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
Deformation

Newman et al., 2001
Crustal container is not, in general, completely rigid and can have elastic and viscoelastic response.
Deformation
Some Thermal Considerations

\[ \frac{\partial H_T}{\partial t} + \frac{\partial}{\partial x_i} (u_i H_T) = \frac{\partial}{\partial x_i} k \left( \frac{\partial}{\partial x_i} T \right) \]

\[
H_T = \rho \int_{T_{ref}}^{T} c_p \, dT + \rho \frac{\partial f}{\partial t} \]

\[
\rho^* \left[ \frac{\partial T^*}{\partial t^*} + u_i^* \frac{\partial T^*}{\partial x_i^*} \right] = \left[ \frac{1}{Pe} \right] \frac{\partial^2 T^*}{\partial x_i^2} - \left[ \frac{1}{Ste} \right] R^* \]

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

Advective/diffusive heat transport

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.

\[
\frac{\partial f}{\partial t} = \frac{1}{T_L - T_s} \frac{\partial T}{\partial t}
\]

\[
C_p^* = C_p + \frac{L}{T_L - T_s}
\]

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**
\[ \frac{\partial}{\partial t} (\phi_k \rho_k) + \frac{\partial}{\partial x_i} (\phi_k \rho_k u_{k,i}) = R_k \]

**Conservation of Momentum**
\[ \frac{\partial (\phi_k \rho_k u_{k,i})}{\partial t} + \frac{\partial (\phi_k \rho_k u_{k,i} u_{k,j})}{\partial x_i} = -\phi_k \frac{\partial P}{\partial x_i} \delta_{ij} + \frac{\partial}{\partial x_i} \left[ \tau_{ij} \right] + D_i + \rho_k \phi_k g_2 \delta_{ij} + R_k u_{k,i} \]

**Conservation of Thermal Energy**
\[ \phi_k \rho_k c_k \left[ \frac{\partial T_k}{\partial t} + u_i \frac{\partial T_k}{\partial x_i} \right] = \delta_{km} \frac{\partial q_k}{\partial x_i} + \pi k_m d \left( \text{Nu} (T_m - T_c) + \phi_k R_k L \right) \]

**Conservation of Chemical Species**
\[ \frac{\partial}{\partial t} \left( \phi_k \rho_k C_{SiO_2} \right) + \frac{\partial}{\partial x_i} \left( \phi_k \rho_k u_{k,i} C_{SiO_2} \right) = \beta_{(f)} \]
Multiphase Equations for Magma Chamber

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Conservation of Thermal Energy

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

Conservation of Chemical Species

\[ \frac{\partial}{\partial t} (\phi_k \rho_k C_{SiO_2}) + \frac{\partial}{\partial x_i} (\phi_k \rho_k u_{k,i} C_{SiO_2}) = \beta_{(f)} \]
**Multiphase Equations for Magma Chamber**

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**Conservation of Momentum**

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\frac{\partial}{\partial t} (\phi_k \rho_k u_{k,i}) + \frac{\partial}{\partial x_i} (\phi_k \rho_k u_{k,i} u_{k,j}) = -\phi_k \frac{\partial P}{\partial x_i} \delta_{ij} + \frac{\partial}{\partial x_i} \left[ \tau_{ij} \right] + D_i + \rho_k \phi_k g_2 \delta_{i2} + R_k u_{k,i}
\]

**Conservation of Thermal Energy**

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

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\frac{\partial}{\partial t} (\phi_k \rho_k C_{SiO_2}) + \frac{\partial}{\partial x_i} (\phi_k \rho_k u_{k,i} C_{SiO_2}) = \beta_{(f)}
\]
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/
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

<table>
<thead>
<tr>
<th></th>
<th>Early eruped Bishop Tuff</th>
<th>Late-erupted Bishop Tuff</th>
<th>Highland Range (HRL 21)</th>
<th>Highland Range (HRL 27)</th>
<th>Peach Spring Tuff (KPST 01D)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>WR*†</td>
<td>WR*†</td>
<td>WR†‡</td>
<td>WR†‡</td>
<td>WR§ Glass§</td>
</tr>
<tr>
<td>SiO₂</td>
<td>77.7</td>
<td>77.5</td>
<td>75.6</td>
<td>75.9</td>
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<tr>
<td>TiO₂</td>
<td>0.07</td>
<td>0.08</td>
<td>0.21</td>
<td>0.12</td>
<td>0.64</td>
</tr>
<tr>
<td>Al₂O₃</td>
<td>12.3</td>
<td>12.5</td>
<td>12.6</td>
<td>12.5</td>
<td>15.9</td>
</tr>
<tr>
<td>FeO</td>
<td>0.70</td>
<td>0.66</td>
<td>1.10</td>
<td>1.12</td>
<td>2.81</td>
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<tr>
<td>MgO</td>
<td>0.01</td>
<td>0.03</td>
<td>0.25</td>
<td>0.10</td>
<td>0.90</td>
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<tr>
<td>CaO</td>
<td>0.45</td>
<td>0.43</td>
<td>0.95</td>
<td>0.64</td>
<td>0.64</td>
</tr>
<tr>
<td>Na₂O</td>
<td>3.91</td>
<td>3.98</td>
<td>3.35</td>
<td>3.27</td>
<td>4.99</td>
</tr>
<tr>
<td>K₂O</td>
<td>4.82</td>
<td>4.88</td>
<td>5.56</td>
<td>5.38</td>
<td>6.40</td>
</tr>
</tbody>
</table>

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)
melts.out

T = 758.50 (C)  P = 1.750 (kbars)  log(10) fO2 = -14.81  delto 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 = -587620.64 (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  C12O-1  F2O-1
73.58  0.11  11.65  0.29  0.00  0.05  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 %)
K8.51Na0.47CaO0.02Al2O3.02S12.9908
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 = 8.00 (gm)  density = 2.56 (gm/cc)  (analysis in mole %)
K8.15Na0.76CaO0.08Al2O3.08S12.9208
G = -130016.02 (J)  H = -113385.22 (J)  S = 17.04 (J/K)  V = 3.16 (cc)  Cp = 9.85 (J/K)
albite  anorthite  sanidine
76.47  3.46  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 = 0.62 (cc)  Cp = 25.39 (J/K)

spinel
mass = 0.39 (gm)  density = 4.97 (gm/cc)  (analysis in mole %)
Fe0.17Mg0.82Fe0.04Al0.08Cr0.007Ti0.1904
G = -2566.95 (J)  H = -1951.80 (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  10.86

water
mass = 3.22 (gm)  density = 0.41 (gm/cc)
H2O
G = -70544.12 (J)  H = -40606.48 (J)  S = 28.03 (J/K)  V = 7.78 (cc)  Cp = 12.87 (J/K)

Total solids
mass = 63.89 (gm)  density = 2.82 (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 = 0.000888283  delta grams = 0.002864
G = -201.91 (J)  H = 21.93 (J)  S = 0.22 (J/K)  V = 77.56 (cc)  Cp = 0.03 (J/K)
Rhyolite MELTS should give results similar to panel C.
Explore MELTS simulations at 12 kbar, with added water.

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

The role of H₂O during crystallization of primitive arc magmas under uppermost mantle conditions and genesis of igneous pyroxenites: an experimental study
### How do your run products compare?

<table>
<thead>
<tr>
<th>Runs</th>
<th>P (GPa)</th>
<th>T(°C)</th>
<th>(h)</th>
<th>H_2O (melt)</th>
<th>H_2O init (wt%±a)</th>
<th>Run products</th>
<th>Phase proportions (wt%±a)</th>
<th>Kd</th>
<th>Δ Φe (%)</th>
<th>ΣP²</th>
<th>capsule (g)</th>
<th>sample (g)</th>
<th>samp/caps ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Basalt (85-44)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td></td>
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<tr>
<td>B690</td>
<td>1.2</td>
<td>1230</td>
<td>25</td>
<td>4.4(3)</td>
<td>~ 3.8</td>
<td>GL, Cpx, Opx</td>
<td>88.9(21):2.8(27):8.2(19)</td>
<td>0.31</td>
<td>0.29</td>
<td>-4.06</td>
<td>0.16</td>
<td>0.1005</td>
<td>0.0089</td>
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<td>B674</td>
<td>1.2</td>
<td>1190</td>
<td>25</td>
<td>4.2(3)</td>
<td>~ 3.8</td>
<td>GL, Cpx, Opx</td>
<td>77.5(25):12.6(30):9.9(21)</td>
<td>0.31</td>
<td>0.29</td>
<td>-0.55</td>
<td>0.22</td>
<td>0.1124</td>
<td>0.0093</td>
</tr>
<tr>
<td>B659</td>
<td>1.2</td>
<td>1150</td>
<td>22</td>
<td>5.7(7)</td>
<td>~ 3.8</td>
<td>GL, Cpx, Opx, SpI</td>
<td>65.3(13):20.5(16):14.1(11):1%</td>
<td>0.28</td>
<td>0.29</td>
<td>-1.88</td>
<td>0.08</td>
<td>0.1212</td>
<td>0.0081</td>
</tr>
<tr>
<td>B681</td>
<td>1.2</td>
<td>1110</td>
<td>27</td>
<td>5.5(2)</td>
<td>~ 3.8</td>
<td>GL, Cpx, Opx, Grt, SpI</td>
<td>49.8(14):31.0(16):13.7(12):4.9(19):0.6(5)</td>
<td>0.32</td>
<td>0.29</td>
<td>1.78</td>
<td>0.55</td>
<td>0.1059</td>
<td>0.0078</td>
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<tr>
<td>B726</td>
<td>1.2</td>
<td>1070</td>
<td>30</td>
<td>6.4(7)</td>
<td>~ 3.8</td>
<td>GL, Cpx, Opx, Grt, Am</td>
<td>39.9(19):27.0(43):8.8(23):13.3(21):8.9(24)</td>
<td>0.31</td>
<td>0.29</td>
<td>0.56</td>
<td>0.34</td>
<td>1.79</td>
<td>0.0832</td>
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<tr>
<td>B714</td>
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<td>1230</td>
<td>24</td>
<td>5.3(2)</td>
<td>~ 5</td>
<td>GL, Cpx, Opx</td>
<td>90.5(38):2.9(26):6.5(33)</td>
<td>0.30</td>
<td>0.30</td>
<td>9.45</td>
<td>0.64</td>
<td>0.0723</td>
<td>0.0060</td>
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<tr>
<td>B686</td>
<td>1.2</td>
<td>1210</td>
<td>26</td>
<td>5.6(4)</td>
<td>~ 5</td>
<td>GL, Cpx, Opx</td>
<td>88.3(13):4.5(17):7.2(12)</td>
<td>0.28</td>
<td>0.27</td>
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<td>0.07</td>
<td>0.0951</td>
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<td>B671</td>
<td>1.2</td>
<td>1190</td>
<td>26</td>
<td>5.3(6)</td>
<td>~ 5</td>
<td>GL, Cpx, Opx</td>
<td>89.6(30):4.1(39):6.3(26)</td>
<td>0.29</td>
<td>0.28</td>
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<td>B665</td>
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<td>1150</td>
<td>26</td>
<td>6.5(4)</td>
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<td>GL, Cpx, Opx</td>
<td>76.0(36):12.5(40):11.4(29)</td>
<td>0.20</td>
<td>0.28</td>
<td>8.34</td>
<td>0.52</td>
<td>0.1078</td>
<td>0.0084</td>
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<tr>
<td>B683</td>
<td>1.2</td>
<td>1110</td>
<td>26</td>
<td>6.0(5)</td>
<td>~ 5</td>
<td>GL, Cpx, Opx, SpI</td>
<td>61.9(29):23.6(33):13.7(2):1.1(9)</td>
<td>0.30</td>
<td>0.28</td>
<td>4.20</td>
<td>0.21</td>
<td>0.1158</td>
<td>0.0088</td>
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<tr>
<td>B704</td>
<td>1.2</td>
<td>1070</td>
<td>32</td>
<td>9.0(3)</td>
<td>~ 5</td>
<td>GL, Cpx, Opx, Grt, Am</td>
<td>46.9(14):19.1(25):10.1(12):0.3(1)</td>
<td>0.30</td>
<td>0.28</td>
<td>0.61</td>
<td>0.33</td>
<td>0.76</td>
<td>0.0128</td>
</tr>
<tr>
<td>B679</td>
<td>1.2</td>
<td>1190</td>
<td>27</td>
<td>3.5(5)</td>
<td>~ 2.5</td>
<td>GL, Cpx, Opx</td>
<td>69.3(25):17.6(46):13.0(31)</td>
<td>0.31</td>
<td>0.29</td>
<td>-8.39</td>
<td>0.49</td>
<td>0.1206</td>
<td>0.0082</td>
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<td>B668</td>
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<td>1150</td>
<td>28</td>
<td>4.5(5)</td>
<td>~ 2.5</td>
<td>GL, Cpx, Opx</td>
<td>53.3(85):23.5(45):16.3(41):5.8(9)</td>
<td>0.28</td>
<td>0.27</td>
<td>-7.25</td>
<td>0.43</td>
<td>0.1104</td>
<td>0.0064</td>
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</tbody>
</table>
PhasePlot --- Available for macs through the app store.
MELTS calculations at grid point: $T = 750.00 \text{ °C}$ and $P = 220.0 \text{ MPa}$

Minimal energy computed.

### Phases in the system:

<table>
<thead>
<tr>
<th>Phase</th>
<th>Mass (g)</th>
<th>Afinitx (mol)</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid</td>
<td>78.78</td>
<td></td>
<td>wt% SiO2 72.47 TiO2</td>
</tr>
<tr>
<td>Sanidine</td>
<td>16.75</td>
<td></td>
<td>K0.70Na0.29Ca0.01...</td>
</tr>
<tr>
<td>Quartz</td>
<td>5.45</td>
<td></td>
<td>SiO2</td>
</tr>
<tr>
<td>Water</td>
<td>0.92</td>
<td></td>
<td>H2O</td>
</tr>
<tr>
<td>Orthopyroxene</td>
<td>0.53</td>
<td></td>
<td>Na0.00Ca0.01Fe*1...</td>
</tr>
<tr>
<td>Spinel</td>
<td>0.14</td>
<td></td>
<td>Fe<em>1.23Mg0.05Fe</em>1...</td>
</tr>
<tr>
<td>Ilmenite ss</td>
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<td>Mn0.00Fe*0.79Mg0...</td>
</tr>
<tr>
<td>Panunzite</td>
<td>(0.00)</td>
<td></td>
<td>Na2.96K0.02Ca0.03...</td>
</tr>
<tr>
<td>WhiteIlkite</td>
<td>(0.00)</td>
<td></td>
<td>Ca3(PO4)2</td>
</tr>
<tr>
<td>Chromite</td>
<td>(0.00)</td>
<td></td>
<td>FeCr2O4</td>
</tr>
<tr>
<td>Actinolite</td>
<td>(0.00)</td>
<td></td>
<td>Ca0.16Fe2.95Mg3.8...</td>
</tr>
<tr>
<td>Apatite</td>
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<td>Ca5(PO4)3OH</td>
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<td>Plagioclase</td>
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<td>K0.70Na0.29Ca0.01...</td>
</tr>
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<td>Augite</td>
<td>(0.00)</td>
<td></td>
<td>Na0.00Ca0.06Fe*1...</td>
</tr>
<tr>
<td>Titanaugite</td>
<td>(0.00)</td>
<td></td>
<td>Na0.00Ca0.06Fe*1...</td>
</tr>
<tr>
<td>Biotte</td>
<td>(83.76)</td>
<td></td>
<td>KFe*0.06Mg0.94...</td>
</tr>
<tr>
<td>Garnet</td>
<td>(164.33)</td>
<td></td>
<td>Na0.00Ca0.06Fe*1...</td>
</tr>
</tbody>
</table>
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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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).
(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/octetave 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.
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’)

![Graphs showing melt fraction and temperature changes](image)
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 too 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:**

**MELT_COMPOSITION:**