]

7

**Compute path**

Save path

filename

Table

csv file

Export references

filename

bibtex file

**Display options**

System unit

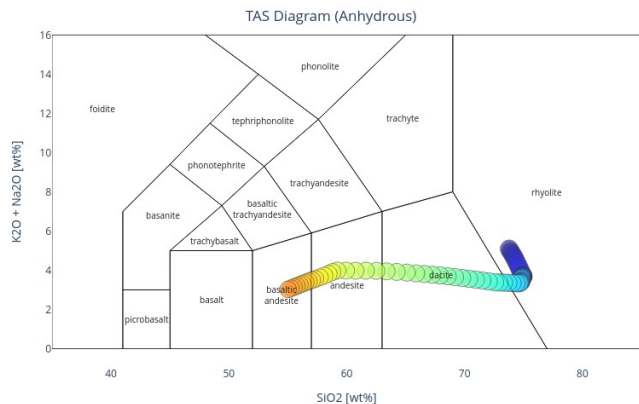
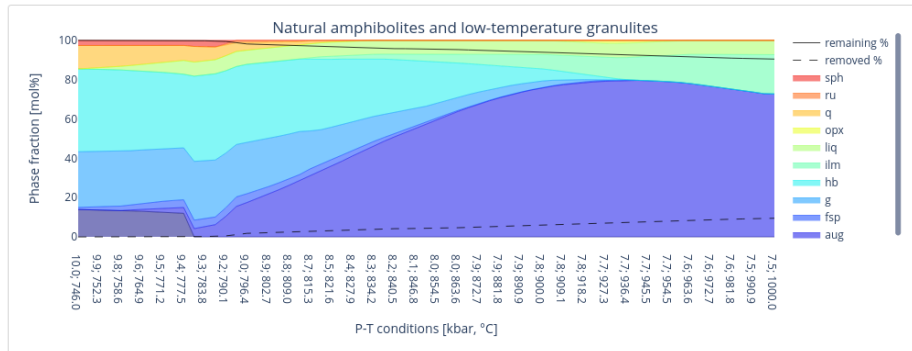
mol%

- Find the solidus at 10kbar and change path definition
- You can add new points by clicking “Add new point”

- Select “Fractional melting”
- Set connectivity threshold to 7% (fraction above which liquid is extracted)
- Compute path!

# MAGEMinApp: PTX path, fractional melting

- If using the predefined bulk-rock composition, this yields:



Path options

Resolution: 32

P-T-X Mode: Fractional melting

Assimilation: false

Connectivity threshold [%]: 7

Compute path

Save path: filename Table **csv file**

Export references: filename bibtext file

Display options

System unit: mol%

- Note that the results of the PTX path can be saved as Table or CSV file in the “Path options” panel

# MAGEMinApp: PTX path, assimilation

- You can also assimilate a fixed composition (second bulk-rock) through the PT path
  - Let's switch back to "Igneous" database
  - Choose "P-T-X mode" = "Equilibrium" and activate assimilation in the "Path options" panel
- Note that when assimilation = true, a third column in the "Path definition" table appears, here you can define the fraction of assimilated material at every point in mol%

**Thermodynamic database** Igneous (Holland et al., 2018)

**Solution phase selection** ☐

☐ Limit Ca-opx 0.5

Buffer no buffer

Solver Hybrid

Verbose none

**Bulk-rock composition**

Drag and drop or select bulk-rock file

Wet Basalt Tonalite 101

oxide	mol_fraction	oxide	mol_fraction
SiO2	50.081	SiO2	66.01
Al2O3	8.6901	Al2O3	11.98
CaO	11.6698	CaO	7.06
MgO	12.1438	MgO	4.16
FeO	7.7832	FeO	5.3
K2O	0.215	K2O	1.57
Na2O	2.4978	Na2O	4.12
TiO2	1.0059	TiO2	0.66
O	0.467	O	0.97
Cr2O3	0.01	Cr2O3	0.01
H2O	5.4364	H2O	50

Igneous (Holland et al., 2018)

**Path definition**

Pressure [kbar] 10

Tolerance [K] 0.01

Find solidus 746.8866348266602

Pressure [kbar] 10

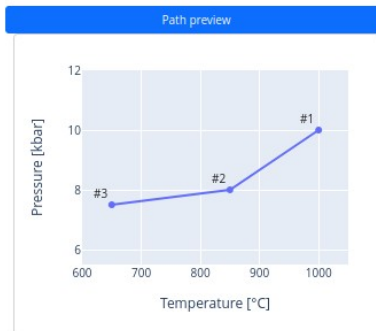
Tolerance [K] 0.01

Find liquidus 1855.734252929687

**Define P-T points**

	P [kbar]	T [°C]	Add [mol%]
x	10	1000	0
x	8	850	10
x	7.5	650	50

Add new point



**Path options**

Resolution 32

P-T-X Mode Equilibrium

Assimilation true

Compute path

Save path filename Table csv file

Export references filename bibtext file

**Display options**

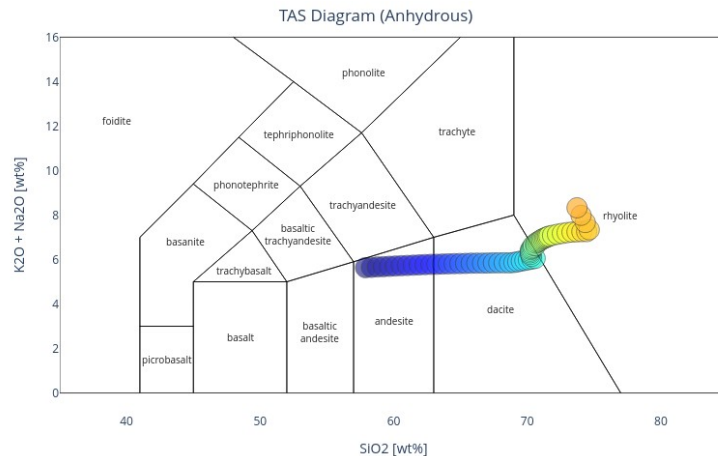
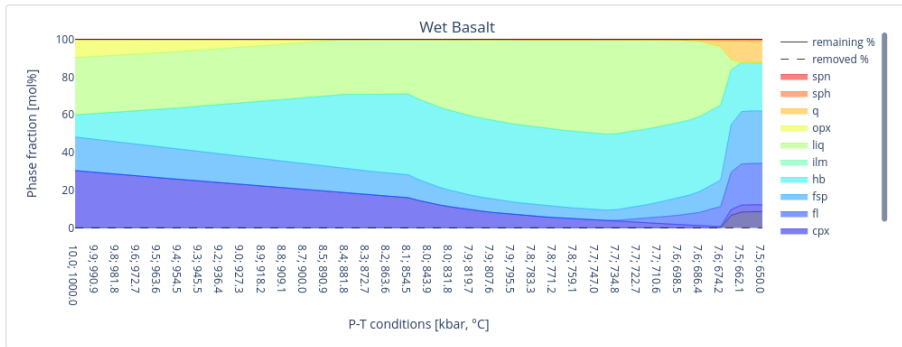
System unit mol%

- Select "Wet basalt" for the left (principal) bulk and "Tonalite 101" for the right (assimilated) bulk
- Update the PT paths points including the fraction of assimilated material
- Compute the path!



# MAGEMinApp: PTX path, assimilation

- This yields with assimilation



- And without assimilation

