Adiabat_1ph: A new public front-end to the MELTS, pMELTS, and pHMELTS models

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[1] The program adiabat_1ph is a simple text-menu driver for subroutine versions of the algorithms MELTS, pMELTS, and pHMELTS [*Asimow et al.*, 2004; *Ghiorso et al.*, 2002; *Ghiorso and Sack*, 1995]. It may be used to calculate equilibrium assemblages along a thermodynamic path set by the user and can simultaneously calculate trace element distributions. The MELTS family of algorithms is suitable for multicomponent systems, which may be anhydrous, water-undersaturated, or water-saturated, with the options of buffering oxygen fugacity and/or water activity. A wide variety of calculations can be performed either subsolidus or with liquid(s) present; melting and crystallization may be batch, fractional, or continuous. The software is suitable for Linux, MacOS X, and Windows, and many aspects of program execution are controlled by environment variables. Perl scripts are also provided that may be used to invoke adiabat_1ph with some command line options and to produce output that may be easily imported into spreadsheet programs, such as Microsoft Excel. Benefits include a batch mode, which allows almost complete automation of the calculation process when suitable input files are written. This technical brief describes version 1.04, which is provided as ancillary material. Binaries, scripts, documentation, and example files for this and future releases may be downloaded at http://www.gps.caltech.edu/~asimow/ adiabat. On a networked computer, adiabat_1ph automatically checks whether a newer version is available.

1. Introduction

[2] Since its release in 1995, MELTS has probably become the most widely used software for thermodynamic calculations in igneous systems [*Ghiorso and Sack*, 1995]. Many other numerical models are publicly available, of course, but generally these are more empirical and involve assumptions that limit their potential for extrapolation, particularly to low melt fractions (e.g., *McKenzie and Bickle* [1988]; *Langmuir et al.* [1992]; *Kinzler and Grove*

[1992]; this list is not intended to be exhaustive). Furthermore, the polybaric melting models are exclusively anhydrous, whereas water-bearing systems are permitted in MELTS. The data set used to calibrate MELTS is heavily biased toward experiments at atmospheric pressure, making it most suitable for studies of magma chamber processes, such as fractional crystallization. Although it captures many features of mantle melting behavior, the limitations of MELTS at higher pressures have been acknowledged [*Hirschmann et al.*, 1998].

The newer parameterization, pMELTS, goes a considerable way toward remedying the problems encountered by MELTS and is intended primarily for melting calculations in peridotite bulk compositions [*Ghiorso et al.*, 2002].

[3] Recently, the MELTS and pMELTS models have been extended to allow small amounts of water to be incorporated into nominally anhydrous minerals, such as olivine and pyroxenes, so that water-undersaturated conditions may be modeled quantitatively [*Asimow et al.*, 2004]. The new model, pHMELTS, has been used to demonstrate that trace amounts of water can have a significant effect on mantle melting behavior [*Asimow et al.*, 2004; *Asimow and Langmuir*, 2003]. The pHMELTS approach is based on the pMELTS calibration for the melting stage and MELTS calibration for crystallization. Here we present the first public release of the pHMELTS model and the software needed to run it.

[4] The program, adiabat_1ph, is a simple text based front end that invokes subroutines from the conventional MELTS or pMELTS models (i.e., hydrous or anhydrous systems) or the modified pHMELTS versions [*Asimow et al.*, 2004; *Ghiorso et al.*, 2002; *Ghiorso and Sack*, 1995]. The command line setup is very flexible and allows a high degree of automation for repetitive calculations, e.g., when testing the effect of a range of water contents or varying the starting pressure-temperature (*P-T*) conditions. We provide a Perl script, run_adiabat.pl, which includes an option to set up batch calculations in adiabat_1ph and also tidies up output. A number of extra features have been added to the adiabat_1ph software, such as simultaneous calculation of trace element distributions, and these are summarized below. The purpose of this report is draw attention to the range of possibilities of the software, whereas detailed instructions on how to perform each type of calculation are given in the accompanying documentation.

[5] Independence from graphical user interfaces also means that the code is portable and has been tested on Linux, MacOS X and Windows systems. Previously, the MELTS package was only available for UNIX/Linux based systems or via a Java/C applet (see http://ctserver.uchicago.edu/). For Windows users this meant that there was no convenient option if their computer network was behind a firewall (as many university-run systems are) or if their Internet connection was slow. Isentropic calculations are not possible with the Java interface and handling of large output data files is imprac-

tical. Although no graphics functions are included in the adiabat_1ph package, users should be able to take advantage of the plotting capabilities of programs such as Matlab or Microsoft Excel (see also the PetroPlot Visual Basic macros for Excel of *Su et al.* [2003]). Since one of the most labor intensive parts of analyzing and plotting results in commercial software is getting the adiabat_1ph output files in the correct format, we provide another simple Perl script that may be used to pick appropriate columns from a variety of files to make a single text table for importing.

2. Thermodynamic Models

[6] The underlying thermodynamic model behind the adiabat_1ph front end is either MELTS [*Ghiorso and Sack*, 1995] or pMELTS [*Ghiorso et al.*, 2002]. Both models share a common set of mineral end-member and solid-solution models. Mixing properties of the silicate liquid phase in MELTS are calibrated on a wide variety of bulk compositions in the system SiO_2-TiO_2-Al_2O_3-Fe_2O_3-Cr_2O_3-FeO-MnO-MgO-NiO-CoO-CaO-Na_2O-K_2O-P_2O_5-H_2O and are suitable at pressures not greater than 3 GPa. pMELTS is intended for peridotite compositions only, in the system SiO_2-TiO_2-Al_2O_3-Fe_2O_3-Cr_2O_3-FeO-MgO-CaO-Na_2O-K_2O-P_2O_5-H_2O, between 1 and 4 GPa. The user may choose either of the thermodynamic models and default maximal pressure ranges will be adjusted to reflect this. We do not recommend using either model outside its intended composition or pressure range.

[7] In MELTS or pMELTS, H_2O is treated as an oxide component, and can partition into melt, pure vapor, or hydrous minerals (including simple amphiboles and micas). In MELTS, the vapor phase standard state properties are derived from the Haar equation of state [*Haar et al.*, 1984], which fails beyond 1 GPa, whereas pMELTS uses the Pitzer and Sterner equation of state for validity to higher pressure [*Pitzer and Sterner*, 1994]. In pHMELTS, the effects of storage of water in nominally anhydrous minerals is approximately modeled [*Asimow et al.*, 2004]. The pHMELTS calculation uses trace element partitioning to distribute H_2O between the system and a "hidden" reservoir representing H_2O dissolved in nominally anhydrous minerals. The partitioning model is adapted from *Hirth and Kohlstedt* [1996]; differences in the details are laid out by *Asimow et al.* [2004]. For pHMELTS calculations, adiabat_1ph should be run in pMELTS mode for mantle melting

calculations and MELTS mode for low-pressure crystallization.

[8] In pHMELTS, there are two ways in which water content may be controlled. The user can specify the total water content of the system and this will be maintained as the calculation proceeds along the chosen *P-T* path. Alternatively, the water buffering procedure described by *Asimow et al.* [2004] may be adopted. In that case, the activity of water (a_{H2O}) is fixed and the appropriate water content is calculated iteratively, by a method similar to that described by *Ghiorso* [1985]. In each case, the water content of the liquid and any vapor phase is tracked by the (p)MELTS algorithm and the water content of the solids is calculated in pHMELTS subroutines by treating the H_2O species as a trace element. An iterative loop is required in the code to ensure that major and trace element compositions converge to the appropriate thermal equilibrium point for the water content of the melt (which is itself a dependent variable).

3. Alternative Garnet Model

[9] The Ca-Mg-Fe garnet solid solution model in MELTS and pMELTS is taken from *Berman and Koziol* [1991]. However, it has just been discovered (P. Luffi, personal communication, 2004) that an error in the printed paper (specifically a missing "3" in Equations 2 and 4) was imported into the original MELTS code and propagated through all subsequent releases of (p)MELTS. The incorrect garnet model is overly nonideal and underestimates the proportion of grossular. This new adiabat_1ph release incorporates, for the first time, an option to use the corrected garnet model.

[10] The MELTS and pMELTS liquid model calibrations included a few garnet-liquid equilibria with the incorrect solid-solution model. Hence using the new garnet code with the (p)MELTS models is not entirely self-consistent and, while garnet chemistry should be improved, the accuracy of other results (e.g., liquid chemistry, melt fraction, modal abundances) may be affected. Certainly, to reproduce previous (p)MELTS calculations requires the old garnet model and this remains the adiabat_1ph default. Unless garnet was excluded, please indicate the choice of garnet model with any published results. We specially emphasize this requirement because previously the underlying model parameters were consistent between different
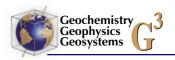
(p)MELTS front-ends, such that calculations could be reproduced exactly on each version.

4. Using Adiabat_1ph

[11] Where possible, we have designed the input files for adiabat_1ph so that they resemble those used in the graphical user interface (GUI) versions of MELTS and pMELTS. Consequently a user familiar with the Linux or Java versions of these programs should have little problem adjusting to this command line version. Many aspects of program execution are controlled by environment variables but these may be read from a text file, as can the command line input, if the Perl script run_adiabat.pl is used. A detailed description of all scripts, input and output files, particularly those specific to the adiabat_1ph version of (pH)MELTS, is given in the documentation, and examples are provided.

[12] In the GUI version of MELTS or pMELTS, a pure liquid trial solution was used and the algorithm progressively added the solid phases required [see *Ghiorso*, 1994]. In adiabat_1ph the initial guess may be superliquidus, as before, or subsolidus [*Asimow and Ghiorso*, 1998]. In the latter case, a norm calculation is used to find the suitable modal proportions for the given composition and suggested phases. Once started, the thermodynamic routines will drop or add phases as needed for chemical equilibrium to be satisfied. Additionally, if conditions are subsolidus or liquid is suppressed, then the approach detailed by *Asimow and Ghiorso* [1998] is used to construct an appropriate redox reaction to solve for the oxygen fugacity (fO_2) of the bulk assemblage. When liquid is present there is a choice as to whether the method of *Asimow and Ghiorso* [1998] is used, regardless. If not, then the parameterization of *Kress and Carmichael* [1991] is used to calculate fO_2 of the liquid, as described by *Ghiorso and Sack* [1995].

[13] The simplest form of calculation is along an adiabat (isentropic), an isotherm or an isobar. In all cases, melting and crystallization may be batch, fractional or continuous. In continuous melting a fixed mass (or volume) proportion of melt is retained in the matrix after extraction. The user must specify which solid phases are to be suppressed for the entire calculation but for liquid there is a function to switch between liquid absent and liquid present calculations so that the potential temperature (T_p) may be determined by equilibration with the prescribed entropy at 1 bar pressure.

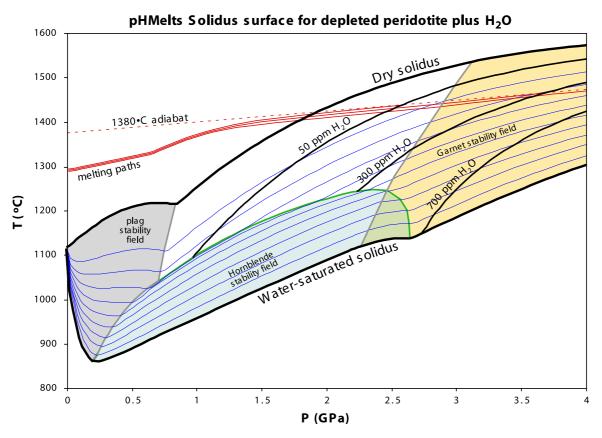**pHMelts Solidus surface for depleted peridotite plus H_2O**

Figure 1. Solidus relations for a depleted peridotite composition (formed by extracting about 1% melt from the fertile lherzolite composition of *Hart and Zindler* [1986]) with variable H_2O contents as predicted from the pHMELTS model using the old garnet model (from *Asimow et al.* [2004]). This illustrates many of the calculations possible with the adiabat_1ph software. The upper heavy black curve is the anhydrous solidus; the lowermost heavy black curve is the water-saturated solidus; both are calculated in pMELTS by tracking the $F = 0$ curve, with and without H_2O included as an oxide component. The blue contours in between are lines of constant activity of water at increments of 0.1 in a_{H2O}, calculated in pHMELTS by turning on the water buffering option. The black curves labeled 50, 300, and 700 show the solidus predicted for these bulk H_2O contents in ppm by weight; these are calculated by imposing the water content in pHMELTS with water buffering switched off. The gray lines delimit the stability of garnet and plagioclase, as calculated using the "phase-diagram mode"; the green boundary delimits the stability of hornblende. The dotted red line is the solid adiabat with a potential temperature of 1380°C, calculated in isentropic mode with liquid suppressed. The solid red curves are the *P-T* trajectories of the adiabatic continuous melting paths for 50, 300, and 700 ppm bulk H_2O in the source.

There is also a phase diagram calculation mode which follows the limit of appearance of a particular phase, either stable or meta-stable, as pressure or temperature is incremented. Alternatively a line of constant melt fraction (*F*, by mass) may be tracked. Finally, *P-T* streamlines input by the user (e.g., from convection models) may be imposed. This range of options for control of the *P-T* path, together with the possibility to automate the process, means that quite complicated phase diagrams may be constructed easily by using our software in tandem with plotting functions, in a spreadsheet program for example, as illustrated by Figure 1. Once appropriate input files for adiabat_1ph and run_adiabat.pl have been created, calculations may

be repeated with small changes (e.g., water content or initial temperature) by simply changing one or two lines in a text file.

5. Trace Element Partitioning

[14] Routines for trace element partitioning between melt and solid phases were introduced in pHMELTS [*Asimow et al.*, 2004]. In this version of adiabat_1ph we have extended the functionality to include user-defined partition coefficients and optional calculation of variable partition coefficients ($D = D(P, T, X)$, where D is the partition coefficient and X the composition) with the method of *Wood and Blundy* [1997]. Part of the motivation for this

Table 1. Allowed Phase-Element Pairs for Calculation of Variable Partition Coefficients Using the Method of *Wood and Blundy* [1997] and References for Expressions and Parameters Used in the Coding of This Method Into Adiabat_1ph
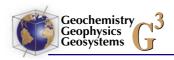
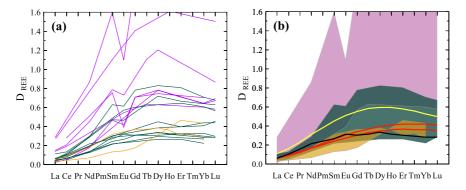| Phase	Reference	Allowed Elements
Clinopyroxene	*Wood and Blundy* [1997]; *Blundy et al.* [1995] (for Na); *Wood et al.* [1999]	Na, K, Sc, Ga, Rb, Sr, Y, Cd, In, Cs, Ba, La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Ra, Ac
Garnet	*van Westrenen et al.* [1999]	Sc, Y, In, La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu
Feldspar	*Blundy and Wood* [1994]	Li, Na, K, Rb, Sr, Y, Cs, Ba, La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu

was a study of the melting of pyroxenite lithologies which can be expected to exhibit quite different trace element partitioning from peridotite, reflecting the compositional variations of both solids and liquids in the two lithologies. Similarly, partition coefficients during fractional crystallization may differ from those during batch crystallization.

[15] The user decides which, if any, phase-element pairs will have variable partition coefficients. For all other phases and elements constant partition coefficients will be used, which can be read in from a file or take default values from the compilations of *McKenzie and O'Nions* [1991, 1995]. We caution against using variable partition coefficients for any combinations not in Table 1, as results may be unpredictable.

[16] One potential drawback with implementing the method of *Wood and Blundy* [1997], together with MELTS or pMELTS, is that solid phase compositions may not be sufficiently accurate and there are systematic temperature offsets compared with experimental data (e.g., ~100°C for the spinel lherzolite solidus in MELTS [*Hirschmann et al.*, 1998] and ~60°C in pMELTS [*Ghiorso et al.*, 2002]). Solid phases are calibrated in systems with limited numbers of components (e.g., 7 for clinopyroxene, 3 for garnet) and additionally there is a tendency for phases, particularly pyroxenes, to undergo phase separation that may lead to more exotic calculated solid phase compositions. The role of rare earth element (REE) partitioning during mantle melting with residual clinopyroxene and garnet has been particularly controversial [e.g., *Hirschmann and Stolper*, 1996; *Blundy et al.*, 1998], so we compare calculated partition coefficients with a selection of published values [*Bacon and Druitt*, 1988; *Dostal et al.*, 1983; *Foley et al.*, 1996; *Fujimaki et al.*, 1984; *Hack et al.*, 1994; *Hart and Dunn*, 1993; *Hauri et al.*, 1994; *Johnson*, 1998; *McKenzie and O'Nions*, 1991; *Ohtani et al.*,

1989; *Reid*, 1983; *Sobolev et al.*, 1996; *Yurimoto and Ohtani*, 1992]. This is not intended as a test of the *Wood and Blundy* [1997] model, which is well established, but simply to ascertain whether application of the model is appropriate here.

[17] For high-pressure, basic magmas the calculated partition coefficients for clinopyroxene are very similar to those of *McKenzie and O'Nions* [1991, 1995] for light and middle REEs and a little higher for heavy REE (Figure 2); note that the *McKenzie and O'Nions* [1991, 1995] values are close to the lower limit of the range exhibited by the compiled data and that the calculated values fall well within this range. For low-pressure magmas of basic to intermediate composition the calculated partition coefficients plot close to the overlap zone between data of basic to intermediate composition. Thus the results for clinopyroxene suggest that model-dependent effects are small compared to the variability in partition coefficients. Furthermore, when phase separation occurs during a calculation, while partition coefficients for individual clinopyroxene phases may be extreme, the weighted mean clinopyroxene partition coefficients remain normal.

[18] For garnet there are no complicated exsolution effects. Calculated partition coefficients fall within the range of published values and the effect of the alternative garnet models is negligible. The calculated values are very similar to *McKenzie and O'Nions* [1991, 1995] for light REE, but calculated values are a little higher for the middle REE and a little lower for the heaviest REE, being approximately equal for Er. Therefore, while the heavy REE are compatible in the modeled garnet composition whether default partition coefficients or the method of *Wood and Blundy* [1997] are used, the middle and heavy REE will be less fractionated relative to each other (e.g., Sm/Lu in the melt) in the latter case. This behavior is inherited from the experimental data

Figure 2. (a) Compiled clinopyroxene partition coefficients for a range of *P-T* conditions, colored according to magma composition; data sources are given in the text. The orange lines are for ultrabasic liquids; green lines are for basic liquids; pink lines are for intermediate compositions. (b) Calculated partition coefficients, compared to ranges for data shown in Figure 2a. Orange region is for ultrabasic liquids; green region is for basic liquids; pink region is for intermediate compositions; black line is from *McKenzie and O'Nions* [1991, 1995], which is the default partition coefficients used if variable partition coefficients are not used. Lower red line is the calculated partition coefficients for melting of the DMM, depleted peridotite, composition of *Workman and Hart* [2005] at 2GPa and 1500 °C, calculated using pMELTS (*F* = 10 wt%) with the old garnet model; upper red line is the calculation, for the same bulk composition and *P-T* conditions, calculated using MELTS (*F* = 2.5 wt%); yellow line is calculated partition coefficients for a melt of G2, the MORB-like pyroxenite composition of *Pertermann and Hirschmann* [2003], at atmospheric pressure and 1150°C (*F* = 50 wt%).

used to calibrate the model of *van Westrenen et al.* [1999] and is not an artifact of MELTS or pMELTS. Note, however, that (pH)MELTS garnet is a Ca-Mg-Fe solid solution; *Pertermann et al.* [2004] recently demonstrated that the TiO_2 content of residual garnet exerts considerable leverage over the REE partitioning during partial melting of MORB-like pyroxenite.

[19] While we believe the calculated partition coefficients to be reasonable, we suggest that the user compares results using variable partition coefficients with similar calculations using (suitable) constant partition coefficients. The variation in melt productivity in MELTS and pMELTS may be more realistic than in empirical models and variations in modal proportions as melting progresses generally parallel experimentally derived variations (e.g., *Hirschmann et al.* [1998] for the MM3 depleted peridotite composition of *Baker and Stolper* [1994]; P. M. Smith et al., manuscript in preparation, for the pyroxenite compositions G2 of *Pertermann and Hirschmann* [2003] and MIX1G of *Hirschmann et al.* [2003]). However, the MELTS and pMELTS calibrations do systematically overestimate the stability of orthopyroxene relative to olivine, garnet may be systematically underestimated relative to clinopyroxene and modal proportions of spinel are particularly sensitive to the Cr_2O_3 content. Still, these offsets (typically a few wt%) are likely to be no greater than the inaccuracies in the residual modes inherent in

empirical models that make assumptions about the melting modes.

6. Other Features

[20] The software includes a source mixing function in which a new source composition may be calculated by combining two (or more) compositions in user-specified proportions. Isotopic ratios and water content of the new source can also be calculated in this way. It is also possible to reproduce the melt focusing calculation described by *Asimow and Stolper* [1999]. This option multiplies the mass of liquid in the system by a fixed factor after each equilibration in order to model the migration of melt in channels or simulate two-dimensional flow with converging melt streamlines. One further option allows major element compositions to be calculated for systems with multiple liquids, although trace element partitioning is not available in this case.

[21] In isentropic mode, the output from adiabat_1ph includes melt fractions and compositions for each pressure. If melting is fractional (or continuous) the melt increments may be integrated for 1-D (column) and 2-D (triangular) melting regimes [*Asimow et al.*, 2001]. This gives the mean extent of melting, in the sense of *Plank et al.* [1995]. The output generated contains the thickness, composition and mean properties of the crust,

as well as aggregated liquids at all depths. A stand alone version of the subroutine that performs the integration, cubicquad2, is also available.

7. Summary

[22] The program adiabat_1ph is a text-menu based front-end to the MELTS, pMELTS and pHMELTS algorithms [*Asimow et al.*, 2004; *Ghiorso et al.*, 2002; *Ghiorso and Sack*, 1995]. A wide variety of calculation modes are included and text output files, suitable for importing into spreadsheets, are generated. The software has been tested on Linux, MacOS X and Windows and is accompanied by a variety of scripts and examples file. As new features and bug fixes are implemented we will make future releases available at http://www.gps.caltech.edu/~asimow/adiabat.

Acknowledgments

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