CIDER

Mathematical and Computational Models of Magmatic Systems: A Primer of Dynamic and Thermodynamic Models

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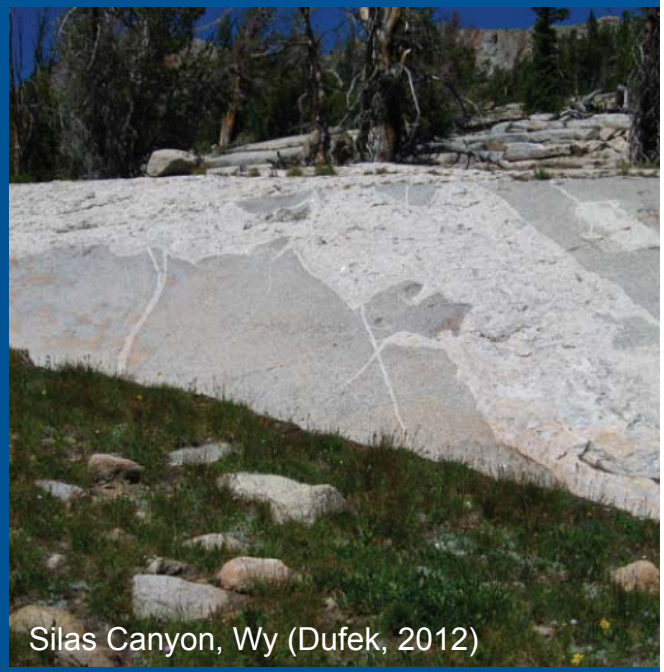
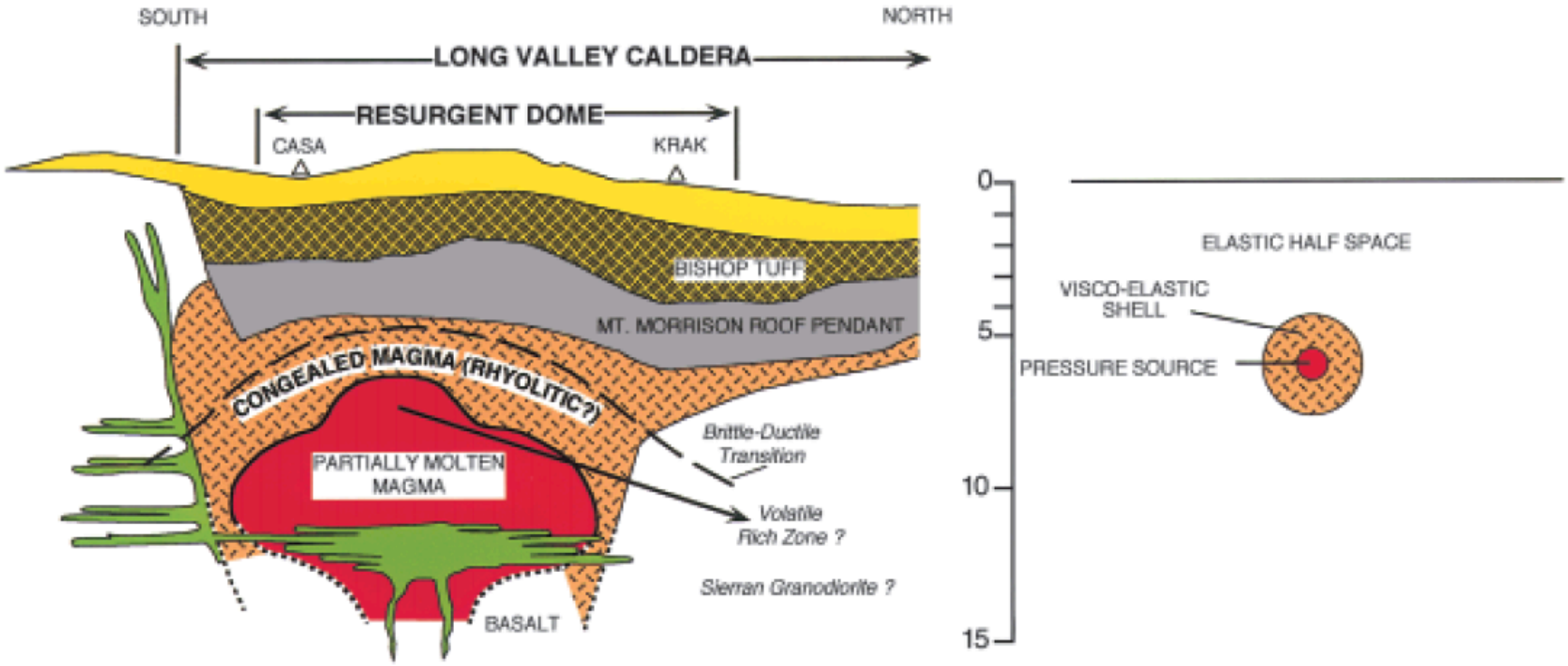
Modeling magmatic processes:

1. Deformation Models
2. Thermal Models
3. Phase Equilibria
4. Magma Dynamics



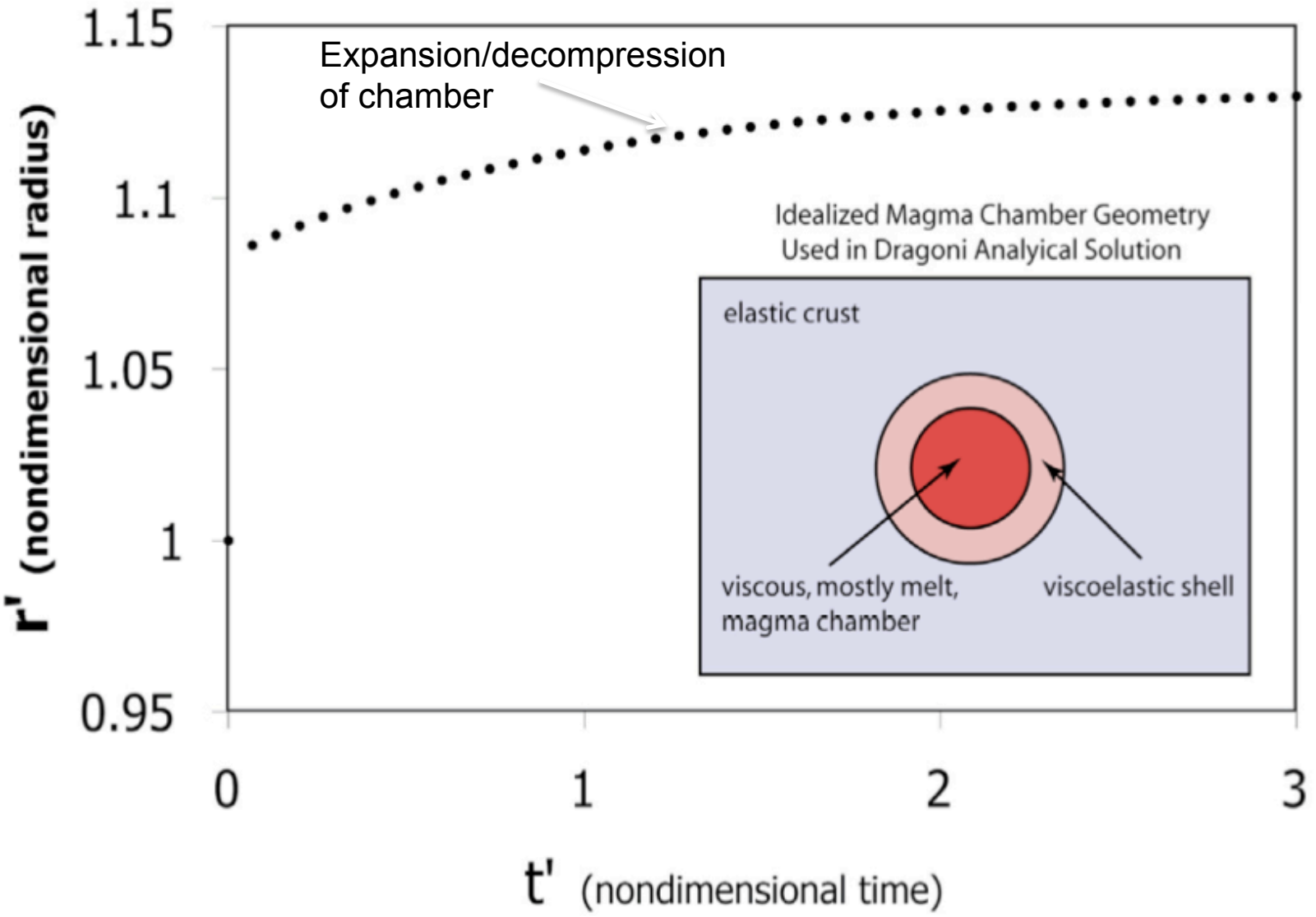
Silas Canyon, Wy (Dufek, 2012)

Deformation

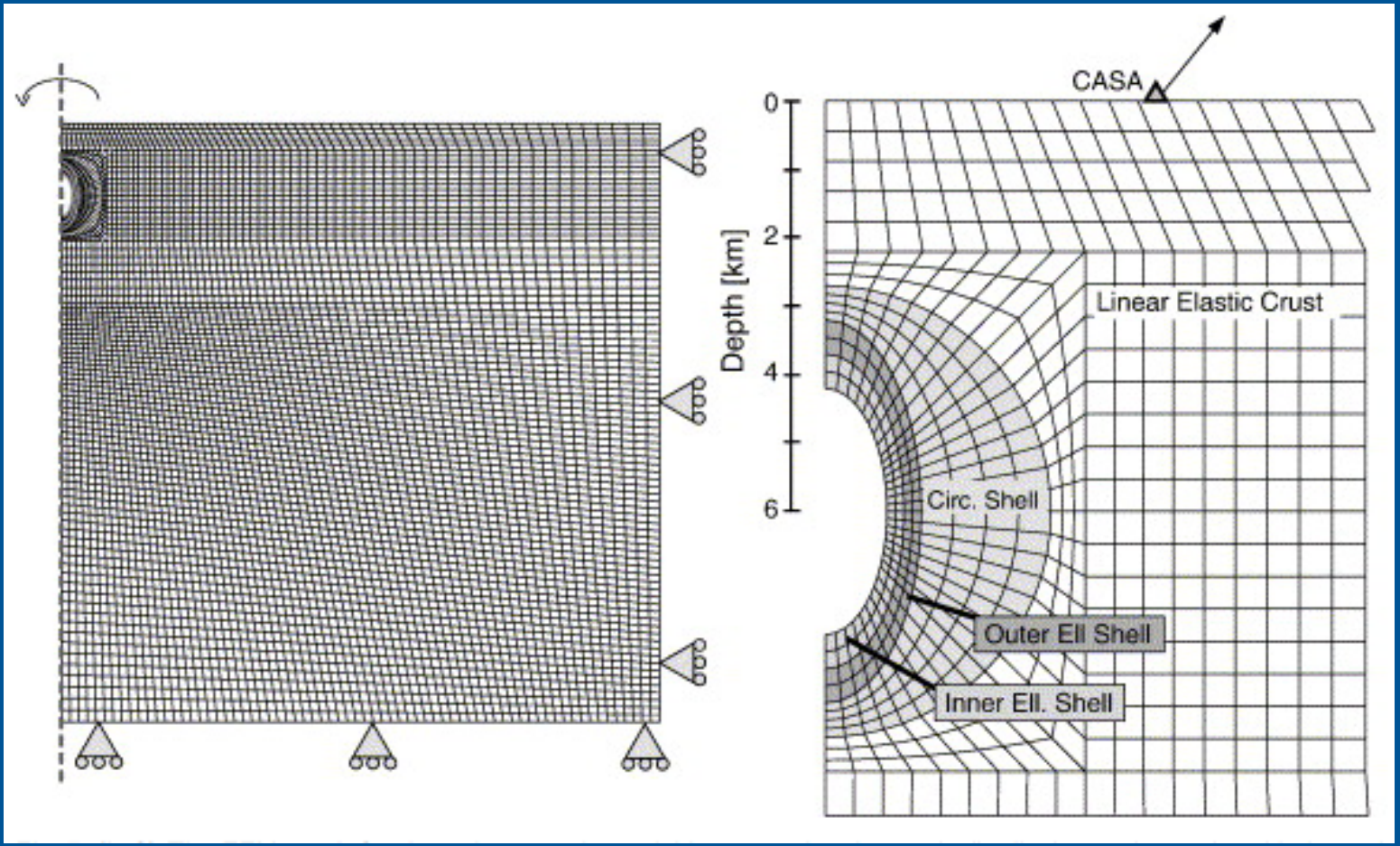


Newman et al., 2001

Crustal container is not, in general, completely rigid and can have elastic and viscoelastic response.



Deformation



Some Thermal Considerations

$$\frac{\partial H_T}{\partial t} + \frac{\partial}{\partial \mathbf{x}_i}\left(\mathbf{u}_i H_T\right) = \frac{\partial}{\partial \mathbf{x}_i} k \left(\frac{\partial}{\partial \mathbf{x}_i} T\right)$$

$$H_T = \overbrace{\rho \int_{\text{Tref}}^{T} c_p dT}^{\text{Sensible Heat}} + \overbrace{\rho\, fL}^{\text{Latent Heat}}$$

$$\rho^* \left[\frac{\partial \mathrm{T}^*}{\partial \mathrm{t}^*} + \mathbf{u}_i^* \frac{\partial \mathrm{T}^*}{\partial \mathrm{x}_i^*}\right] = \left[\frac{1}{\mathrm{Pe}}\right] \frac{\partial^2 \mathrm{T}^*}{\partial \mathrm{x}_i^{2*}} - \left[\frac{1}{\mathrm{Ste}}\right] R^*$$

$$R^* = \rho^* \frac{\partial f}{\partial t^*}$$

Dimensionless rate of production of melt

$$\mathrm{Pe} = \left[\frac{c_p \rho_0 \delta}{k}\right] \mathbf{u}_0$$

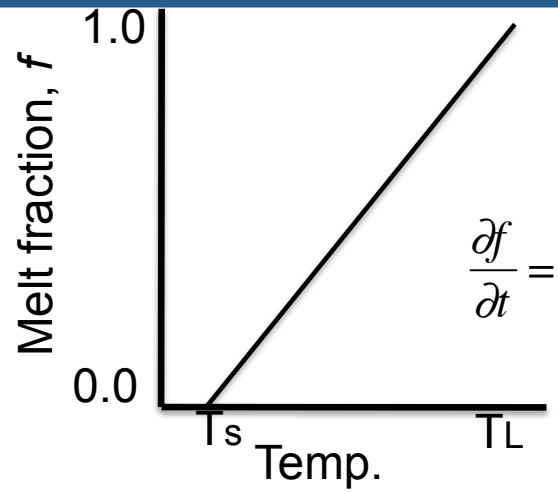
Advective/diffusive heat transport

$$\mathrm{Ste} = \frac{c_p T_0}{L}$$

Sensible/latent heat contribution

Numerous modeling approaches applied to the magmatic problem from 1-D conduction to 3D multiphase dynamic simulations

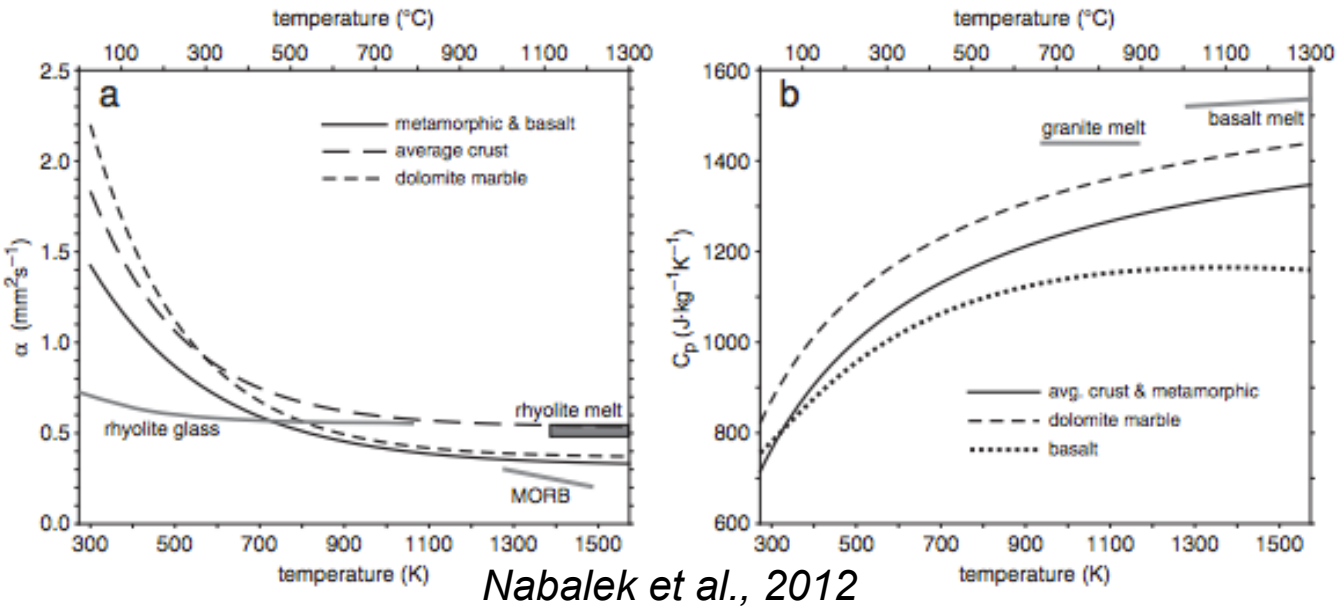
Effect of latent heat --- Often treated with a linearization of MF vs. Temp.



$$\frac{\partial f}{\partial t} = \left[\frac{1}{T_L - T_S}\right]\frac{\partial T}{\partial t}$$

$$c_p^* = c_p + \frac{L}{T_L - T_s}$$

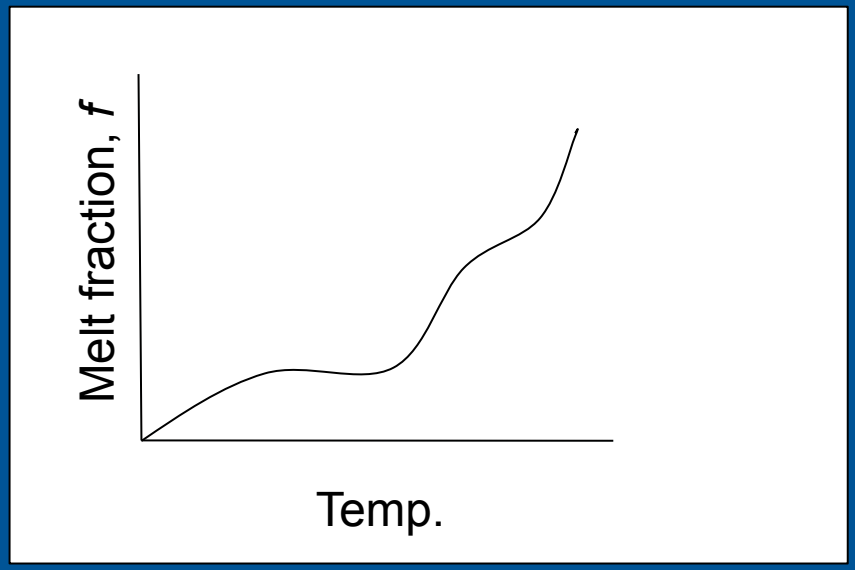
Can have an even greater influence that temperature dependent diffusivities --- something we know to be important for the thermal evolution of plutons.



Nabalek et al., 2012

Non-linear Melt Fraction to temperature relationship (but still assuming that different phases have the same latent heat).

--- in general need to use an iterative approach (e.g. Prakash and Voller)



Magma Dynamics

Single (Eulerian)

Single phase with modified density due to local composition, temp., melt fraction, etc. (no relative motion between phases)

Multiphase (Eulerian-Eulerian, Eulerian-Lagrangian, Eulerian-Eulerian-Lagrangian)

Relative motion between phases.

Multiphase Equations for Magma Chamber

Volume fraction of all phases equals 1

$$\sum_k \phi_k = 1$$

Conservation of Mass

$$\frac{\partial}{\partial t}\left(\phi_k \rho_k\right) + \frac{\partial}{\partial \mathbf{x_i}}\left(\phi_k \rho_k \mathbf{u_{k,i}}\right) = R_k$$

Conservation of Momentum

$$\frac{\partial(\phi_k \rho_k \mathbf{u_{k,i}})}{\partial t} + \frac{\partial(\phi_k \rho_k \mathbf{u_{k,i}} \mathbf{u_{k,j}})}{\partial \mathbf{x_i}} =$$

$$-\phi_k \frac{\partial P}{\partial \mathbf{x_i}} \delta_{ij} + \frac{\partial}{\partial \mathbf{x_i}}\left[\tau_{\mathbf{ij}}\right] + \mathbf{D}_i + \rho_k \phi_k \boldsymbol{g}_2 \delta_{\mathbf{i2}} + R_k \mathbf{u_{k,i}}$$

Conservation of Thermal Energy

$$\phi_k \rho_k c_k \left[\frac{\partial \mathrm{T_k}}{\partial \mathrm{t}} + \mathbf{u_i} \frac{\partial \mathrm{T_k}}{\partial \mathbf{x_i}}\right] = \delta_{\mathrm{km}} \frac{\partial \mathrm{q_k}}{\partial \mathbf{x_i}} + \pi k_m \mathrm{d}\ \mathbf{Nu}\left(\mathrm{T}_m - \mathrm{T_c}\right) + \phi_k R_k L$$

Conservation of Chemical Species

$$\frac{\partial}{\partial t}\left(\phi_k \rho_k C_{SiO_2}\right) + \frac{\partial}{\partial \mathbf{x_i}}\left(\phi_k \rho_k \mathbf{u_{k,i}} C_{SiO_2}\right) = \beta_{(f)}$$

Multiphase Equations for Magma Chamber

Volume fraction of all phases equals 1

$$\sum_k \phi_k = 1$$

Conservation of Mass

$$\frac{\partial}{\partial t}\left(\phi_k \rho_k\right) + \frac{\partial}{\partial \mathbf{x_i}}\left(\phi_k \rho_k \mathbf{u_{k,i}}\right) = R_k$$

Crystals and magma have distinct sets of conservation equations (denoted by *k* in these equations)

Conservation of Momentum

$$\frac{\partial(\phi_k \rho_k \mathbf{u_{k,i}})}{\partial t} + \frac{\partial(\phi_k \rho_k \mathbf{u_{k,i}} \mathbf{u_{k,j}})}{\partial \mathbf{x_i}} =$$

$$-\phi_k \frac{\partial P}{\partial \mathbf{x_i}} \delta_{ij} + \frac{\partial}{\partial \mathbf{x_i}}\left[\tau_{\mathbf{ij}}\right] + \mathbf{D}_i + \rho_k \phi_k \boldsymbol{g}_2 \delta_{\mathbf{i2}} + R_k \mathbf{u_{k,i}}$$

Conservation of Thermal Energy

$$\phi_k \rho_k c_k \left[\frac{\partial \mathrm{T_k}}{\partial \mathrm{t}} + \mathbf{u_i} \frac{\partial \mathrm{T_k}}{\partial \mathbf{x_i}}\right] = \delta_{\mathrm{km}} \frac{\partial \mathrm{q_k}}{\partial \mathbf{x_i}} + \pi k_m \mathrm{d}\ \mathbf{Nu}\left(\mathrm{T}_m - \mathrm{T_c}\right) + \phi_k R_k L$$

Conservation of Chemical Species

$$\frac{\partial}{\partial t}\left(\phi_k \rho_k C_{SiO_2}\right) + \frac{\partial}{\partial \mathbf{x_i}}\left(\phi_k \rho_k \mathbf{u_{k,i}} C_{SiO_2}\right) = \beta_{(f)}$$

Multiphase Equations for Magma Chamber

Volume fraction of all phases equals 1

$$\sum_k \phi_k = 1$$

Conservation of Mass

$$\frac{\partial}{\partial t}\left(\phi_k \rho_k\right) + \frac{\partial}{\partial \mathbf{x_i}}\left(\phi_k \rho_k \mathbf{u_{k,i}}\right) = \boxed{R_k}$$

Conservation of Momentum

$$\frac{\partial(\phi_k \rho_k \mathbf{u_{k,i}})}{\partial t} + \frac{\partial(\phi_k \rho_k \mathbf{u_{k,i}} \mathbf{u_{k,j}})}{\partial \mathbf{x_i}} =$$

$$-\phi_k \frac{\partial P}{\partial \mathbf{x_i}} \delta_{ij} + \frac{\partial}{\partial \mathbf{x_i}}\left[\tau_{\mathbf{ij}}\right] + \mathbf{D}_i + \rho_k \phi_k \boldsymbol{g}_2 \delta_{\mathbf{i2}} + \boxed{R_k \mathbf{u_{k,i}}}$$

Conservation of Thermal Energy

$$\phi_k \rho_k c_k \left[\frac{\partial \mathrm{T_k}}{\partial \mathrm{t}} + \mathbf{u_i} \frac{\partial \mathrm{T_k}}{\partial \mathbf{x_i}}\right] = \delta_{\mathrm{km}} \frac{\partial \mathrm{q_k}}{\partial \mathbf{x_i}} + \pi k_m \mathrm{d}\ \mathbf{Nu}\left(\mathrm{T}_m - \mathrm{T_c}\right) + \boxed{\phi_k R_k L}$$

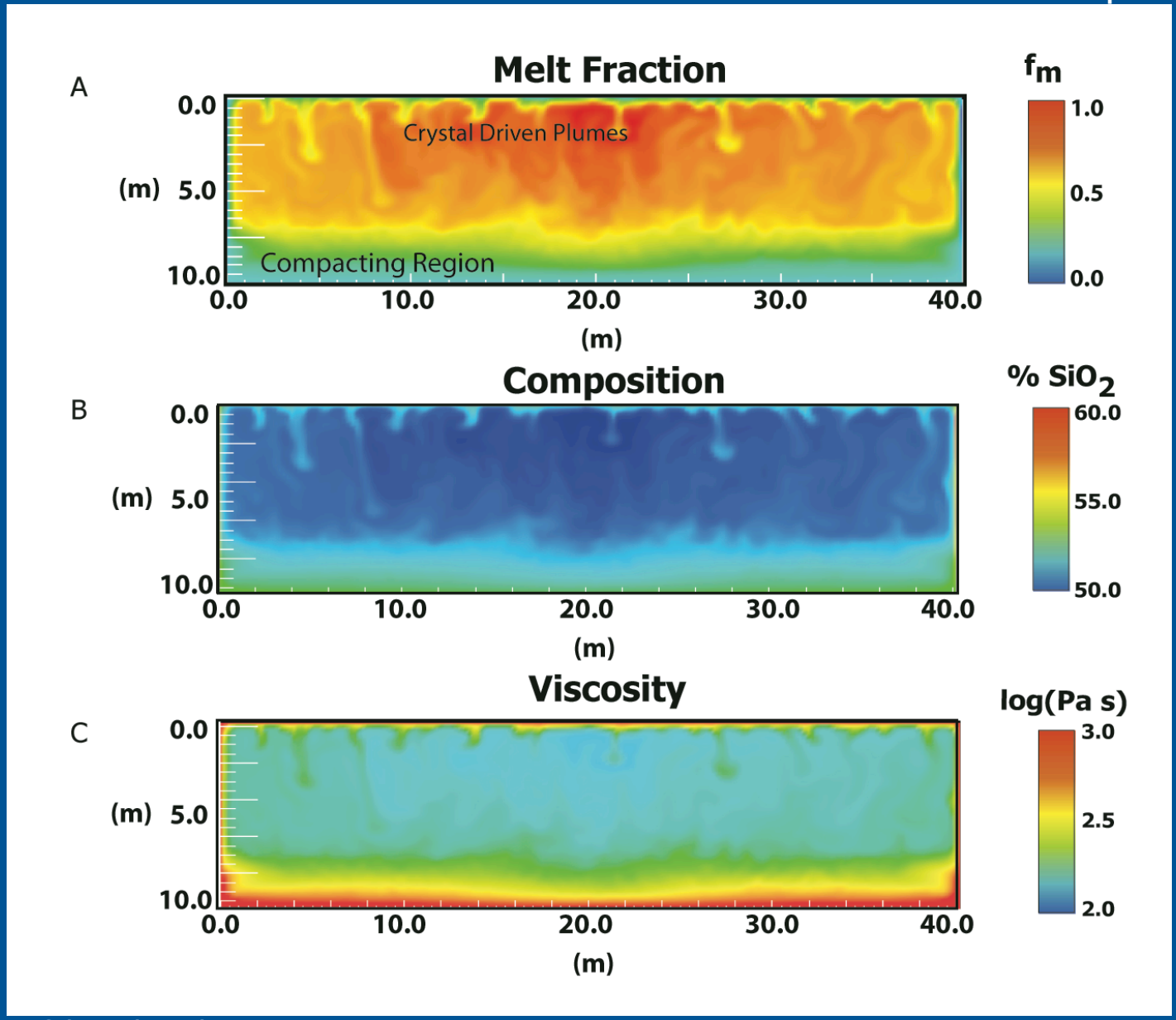
Conservation of Chemical Species

$$\frac{\partial}{\partial t}\left(\phi_k \rho_k C_{SiO_2}\right) + \frac{\partial}{\partial \mathbf{x_i}}\left(\phi_k \rho_k \mathbf{u_{k,i}} C_{SiO_2}\right) = \boxed{\beta_{(f)}}$$

Crystallization

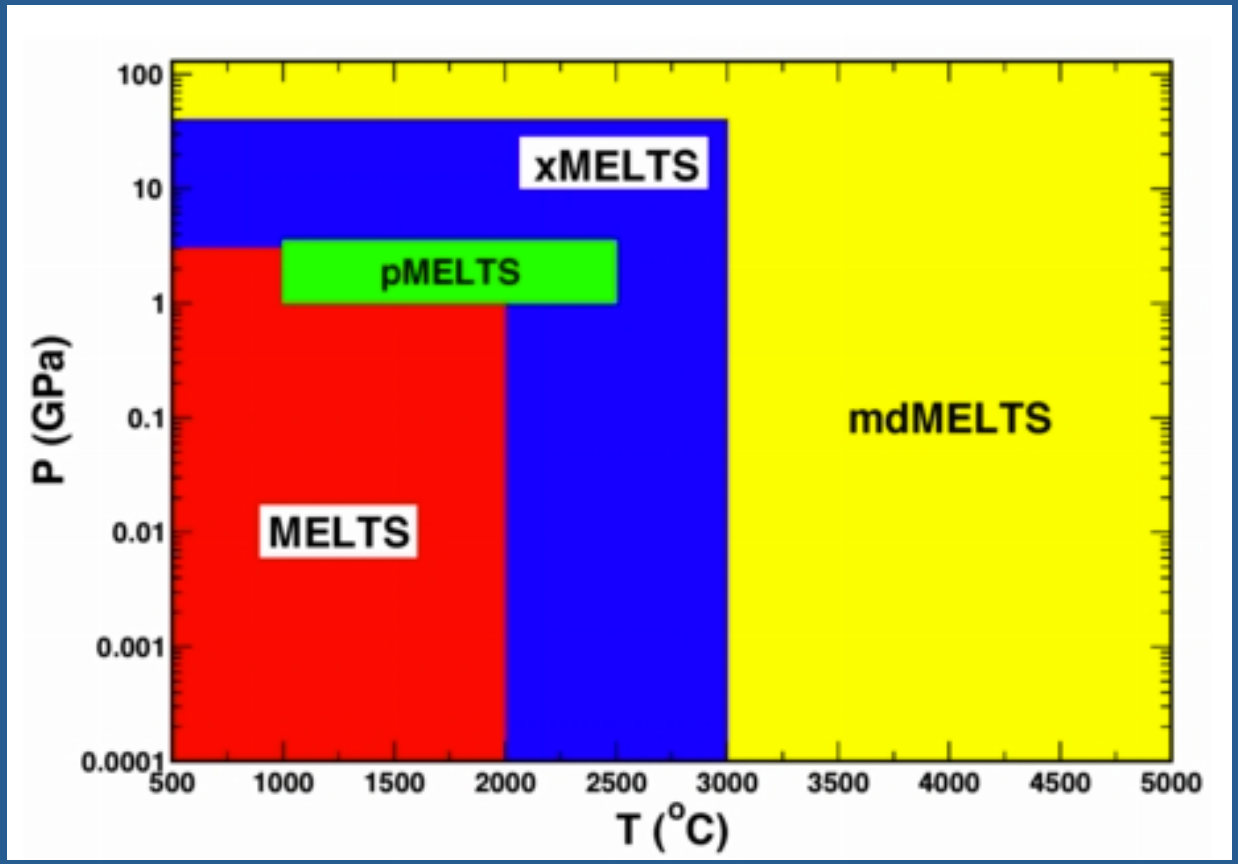
An Example Simulation:

Basaltic intrusion, modeled intrusion depth: 24 km



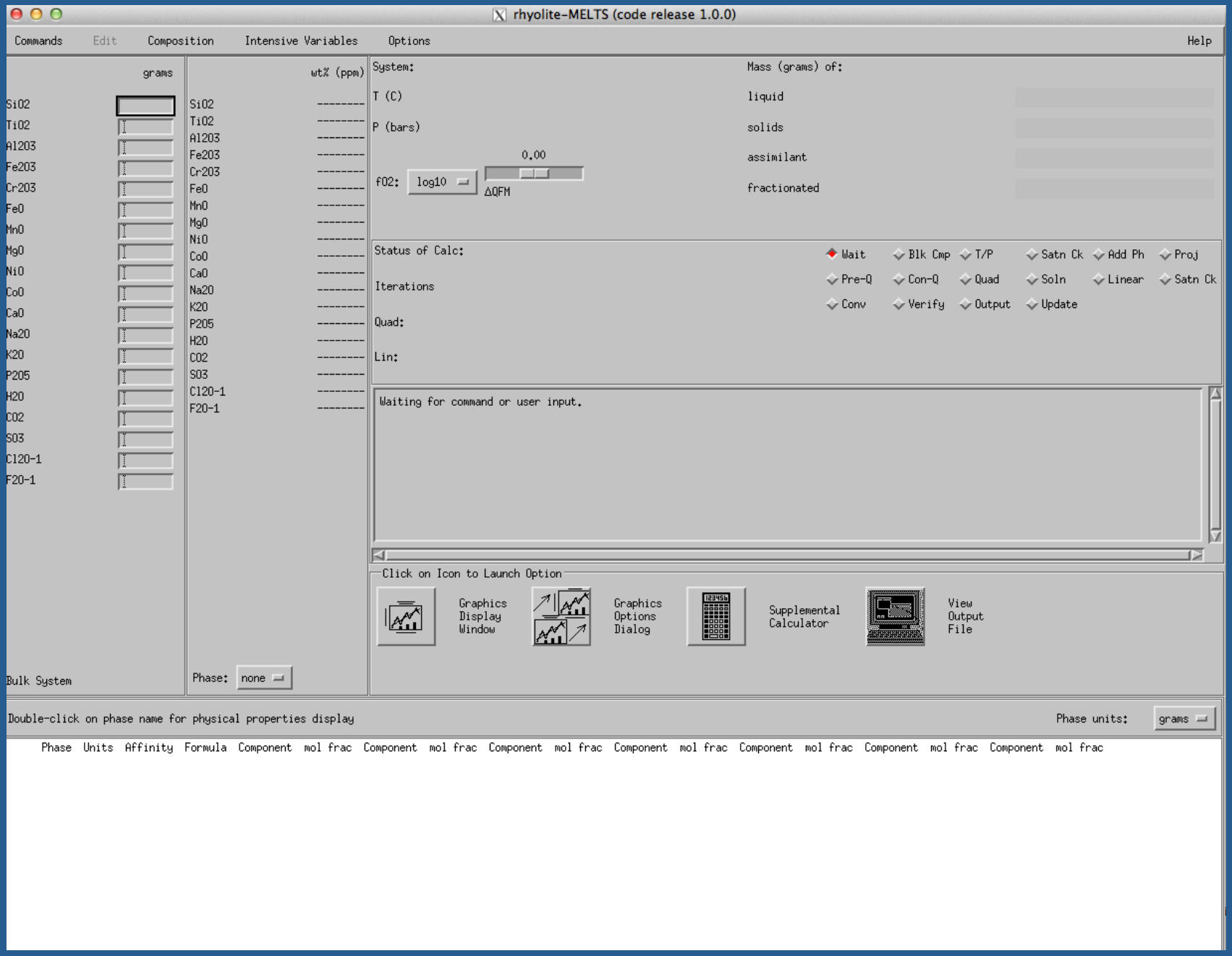
Dufek and Bachmann, 2010

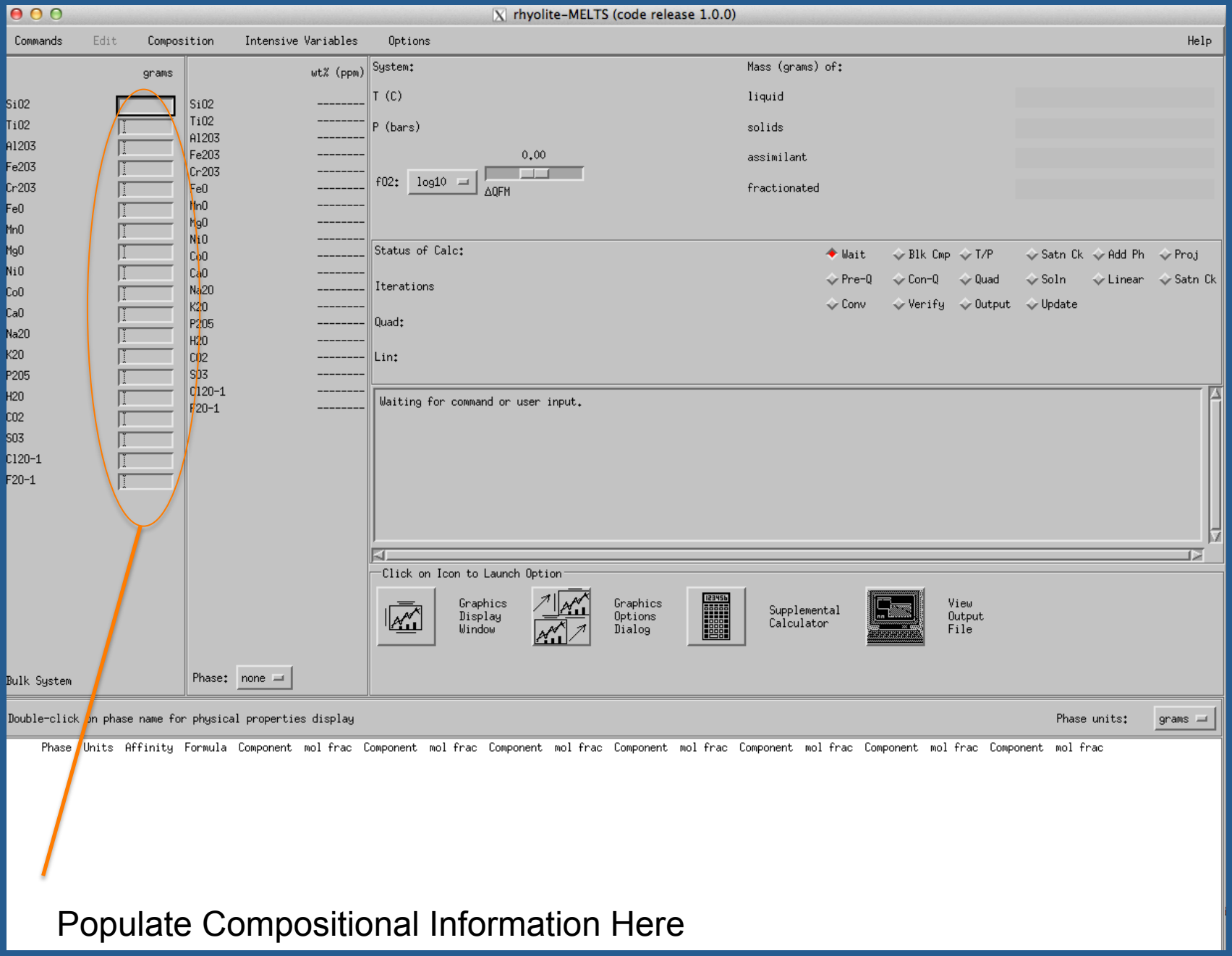
Thermodynamic Modeling with MELTS (Mark Ghiorso's website: http://melts.ofm-research.org/



Download and install rhyolite-MELTS (if using a mac or linux box you can download the appropriate version. You can also download via the virtualBox running linux.

http://melts.ofm-research.org/


rhyolite-MELTS (code release 1.0.0)
Commands
Edit
Composition
Intensive Variables
Options
Help
grams
wt% (ppm)
SiO2
TiO2
Al2O3
Fe2O3
Cr2O3
FeO
MnO
MgO
NiO
CoO
CaO
Na2O
K2O
P2O5
H2O
CO2
SO3
C12O-1
F2O-1
Bulk System
Phase: none
System:
T (C)
P (bars)
0.00
fO2: log10
ΔQFM
Mass (grams) of:
liquid
solids
assimilant
fractionated
Status of Calc:
Iterations
Quad:
Lin:
Wait
Blk Cmp
T/P
Satn Ck
Add Ph
Proj
Pre-Q
Con-Q
Quad
Soln
Linear
Satn Ck
Conv
Verify
Output
Update
Waiting for command or user input.
Click on Icon to Launch Option
Graphics Display Window
Graphics Options Dialog
Supplemental Calculator
View Output File
Double-click on phase name for physical properties display
Phase units: grams
Phase Units Affinity Formula Component mol frac Component mol frac Component mol frac Component mol frac Component mol frac Component mol frac Component mol frac



Populate Compositional Information Here

Example 1: Early Bishop Tuff

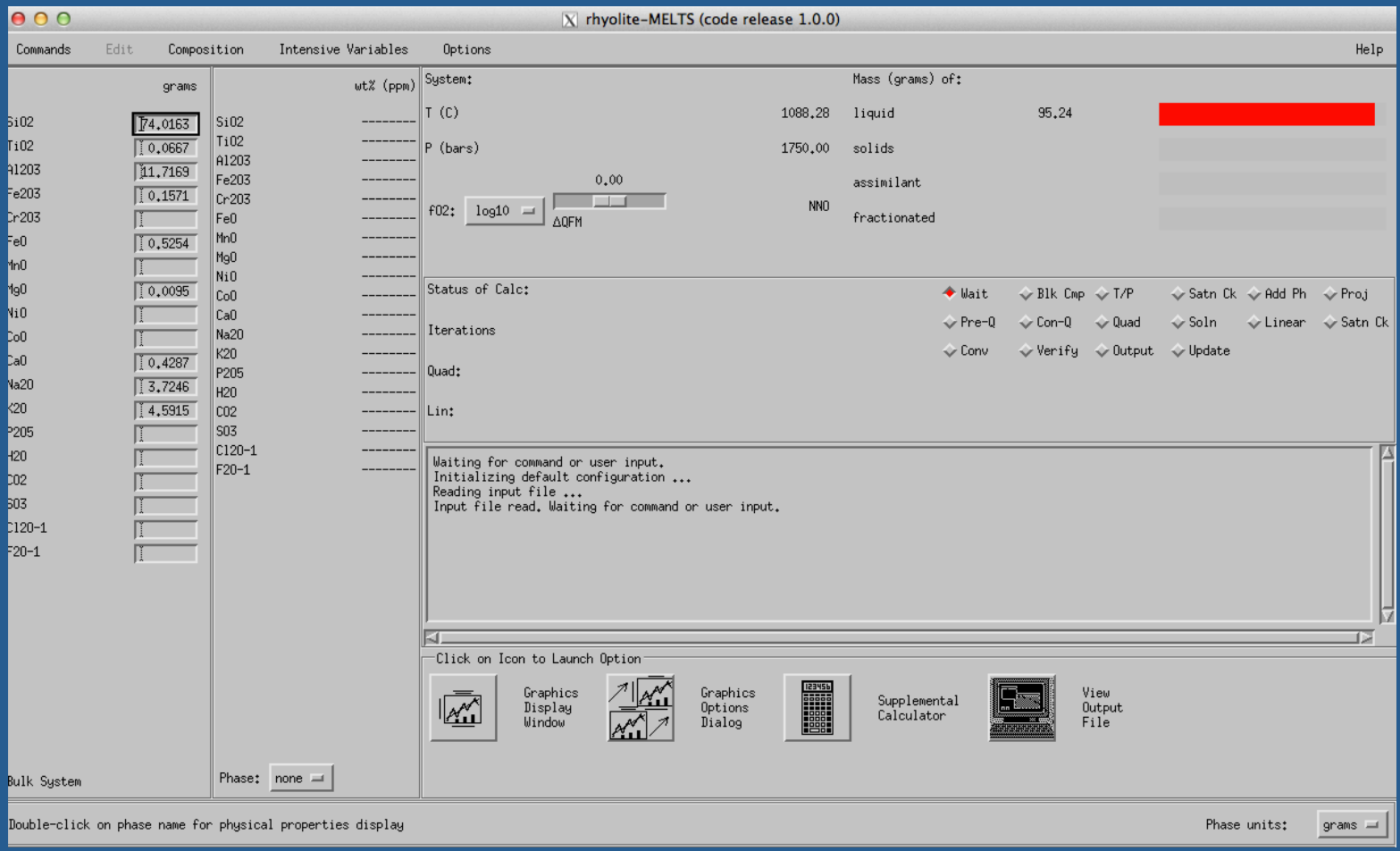
For further information see Gualda et al., 2012

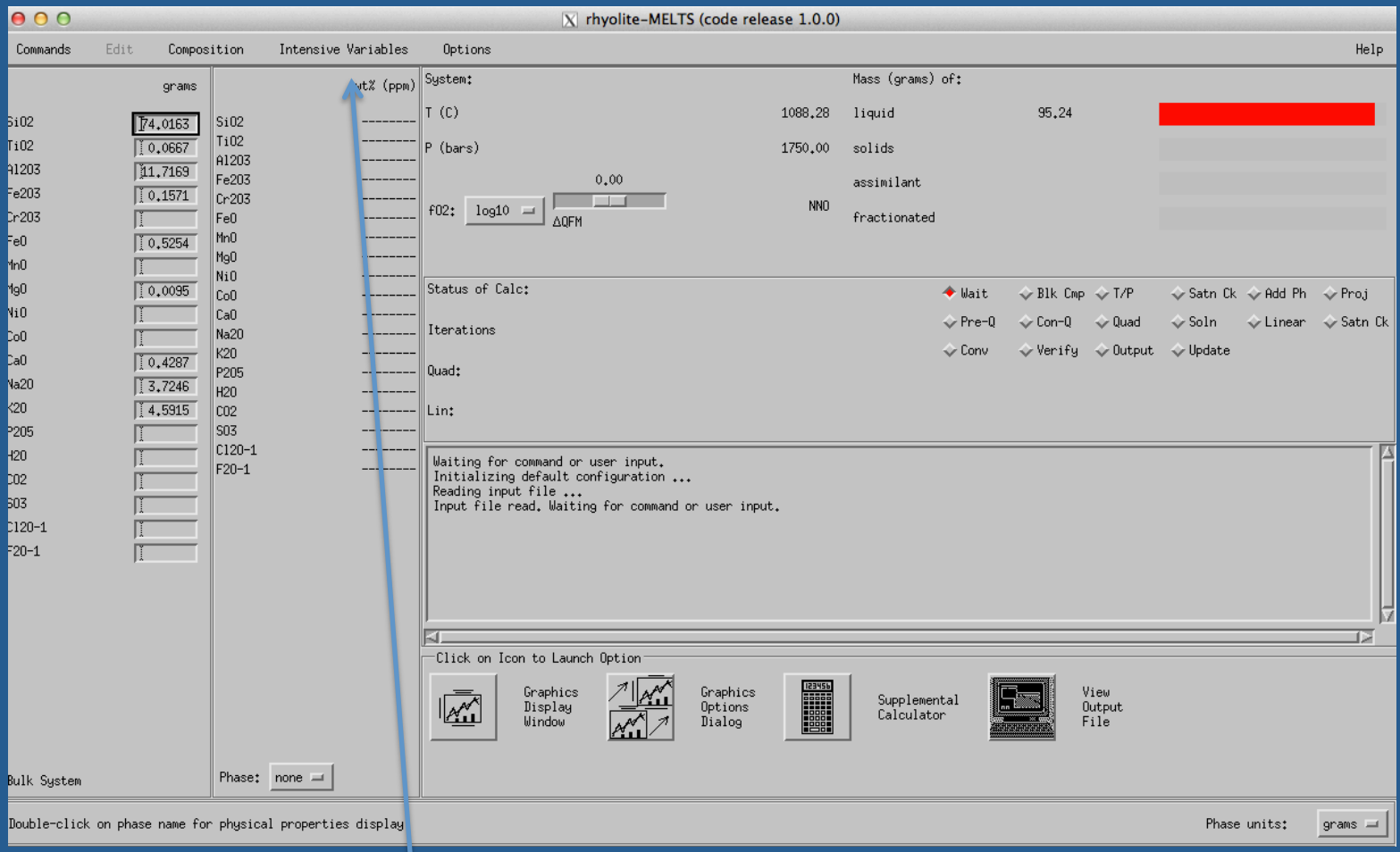
1. Demonstrates basic functioning of MELTS.
2. Demonstrates calibration for hydrous, silicic systems.

Table 1: Whole-rock (WR), melt inclusion (MI), and glass compositions used in simulations

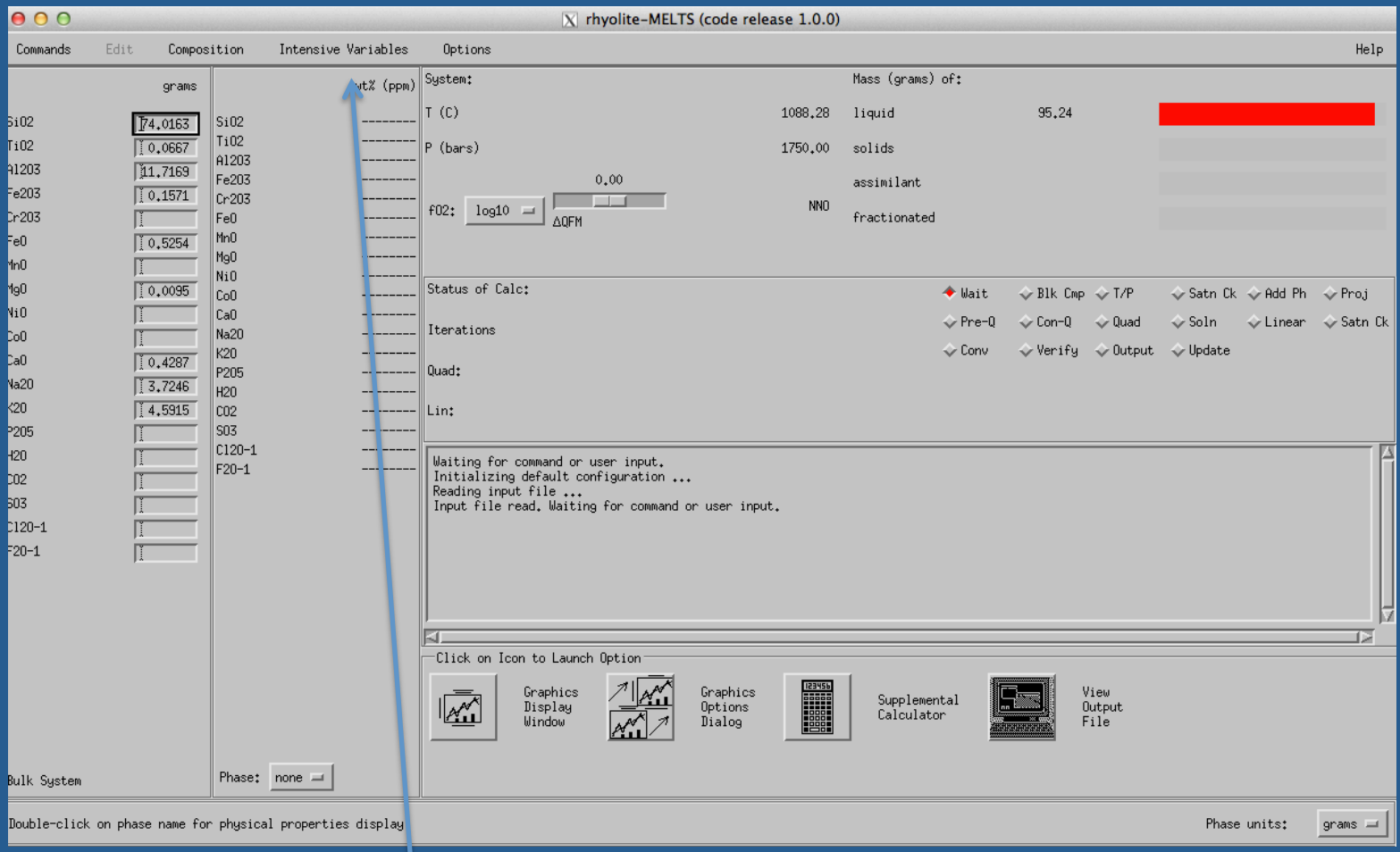
	Early erupted Bishop Tuff		Late-erupted Bishop Tuff		Highland Range (HRL 21)		Highland Range (HRL 27)		Peach Spring Tuff (KPST 01D)	
	WR*	MI†	WR*	MI†	WR‡	Glass‡	WR‡	Glass‡	WR§	Glass§
SiO_2	77·7	77·5	75·6	77·7	77·5	77·9	68·3	75·6	75·6	76·7
TiO_2	0·07	0·08	0·21	0·09	0·12	0·12	0·64	0·28	0·19	0·14
Al_2O_3	12·3	12·5	13·0	12·0	12·5	12·5	15·9	14·2	13·2	12·7
FeO	0·70	0·66	1·10	0·65	0·62	0·45	2·81	0·22	0·96	0·69
MgO	0·01	0·03	0·25	0·04	0·10	0·05	0·90	0·00	0·20	0·06
CaO	0·45	0·43	0·95	0·45	0·64	0·48	2·22	0·30	0·75	0·42
Na_2O	3·91	3·98	3·35	3·70	2·64	3·27	4·99	4·07	2·72	3·30
K_2O	4·82	4·88	5·55	5·36	5·93	5·27	4·20	5·35	6·40	5·93

*Hildreth (1979).
†Anderson *et al.* (2000).
‡Colombini *et al.* (2011).
§Carley (2010).

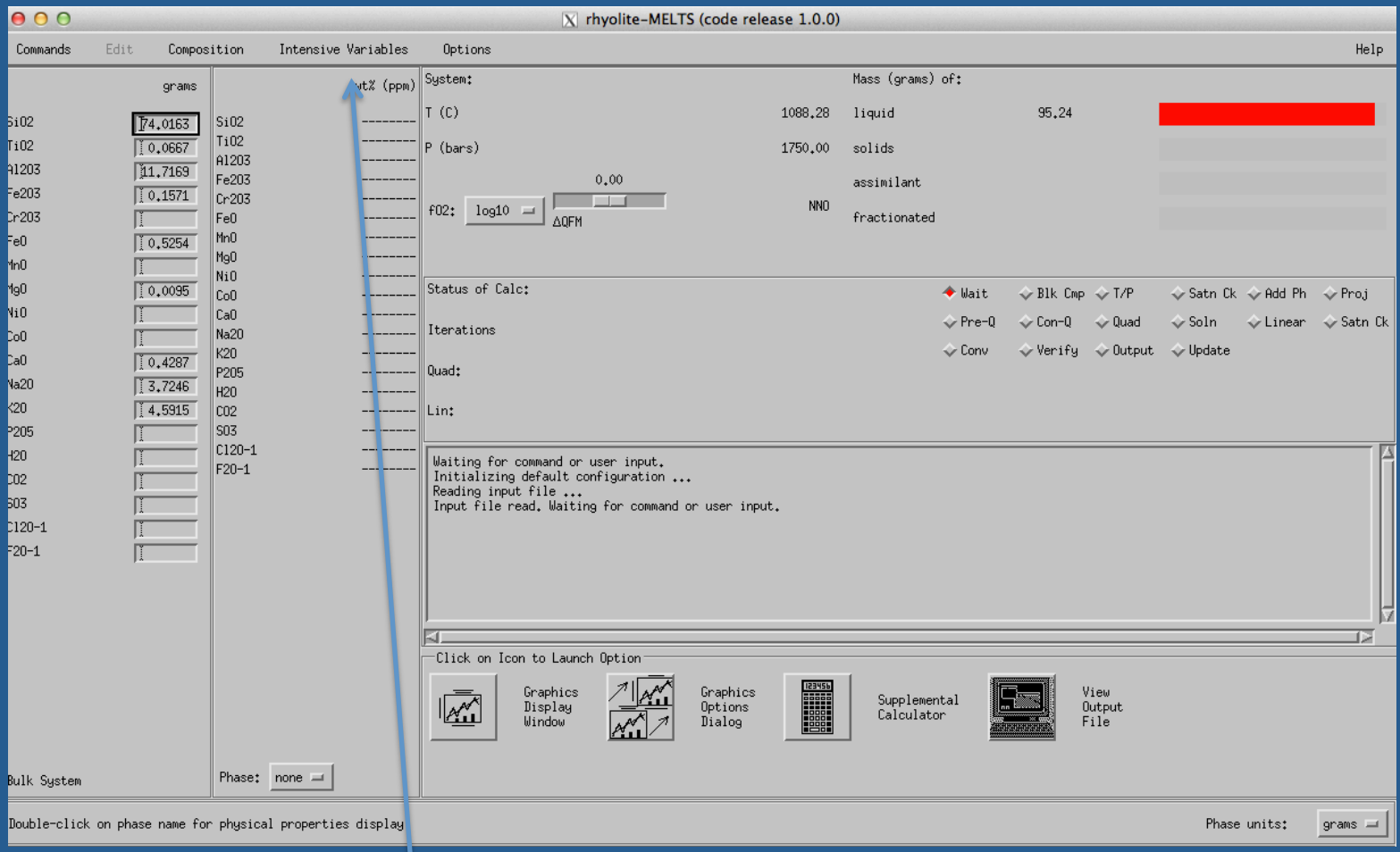

rhyolite-MELTS (code release 1.0.0)
Commands
Edit
Composition
Intensive Variables
Options
Help
grams
SiO2 74.0163
TiO2 0.0667
Al2O3 11.7169
Fe2O3 0.1571
Cr2O3
FeO 0.5254
MnO
MgO 0.0095
NiO
CoO
CaO 0.4287
Na2O 3.7246
K2O 4.5915
P2O5
H2O
CO2
SO3
Cl2O-1
F2O-1
Bulk System
wt% (ppm)
SiO2 --------
TiO2 --------
Al2O3 --------
Fe2O3 --------
Cr2O3 --------
FeO --------
MnO --------
MgO --------
NiO --------
CoO --------
CaO --------
Na2O --------
K2O --------
P2O5 --------
H2O --------
CO2 --------
SO3 --------
Cl2O-1 --------
F2O-1 --------
Phase: none
System:
T (C) 1088.28
P (bars) 1750.00
0.00
fO2: log10
ΔQFM
NNO
Mass (grams) of:
liquid 95.24
solids
assimilant
fractionated
Status of Calc:
Iterations
Quad:
Lin:
Wait
Blk Cmp
T/P
Satn Ck
Add Ph
Proj
Pre-Q
Con-Q
Quad
Soln
Linear
Satn Ck
Conv
Verify
Output
Update
Waiting for command or user input.
Initializing default configuration ...
Reading input file ...
Input file read. Waiting for command or user input.
Click on Icon to Launch Option
Graphics Display Window
Graphics Options Dialog
Supplemental Calculator
View Output File
Double-click on phase name for physical properties display
Phase units: grams



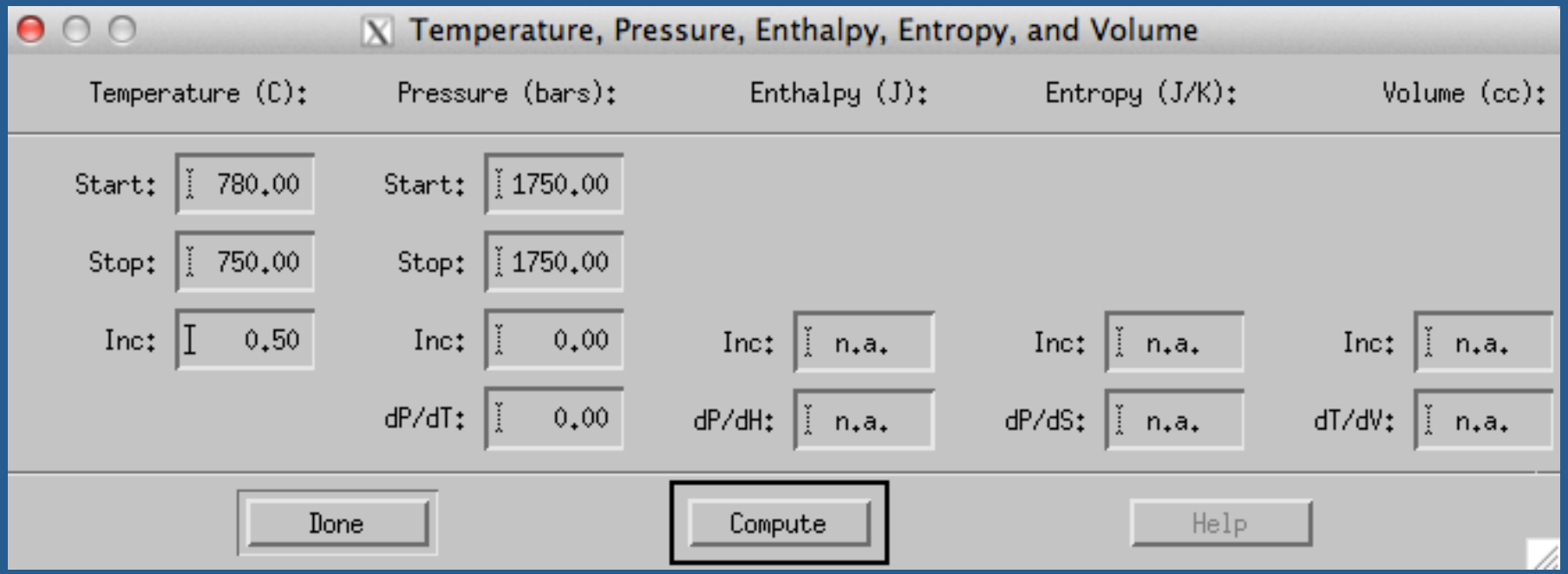
Now set the oxygen fugacity to Ni-NiO, here



Now set the oxygen fugacity to Ni-NiO, here



Set the intensive variables



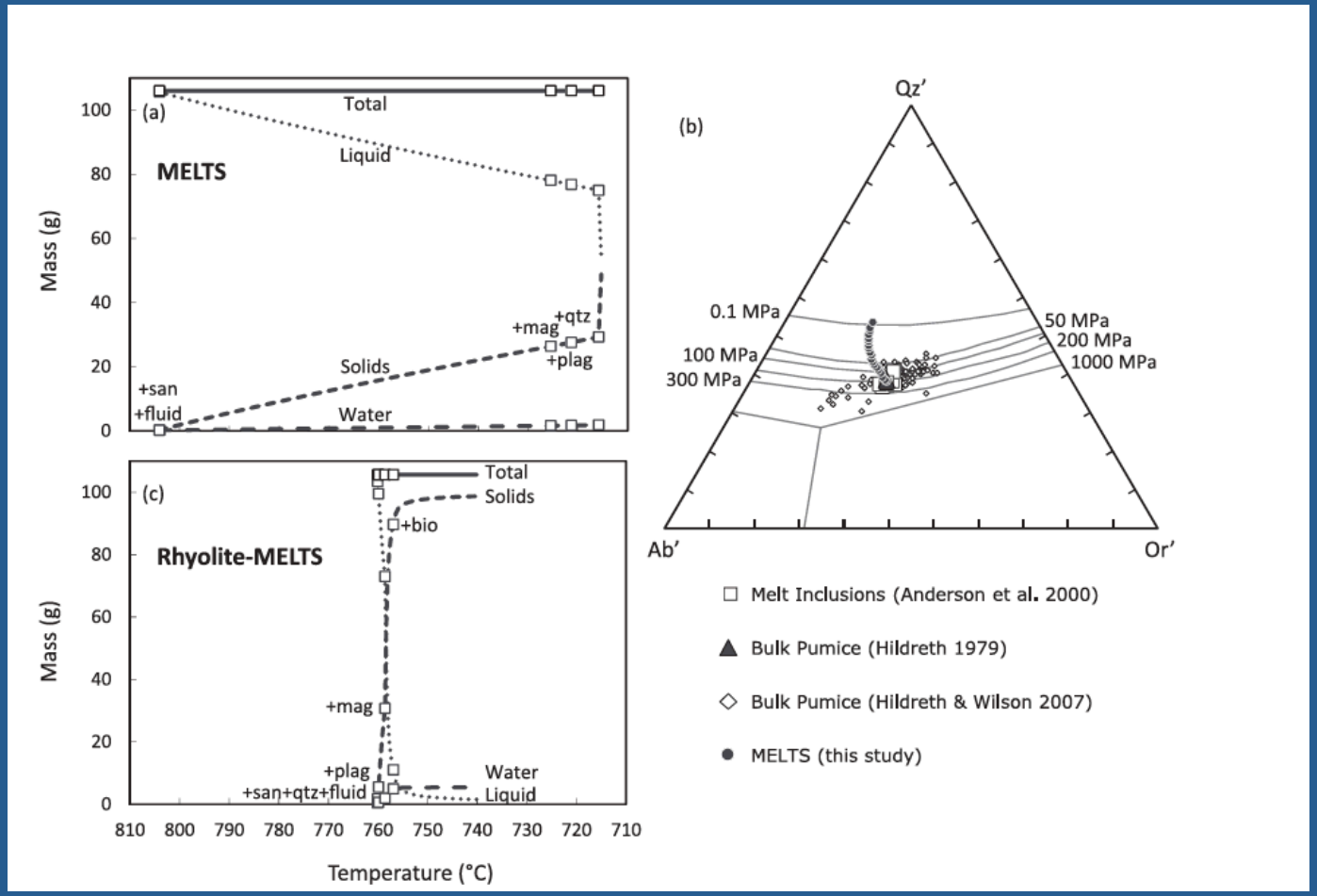
Add 5% water, and compute redox state and normalize (under Composition tab)

```
josef-dufeks-macbook-2:~ dufek$ ls *tbl melts.out
clinopyroxene.tbl       leucite-ss.tbl          melts.out               orthopyroxene.tbl       rhm-oxide.tbl           water.tbl
feldspar.tbl            melts-liquid.tbl        olivine.tbl             quartz.tbl              spinel.tbl              whitlockite.tbl
```

melts.out

```
T = 758.50 (C)  P = 1.750 (kbars)  log(10) f O2 = -14.81  delta HM = -5.17  NNO = 0.00  QFM = 0.41  COH = 1.90  IW = 4.74

Constraint Flags: fO2 path = NNO

Liquid           mass = 36.13 (gm)  density = 2.20 (gm/cc)  viscosity = 6.38 (log 10 poise)     (analysis in wt %)
                G = -587620.04 (J)  H = -493076.62 (J)  S = 91.64 (J/K)  V = 16.40 (cc)  Cp = 48.27 (J/K)
        SiO2   TiO2  Al2O3  Fe2O3  Cr2O3    FeO    MnO    MgO    NiO    CoO    CaO   Na2O    K2O   P2O5    H2O    CO2    SO3 Cl2O-1  F2O-1
       73.50   0.11  11.65   0.29   0.00   0.65   0.00   0.02   0.00   0.00   0.51   3.76   4.62   0.00   4.89   0.00   0.00   0.00   0.00

feldspar         mass = 30.28 (gm)  density = 2.52 (gm/cc)     (analysis in mole %)
                 K0.51Na0.47Ca0.02Al1.02Si2.98O8
                 G = -481019.45 (J)  H = -415931.57 (J)  S = 63.09 (J/K)  V = 12.00 (cc)  Cp = 36.16 (J/K)
              albite     anorthite      sanidine
               47.27          1.56         51.17

feldspar         mass = 8.08 (gm)  density = 2.56 (gm/cc)     (analysis in mole %)
                 K0.15Na0.76Ca0.08Al1.08Si2.92O8
                 G = -130816.62 (J)  H = -113235.22 (J)  S = 17.04 (J/K)  V = 3.16 (cc)  Cp = 9.85 (J/K)
              albite     anorthite      sanidine
               76.47          8.46         15.06

quartz           mass = 21.91 (gm)  density = 2.54 (gm/cc)
                 SiO2
                 G = -358160.09 (J)  H = -313151.20 (J)  S = 43.17 (J/K)  V = 8.62 (cc)  Cp = 25.39 (J/K)

spinel           mass = 0.39 (gm)  density = 4.97 (gm/cc)     (analysis in mole %)
                 Fe''1.17Mg0.02Fe'''1.54Al0.08Cr0.00Ti0.19O4
                 G = -2566.95 (J)  H = -1851.80 (J)  S = 0.69 (J/K)  V = 0.08 (cc)  Cp = 0.35 (J/K)
            chromite     hercynite     magnetite        spinel    ulvospinel
                0.00          2.03         77.19          1.92         18.86

water            mass = 3.22 (gm)  density = 0.41 (gm/cc)
                 H2O
                 G = -70544.12 (J)  H = -40696.48 (J)  S = 28.93 (J/K)  V = 7.78 (cc)  Cp = 12.87 (J/K)

Total solids     mass = 63.89 (gm)  density = 2.02 (gm/cc)
                 G = -1043107.23 (J)  H = -884866.27 (J)  S = 152.93 (J/K)  V = 31.64 (cc)  Cp = 84.61 (J/K)

Viscosity of the System cannot be computed.

System           mass = 100.01 (gm)  density = 2.08 (gm/cc)
                 G = -1630727.27 (J)  H = -1377942.89 (J)  S = 244.57 (J/K)  V = 48.04 (cc)  Cp = 132.88 (J/K)

Oxygen           delta moles = 0.000883283  delta grams = 0.028264
                 G = -201.91 (J)  H = 21.03 (J)  S = 0.22 (J/K)  V = 75.76 (cc)  Cp = 0.03 (J/K)
```

Rhyolite MELTS should give results similar to panel C.



Contrib Mineral Petrol (2001) 141: 643–658
DOI 10.1007/s004100100266

Othmar Müntener · Peter B. Kelemen · Timothy L. Grove

The role of H_2O during crystallization of primitive arc magmas under uppermost mantle conditions and genesis of igneous pyroxenites: an experimental study

Table 1 Starting material for high pressure experiments, analyzed and reported by Baker et al. (1994)

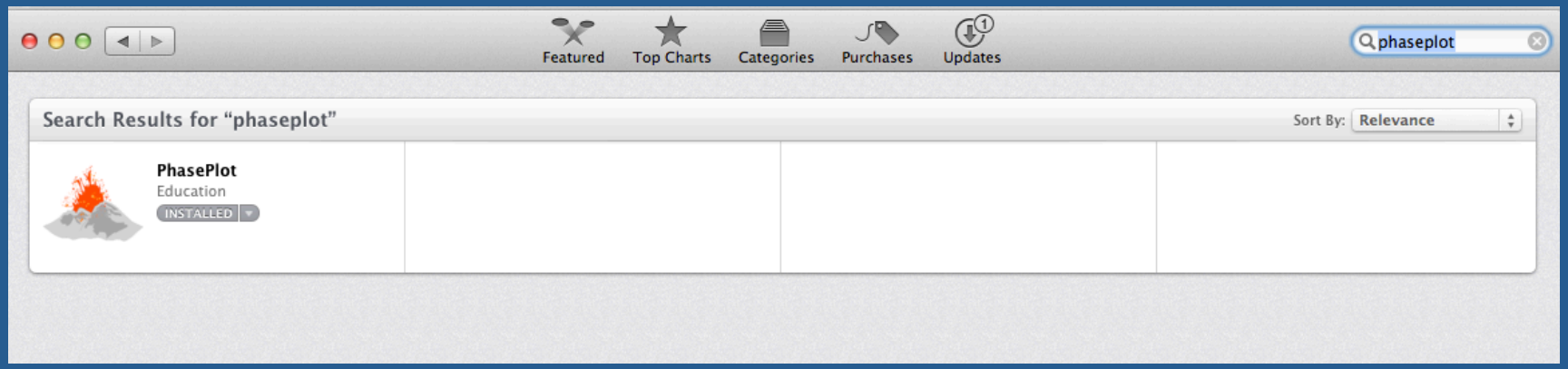
Sample	SiO_2	TiO_2	Al_2O_3	FeO	MnO	MgO	CaO	Na_2O	K_2O	P_2O_5	Cr (ppm)	Ni (ppm)	Mg#
85–44	51.68	0.60	16.40	7.93	0.16	10.79	9.67	2.24	0.42	0.11	693	230	0.707
85–41c	57.79	0.60	14.46	5.74	0.11	9.14	8.17	3.11	0.71	0.15	590	121	0.738

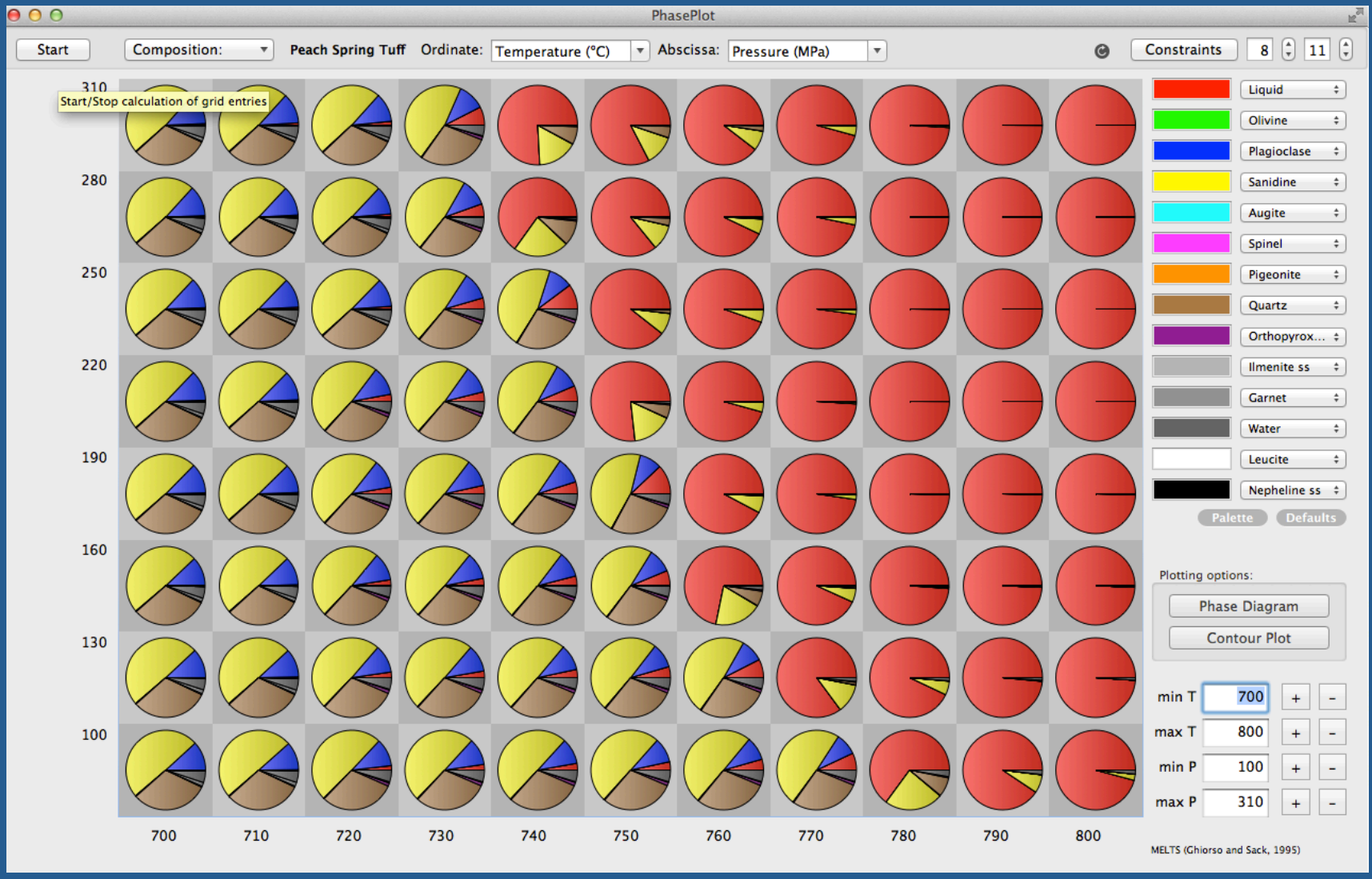
Explore MELTS simulations at 12 kbar, with added water.

Runs	P (GPa)	T(°C)	(h)	H_2O (melt)	H_2O init (wt%a)	Run products	Phase proportions (wt%)	Kd						Δ Φε (%)	ΣP2	capsule (g)	sample (g)	samp/caps ratio
								Cpx	Opx	OI	Spi	Grt	Am					
Basalt (85-44)																		
B690	1,2	1230	25	4.4(3)	~3.8	Gl, Cpx, Opx	88.9(21):2.8(27):8.2(19)	0,31	0,29					–4,08	0,16	0,1005	0,0089	0,08806
B674	1,2	1190	25	4.2(3)	~3.8	Gl, Cpx, Opx	77.5(25):12.6(30):9.9(21)	0,31	0,29					–0,55	0,22	0,1124	0,0093	0,08230
B659	1,2	1150	22	5.7(7)	~3.8	Gl, Cpx, Opx, Spl	65.3(13):20.5(16):14.1(11):tr.	0,28	0,29					–1,88	0,08	0,1212	0,0081	0,06686
B681	1,2	1110	27	5.5(2)	~3.8	Gl, Cpx, Opx, Grt, Spi	49.8(14):31.0(16):13.7(12):4.9(19):0.6(5)	0,32	0,29		1,78	0,55		0,38	0,04	0,1059	0,0078	0,07365
B726	1,2	1070	30	6.4(7)	~3.8	Gl, Cpx, Opx, Grt, Am	39.9(19):27.0(43):8.8(23):15.3(51):8.9(24)	0,31	0,29			0,56	0,34	1,79	0,09	0,0832	0,0078	0,09375
B714	1,2	1230	24	5.3(2)	~5	Gl, Cpx, Opx	90.5(38):2.9(26):6.5(33)	0,30	0,30					9,45	0,64	0,0723	0,0060	0,08299
B686	1,2	1210	26	5.6(4)	~5	Gl, Cpx, Opx	88.3(13):4.5(17):7.2(12)	0,28	0,27					1,48	0,07	0,0951	0,0083	0,08728
B671	1,2	1190	26	5.3(6)	~5	Gl, Cpx, Opx	89.6(30):4.1(35):6.3(26)	0,29	0,28					6,81	0,38	0,1151	0,0090	0,07823
B665	1,2	1150	26	6.5(4)	~5	Gl, Cpx, Opx	76.0(36):12.5(40):11.4(29)	0,29	0,28					8,34	0,52	0,1078	0,084	0,07746
B683	1,2	1110	26	6.0(5)	~5	Gl, Cpx, Opx, Spi	61.9(29):23.6(33):13.7(21):1.1(9)	0,30	0,28		0,70			4,20	0,21	0,1158	0,0088	0,07599
B704	1,2	1070	32	9.0(3)	~5	Gl, Cpx, Opx, Grt, Am	46.9(14):19.1(25):10.1(12):0.1(31):23.9(6)	0,30	0,28				0,61 0,33	0,76	0,05	0,1128	0,0080	0,07092
B679	1,2	1190	27	3.5(5)	~2.5	Gl, Cpx, Opx	69.3(35):17.6(46):13.0(31)	0,31	0,29					–8,39	0,49	0,1206	0,0082	0,06799
B668	1,2	1150	28	4.5(5)	–2.5	Gl, Cpx, Opx, Pl	53.3(85):23.5(45):16.2(41):6.0(50)	0,28	0,27					–7,25	0,43	0,1104	0,0104	0,09420

How do your run products compare?

PhasePlot --- Available for macs through the app store.

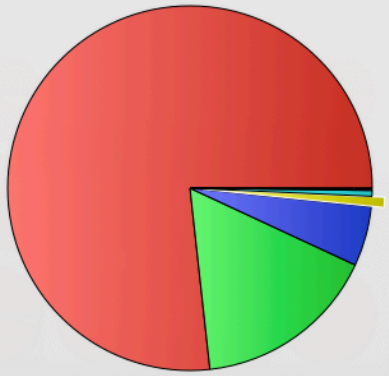



PhasePlot
Start
Composition:
Peach Spring Tuff
Ordinate:
Temperature (°C)
Abscissa:
Pressure (MPa)
Constraints
8
11
Start/Stop calculation of grid entries
310
280
250
220
190
160
130
100
700
710
720
730
740
750
760
770
780
790
800
Liquid
Olivine
Plagioclase
Sanidine
Augite
Spinel
Pigeonite
Quartz
Orthopyrox...
Ilmenite ss
Garnet
Water
Leucite
Nepheline ss
Palette
Defaults
Plotting options:
Phase Diagram
Contour Plot
min T
700
max T
800
min P
100
max P
310
MELTS (Ghiorso and Sack, 1995)

MELTS calculations at grid point: T = 750.00 °C and P = 220.0 MPa

Minimal energy computed.

Phase Display:



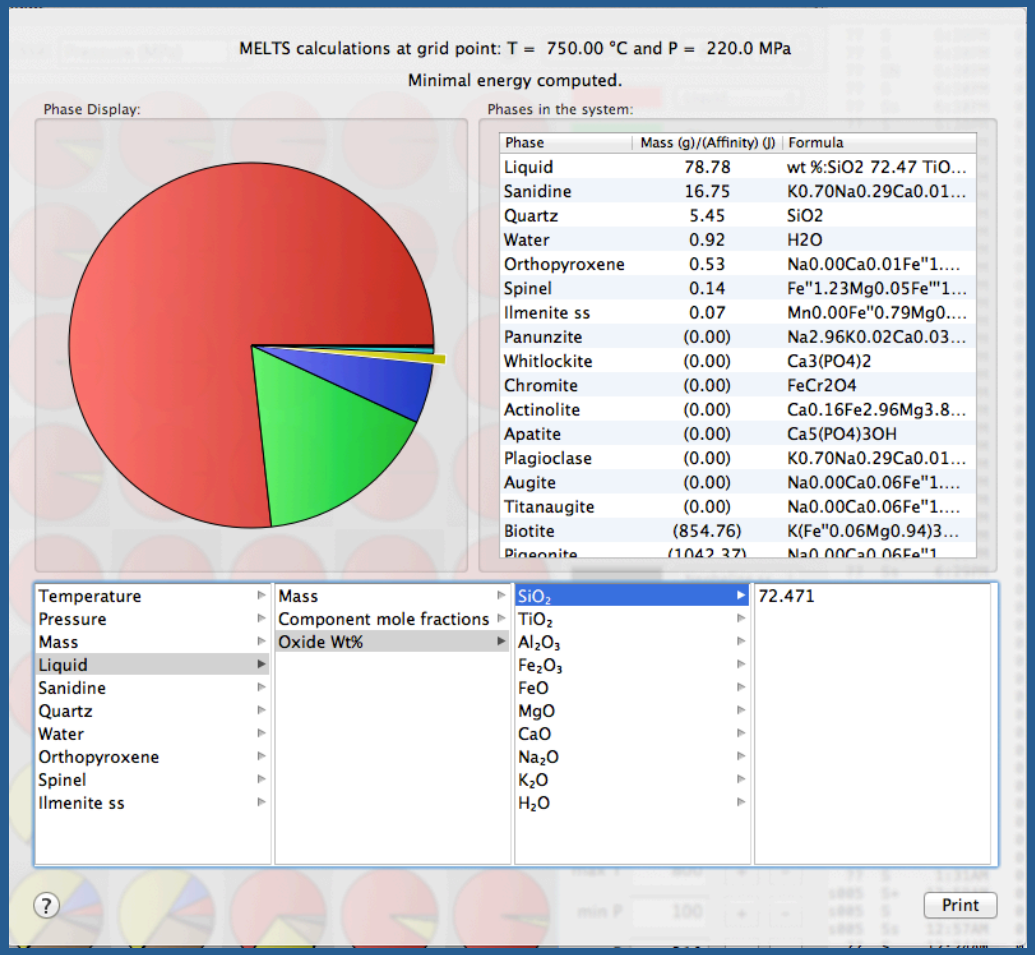
Phases in the system:

Phase	Mass (g)/(Affinity) (J)	Formula
Liquid	78.78	wt %:SiO2 72.47 TiO...
Sanidine	16.75	K0.70Na0.29Ca0.01...
Quartz	5.45	SiO2
Water	0.92	H2O
Orthopyroxene	0.53	Na0.00Ca0.01Fe"1....
Spinel	0.14	Fe"1.23Mg0.05Fe'"1...
Ilmenite ss	0.07	Mn0.00Fe"0.79Mg0....
Panunzite	(0.00)	Na2.96K0.02Ca0.03...
Whitlockite	(0.00)	Ca3(PO4)2
Chromite	(0.00)	FeCr2O4
Actinolite	(0.00)	Ca0.16Fe2.96Mg3.8...
Apatite	(0.00)	Ca5(PO4)3OH
Plagioclase	(0.00)	K0.70Na0.29Ca0.01...
Augite	(0.00)	Na0.00Ca0.06Fe"1....
Titanaugite	(0.00)	Na0.00Ca0.06Fe"1....
Biotite	(854.76)	K(Fe"0.06Mg0.94)3...
Pigeonite	(1042.37)	Na0.00Ca0.06Fe"1

- Temperature
- Pressure
- Mass
- Liquid
- Sanidine
- Quartz
- Water
- Orthopyroxene
- Spinel
- Ilmenite ss

?

Print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Minimal energy computed.
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Ilmenite ss 0.07 Mn0.00Fe"0.79Mg0....
Panunzite (0.00) Na2.96K0.02Ca0.03...
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Chromite (0.00) FeCr2O4
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Plagioclase (0.00) K0.70Na0.29Ca0.01...
Augite (0.00) Na0.00Ca0.06Fe"1....
Titanaugite (0.00) Na0.00Ca0.06Fe"1....
Biotite (854.76) K(Fe"0.06Mg0.94)3...
Temperature
Pressure
Mass
Liquid
Sanidine
Quartz
Water
Orthopyroxene
Spinel
Ilmenite ss
Mass
Component mole fractions
Oxide Wt%
SiO2
TiO2
Al2O3
Fe2O3
FeO
MgO
CaO
Na2O
K2O
H2O
72.471
?
Print

Directly coupling MELTS with multiphase dynamics calculations

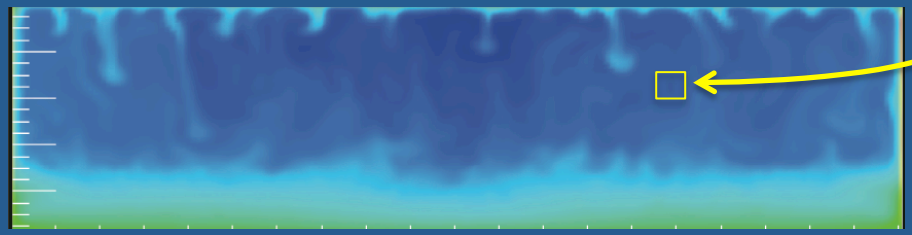
- Conservation of mass, enthalpy and momentum is solved for discrete phases, and the phase equilibria, melt composition, thermodynamic variables are solved at each position and time.

- More accurate computation of the sensible to latent heat partitioning than is available with other approaches.

- Provides detailed assessment of geochemistry.

- Allows calculation of wide parameter space of enthalpy, pressure, and water contents

- Implemented in a parallel computational architecture.



From enthalpy, pressure and composition MELTS provides phase equilibria, temperature, and thermodynamic variables

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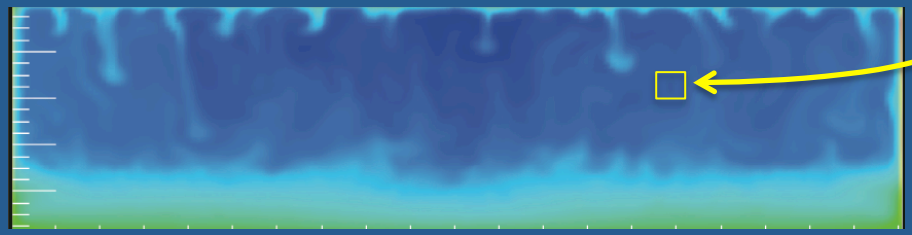

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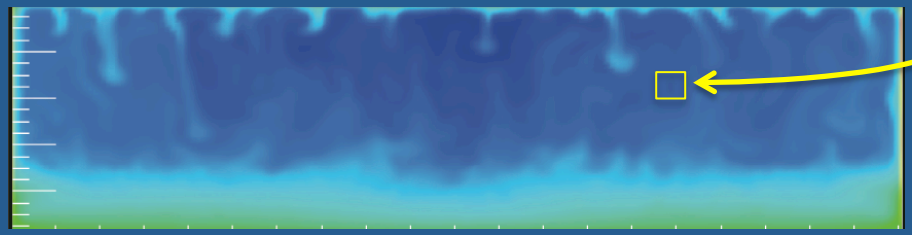

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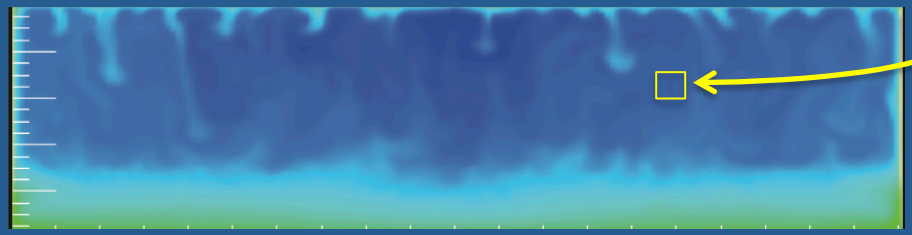

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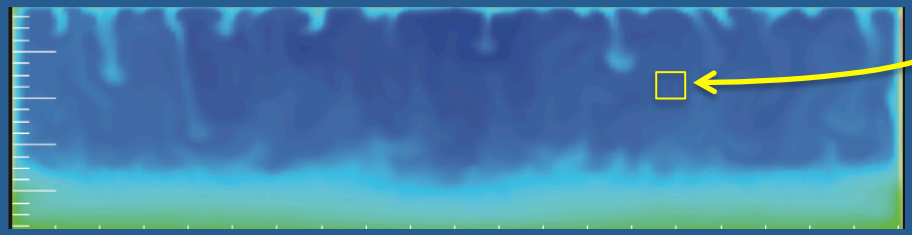

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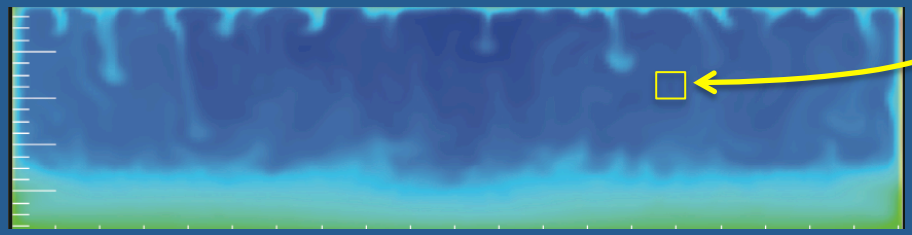

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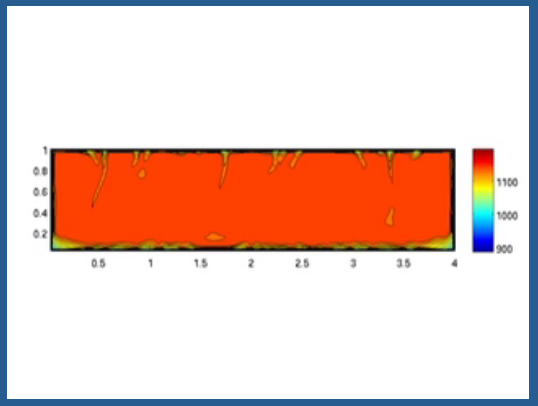
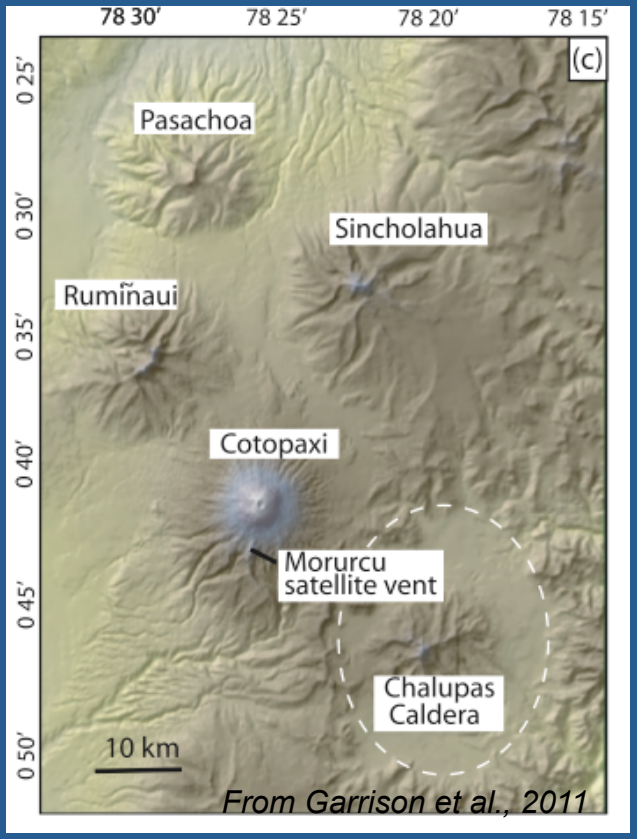
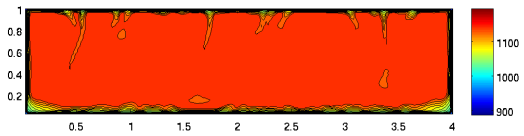
Intrusion of Cotopaxi Andesite



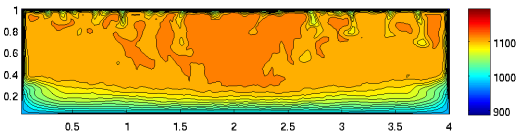


Cotopaxi is dominated by andesitic and rhyolitic volcanism.

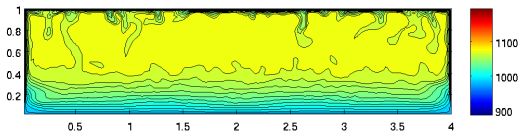
We explored the melt extraction probability for an initial andesitic body using a combined dynamics+melts approach (we explored a range of conditions, but shown here are those for a 500 m thick body with a 250 m think partial melt zone zone (viscoelastic layer).



2500 yrs

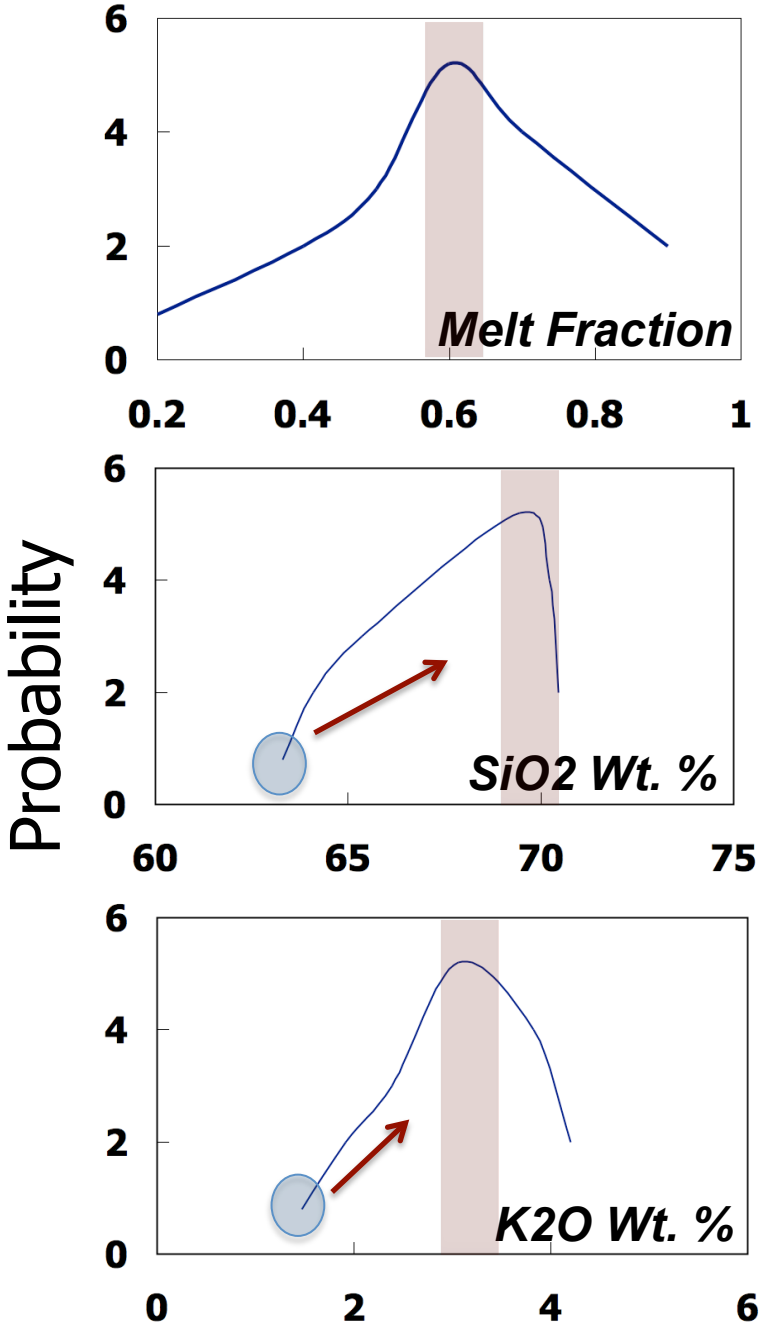


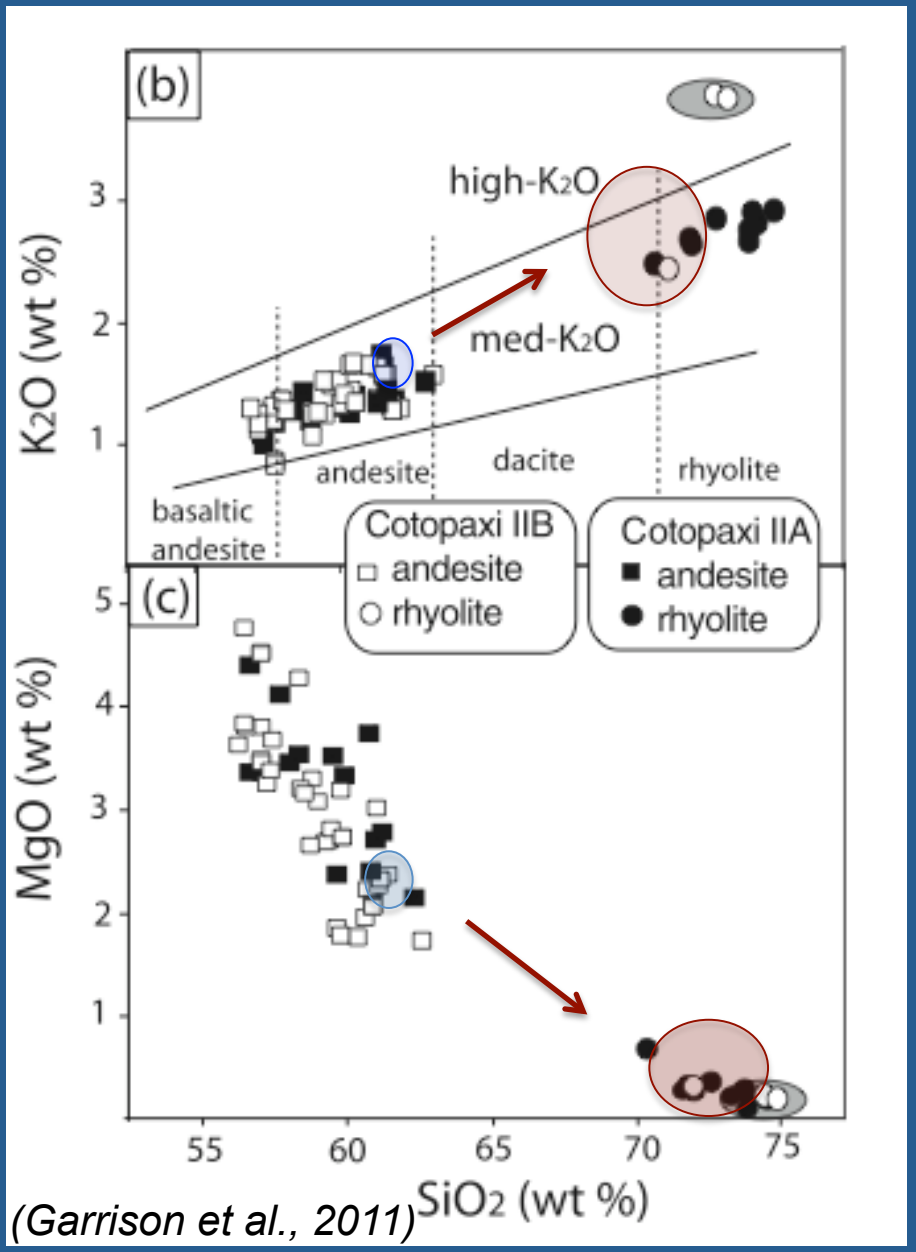
5000 yrs



7500 yrs

Model Extraction Probabilities





(Garrison et al., 2011)

Using VirtualBox we can explore some uses of MELTS as a constitutive property engine and latent heat effects.

On my website download the tarred directory:
http://shadow.eas.gatech.edu/~dufek/MELTING_1D.tar.gz

This can be downloaded from your browser in VirtualBox.

Then: tar –xvf MELTING_1D.tar.gz

In this directory is an executable ‘melt_1D.exe’ , and three input files that can be modified in a text editor:

INPUT: general simulation parameters
INTRUSION_INPUT: composition of oxides in intrusion
COUNTRY_ROCK_INPUT: surrounding rock composition

This code is a simplified 1D code using MELTS as a thermodynamic engine

Features:
-Variable composition for the country-rock and intrusion.

-Enthalpy conservation is maintained and MELTS provides the information about sensible and latent balance.

-An initial 1D intrusion ‘sill’ is intruded at its liquidus.

-MELTS can go unstable near and below the solidus, and enthalpy below the solidus is calculated using the derivative of the heat capacity with respect to temperature at the solidus and projecting the modified heat capacity.

-Physical properties are composition, temperature dependent.

-Model also calculates a simplified change in pressure in the chamber as a result of volume change during phase change.

-There are a few matlab/octave scripts for visualization if you have matlab/ octave installed, otherwise there are some fairly easy to examine text files. To install the octave package on VirtualBox type ‘octave’ and detailed instructions will follow.

After selecting the INPUT parameters that you want you can run this program from the command line using:

./melt_1D.exe &> /dev/null &

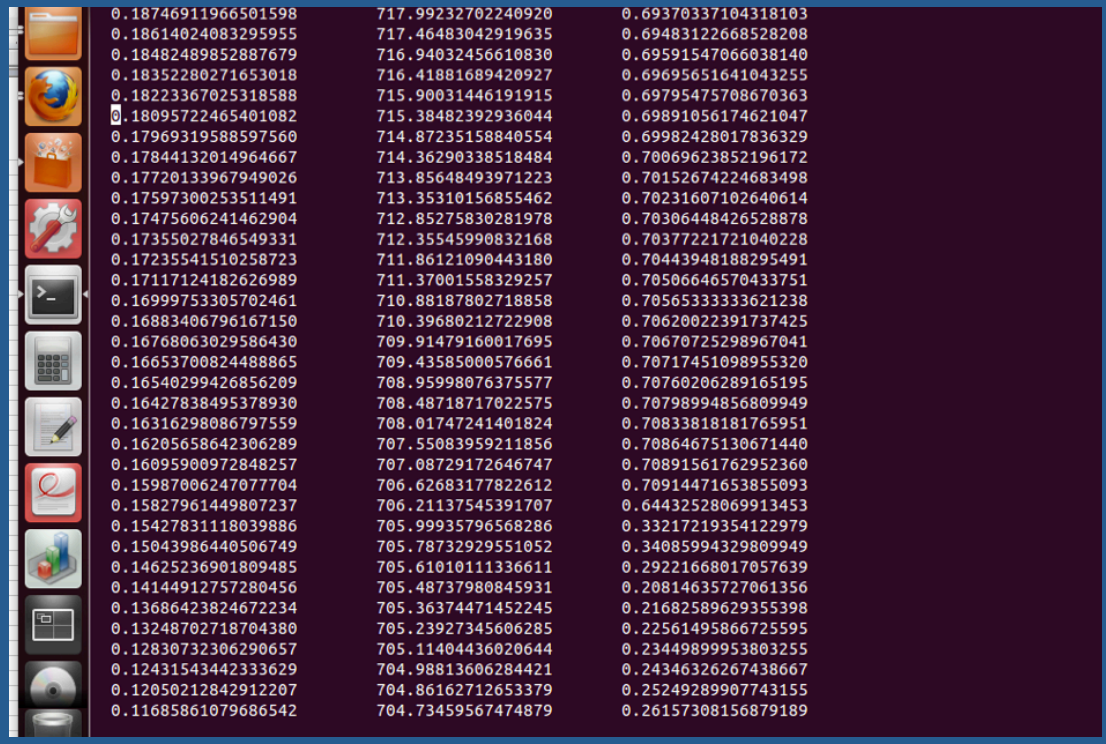
The program can be a little sluggish in virtualBox (may take a few minutes). After 1-2 minutes of initialization you should see a count progressing in TIMESTEPS (ls –l TIMESTEPS will show you if it has recently written).

To edit the inputs you can used standard text editors (vi, emacs).

Example 1: Sensible vs. Total Heat

-Using the initial parameters in the INPUT files, run the code.

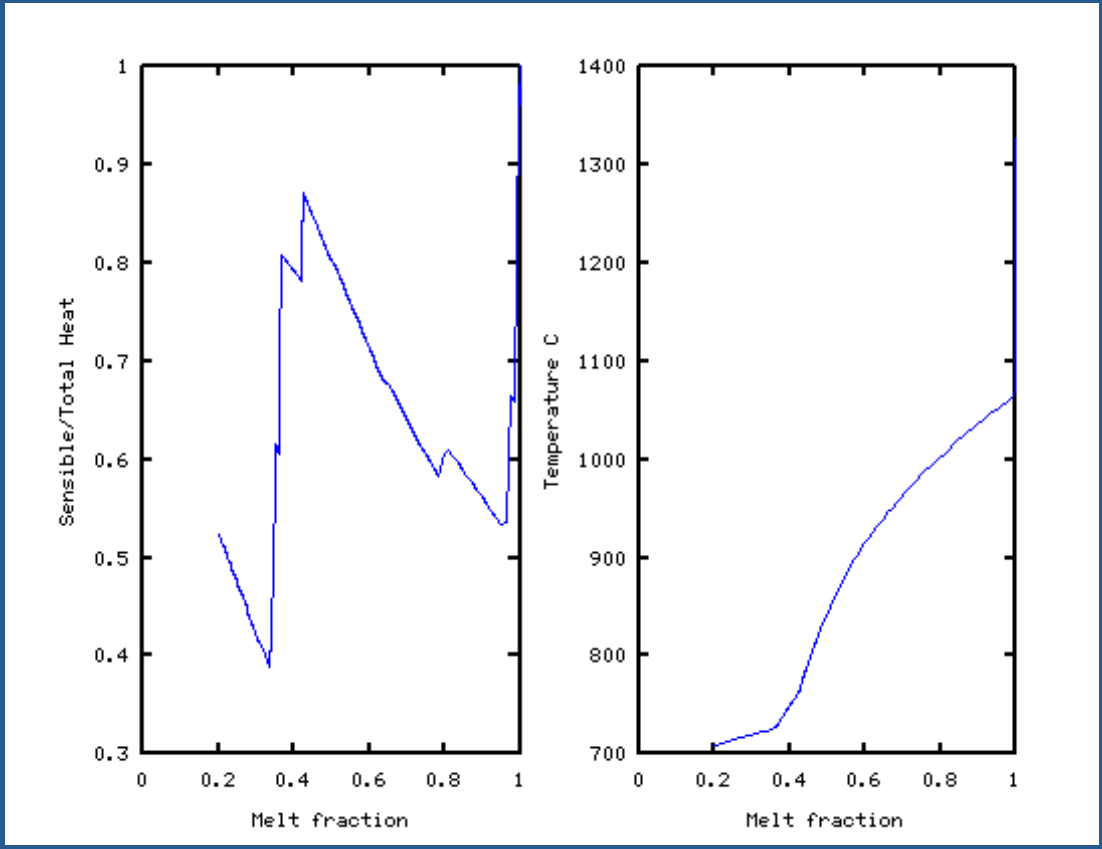
-In the file ‘SENSIBLE’, there should be three columns, melt fraction, temperature (C) and the ratio of sensible heat to total enthalpy drop from the previous value. The smaller this last ratio is the more important latent heat is in buffering the temperature.



0.18746911966501598	717.99232702240920	0.69370337104318103
0.18614024083295955	717.46483042919635	0.69483122668528208
0.18482489852887679	716.94032456610830	0.69591547066038140
0.18352280271653018	716.41881689420927	0.69695651641043255
0.18223367025318588	715.90031446191915	0.69795475708670363
0.18095722465401082	715.38482392936044	0.69891056174621047
0.17969319588597560	714.87235158840554	0.69982428017836329
0.17844132014964667	714.36290338518484	0.70069623852196172
0.17720133967949026	713.85648493971223	0.70152674224683498
0.17597300253511491	713.35310156855462	0.70231607102640614
0.17475606241462904	712.85275830281978	0.70306448426528878
0.17355027846549331	712.35545990832168	0.70377221721040228
0.17235541510258723	711.86121090443180	0.70443948188295491
0.17117124182626989	711.37001558329257	0.70506646570433751
0.16999753305702461	710.88187802718858	0.70565333333621238
0.16883406796167150	710.39680212722908	0.70620022391737425
0.16768063029586430	709.91479160017695	0.70670725298967041
0.16653700824488865	709.43585000576661	0.70717451098955320
0.16540299426856209	708.95998076375577	0.70760206289165195
0.16427838495378930	708.48718717022575	0.70798994856809949
0.16316298086797559	708.01747241401824	0.70833818181765951
0.16205658642306289	707.55083959211856	0.70864675130671440
0.16095900972848257	707.08729172646747	0.70891561762952360
0.15987006247077704	706.62683177822612	0.70914471653855093
0.15827961449807237	706.21137545391707	0.64432528069913453
0.15427831118039886	705.99935796568286	0.33217219354122979
0.15043986440506749	705.78732929551052	0.34085994329809949
0.14625236901809485	705.61010111336611	0.29221668017057639
0.14144912757280456	705.48737980845931	0.20814635727061356
0.13686423824672234	705.36374471452245	0.21682589629355398
0.13248702718704380	705.23927345606285	0.22561495866725595
0.12830732306290657	705.11404436020644	0.23449899953803255
0.12431543442333629	704.98813606284421	0.24346326267438667
0.12050212842912207	704.86162712653379	0.25249289907743155
0.11685861079686542	704.73459567474879	0.26157308156879189

You can plot the results in octave used the included script.

-Open octave, and type ‘sensible_plot’. (For those of you familiar with matlab you can edit these simple plotting scripts in a similar way, for instance here you could edit with ‘vi sensible_plot.m’)



Other files of interest are:

TEMP - 1D temperature profile, writes out every specified time interval wraps in one long array.

CRUSTAL_MELT – 1D melt fraction profile, writes out every specified time interval wraps in one long array.

MELT_LENGTH – gives the total amount of melt integrated over the 1D column.

MELT_COMPOSITION – Gives the melt fraction, depth, time and composition of evolving melt.

PHASES – List of phases present at depth/time.

Some useful octave scripts: sensible_plot, temp,

Exercise 2 Modify minimum melt fraction and monitor MAXTEMP to further examine latent heat.

In the INPUT file is listed a minimum melt fraction that is tracked in the simulations. Below this value the code uses the derivative of the heat capacity (temp. dependent) but has no latent heat contribution.

Vary this parameter (from 0 to 1) and examine the result in temperature (going all the way to 0 will probably take to long, so just going to .1 or .2 should be fine to illustrate the effect). If you have matlab/octave use the provided script temp.m to plot a temperature profile, or look at the TEMP file for the series of 1D profiles. Also the file MAXTEMP records the maximum temperature in each timestep and may be easier if you are just looking at text files (rather than plotting).

How does MAXTEMP vary in time as more the latent heat contribution is decreased?

For any of these simulations you can examine the phases present and the melt composition:

PHASES:

```
numphases                 7
DEPTH (m) =    6200.0000000000000
TIME (yr) =   10.000000000000000
system^@^@^@^@^@^@^@^@^@^@^@^@^@^@   1.0000000000000000
liquid^@^@^@^@^@^@^@^@^@^@^@^@^@^@  0.43954248553078684
olivine^@^@^@^@^@^@^@^@^@^@^@^@^@^@  7.56275958479449700E-002
fayalite^@^@^@^@^@^@^@^@^@^@^@^@^@^@  1.10355168963640147E-002
sphene^@^@^@^@^@^@^@^@^@^@^@^@^@^@  0.46320616367940859
garnet^@^@^@^@^@^@^@^@^@^@^@^@^@^@  5.56553865230703920E-003
melilite^@^@^@^@^@^@^@^@^@^@^@^@^@  5.02269939318869280E-003
numphases           4
DEPTH (m) =    6000.0000000000000
TIME (yr) =   10.000000000000000
system^@^@^@^@^@^@^@^@^@^@^@^@^@^@   1.0000000000000000
liquid^@^@^@^@^@^@^@^@^@^@^@^@^@^@  0.97624915766158793
olivine^@^@^@^@^@^@^@^@^@^@^@^@^@^@  1.18029143371791006E-004
fayalite^@^@^@^@^@^@^@^@^@^@^@^@^@^@  2.36328131950403648E-002
numphases           3
DEPTH (m) =    5800.0000000000000
```

MELT_COMPOSITION:

```
DEPTH (m) =    6000.0000000000000
TIME (yr) =   10.000000000000000
MELT FRACTION =   0.97624915766158793
MELT COMPOSITION SiO2^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@=   62.586005068826161
MELT COMPOSITION TiO2^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@=  0.67706615072850862
MELT COMPOSITION Al2O3^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@=   17.516998669099962
MELT COMPOSITION Fe2O3^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@=  0.82761292669003228
MELT COMPOSITION Cr2O3^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@=   0.0000000000000000
MELT COMPOSITION FeO^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@=   4.3331814171245231
MELT COMPOSITION MnO^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@=  9.21895801842007589E-002
MELT COMPOSITION MgO^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@=   2.2797807883393770
MELT COMPOSITION NiO^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@=   0.0000000000000000
MELT COMPOSITION CoO^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@=   0.0000000000000000
MELT COMPOSITION CaO^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@=   5.2555090444415703
MELT COMPOSITION Na2O^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@=   4.3238338965605072
MELT COMPOSITION K2O^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@=   1.6966022627377511
MELT COMPOSITION P2O5^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@=  0.24379022315376928
MELT COMPOSITION H2O^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@=   2.0486573374266510
MELT COMPOSITION CO2^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@=   0.0000000000000000
MELT COMPOSITION SO3^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@=   0.0000000000000000
MELT COMPOSITION Cl2O-1^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@=   0.0000000000000000
MELT COMPOSITION F2O-1^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@=   0.0000000000000000
```