Petrolog3: Integrated software for modeling crystallization processes

Leonid V. Danyushevsky
CODES and School of Earth Sciences, University of Tasmania, Private Bag 79, Hobart, Tasmania 7001, Australia (l.dan@utas.edu.au)

Pavel Plechov
Petrology Department, Geology Faculty, Moscow State University, Vorob'evy Gory, Moscow, Russia (pavel@ueb.ru)

[1] This paper introduces Petrolog3, software for modeling (1) fractional and equilibrium crystallization, (2) reverse fractional crystallization at variable pressure, melt oxidation state and melt H2O contents, and (3) postentrapment reequilibration of melt inclusions in olivine. Petrolog3 offers an algorithm that allows calculations with a potentially unlimited number of (1) mineral-melt equilibrium models for major and trace elements and (2) models describing melt physical parameters such as density and viscosity, melt oxidation state, and solubility of fluid components in silicate melts. The current version of the software incorporates 46 mineral-melt equilibrium models for 8 minerals; 3 models describing distribution of trace elements between minerals and melt; 4 models of melt oxidation state; 1 model for H2O solubility in silicate melts; and 4 models describing melt density and viscosity. The idea behind the program is to provide the community of igneous petrologists and geochemists with a user-friendly interface for using any combinations of available mineral-melt equilibrium models for computer simulation of the crystallization process.

Components: 16,600 words, 27 figures.

Keywords: crystallization modeling; igneous petrology; melt inclusions; peritectic; reverse fractional crystallization.

Index Terms: 3610 Mineralogy and Petrology: Geochemical modeling (1009, 8410); 3618 Mineralogy and Petrology: Magma chamber processes (1036); 3640 Mineralogy and Petrology: Igneous petrology.

Received 13 January 2011; Revised 17 March 2011; Accepted 6 April 2011; Published 29 July 2011.


1. Introduction

[2] Crystal fractionation is one the main mechanisms of magma evolution leading to generation of magmatic series. The extensive sets of experimental data on crystallization of natural magmas built over the last several decades [e.g., Ariskin et al., 1996; Hirschmann et al., 2008] form the foundation for a number of computer models describing mineral-melt equilibria during magma evolution. The most popular algorithms include MELTS and its derivatives [e.g., Ghiorso et al., 1983, 2002; Smith and Asimow, 2005], based on the principle of minimization of free energy, and COMAGMAT [Frenkel and Ariskin, 1984; Ariskin et al., 1993], based on the principle of pseudoliquidus temperatures [e.g., Nathan and Van Kirk, 1978].

[3] At the same time, the number of alternative models describing equilibrium between silicate melts and specific minerals has grown continuously.
For example, over 20 different models have been published to date that describe equilibrium between olivine and melt (see Appendix A for references), posing the question of which model to choose for a particular modeling task at hand. To facilitate comparison of different models by calculating fractionation paths using different combinations of existing models, Petrolog2 has been developed [Danyushevsky, 2001; http://www.geol.utas.edu.au/~leonid/Petrolog.html] which simulates melt evolution during fractional crystallization.

As different models are based on different numbers of mineral and melt components, and different formulations for their chemical activity-compositional relationships, an algorithm for simulating crystallization using such models must rely only on model outputs (i.e., temperature of equilibrium and liquidus mineral compositions) and thus has to be effectively independent of the model formulations. Petrolog2 was restricted to modeling fractional crystallization only, as a model-independent algorithm for describing equilibrium crystallization, including peritectic reactions, had not been developed at the time.

This paper introduces Petrolog3 (see Software S1 in the auxiliary material), a software for modeling fractional, equilibrium and semifractional crystallization mechanisms using a model-independent algorithm which we developed (the program can be downloaded from the Petrolog3 home page http://petrolog.web.ru/; Petrolog3 works under Windows operating system). The idea behind the software is to provide the community of igneous petrologists and geochemists with a user-friendly interface for using any combinations of available mineral-melt equilibrium models for computer simulation of the crystallization process. The user interface of the software is described in the Petrolog3 manual (Appendix B). Note that Petrolog3 is not designed to generate new models of mineral-melt equilibrium.

2. The Algorithm

Petrolog3 incorporates published mineral-melt equilibrium models for individual minerals. Models that can be included in Petrolog3 must calculate, for a given melt composition at a given pressure and oxidation state, both the temperature at which the mineral appears on the liquidus of this melt, and the composition of the mineral. Currently, Petrolog3 incorporates 46 models for 8 different minerals (Appendix A), which are effectively restricted to anhydrous minerals in mafic and andesitic systems, as no models for other minerals are currently available. The modular structure of the code allows for a large number of minerals and models for each mineral to be included in the software as new models become available.

A large number of published models of mineral-melt equilibrium do not incorporate pressure and are applicable only at 1 atm, anhydrous conditions; some others are capable of modeling at elevated pressures, but do not incorporate hydrous conditions. To enable the use of such models for calculations at elevated pressures and hydrous conditions, Petrolog3 offers an option of introducing user-defined corrections to calculated temperatures as a function of pressure (in the form dT/dP, degrees/kbar) and melt H2O content (in the form dT = A * H2O(wt %)B [Falloon and Danyushevsky, 2000; Médard and Grove, 2008]). The software provides default values for these corrections based on the currently preferred values, but also allows the user to change these values if desired. Note that these corrections would not apply to the calculated mineral composition which would remain the same as if calculated at 1 atm anhydrous.

For modeling crystallization, the user must specify a particular model that will be used for each mineral involved in the calculation. The same calculation can be repeated with a different set of models to assess the robustness of the crystallization paths produced.

2.1. Modeling Crystallization Within the Stability Field of a Single Mineral

For a given melt composition, the calculated liquidus temperature of the mineral is taken to be the crystallization temperature. The amount of the mineral to be subtracted from the melt is determined by the calculation step which is set as a fraction of the amount of melt. Accurate modeling of pure fractional crystallization using this approach generally requires that the calculation step is significantly (orders of magnitude) smaller than the total extent of crystallization to be modeled.

Modeling of fractional crystallization requires that the mineral (M0) which crystallizes from the melt (L0) during each step is in equilibrium with a melt composition (L1) residual after the formation of the mineral:

\[ C_{L0} = X \cdot C_{M0} + (1 - X) \cdot C_{L1}, \]  

(1)
where X is the calculation step and C$_i$ is the concentration of element “i” in either mineral or melt.

[11] In Petrolog3, this is solved through an iterative procedure that determines a mineral composition that is perfectly mass balanced following equation (1), but can differ from the composition in equilibrium with L$_1$ by less than the value of a set threshold (10$^{-8}$ wt % of any major element in the mineral composition).

[12] When modeling pure fractional crystallization, a mineral is “removed” from contact with melt and placed into the “cumulate” part of the system, thus retaining its original composition. The procedure is then repeated with the composition L$_1$. Petrolog3 records the evolution of the melt composition, the instantaneous composition of the crystallizing mineral, and the average composition of the “cumulate.”

[13] When modeling equilibrium crystallization, the total amount of the crystallized mineral remains in equilibrium with the residual melt, thus continuously changing its composition. A general mass balance requirement for equilibrium crystallization can be expressed as

$$X_{old}^M * C_{Mold} + X_{old}^L * C_{Lold} = (X_{old}^M + X) * C_{Mnew} + (X_{old}^L - X) * C_{Lnew}, \quad (2)$$

where $X_{old}^M$ and $X_{old}^L$ are the weight fractions of mineral and melt on the previous step, respectively; X is the calculation step; C$^i$ is the concentration of element “i” in either mineral or melt; M$_{old}$ is in equilibrium with L$_{old}$; and M$_{new}$ is in equilibrium with L$_{new}$. On each step, equation (2) is solved through an iterative procedure as described for equation (1).

[14] During equilibrium crystallization, Petrolog3 records the evolution of melt composition and the composition and amount of the mineral on each step. No “cumulate” is formed during equilibrium crystallization. The combined composition of the melt and mineral is referred to as “magma.”

[15] During crystallization of natural magmas, an intermediate scenario is likely, which can be referred to as “semifractional” crystallization, in which a certain proportion of a crystallizing mineral reequilibrates with the continuously evolving melt, whereas the remainder of the mineral is “removed” from contact with the melt at each step. This is achieved either by crystal settling from the magma into cumulate layers, or by shielding of the mineral by the newly grown rim. In Petrolog3, the extent of fractionation can be specified as a proportion of the mineral that is removed from contact with the melt at each step, which can vary between 100 (pure fractional crystallization) and 0 (pure equilibrium crystallization). When the extent of fractionation is set between 0 and 100, the mineral is present in both the “magma” and the “cumulate” (Figure 1).

2.2. Modeling Cotectic Crystallization

[16] A combination of mineral-melt equilibrium models for different minerals can be used to describe crystallization of silicate melts [e.g., Nathan and Van Kirk, 1978; Nielsen and Dungan, 1983; Frenkel and...
The essence of the approach is, for a given melt composition, to calculate liquidus temperatures for all mineral phases involved in the calculation. Such temperatures are commonly called “pseudoliquidus” temperatures (PLT) as only the phase with the highest calculated temperature is the true liquidus phase.

If two or more minerals have the same PLT for a given melt composition, and this temperature is the highest of all PLTs for minerals involved in the calculation, this indicates that those minerals with the same PLT should be crystallizing together. The relationship between simultaneously crystallizing minerals may be determined by the slopes of their PLTs as a function of composition. If the slopes are opposing (i.e., a change of melt composition due to subtraction of one mineral, resulting in a decrease of its PLT, leads to an increase of the PLT of another mineral), then it is assumed that the cocrystallizing minerals are in a cotectic relationship. A common example of a two-mineral cotectic crystallization is an olivine-plagioclase cotectic in anhydrous basaltic systems (Figure 2).

Consider a case for which melt composition is in the olivine-only field immediately adjacent to the olivine-plagioclase cotectic (Figure 2c). As olivine is the liquidus phase of such a melt, its composition will be subtracted from the melt at the next step. The resultant melt composition is in the plagioclase-only field (Figure 2c). Thus, at the next step, plagioclase will be removed from the melt, shifting the melt composition back toward the olivine-only field (Figure 2c). In other words, cotectic crystallization is modeled by consecutive steps, each involving the removal of a single mineral from the melt. This algorithm yields the proportions of the crystallizing phases along the cotectic as an independent parameter, which is dependent on the set of models used in the calculations. Such proportions are determined by the slope of the liquidus surface for each mineral in a direction away from the mineral apex, which is model-specific. Thus, a possible criterion for the suitability of the models chosen for describing crystallization of the composition of interest is whether the resultant proportions of the cocrystallizing minerals correspond to those observed in natural samples or experimental studies of crystallization of similar compositions (Figure 2).

When modeling pure fractional cotectic crystallization, the amount of mineral removed from the melt at each step equals the calculation step. When modeling semifractional or equilibrium crystallization, the amount of mineral in equilibrium with the melt equals the total amount of this mineral in the “magma.”

Although the above algorithm has been widely used to model fractional cotectic crystallization [e.g., Nathan and Van Kirk, 1978; Nielsen, 1988], it is used here for the first time to model equilibrium crystallization. The validity of this algorithm for modeling equilibrium cotectic crystallization is demonstrated by comparing the results of calculations performed at different calculation steps (Figure 3). If calculations are performed with an infinitely small step, the algorithm would effectively reproduce simultaneous crystallization of cotectic minerals. If no systematic shift in the cotectic position is observed with increasing size of the calculation step, this would imply that the algorithm is step independent and can successfully reproduce cotectic crystallization. As can be seen from Figure 3, there is no systematic difference between cotectics calculated for a single starting composition under the same conditions, but using variable calculations steps. However, larger calculation steps clearly result in poorer precision. Modeling a cotectic using a calculation step of 0.01 wt % results in a precision of ~0.2°C and ~0.01 wt %, for the crystallization temperature and melt major element concentrations, respectively (Figure 3b). Decreasing the calculation step further would result in significantly longer calculation times, but would not produce any geologically significant improvement in precision.

Figure 2d demonstrates an application of the new algorithm to modeling an experimentally derived equilibrium olivine-plagioclase-clinopyroxene cotectic crystallization of a basaltic composition. This example demonstrates that the algorithm reproduces experimentally derived cotectics, but also illustrates differences arising from using different mineral-melt equilibrium models.

### 2.3. Modeling Crystallization Involving Peritectic Reactions

When two or more minerals on the liquidus of a melt are characterized by liquidus surfaces with slopes in the same direction (i.e., a change of melt composition due to subtraction of one mineral, resulting in a decrease of its PLT, also leads to a decrease of the PLT of the other mineral), it is assumed that the cocrystallizing minerals are in a peritectic relationship. A peritectic relationship occurs if a melt corresponding in composition to one of the minerals, has another mineral on its
Figure 2
liquidus. A peritectic relationship can be generally described as:

$$M_1 + L_1 \rightarrow M_2 + L_2,$$

(3)

where $M$ and $L$ are mineral and melt, respectively.

[23] The mineral with the shallower slope of the liquidus surface crystallizes ($M_2$), whereas the mineral with the steeper slope dissolves ($M_1$). Note that the peritectic relationship only occurs if $M_1$ reequilibrates with the melt, whereas $M_2$ can crystallize in either equilibrium or fractional manner. A common example of a two-mineral peritectic reaction is an olivine-orthopyroxene peritectic in basaltic systems (Figure 4).

[24] In real cases of multimineral crystallization, a cotectic relationship between some minerals may be accompanied by peritectic reactions among others. In such cases the dissolving phase is taken to be one with the steepest slope of the liquidus surface in the direction away from the composition of the mineral that is produced during the peritectic reaction.

2.4. Modeling Trace Elements During Crystallization

[25] Petrolog3 considers an element to be a trace element if its concentration is not used in calculations of activities of mineral and/or melt components by the mineral-melt equilibrium models included in the software. The behavior of such elements is modeled through partition coefficients ($K_d$) between the minerals and melt. Petrolog3 offers two alternative options for defining $K_d$. The first option is to set a constant $K_d$ value, which is used through the entire course of the calculation. The second option allows for using empirical and/or thermodynamically sound models which define $K_d$ values as a function of melt composition, temperature, mineral composition, and so on. The modular structure of the software allows for a potentially unlimited number of such models for each element in each mineral. The $K_d$ models available in Petrolog3 are listed in Appendix A.

3. Use of Intensive Parameters

3.1. Modeling Polybaric Crystallization

[26] Petrolog3 offers several options for modeling crystallization at elevated pressure. Pressure can be set at a fixed value. Alternatively, polybaric crystallization can be modeled either as continuous ascent of the magma at a constant rate set as a $dP/dT$ value (bar/degree), or in several steps (maximum of 5), each characterized by a separate $dP/dF$.

Figure 2. Examples of an olivine-plagioclase cotectic fractional crystallization (Figures 2a, 2b, and 2c) and an olivine-plagioclase-clinopyroxene cotectic equilibrium crystallization calculated with a range of mineral-melt equilibrium models (Figure 2d). For the case of fractional crystallization, crystallization of a basaltic composition, calculated using the olivine and plagioclase models of Danyushevsky [2001], was modeled with a calculation step of 0.01 wt %; the total extent of crystallization is 17 wt %; the results were recorded at intervals of 1 wt % total crystallization. The average calculated weight proportion of plagioclase to olivine along this cotectic is 2.6. Thick arrows on Figures 2b and 2c show the direction of temperature decrease along the cotectic. (a) A normative CIPW olivine-plagioclase-diopside projection showing the starting composition and the position of the calculated olivine-plagioclase cotectic. (b) An enlarged portion of the normative CIPW olivine-plagioclase-diopside projection showing the calculated olivine-plagioclase cotectic. Open circles correspond to 1 wt % fractionation intervals. (c) An enlarged portion of the calculated olivine-plagioclase cotectic showing individual calculation steps (black dots) between two intermediate outputs (open circles). (d) Modeling an experimentally derived equilibrium crystallization trend. Four plots display changes in melt $Al_2O_3$ and TiO$_2$ contents, extent of crystallization (F) and experimental temperatures, all plotted against melt MgO content. Curve 1 is experimental data from Torney et al. [1987]; 1 atm crystallization experiments with starting composition AI96-18-1, producing a crystallization sequence of olivine, olivine + plagioclase, olivine + plagioclase + clinopyroxene. Experimental constraints indicate plagioclase first appearance at melt MgO between 8.2 and 7.9 wt %; clinopyroxene first appearance at MgO between 7.2 and 6.9 wt %. Curve 2 is crystallization trend calculated using olivine, plagioclase, and clinopyroxene models of Ariskin et al. [1993]. Curve 3 is crystallization trend calculated using olivine, plagioclase, and clinopyroxene models of Danyushevsky [2001]. Curve 4 is crystallization trend calculated using olivine, plagioclase, and clinopyroxene models of Langmuir et al. [1992]. Curve 5 is crystallization trend calculated using olivine model of Ford et al. [1983], plagioclase model of Pletchov and Gerya [1998], and clinopyroxene models of Nielsen [1988]. The first kink on all model trends (MgO 8.1–7.8 wt %) reflects appearance of plagioclase on the liquidus; the second kink (MgO 7.4–6.8 wt %) corresponds to the appearance of clinopyroxene on the liquidus. Two shaded areas on the $Al_2O_3$ versus MgO plot indicate the range of melt compositions at predicted first appearances of plagioclase and clinopyroxene, when using different mineral-melt equilibrium models.
value (where F is the degree of crystallization in percent).

3.2. Modeling Crystallization of Hydrous Compositions

Some of the models available in Petrolog3 incorporate the effect of melt H₂O content on crystallization temperature and/or composition of crystallizing minerals [Pletchov and Gerya, 1998; Danyushevsky, 2001; Putirka, 2005]. As described above, Petrolog3 allows the user to introduce corrections to the “anhydrous” models to account for the effect of H₂O on crystallization temperatures. [28] During calculations, the solubility of H₂O in the melt at a given T and P is calculated after the model of Moore et al. [1998]. When the amount of H₂O in the melt exceeds the solubility value, excess H₂O is assigned to a separate “fluid” phase.

Figure 3. An example of an olivine-plagioclase cotectic equilibrium crystallization of a basaltic composition, calculated using olivine and plagioclase models of Danyushevsky [2001]. The calculations were performed with a set of different calculation steps as indicated in the legend. Tolivine, olivine PLT; Tplagioclase, plagioclase PLT. (a) Melt evolution path and change in temperature along the cotectic for a total extent of crystallization of 17 wt %. The results were recorded at intervals of 1 wt % total crystallization. (b) Same as Figure 3a but for 1 wt % of crystallization with every individual step shown. Note that increasing the calculation step leads to worse precision of the modeled cotectic but does not produce a systematic shift in the position of the cotectic. See text for discussion.
Petrolog3 models degassing in a closed system, i.e., it is assumed that “fluid” remains within the “magma.” Petrolog3 also offers an option to perform the entire calculation under H$_2$O-saturated conditions.

Petrolog3 also offers an option of forcing the starting composition on an olivine-plagioclase (±clinopyroxene) cotectic by adjusting melt H$_2$O content, following the method of Danyushevsky [2001]. The essence of the approach is to first calculate the amount of H$_2$O which is required for the starting composition to lie on an olivine-plagioclase cotectic, and then to model crystallization as described in section 3.1 (see Danyushevsky[2001] for a detailed description of the approach). This option is limited to the mineral–melt models of Danyushevsky [2001] and should only be used for modeling crystallization of mid-ocean ridge and back-arc basin basalt compositions. When using this option, calculation pressure should be set at a value that ensures that the melt H$_2$O content required is less than the saturation value.

### 3.3. Mass Balance Considerations and Modeling Melt Oxidation State

Petrolog3 models crystallization as a closed system process for all cations. In general, the system consists of “magma,” “cumulate” and “fluid”...
(see above for the definitions of these terms). Thus, for every cation, mass balance requirements can be described as

\[ C_0 = C_m \cdot X_m + \sum_{k=1}^{k} C_{ph}^{k} \cdot X_{ph}^{k} + \sum_{k=1}^{k} C_{cum}^{k} \cdot X_{cum}^{k} + C_f \cdot X_f, \]

(4)

where \( C_0 \) is the initial concentration of cation \( i \); \( C_m \) and \( C_f \) are concentrations of this cation in the melt and “fluid,” respectively; \( k \) is the number of minerals in the system; \( C_{ph} \) and \( C_{cum} \) are concentrations of this cation in minerals in the “magma” (phenocrysts) and “cumulate,” respectively; \( X_m, X_{ph}, X_{cum}, X_f \) are weight fractions of all phases in the system.

[31] Thus, at any stage of crystallization the concentration of a cation in a magma can be described as

\[ C_{magma} = \frac{C_m \cdot X_m + \sum_{k=1}^{k} C_{ph}^{k} \cdot X_{ph}^{k}}{1 - X_f - X_{cum}}, \]

(5)

where

\[ X_{cum} = \sum_{k=1}^{k} X_{cum}^{k}. \]

Unlike for cations, the system is not closed for oxygen to allow for buffering of melt oxidation state. Petrolog3 offers several options for defining the melt oxidation state during calculations, which is expressed as the value of \( \text{Fe}^{2+}/\text{Fe}^{3+} \). It is assumed that Fe is the only cation with variable valency which is dependent on oxygen fugacity. The melt oxidation state can be modeled either as a function of oxygen fugacity that evolves along an oxygen buffer (e.g., nickel-nickel oxide), or as a constant melt \( \text{Fe}^{2+}/\text{Fe}^{3+} \) value.

[32] Crystallization can also be modeled assuming that the system is closed for oxygen, thus keeping constant the initial amounts of \( \text{Fe}^{2+} \) and \( \text{Fe}^{3+} \). In this case, changes in oxygen fugacity in the system during crystallization are determined by changes in the melt \( \text{Fe}^{2+}/\text{Fe}^{3+} \) value during melt evolution.

4. Additional Modeling Options in Petrolog3

[33] In addition to modeling crystallization, Petrolog3 offers several unique options such as determination of melt liquidus association, modeling reverse fractional crystallization and modeling postentrapment reequilibration of melt inclusions in olivine with their host mineral.

4.1. Determination of Melt Liquidus Association

[34] This option allows, for a given melt composition, simultaneous calculation of PLTs and compositional parameters for all minerals using any number of models available for each mineral. An example of such a calculation is shown in Figure 5.

[35] Such calculations can be used for two purposes. First they may be used to assess the suitability of specific models for modeling crystallization within a particular compositional range. For this purpose, calculations can be performed for experimentally derived compositions within the compositional range of interest, in order to determine which models reproduce best the experimental temperatures and mineral compositions in this compositional range. Such calculations can also be used to determine the values of corrections for the effects of pressure and/or melt H\(_2\)O contents that may be required to improve model performance.

[36] Second, if a set of preferred models is known, this option can be used to assess whether a specific composition lies within a single-mineral crystallization field, or on a cotectic/peritectic (see Appendix B for more details).

4.2. Modeling of Reverse Fractional Crystallization

[37] Modeling of reverse fractional crystallization can be used to restore the compositions of less fractionated parental melts from the compositions of evolved erupted lavas [e.g., Danyushevsky et al., 2000b, 2004] and for restoring the original trapped compositions of melt inclusions in phenocrysts (see Danyushevsky et al. [2000a] for a detailed description of the technique). It is only possible to reverse the results of fractional crystallization, as during equilibrium crystallization no record is preserved of the proportions of crystallizing minerals.

[38] The principle behind calculating reverse fractional crystallization is adding minerals that crystallized from the melt back into the melt composition thus moving it up along the liquid line of descent toward more primitive compositions. Unlike fractionation calculations, in which the mineral with the highest PLT is subtracted from the melt composition, the mineral with the lowest PLT is added to the
Estimation of Melt liquidus assemblage

Minerals and models chosen for calculations are:

- Clinopyroxene (Cpx): Bolotkova et al., 1995, Beattie, 1983
- Plagioclase (Plg): Nielsen, 1988, Ariskin et al., 1993
- Ilmenite (Ilm): Nielsen, 1985
- Magnetite (Mgt): Ariskin, Barmina 1999

Fe2O3 in the melt is calculated using QFM buffer of oxygen fugacity following the model of Borisov and Shapkin, 1990

Pressure = 0.001 kbar

<table>
<thead>
<tr>
<th>OLv</th>
<th>OLv</th>
<th>OLv</th>
<th>OLv</th>
<th>OLv</th>
<th>Flg</th>
<th>Flg</th>
<th>Flg</th>
<th>Cpx</th>
<th>Cpx</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ford83</td>
<td>Arisk86</td>
<td>RoaEms70</td>
<td>Gaetani01</td>
<td>Arisk93</td>
<td>Weaver90</td>
<td>Nielsen85</td>
<td>Arisk90</td>
<td>Arisk93</td>
<td>Weaver90</td>
</tr>
<tr>
<td>1203.8</td>
<td>1200.6</td>
<td>1208.4</td>
<td>1195.9</td>
<td>1202.8</td>
<td>1202.2</td>
<td>1179.4</td>
<td>1190.6</td>
<td>1175.5</td>
<td>1191.0</td>
</tr>
<tr>
<td>Fo</td>
<td>Fo</td>
<td>Fo</td>
<td>Fo</td>
<td>Fo</td>
<td>An</td>
<td>An</td>
<td>An</td>
<td>Mg#Cpx</td>
<td>Mg#Cpx</td>
</tr>
<tr>
<td>85.17</td>
<td>84.52</td>
<td>85.26</td>
<td>85.09</td>
<td>84.79</td>
<td>74.71</td>
<td>69.05</td>
<td>74.03</td>
<td>86.03</td>
<td>86.85</td>
</tr>
<tr>
<td>Cpx</td>
<td>Cpx</td>
<td>Flg</td>
<td>Flg</td>
<td>Spl</td>
<td>Spl</td>
<td>Ilm</td>
<td>Mgt</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nielsen88</td>
<td>Bolikh96</td>
<td>Beatt83</td>
<td>Nielsen88</td>
<td>Arisk93</td>
<td>Nielsen85</td>
<td>Arisk93</td>
<td>Nielsen85</td>
<td>Arisk99</td>
<td></td>
</tr>
<tr>
<td>1195.7</td>
<td>1185.2</td>
<td>1183.4</td>
<td>1168.3</td>
<td>1172.4</td>
<td>1433.0</td>
<td>1268.1</td>
<td>765.1</td>
<td>1031.2</td>
<td></td>
</tr>
<tr>
<td>Mg#Cpx</td>
<td>Mg#Cpx</td>
<td>Mg#Cpx</td>
<td>Mg#Flg</td>
<td>Mg#Flg</td>
<td>Cr#Spl</td>
<td>Cr#Spl</td>
<td>Mg#Ilm</td>
<td>Mg#Mgt</td>
<td></td>
</tr>
<tr>
<td>87.15</td>
<td>85.90</td>
<td>85.44</td>
<td>81.93</td>
<td>84.35</td>
<td>31.06</td>
<td>55.66</td>
<td>42.56</td>
<td>36.02</td>
<td></td>
</tr>
</tbody>
</table>

Figure 5. An example of Petrolog3 output for calculations of the melt liquidus association.

The approach is least ambiguous when used with compositions that lie within the crystallization field of a single mineral rather than on a cotectic. This is because, unlike when modeling fractionation, the algorithm requires additional information to determine when minerals appeared on the liquidus of the evolving melt during forward fractionation (Figure 6).

Petrolog3 offers several options to specify when the melt composition should leave the cotectic, which include temperature, melt composition and mineral composition. In practice, the mineral composition is the easiest to determine, as the record of fractional crystallization is preserved in the range of compositions of phenocrysts formed, and those are often present in erupted lavas. Setting the least fractionated mineral compositions present in lavas as the compositions corresponding to the moment when minerals occurred on the liquidus, enables quantitative reconstructions of fractionation trends using reverse fractionation calculations.

Examples shown on Figure 6 illustrate two important points. First, unlike fractionation calculations, in which crystallization of any number of minerals can be modeled for any starting composition, with the algorithm determining which minerals actually crystallize from the melt, the minerals that are included in reverse fractionation calculations must be on the liquidus of the starting composition at the calculation parameters chosen. Second, the shape of the calculated trend is dependent on the conditions at which minerals are excluded from calculations to force the trend off a cotectic.

4.3. Modeling Postentrapment Reequilibration of Melt Inclusions in Olivine

Reequilibration of Fe and Mg between melt inclusions and their host olivine phenocrysts is
described in detail by Danyushevsky et al. [2000a, 2002], with the main points summarized briefly below. The underlying assumption in these considerations is that the composition of the host olivine does not change after trapping of the melt inclusion.

[44] Cooling of an inclusion after trapping results in crystallization of olivine from the trapped melt, forming an olivine rim on the walls of the inclusion. The crystallizing olivine rim is progressively enriched in Fe and depleted in Mg, i.e., decreases in forsterite component, resulting in a compositional gradient within the rim. The existence of this compositional gradient causes reequilibration of the inclusion with its host. This reequilibration is achieved by diffusion of Fe out of, and Mg into the initial volume of the inclusion. This leads to a rapid decrease in Fe content of the residual melt inside the inclusion, a process referred to as “Fe loss” by Danyushevsky et al. [2000a].

[45] Conversely, if an olivine grain containing a melt inclusion is heated over the temperature of inclusion entrapment, host olivine around the inclusion would melt, increasing the Mg# of the melt inside the inclusion and resulting in disequilibrium between the melt and host olivine. This leads to reequilibration of the melt with the host, which is achieved by diffusion of Fe into, and Mg out of the melt inside the inclusion. This leads to a

![Figure 6. An example of forward and reverse modeling of an olivine-plagioclase cotectic fractional crystallization of a basaltic composition, calculated using the olivine and plagioclase models of Ariskin et al. [1993] and plotted on a normative CIPW olivine-plagioclase-diopside projection. The calculations were performed with a calculation step of 0.01 wt %; the total extent of crystallization is 19 wt %; the results were recorded at intervals of 1 wt % total crystallization. (a) Forward modeling of fractional crystallization. Starting composition (large circle) is in the olivine-only field and has a liquidus temperature of 1254°C. After ~4 wt % crystallization of olivine at 1202°C, the melt composition is saturated in plagioclase, and crystallization continues along an olivine-plagioclase cotectic to 1175°C; thick arrow shows the direction of temperature decrease along the cotectic. (b) Reverse modeling of fractional crystallization. The starting composition (large square) is evolved from the forward calculated cotectic to 1202°C but then continues along the cotectic and does not reproduce the original trend in the olivine-only field. The final temperature after the 19 wt % of fractionation is 1209°C. This demonstrates that the algorithm for modeling of reverse fractionation does not have a built-in mechanism to determine when minerals appear on the liquidus during fractionation; thus, these conditions should be set by the user. Open squares show the result of calculations of the reverse of 19 wt % of olivine-plagioclase cotectic crystallization. The trend first follows the forward calculated cotectic to 1202°C but then continues along the cotectic and does not reproduce the original trend in the olivine-only field. The final temperature after the 19 wt % of fractionation is 1209°C. This demonstrates that the algorithm for modeling of reverse fractionation does not have a built-in mechanism to determine when minerals appear on the liquidus during fractionation; thus, these conditions should be set by the user. Open squares show the result of calculations of the reverse of 19 wt % of olivine-plagioclase cotectic crystallization, where plagioclase is excluded at 1202°C, thus allowing the melt composition to enter the olivine-only field, fully reproducing the original fractionation trend for the total of 19 wt % reverse fractionation. Black dots show the result of calculation of the reverse of 19 wt % of fractionation of the same starting composition for the case when pigeonite is also included in calculations. The resultant trend is very different to the original fractionation trend of melt. This is because pigeonite was not on the liquidus of the starting composition (i.e., its PLT is lower than that for olivine and plagioclase), and thus the algorithm is adding pigeonite to the melt until another mineral (plagioclase in this case) has the lowest PLT. The model chosen for pigeonite is that of Ariskin et al. [1993].
rapid increase in Fe content of the melt, a process that can be referred to as “Fe gain.”

Petrolog3 offers an option of reconstructing the initially trapped melt composition by reversing the reequilibration process, provided that the user specifies the FeO* content in the initially trapped melt. In cases when the FeO* content in the trapped melt cannot be independently constrained, calculations can be performed using a number of different FeO* values in order to estimate the effect this parameter has on the derived trapped composition.

Known values of the diffusion coefficient for Fe-Mg interdiffusion in olivine [e.g., Chakraborty, 1997] allow calculation of the time required for reequilibration to occur. If an inclusion is completely reequilibrated, it is possible to calculate the minimum time that the host phenocryst spent at temperatures between trapping and diffusion closure. However, if reequilibration is not complete when the closure temperature is reached and a diffusion profile around an inclusion is preserved, a quantitative time estimate can be made.

Note that this technique does not allow an estimate of the residence time at (or close to) the trapping temperature, since at these conditions there is no crystallization within the inclusion.

Petrolog3 offers an option for forward modeling the reequilibration process under both anhydrous and hydrous conditions. This modeling can be performed either for the case of instant cooling, or for the case of cooling with a specific cooling rate. In the case of instant cooling, the zoned rim on the walls of the inclusion grows first without reequilibration, and then reequilibration occurs at a constant temperature. In the second case, reequilibration and growth of the rim occur simultaneously. During this modeling it is assumed that olivine is the only crystallizing phase. This allows for a faster calculation, but does not introduce any extra uncertainty into the results, as the reequilibration process is controlled entirely by the thermodynamics of olivine-melt equilibrium. The algorithm takes into account the difference in the thermal expansion coefficients between melt and olivine and the effect of the reequilibration processes on the amount of olivine crystallized on the walls of the inclusion during cooling.

5. Summary

Petrolog3 offers a model-independent algorithm for describing fractional and equilibrium crystallization and reverse fractional crystallization at variable pressure, melt oxidation state and melt H2O contents, and for modeling postentrapment reequilibration of melt inclusions in olivine. The algorithm allows for a potentially unlimited number of mineral-melt equilibrium models for major and trace elements; of models describing melt physical parameters, such as density and viscosity; of models for solubility of fluid components in silicate melts; and of model for melt oxidation state. The current version of the software incorporates 46 mineral-melt models for 8 minerals; 3 models describing distribution of trace elements between minerals and melt; 4 models of melt oxidation state; one model for H2O solubility in silicate melts; and 4 models describing melt density and viscosity.

The software is freely available from the Petrolog3 home page at http://petrolog.web.ru/. The Webpage also provides an opportunity for users’ feedback including suggestions for additional models to be included in the future versions.

Appendix A: List of Models Included in Petrolog3


A2. Olivine-Melt Equilibrium Models Based on Exchange Coefficient Values

The olivine-melt equilibrium models based on exchange coefficient values are from Sobolev and Danyushevsky [1994] and Toplis [2005].

A3. Plagioclase-Melt Equilibrium Models

A4. Clinopyroxene-Melt Equilibrium Models


A5. Orthopyroxene-Melt Equilibrium Models

[56] The orthopyroxene-melt equilibrium models are from Ariskin et al. [1993], Beattie [1993], Bolikhovskaya et al. [1995], and Nielsen and Drake [1979].

A6. Pigeonite-Melt Equilibrium Models

[57] The pigeonite-melt equilibrium models are from Ariskin et al. [1986, 1993], Bolikhovskaya et al. [1995], and Nielsen [1988].

A7. Spinel-Melt Equilibrium Models

[58] The spinel-melt equilibrium models are from Ariskin and Nikolaev [1996] and Nielsen [1985].

A8. Ilmenite-Melt Equilibrium Models

[59] The ilmenite-melt equilibrium models are from Ariskin and Barmina [1999] and Nielsen [1985].

A9. Magnetite-Melt Equilibrium Model

[60] The magnetite-melt equilibrium model is from Ariskin and Barmina [1999].

A10. Models for Trace Elements

[61] The models for trace elements are from Beattie et al. [1991], Kinzler et al. [1990], and Blundy and Wood [1991].

A11. Models of Melt Oxidation State

[62] The models of melt oxidation state are from Borisov and Shapkin [1990], Kilinc et al. [1983], Kress and Carmichael [1988], and Sack et al. [1980].

A12. Models of Melt Density and Viscosity

[63] The models of melt density and viscosity are from Bottinga and Weill [1972], Giordano and Dingwell [2003], Lange and Carmichael [1987], and Nelson and Carmichael [1979].

Appendix B: Petrolog3 Manual

B1. Overview of Petrolog3

[64] Petrolog3 is software for modeling fractional and equilibrium crystallization and reverse of fractional crystallization at variable pressure, melt oxidation state and melt H2O contents, and for modeling postentrapment reequilibration of melt inclusions in olivine.

[65] Modeling of crystallization in Petrolog3 is based on the concept of pseudoliquidus temperatures [Nathan and Van Kirk, 1978; Nielsen and Dungan, 1983; Ariskin et al., 1986]. The method relies on the ability of the mineral-melt equilibria models to calculate liquidus temperature not only for the range of melt compositions where the minerals are stable, but also in the metastable regions of melt compositions for each phase (i.e., pseudoliquidus temperatures).

[66] The essence of the technique is to compare calculated pseudoliquidus temperatures for a number of minerals that may crystallize from a given melt composition. The mineral with the highest calculated temperature is the mineral on the liquidus of the melt, and this mineral is subtracted from melt, after which the process is repeated. Calculated temperatures for nonliquidus minerals are pseudoliquidus temperatures, as these minerals are not actually on the liquidus of the melt.

[67] Petrolog3 offers a model-independent algorithm, which can incorporate a potentially unlimited number of mineral-melt equilibria models for major and trace elements; and of models describing melt physical parameters, such as density and viscosity, solubility of fluid components in silicate melts, melt oxidation state.

[68] Note that mineral-melt equilibrium models that can be included in Petrolog3 must calculate, for a given melt composition at a given pressure and oxidation state, both the temperature at which the mineral appears on the liquidus of this melt, and the composition of the mineral.

[69] Petrolog3 runs under Windows operating system (XP or higher). Screen resolution should be set to higher than 800 × 600 pixels.

[70] Note that Petrolog3 requires that the DPI setting of Windows operating system is set to
“Normal size” at Display Properties/Settings/Advanced/General. To check/change this setting, go to the Control Panel, choose Display properties option, then choose the Settings tab, and press the Advanced button at the right-hand corner of the tab. Changing this setting requires rebooting the operating system.

Petrolog3 can be used to perform four general types of calculations: Modeling of Crystallization, Modeling of Reverse of Crystallization, Estimating Melt Liquidus Association, and Modeling of Melt Inclusions in Olivine.

Each calculation type can be selected by choosing the appropriate tab from the main window of the software, which opens when the program is loaded. Four tabs corresponding to the four calculation types are called “Crystallisation,” “Reverse Crystallisation,” “Melt Liquidus Association” and “Olivine MI.”

The “Modeling of Crystallization” tab is shown on Figure B1.

Each tab window has three main parts: the top part (gray background) is used to set calculation parameters (Parameters Section); the middle part (white background) is for the output of calculation results (Output Section); and the bottom part (gray background) is for the output of noncritical debugging messages and warnings (Debug Section).

The Parameters Section has a number of boxes with white background (e.g., “Calculation step” or “Initial pressure”), in which parameter values can be typed in, and a number of settings in blue, which can be changed by clicking on them and choosing a different setting in a pop-up window.

When parameters are set, calculations are started by pressing the “Start Calculations” button at the right-hand corner of the Parameters Section. The Output Section will list the set of parameters chosen for calculation and calculation results. Text in the Output Section can be highlighted and copied into the Windows clipboard by pressing Ctrl+C, and then pasted into a text editor.
When calculations start, the “Start Calculations” button changes to the “Interrupt Calculations” button, which can be used to abort the current run.

The program is loaded with a default set of parameters and a default starting composition (PetrologDefault), and thus pressing “Start Calculations” button straight after the program is loaded would result in a default calculation.

B2. Modeling of Crystallization

To model crystallization, chose “Crystallisation” tab of the Main Window (Figure B1).

B2.1. Starting Composition

The starting composition is set in the “Starting Melt Composition” subsection of the Parameters Section.

Petrolog3 allows the starting composition to be entered manually or loaded from a file.

B2.1.1. Manual Entry of the Starting Composition

When the program is loaded, the “Starting melt composition” subsection of the Parameters Section contains the default starting composition PetrologDefault. This composition can be edited directly within this section. The concentrations of major elements are in wt % oxides.

Trace element contents and values for trace element distribution coefficients for each mineral are set and/or edited by clicking on “Set trace elements” label, which opens the “Trace Elements” pop-up window (Figure B2).

The concentrations of trace elements of interest (in ppm) are entered into the first column “Value in ppm.” All elements which concentrations are not zero will be included in calculations. To reset all concentration values to zero press “Set all traces to 0” button.

Petrolog3 provides two options for defining values of distribution coefficients (Kd,min = Ci,min/ Ci,melt, where “Ci” is concentration in units of weight of element “i” in mineral (min; e.g., olivine, plagioclase, etc) and melt).

The first option is to set a constant Kd value, which is then used through the entire course of the calculation. To set a value, click on the cell corresponding to the element in the mineral. A pop-up window appears (Figure B2) where Kd value can be set. All Kd values can be set without closing the pop-up window by clicking consequently on different cells of the Kd table. To close the pop-up window press “Ok” button or click on the concentration column.

The second option allows for using empirical and/or thermodynamically sound models which define Kd values as a function of parameters, such as melt composition, temperature, mineral compo-
sition, and so on. If $K_d$ models are available for the mineral, they will be listed in the pop-up window together with names of elements which the model applies to (Figure B2). Clicking on the list of elements (not the name of the model) will apply the model to all elements in the list. If required, $K_d$ values for individual elements in the list can be later set to constant values without affecting the application of the chosen model to the remaining elements in the list.

$K_d$ models available in the current version of Petrolog3 are Beattie et al. [1991], Kinzler et al. [1990], and Blundy and Wood [1991].

To save the chosen set of $K_d$ values and models, press “Save this set” button. In the dialog window enter a file name and extension, if desired.

Note that Petrolog3 does not assign an extension to files which contain sets of $K_d$ values.

To load a saved set of $K_d$ values, press “Load $K_d$’s from file” button and chose the file name in the dialog window.

Note that to display all files on disk, choose “all files” in the “Save as file type” field. Press “Save” button to load the chosen set.

To finish editing trace element values and $K_d$ values, close the “Trace elements” window by pressing the white-on-red cross at the top right corner.

Note that if concentrations of at least one trace element are set to a nonzero value, a star appears next to the “Set trace elements” label in the “Starting melt composition” subsection.

**B2.1.2. Loading Starting Composition(s) From File**

The starting composition(s) can also be loaded from a file by using the “Open data file” option of the File menu. The data file should contain analyses stored as rows with the first row containing element names. The program can read delimited text files, with “tabs,” blank spaces, and commas used as delimiters.

Note that the order of elements in the file is not prescribed. Petrolog3 identifies elements by analyzing the first row of the data file.

The following abbreviations should be used for major and trace elements (not case sensitive): SiO$_2$, TiO$_2$, Al$_2$O$_3$, Fe$_2$O$_3$, FeO, FeO*, MnO, MgO, CaO, Na$_2$O, K$_2$O, P$_2$O$_5$, Cr$_2$O$_3$, B, Be, Sc, V, Co, Ni, Cu, Zn, Ga, Rb, Sr, Y, Zr, Nb, Cs, Ba, La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Hf, Ta, Re, Os, Pb, Th, U. Concentrations of major elements should be supplied in wt % oxides, for trace elements in ppm.

When a file is loaded, the first analysis in the file is displayed in the “Starting melt composition” subsection. The values in this analysis can be edited in Petrolog3 without affecting the data file on disk. When the “Start calculations” button is pressed, the calculations will start using the composition displayed in the “Starting melt composition” subsection.

Note that the starting composition in the “Starting melt composition” subsection does not change during calculations and can be used in subsequent calculations if required.

Note that when a file is loaded, its name and full path are displayed at the top of the Petrolog3 window.

If the data file contains more than one analysis, it is possible to choose another analysis by clicking on the “Select another analysis” label in the “Starting melt composition” subsection, which becomes active. In the pop-up window that appears, double-click on the analysis required. The concentration values for this analysis appear in the “Starting melt composition” subsection. To close the “Select analysis” window click on the cross at the top right corner.

**B2.1.2.1. Calculating Multiple Analyses From File**

Petrolog3 offers an option of calculating all analyses in the data file using the same set of calculation parameters. When a data file is loaded, the “Use whole file” check box becomes active, if there is more than one analysis in the file. When the “Use whole file” box is checked, Petrolog3 ignores the composition in the “Starting melt composition” subsection, an instead reads consequently analyses from the data file specified.

**B2.2. Setting Calculation Parameters**

The following calculation parameters can be set before starting calculations: (1) the set of minerals involved in calculations; (2) mineral-melt equilibrium model for each mineral; (3) proportion of fractionation for each mineral; (4) pressure; (5) melt oxidation state; (6) calculation step; (7) conditions to stop calculations; and (8) conditions for the output of intermediate results during calculation. These are described in detail below.

Minerals and models are chosen in the “Mineral-melt models” subsection of the Parameters Section (Figure B1).

When “press to Select” is written in the “Model” field next to a mineral name when “Start calculations” button is pressed, this mineral will not be included in calculations. If a model abbreviation is written next to a mineral name (e.g., Ford et al. [1983] next to Olivine on Figure B1), the mineral will be included in calculations.

To choose a model for a mineral, click on the “Model” field for that mineral. A pop-up window with a list of models available for this mineral will appear (Figure B3).

This window is a table with 5 columns. The “Model” column lists model abbreviations.

Column “P” indicates if a model incorporates the effect of pressure on mineral-melt equilibrium, or alternatively is designed for the atmospheric pressure only. If the “P” cell for a model is blue, this indicates that the model incorporates pressure.

Column “W” indicates if a model incorporates the effect of H₂O on mineral-melt equilibrium, or alternatively is designed for anhydrous conditions only. If the “W” cell for a model is blue, this indicates that the model was developed for both anhydrous and hydrous conditions.

Column “TR” indicates if a model incorporates any trace elements. If the “TR” cell for a model is blue, this indicates that the model incorporates some trace elements.

Blue rectangle to the left of the Ford et al. [1983] model (Figure B3) indicates that this model is currently chosen for calculations.

When choosing a model for olivine-melt equilibrium, the “Use Kd for composition” check box at the bottom of the form can be used to set an olivine-melt Fe-Mg exchange Kd value to calculate olivine composition. When the box is checked, a pop-up window appears that is used to set a Kd values (Figure B4).

Four options are available for calculating Kd values:

1. Kd = const. If this option is chosen, a Kd value must be specified that will be used in calculations.

2. Ln(Kd) = A/T(K) + B * P(kbar)/T(K) + C. If this option is chosen, values for coefficients A, B and C must be provided. The default values correspond to Kd = 0.3.

3. When the Sobolev and Danyushevsky [1994] option is chosen, Kd values will be calculated following the method described in the Appendix 1 of Sobolev and Danyushevsky [1994].

4. When the Toplis [2005] option is chosen, Kd values will be calculated using the method of Toplis [2005].

Note that when calculating olivine composition using a Kd value, the olivine-melt equilibrium model chosen in the “Select models for Olivine” window (Figure B3) is used for calculating olivine crystallization temperature, whereas olivine composition is calculated using the specified Kd value.

To close the “Choose Kd Model” window, press the cross at the top right corner.
To deselect the Kd option, uncheck the “Use Kd for composition” box by clicking on it when it is checked.

The current version of Petrolog3 includes the following mineral-melt equilibrium models:


- Orthopyroxene-melt equilibrium models are from Ariskin et al. [1993], Beattie [1993], Bolikhovskaya et al. [1995], and Nielsen and Drake [1979].

- Pigeonite-melt equilibrium models are from Ariskin et al. [1986, 1993], Bolikhovskaya et al. [1995], and Nielsen [1988].

- Spinel-melt equilibrium models are from Ariskin and Nikolaev [1996] and Nielsen [1985].

- Ilmenite-melt equilibrium models are from Ariskin and Barmina [1999] and Nielsen [1985].

Magnetite-melt equilibrium model is from Ariskin and Barmina [1999].

### B2.2.1. Setting a Pressure Correction

Petrolog3 offers an option to introduce a user-defined linear correction for the effect of pressure on crystallization (liquidus) temperature calculated by a model. A separate correction value can be set for each mineral involved in calculations. To set a correction, click on the “P” cell next to the chosen model. This opens a pop-up window where a correction value in degrees/kbar can be set (Figure B5).

Note that a correction can be set to the calculated temperature regardless of whether the chosen model incorporates pressure.

Note that a correction, once chosen, applies to all models, i.e., if the mineral-melt model is changed after the correction is set, the correction will apply automatically to the new model. To remove the correction, open the “Pressure correction” window again and uncheck the “Correct for Pressure” box. If correction is set, small letter “c” appears in the “P” cell next (Figure B6).

Note that setting a user-defined correction for the effect of pressure on the liquidus temperature, does not affect the mineral composition that the chosen model calculates.
B2.2.1.2. Setting an H2O Correction

As only a few models available in Petrolog3 incorporate the effect of melt H2O content on crystallization temperature and/or composition of crystallizing minerals [Pletchov and Gerya, 1998; Danyushevsky, 2001; Putirka, 2005], Petrolog3 allows the user to introduce corrections to the “anhydrous” models for the effect of H2O on crystallization temperatures, to enable calculations under hydrous conditions with models developed for anhydrous conditions only. Similarly to the pressure correction described above, such a correction does not affect the calculated mineral compositions.

To set a correction, click on the “W” cell next to the chosen model. This opens a pop-up window (Figure B7) where a correction can be set in a form \[ dT (\degree C) = A \times (H2O \text{ wt} \%)^B \] [Falloon and Danyushevsky, 2000], which can also be used to introduce a linear correction, when B is set to 1.

Note that a correction can be set to the calculated temperature regardless of whether the chosen model incorporates H2O.

Note that a correction, once chosen, applies to all models, i.e., if the mineral-melt model is changed after the correction is set, it will apply automatically to the new model. To remove the correction, open the “Correction for H2O content” window again and press the “Remove” button. If a correction is set, small letter “c” appears in the “W” cell next (Figure B8).

The “Mineral-melt models” subsection of the Parameters Section (Figure B1) display the models chosen for each mineral and uses columns “P,” “W,” and “Tr” to indicate whether the chosen models incorporate effects of pressure and/or H2O, and/or trace elements, and whether any user-defined correction are set for the effects of pressure and/ or melt H2O contents. Capital “Y” is used to indicate that a model includes a corresponding effect, whereas “c” is used to indicate that a correction is set (Figure B9).

B2.2.1.3. Hydrous Calculations

Petrolog3 uses the model of Moore et al. [1998] to determine the solubility of H2O in the melt at a given T and P. When the amount of H2O in the
melt exceeds the solubility value, excess H$_2$O is assigned to a separate “fluid” phase. Petrolog3 models degassing in a closed system, i.e., it is assumed that “fluid” remains within the “magma.” Petrolog3 also offers an option to perform the entire calculation under H$_2$O-saturated conditions. To use this option, check the “H$_2$O saturated” box within the “Starting melt composition” subsection of the Parameters Section of the main form (Figure B1).

### B2.2.1.4. Calculating an Olivine-Plagioclase ± Clinopyroxene Cotectic

Petrolog3 offers an option of forcing the starting composition on an olivine-plagioclase (±clinopyroxene) cotectic by adjusting melt H$_2$O content, following the method of Danyushevsky [2001]. The essence of the approach is to first calculate the amount of H$_2$O which is required for the starting composition to lie on an olivine-plagioclase cotectic, and then to model crystallization with this H$_2$O content in the starting composition, so that the composition is cotectic from the onset of crystallization (see Danyushevsky [2001] for a detailed description of the approach). The set of minerals is limited to olivine, plagioclase and clinopyroxene, and the set of models is limited to those from Danyushevsky [2001].

To use this option, check the “As Pl-Ol cotectic” box within the “Mineral-melt models” subsection of the Parameters Section (Figure B9).

Note that this option should be used for MORB and BABB compositions only, as the models of Danyushevsky [2001] have not been calibrated outside this compositional range.

### B2.2.2. Setting the Extent of Fractionation for Each Mineral

Petrolog3 allows for a specific extent of fractionation to be set for each mineral using the “% of frac. crystallization” subsection of the Parameters Section (Figure B1). By default, a value of 100% is assigned to each mineral, corresponding to the case of pure fractional crystallization. When modeling pure fractional crystallization, a mineral is “removed” from contact with melt and placed into the “cumulate” part of the system, thus retaining its original composition.

If 0% is assigned to a mineral, this corresponds to pure equilibrium crystallization. When modeling equilibrium crystallization, the total amount of the crystallized mineral remains in equilibrium with the residual melt, thus continuously changing its composition. No “cumulate” is formed during equilibrium crystallization.

When a number between 0 and 100 is entered for a mineral, this proportion of the mineral is continuously “removed” from contact with the melt preserving its composition, whereas the remainders of the mineral reequilibrates with the continuously evolving melt.

### B2.2.3. Setting Calculation Pressure

A value of pressure to be used during calculations is set in the “Initial P” subsection of the Parameters Section (Figure B1). A value at the onset of calculations (in kbar) can be set in the text box within this subsection. To determine how pressure changes during calculations, click on the blue text label next to the text box in this subsection. This will open the “Pressure settings” pop-up window (Figure B10).

By default, the “Keep pressure constant” option is chosen.

The “dP/dT gradient” option allows for pressure to be continuously changed at a fixed rate as a function of decreasing temperature. A positive value corresponds to decreasing pressure during crystallization. If pressure reaches 1 bar before the end of the calculations, it would remain at 1 bar for the remainder of the calculations. Setting a negative
The “Pressure steps” option allows for changing pressure during calculations as a function of the degree of fractionation. Up to four intervals with specific dP/dF values can be set. The dP/dF value for an interval is calculated from the P and F values set as the boundary conditions for this interval. The dP/dF value can equal 0 (pressure is constant) for any number of intervals. To set it to 0, the P,kb value should be the same at the start and end of the interval.

B2.2.4. Setting Calculation Step

A value for the calculation step is set in the “Calculation step” text box in the Parameters Section (Figure B1). The calculation step determines the amount (in wt %) by which the crystal mass increases at each step of the calculations. The smaller the calculation step is, the longer the same calculation would take. The default value is 0.01% of the amount of melt on each step. It is not recommended to increase the calculation step.

Note that the algorithm behind Petrolog3 is designed with an assumption that the output of the intermediate states of the system would occur at frequencies which are at least 2 orders of magnitude larger than the calculation step. For examples, if the calculation step is set to 0.01%, the smallest recommended output frequency is 1%.

B2.2.5. Setting Conditions for Intermediate Output

Petrolog3 offers several options for defining conditions for the output of the intermediate states of the system during calculations. The default setting is 1 wt % of crystallization. To change this setting, click on the blue text label “Intermediate output” in the Parameters Section (Figure B1). The “Conditions for intermediate output” window would pop-up (Figure B11). Several different options can be set simultaneously and the program will display the intermediate states of the system satisfying all of the criteria selected.

B2.2.6. Setting Conditions to Stop Calculations

Petrolog3 offers several options for defining conditions for stopping the calculations. The default setting is 0 wt % of crystallization, indicating that no crystallization calculation is performed. To change this setting, click on the blue text label “Stop at 0% percent of fractionation” in the “Conditions to stop calculations” subsection of the Parameters Section (Figure B1). The “Conditions for stopping calculations” window would pop-up (Figure B12). Any one option can be set at a time. To close the window and save your choice, press the cross at the top right corner of the window.

B2.2.7. Setting Melt Oxidation State

The melt oxidation state (i.e., the proportion of Fe³⁺ and Fe²⁺ in the melt) during calculations is set in the “Initial oxidation state” subsection of the Parameters Section (Figure B1): (1) calculation along an oxygen buffer; (2) calculation with a constant Fe²⁺/Fe³⁺ value; (3) calculation assuming a closed system for oxygen, and (4) defining melt oxidation state as a function of liquidus olivine composition.

The default option is calculating along a QFM buffer of oxygen fugacity. Clicking on blue text label “Buffer: ‘QFM’” opens the “Oxygen fugacity advanced options” pop-up window (Figure B13).

This window allows choosing one of the four options for controlling oxygen fugacity, changing the oxygen buffer used, and setting a model to cal-
Calculate the melt oxidation state as a function of melt composition, temperature and oxygen fugacity.

[158] Click on blue text label “QFM” to open the “Oxygen Buffers” pop-up window (Figure B14).

[159] Petrolog3 offers eight oxygen fugacity buffers. To choose a buffer click on one of the check boxes next to the buffer name. You can also specify a shift from the buffer in log10 units of \( f\text{O}_2 \) by specifying a positive or negative value in the “Buffer shift (log units)”: text box. The following oxygen buffers are available in Petrolog3:

- Ni–NiO \( \ln(f\text{O}_2) = -57.403.5/T(K) + 21.55; \)
- QFM \( \ln(f\text{O}_2) = -56.280/T(K) + 19.09; \)
- WM \( \ln(f\text{O}_2) = -85.083/T(K) + 37.04; \)
- FeW \( \ln(f\text{O}_2) = -61.790/T(K) + 14.9; \)
- MH \( \ln(f\text{O}_2) = -54.912/T(K) + 31.03; \)
- Co-CoO \( \ln(f\text{O}_2) = -57.726/T(K) + 18.27; \)
- \( \text{Fe}^{3+} = 0; \)
- QFFe \( \ln(f\text{O}_2) = -63.362.5/T(K) + 14.73; \)

Close this window by pressing the “Ok” button.

[160] You need also to choose a model that defines melt oxidation state as a function of melt composition, temperature and oxygen fugacity. The default model is from Borisov and Shapkin [1990]. Click on the blue text label “Borisov and Shapkin, 1990” on the “Oxygen fugacity advanced options” pop-up window (Figure B13), to open the “Melt oxidation state model” pop-up window (Figure B15).

[161] Choose a model by clicking on a check box next to the preferred model. The following four models are available in Petrolog3: Sack et al. [1980], Kilinc et al. [1983], Kress and Carmichael [1988], and Borisov and Shapkin [1990].

[162] Alternatively, the “Melt oxidation state model” pop-up window (Figure B15) can be opened directly from “Initial oxidation state” subsection of the Parameters Section (Figure B1).

[163] When using an oxygen buffer to define melt oxidation state, the \( \text{Fe}^{2+}/\text{Fe}^{3+} \) value in the melt will be calculated from the oxygen fugacity value corresponding to the chosen buffer, following the chosen model for the oxidation state.

[164] When using a constant \( \text{Fe}^{2+}/\text{Fe}^{3+} \) value to set melt oxidation state, oxygen fugacity is calculated...
from the Fe$^{2+}$/Fe$^{3+}$ value of the melt following the chosen model for the oxidation state (Figure B15).

When calculating assuming a closed system for oxygen, the Fe$_2$O$_3$ and FeO in the starting composition are treated as “independent” elements. Oxygen fugacity is calculated from the Fe$^{2+}$/Fe$^{3+}$ value of the melt following the chosen model for the oxidation state (Figure B15).

If the melt oxidation state is defined as a function of liquidus olivine composition (Figure B13), you should specify values for coefficients A and B for the equation (Fe$^{2+}$/Fe$^{3+}$)$_{\text{melt}} = A \cdot \text{Fo} + B$, where Fo is the proportion of forsterite in the liquidus olivine in mol%. For a detailed description of this technique, see Danyushevsky and Sobolev [1996].

Note that this option is only available when olivine has been chosen for calculations in the “Mineral-melt models” window.

When using this option to define melt oxidation state, oxygen fugacity will be calculated from the Fe$^{2+}$/Fe$^{3+}$ value of the melt following the chosen model for the oxidation state (Figure B15).

**B2.2.8. Choosing Models to Calculate Melt Physical Properties**

Petrolog3 calculates melt density and viscosity during fractionation. To choose from the available models, click on the blue text labels within the “Physical properties” subsection of the Parameters Section (Figure B1). Clicking on the blue text next to “Density” opens the “Density models” pop-up window (Figure B16). Chose the desired model by pressing on one of the radio buttons next to model names. Petrolog3 offers two models for calculating melt density: Lange and Carmichael [1987] and Nelson and Carmichael [1979]. Close the window by pressing the “Ok” button.

Clicking on the blue text next to “Viscosity” opens the “Models for Viscosity” pop-up window (Figure B17). Choose the desired model by pressing on one of the radio buttons next to model names. Petrolog3 offers two models for calculating melt viscosity: Bottinga and Weill [1972] and Giordano and Dingwell [2003]. Close the window by pressing the “Ok” button.

**B2.3. Output of Results**

Petrolog3 offers three options for saving calculation results for future use.

1. During calculations, Petrolog3 prints the output into the Output Section of the Main Form (Figure B1). This output can be highlighted with the window copied (Ctrl+C) in to the clipboard to be used in a text editor.

2. Petrolog3 can save the output into a number of comma-separated values files (.csv) with a user specified name. To specify the file name, go to the File option of the Main Menu on the main form (Figure B1) and use the “File for output...” option. A general form of the file names generated by Petrolog3 then is “UserSpecifiedName_*.csv.” The user-specified file name and its full path are displayed on the main form (Figure B1) right above the Output Section of the Main form.

These files can either be opened manually after the calculation is finished, or can be exported into Excel by using the “Export to MS Excel” option of the Main menu on the main form (Figure B1), and choosing the “Results of previous calculations” options. A dialog window pops up where the user should select file “UserSpecifiedName_FRAC.csv.” This will create an Excel workbook with...
several worksheets containing all the details of the calculation.

Note that “FRAC” in the Petrolog3 output file names denotes files produced during calculations using the Crystallization Option of the Main Menu (Figure B1).

Note that Petrolog3 generates a new instance of Excel every time it exports calculation results.

Note that if the user-specified file name is not changed before the next calculation, the results of the previous calculation saved in the .csv files would be overwritten.

3. If a user specified name is not provided, Petrolog3 saves the result into a number of comma-separated values files (.csv) which names always start with “Petrolog_output_” A general form of the files name is “Petrolog_output_FRAC*.csv.” These files can either be opened manually after the calculation is finished, or can be exported into Excel by using the “Export to MS Excel” option of the main menu on the main form and choosing the “Results of the last calculation” option. Since every calculation produces files with the same name, they are overridden at the beginning of calculation.

B3. Melt Liquidus Association

To determine melt liquidus association, choose “Melt liquidus association” tab of the Main Window (Figure B18).

Note that it is recommended that you read section B2 of this manual before reading this section.

In this option, Petrolog3 does not model a crystallization path but calculates pseudoliquidus temperatures and liquidus mineral compositions for a chosen set of minerals and mineral-melt equilibrium points. The following mineral compositional parameters are also calculated: olivine, mol % forsterite (Fo); plagioclase, mol % anorthite (An); clinopyroxene, orthopyroxene, pigeonite, ilmenite, and magnetite, Mg# (100 * Mg/(Mg + Fe)); and spinel: Cr# (100 * Cr/(Cr + Al)).
[182] By comparing calculated temperatures for different minerals, the liquidus association of a melt composition can be established. As the stated errors for most models are \(\sim15^\circ\text{C} – 20^\circ\text{C}\), the liquidus association should include the mineral with the highest calculated temperature and also minerals which pseudoliquids temperatures are within \(\sim20^\circ\text{C}\) of the calculated liquidus temperature.

[183] Note that during melt liquidus association calculations it is possible to choose any number of models for each mineral. This allows a comparison to be made between different models.

[184] If models of Danyushevsky [2001] for olivine and plagioclase are chosen, Petrolog3 will automatically estimate the \(\text{H}_2\text{O}\) content in the melt which is required for this composition to lie on an olivine + plagioclase cotectic.

[185] If models of Danyushevsky [2001] for olivine and clinopyroxene are chosen, Petrolog3 will automatically estimate crystallization pressure at which the melt composition is saturated with both olivine and clinopyroxene.

[186] Note that models of Danyushevsky [2001] are calibrated for MORB and BABB compositions only.

[187] Since crystallization calculations are not performed under this Option, the number of calculation parameters is that can be set is limited.

[188] Handling of both the starting compositions and calculation output is the same as for the Crystallization option (see section B2.1 and B2.3 of this manual).

[189] Note that “MLA” in the Petrolog3 output file names denotes files produced during calculations using the Melt Liquidus Association Option of the Main Menu (Figure B18).

[190] Corrections to the calculated liquidus temperatures for the effects of pressure and melt \(\text{H}_2\text{O}\) contents can be set in the same way as during the crystallization calculations (see sections B2.2.1.1 and B2.2.1.2 of this manual).

[191] The melt oxidation state (i.e., the proportion of \(\text{Fe}^{3+}\) and \(\text{Fe}^{2+}\) in the melt) during calculations can be set in the “Initial oxidation state” subsection of the Parameters Section (Figure B18) in the exactly the same way as during Crystallization calculations (see section B2.2.7 of this manual).

[192] A value of pressure to be used during calculations is set in the “Pressure (in Kbar)” subsection of the Parameters Section (Figure B18).

B4. Reverse of Fractional Crystallization

[193] To model reverse of fractional crystallization, choose “Reverse Crystallisation” tab of the Main Window (Figure B19).

[194] Note that it is recommended that you read sections B2 and B3 of this manual before reading this section.

[195] The principle behind calculating the reverse of fractional crystallization is adding minerals that crystallized from the melt back to the melt composition thus moving it up along a cotectic (a liquid line of descent) toward more primitive compositions. Unlike crystallization calculations, where the mineral with the highest pseudoliquids temperature is subtracted from the melt composition, the mineral with the lowest pseudoliquids temperature is added to the melt composition during the reverse of fractionation calculations. The technique is least ambiguous when used with compositions that lie within a single phase saturation field.

[196] Note that fractional crystallization only can be reversed, as equilibrium crystallization does not preserve sufficient information on the crystallization history to enable reverse calculations.

[197] Unlike crystallization calculations, when crystallization of any number of minerals can be modeled for any starting composition, with the program determining which minerals actually crystallize from the melt, the minerals that are included in the reverse of fractionation calculations must be on the liquidus of the starting composition at the calculation parameters chosen. Which minerals are present on the liquidus of a starting composition can be checked using the “Melt liquidus association” option (see section B3 of this manual).

[198] Also unlike crystallization calculations, the algorithm for modeling the reverse of fractionation does not have a built-in mechanism for determining when minerals appeared on the liquidus during fractionation, and thus these conditions should be set by the user. Consider an example with a melt composition having the following crystallization sequence: first olivine, then plagioclase after 5% crystallization (crystallization along an olivine + plagioclase cotectic), and then clinopyroxene after 15% crystallization (crystallization along an olivine + plagioclase + clinopyroxene cotectic), with a total extent of crystallization of 25%. Reversing this crystallization sequence using the evolved melt composition formed after 25% of crystallization
would start with reversing crystallization along the olivine + plagioclase + clinopyroxene cotectic. However, the algorithm cannot determine when clinopyroxene (or plagioclase) appeared on the liquidus during fractionation, and the timing of these events should be set by the user. Thus the exact form of the calculated trend of melt evolution is dependent on the conditions at which minerals are excluded from calculations to force the trend off a cotectic.

The parameters at which the melt moves of a given cotectic (i.e., parameters for mineral exclusion) are set in the “Parameters for Exclusion” subsection of the Parameters Section of the main window (Figure B19). Click on the blue text label (“press to set”) next to the desired mineral to open the “Conditions for exclusion” pop-up window for this mineral (Figure B20).

Petrolog3 offers four different options for setting the timing of mineral exclusion: (1) temperature; (2) melt MgO content; (3) composition of liquidus olivine; and (4) the composition of the mineral to be excluded. Several options can be set simultaneously and the mineral will be excluded when any of the set conditions are met.

All other parameters for the reverse of fractional crystallization calculations are set in exactly the same way as for forward crystallization.
the same way as for the crystallization calculation (see section B2 of this manual).

Handling of both the starting compositions and calculation output is the same as for the Crystallization option (see sections 2.1 and 2.3 of this manual).

Note that “REV” in the Petrolog3 output file names denotes files produced during calculations using the Reverse of Fractional Crystallization Option of the Main Menu (Figure B19).

B5. Modeling Postentrapment Reequilibration of Melt Inclusions in Olivine

To model postentrapment reequilibration of melt inclusions in olivine, chose “Olivine MI” tab of the Main Window (Figure B21).

Note that it is recommended that you read sections B2, B3 and B4 of this manual before reading this section.

B5.1. Reconstructing the Initial Trapped Composition of the MI

Reequilibration of Fe and Mg between melt inclusions and their host olivine phenocrysts is described in detail by Danyushevsky et al. [2000a, 2002], with the main points summarized briefly below. The underlying assumption in these considerations is that the composition of the host olivine does not change after trapping of the melt inclusion.

Cooling of an inclusion after trapping results in crystallization of olivine from the trapped melt, forming an olivine rim on the walls of the inclusion. The crystallizing olivine rim is progressively enriched in Fe and depleted in Mg, i.e., decreases in forsterite component, resulting in a compositional gradient within the rim. The existence of this compositional gradient causes reequilibration of the inclusion with its host. This reequilibration is achieved by diffusion of Fe out of, and Mg into the initial volume of the inclusion. This leads to a rapid decrease in Fe content of the residual melt inside
the inclusion, a process referred to as “Fe loss” by Danyushevsky et al. [2000a].

Conversely, if an olivine grain containing a melt inclusion is heated over the temperature of inclusion entrapment, host olivine around the inclusion would melt, increasing the Mg# of the melt inside the inclusion and resulting in disequilibrium between the melt and host olivine. This leads to reequilibration of the melt with the host, which is achieved by diffusion of Fe into, and Mg out of the melt inside the inclusion. This leads to a rapid increase in Fe content of the melt, a process that can be referred to as “Fe gain.”

Petrolog3 offers an option of reconstructing the initially trapped melt composition, providing that the user specifies the FeO* content of the trapped melt. The algorithm simulates the following experimental procedure:

1. An olivine grain containing an inclusion is kept at a given temperature until the inclusion is in complete equilibrium with the host. Within the algorithm, this temperature corresponds to the olivine liquidus temperature of the melt inclusion composition provided (starting melt composition). The algorithm simulates exchange of Fe and Mg between melt and olivine, which occurs during the reequilibration process. Reequilibration maybe accompanied by either melting or crystallization of the host olivine at the inclusion wall.

2. Once equilibrium is reached, the algorithm compares the FeO* content of the melt with the user-specified FeO* content of the trapped melt.

3. If the user-specified FeO* content is higher than the FeO* content of the melt, the algorithm simulates increasing experimental temperature while keeping the melt inclusion and its host in equilibrium. If the user-specified FeO* content is lower than the FeO* content of the melt, the algorithm simulates decreasing experimental temperature while keeping the melt inclusion and its host in equilibrium. In both cases this continues until the FeO* content within the melt inclusion equals the user-specified value. The algorithm simulates melting or crystallization of olivine and the exchange of Fe and Mg between melt and olivine, which occurs during this process.

To use this option, click on the “Reconstruct MI composition” radio button in the Parameters Section of the main menu (Figure B21).

The user must provide the measured composition of the melt inclusion, the composition of the host olivine (Fo, mol %), and the FeO* content of the trapped melt. These parameters are set within the “Reconstructing MI composition to a given FeO* value” part of the Parameters Section of the main window (Figure B21).

Note that data files in this option are handled in the same way as described in section B2.1 of this manual. The host olivine composition and the FeO* content of the trapped melt must be present in the data file for each analysis, if the “calculate whole file” option is used. The column names for these two parameters should read “Fo_h” and “FeO_final”, respectively (not case sensitive).

User-specified calculation parameters for this option include: olivine-melt equilibrium model; melt oxidation state, model for calculating melt density, and a model for calculating minor element contents (Ca, Mn, Cr) in olivine. The first three parameters are set in the exactly the same way as described in section B2 of this manual.

The last parameter allows the user to introduce minor elements into the calculated olivine composition. The contents of these elements are calculated as a function of olivine Fo content, and are set to typical values for either komatiites, or high-Ca boninites, or MORB/BABB. If the contents of these elements in olivine are set to 0 (None), they are modeled as perfectly incompatible elements.

Note that all calculations within this option are performed at a pressure of 1 atm.

During calculations, Petrolog3 records intermediate output in the Output Section of the main window. This output is provided mainly to keep the user informed on the progress of the calculations. Petrolog3 writes the results of calculations into a .csv file.

For each inclusion, Petrolog3 writes 3 lines into the output file. The first line, marked by value “1” in the “No.” column, corresponds to the starting composition. The second line, marked by value “2” in the “No.” column, corresponds to the moment when inclusion reaches equilibrium with the host (and of step 1 above). The third line, marked by value “3” in the “No.” column, corresponds to the final result of the calculation, when inclusion is in equilibrium with the host and the FeO* in the melt matches the user-defined value.

Note that the output files in this option are handled in the same way as described in section B2.3 of this manual. “IRL” in the Petrolog3 output file
names denotes files produced during calculations using this option.

B5.2. Modeling Diffusive Reequilibration During “Fe Loss”

[222] Known values of the diffusion coefficient for Fe-Mg interdiffusion \( (D_{Fe-Mg}) \) in olivine [e.g., Chakraborty, 1997] allow calculation of the time required for reequilibration to occur. If an inclusion is completely reequilibrated, it is possible to calculate the minimum time that the host phenocryst spent at temperatures between trapping and diffusion closure. However, if reequilibration is not complete when the closure temperature is reached, and thus a diffusion profile around the inclusion is preserved, a quantitative time estimate can be made.

[223] Note that this technique does not allow an estimate of the residence time at (or close to) the trapping temperature, since at these conditions there is no (or very little) crystallization within the inclusion.

[224] Petrolog3 offers an option for forward modeling of the reequilibration process during cooling after entrainment (i.e., for the case of “Fe loss”). To choose this option, press the “Model diffusion” radio button in the Parameters Section of the main window (Figure B21).

[225] The user must provide the trapped inclusion composition, the inclusion radius (microns) and the length of the cooling interval (in °C). These parameters are set within the “Diffusion profile modeling” section of the Parameters Section of the main window (Figure B21).

[226] Note that in this option, the starting composition cannot be imported from a data file.

[227] User-specified calculation parameters for this option include: olivine-melt equilibrium model; melt oxidation state, model for calculating melt density, and a model for calculating minor element contents (Ca, Mn, Cr) in olivine. The first three parameters are set in the exactly the same way as described in section B2.3 of this manual.

[228] The last parameter allows the user to introduce minor elements into the calculated olivine composition. The contents of these elements are calculated as a function of olivine Fo content, and are set to typical values for either komatiites, or high-Ca boninites, or MORB/BABB. If the contents of these elements in olivine are set to 0, they are modeled as perfectly incompatible elements.

[229] Note that all calculations within this option are performed at a pressure of 1 atm.

[230] Diffusion modeling can be performed either for the case of instant cooling, or for the case of cooling with a specific cooling rate.

[231] In the case of instant cooling, the zoned rim on the walls of the inclusion grows first and then reequilibration occurs while the grain resides at the lower end of the cooling interval. To use this option, click on the “Instant cooling” radio button in the “Select type of calculations” part within the Parameters Section of the main window (Figure B21). For this option, the user needs to specify the extent of reequilibration, a parameter that will be used to determine when diffusion calculations are completed. This parameter is set in the text box next to the “Instant cooling” radio button. The degree of reequilibration, i.e., the extent of “Fe loss,” can be defined as the amount of FeO* “lost” by the residual melt relative to the amount that is “lost” in the case of complete reequilibration.

[232] The output file generated within this option contains the melt compositions and diffusion profiles generated at different stages of calculations. The diffusion profiles are expressed as values of FeO* concentration in olivine over distance from the center of the melt inclusion. The melt compositions recorded correspond to (1) the starting composition, (2) the composition of the melt after instant cooling (0% reequilibration), (3) the composition of the melt in the case of complete reequilibration (100%), and (4) the composition of the melt at the required extent of reequilibration. The FeO* profiles recorded correspond to the initial rim profile after the instant cooling, and to the resultant FeO* profile after the calculations are completed.

[233] Note that the output files in this option are handled in the same way as described in section B2.3 of this manual. “PIC” in the Petrolog3 output file names denotes files produced during calculations using this option.

[234] In the case of cooling with a specific cooling rate, reequilibration and cooling occur simultaneously. To use this option, click on the “Cooling Rate” radio button in the “Select type of calculations” part within the Parameters Section of the main window (Figure B21). For this option, the user needs to specify the cooling rate, and the calculations will simulate cooling with the specified rate from the start to the end of the cooling interval. This
parameter is set in the text box next to the “Cooling Rate” radio button.

[235] Modeling of diffusion under this option is performed in 10°C steps, with each step modeled as a separate instant cooling calculation. The program generates two output files. One file contains a record of diffusion profiles at the end of each 10° step, and the second file contains melt compositions at the end of each step.

[236] Note that the output files in this option are handled in the same way as described in section B2.3 of this manual. “PCR” in the Petrolog3 output file names denotes files produced during calculations using this option. “PR” at the end of the file name denotes files containing calculated FeO profiles. “COMP” at the end of the file name denotes files containing calculated melt compositions.

[237] To enable modeling of complex cooling histories, Petrolog3 allows for using the result of the last calculation as the starting point for the next calculation. For this purpose, after each diffusion modeling calculation Petrolog3 saves both the final profile and the final melt composition into a file called “LAST_RES.DAT.” In order to use the results of the last calculation as the starting point for the following calculation, check the “Load last result” checkbox in the “Diffusion profiles modeling” part of the Parameters Section of the main window (Figure B21).

[238] Note that loading the results of the last calculation automatically sets the size for the inclusion radius, which should be changed.

[239] Note that it is recommended that the user does not delete file “LAST_RES.DAT” from the directory which contains the Petrolog3 executable (i.e., “Petrolog.exe” file).

[240] Calculation under both options can simulate a reheating experiment with the melt inclusions, an optional calculation performed at the end of diffusion modeling. To include this calculation, check the “Simulate reheating experiment” checkbox within the “Diffusion profiles modeling” part of the Parameters Section of the main window (Figure B21). The user is then also required to provide a temperature value for the reheating experiment. The temperature is set in the “T exp (°C)” text box next to the “Simulate reheating experiment” checkbox.

[241] Using this option allows Petrolog3 to reproduce the following scenario: 1) inclusion is trapped; 2) after entrapment, inclusion is cooled within the plumbing system prior to eruption; 3) the grain with the inclusion is experimentally reheated to a certain temperature and quenched. The results of diffusion modeling can then be directly compared with the analyzed composition of the experimentally quenched inclusion.

[242] To facilitate combining calculations of the initial trapped inclusion compositions with diffusion modeling, Petrolog3 populates the Starting melt composition for the “Diffusion profile modeling” option with the result of the calculation performed with the “Reconstructing MI composition to a given FeO* value” option. Temperature value for experimental reheating is also set to correspond to the olivine liquidus temperature of the starting composition for the “Reconstructing MI composition to a given FeO* value.”

[243] Note that it is recommended that the user contact the authors if an advanced use of the diffusion modeling is intended.

[244] Note that if the results of a diffusion modeling calculation are intended to be used in the following calculation, simulation of the reheating experiment should not be performed.

Acknowledgments

[245] This research was supported by the Australian Research Council through the operational grant to CODES, a Centre of Excellence in Ore Deposits at the University of Tasmania. The authors are grateful to Alexey Ariskin for stimulating discussions of modeling algorithms and Kyrill Bychkov for assistance with programming of the Petrolog3 interface. L.V.D. offers special thanks to Alex Sobolev for introducing him to computer modeling of crystallization processes while L.V.D. was a postgraduate student at the Vernadsky Institute in 1980s. The original manuscript has benefited significantly from constructive reviews by Peter Luffi, Nicolas Arndt, and two anonymous reviewers and editorial handling by Joel Baker and Kazuhito Ozawa.

References


Danyushevsky, L. V., F. N. Della‐Danya (2001), The effect of small amounts of
Danyushevsky, L. V., S. Sokolov, and T. J. Falloon (2002),
Ariskin, A. A., G. S. Barmina, and M. Y. Frenkel (1986),
Chakraborty, S. (1997), Rates and mechanisms of Fe
Mg‐
Ariskin, A. A., M. Y. Frenkel, G. S. Barmina, and R. Nielsen
Ariskin, A. A., G. S. Barmina, S. S. Meshalkin, G. S. Nikolaev,
Bolikhovskaya, S.V., M.O. Vasil
Beattie, P., C. Ford, and D. Russell (1991), Partition

Beattie, P., C. Ford, and D. Russell (1991), Partition

Blundy, J. D., and B. J. Wood (1991), Crystal-chemical
controls on the partitioning of Sr and Ba between plagioclase
feldspar, silicate melts, and hydrothermal solutions, Geochim.

Bolikhovskaya, S.V., M.O. Vasil’eva, E.V. Koptev-Dvornikov
(1995), Modelling of low-Ca pyroxene crystallisation in basic
systems (New versions of geothermometers), Geokhimia, 12,
1710–1727.

Borisov, A. A., and A. I. Shapkin (1990), A new empirical
equation rating Fe3+/Fe2+ in magmas to their composition,

Bottinga, Y., and D. F. Weill (1972), The viscosity of
magnetic silicate liquids: A model for calculation, Am. J. Sci.,

Chakraborty, S. (1997), Rates and mechanisms of Fe-Mg
interdiffusion in olivine at 980°–1300°, J. Geophys. Res.,

Danyushevsky, L. V. (2001), The effect of small amounts of
H2O on crystallisation of mid-ocean ridge and backarc basin
magmas, J. Volcanol. Geotherm. Res., 110, 265–280,
doi:10.1016/S0377-0273(01)00213-X.

Danyushevsky, L. V., and A. V. Sobolev (1996), Ferric-
ferrous ratio and oxygen fugacity calculations for primitive
mantle-derived melts: Calibration of an empirical technique,

Danyushevsky, L. V., F. N. Della-Pasqua, and S. Sokolov
(2000a), Re-equilibration of melt inclusions trapped by mag-

Danyushevsky, L. V., S. M. Egins, T. J. Falloon, and
D. Christie (2000b), H2O abundance in depleted to moder-
amely enriched mid-ocean ridge magmas, Part I: Incompatible
behaviour, implications for mantle storage, and origin of regional variations, J. Petrol., 41, 1329–1364, doi:10.1093/
petrology/41.8.1329.

Danyushevsky, L. V., S. Sokolov, and T. J. Falloon (2002),
Melt inclusions in olivine phenocrysts: Using diffusive
re-equilibration to determine the cooling history of a crystal,
with implications for the origin of olivine-phryic volcanic

Danyushevsky, L. V., R. A. J. Leslie, A. J. Crawford, and
P. Durance (2004), Melt inclusions in primitive olivine
phenocrysts: The role of localised reaction processes in
the origin of anomalous compositions, J. Petrol., 45,

(76)90011-9.

Falloon, T. J., and L. V. Danyushevsky (2000), Melting of
refractory mantle at 1.5, 2.0 and 2.5 GPa under H2O-
undersaturated conditions: Implications for the petrogenesis
of high-Ca boninites and the influence of subduction compo-
petrology/41.2.257.

Ford, C. E., D. G. Russell, J. A. Groven, and M. R. Fisk
(1983), Distribution coefficients of Mg2+, Fe2+, Ca2+ and
Mn2+ between olivine and melt, J. Petrol., 24, 256–265.

Frenkel, M. Y., and A. A. Ariskin (1984), A computer
algorithm for equilibration in a crystallizing basalt magma,

major-element evolution of olivine-hosted melt inclusions,
00370-9.

Ghiorso, M. S., J. S. E. Carmichael, and M. L. Rivers (1983),
The Gibbs free energy of mixing of natural silicate liquids,

Ghiorso, M. S., M. M. Hirschmann, P. W. Reiners, and
V. C. Kress (2002), The PMELT: A revision of MELTS for
improved calculation of phase relations and major element
partitioning related to partial melting of the mantle to

Giordano, D., and D. B. Dingwell (2003), Non-Arrhenian
multicomponent melt viscosity: A model, Earth Planet. Sci.

Herzberg, C., and M. J. O’Hara (2002), Plume-associated
ultramafic magmas of phanerozoic age, J. Petrol., 43,

Hirschmann, M. M., M. S. Ghiorso, F. A. Davis, S. M. Gordon,
S. Mukherjee, T. L. Grove, M. Krawczynski, E. Médard, and
C. B. Till (2008), Library of Experimental Phase Relations
(LEPR): A database and Web portal for experimental mag-
matic phase equilibria data, Geochim. Cosmochim. Geosyst., 9,

Kilinc, A., I. S. E. Carmichael, M. L. Rivers, and R. O. Sack
(1983), The ferric-ferrous ratio of natural silicate liquids
equilibrated in air, Contrib. Mineral. Petrol., 83, 136–140,
doi:10.1007/BF00373086.

Kinzler, R. J., T. L. Grove, and S. I. Recca (1990), An
experimental study on the effect of temperature and melt composi-
tion on the partitioning of nickel between olivine and silicate melt, Geochim. Cosmochim. Acta, 54, 1265–1265,
doi:10.1016/0016-7037(90)90151-A.

Kress, V. C., and I. S. E. Carmichael (1988), Stoichiometry of
the iron oxidation reaction in silicate melts, Am. Mineral.
73, 1267–1274.

Lange, R. A., and I. S. E. Carmichael (1987), Densities of
Na2O-K2O-CaO-MgO-FeO-Fe2O3-Al2O3-TiO2-SiO2
liquids: New measurements and derived partial molar prop-

systematics of mid-ocean ridge basalts: Constraints on melt
generation beneath ocean ridges, in Mantle Flow and Melt
Generation at Mid-ocean Ridges, Geophys. Monogr. Ser.,


