MELTS_Excel: A Microsoft Excel-based MELTS interface for research and teaching of magma properties and evolution

Guilherme A. R. Gualda, Earth & Environmental Sciences, Vanderbilt University, Nashville, Tennessee, USA.

Mark S. Ghiorso, OFM Research - West, Seattle, Washington, USA.

Corresponding author: G. A. R. Gualda, Earth & Environmental Sciences, Vanderbilt University, Nashville, TN 37235, USA. (g.gualda@vanderbilt.edu)

Key points

- Rhyolite-MELTS interface based on Microsoft Excel

Abstract

The thermodynamic modeling software MELTS is a powerful tool for investigating crystallization and melting in natural magmatic systems. Rhyolite-MELTS is a recalibration of MELTS that better captures the evolution of silicic magmas in the upper crust. The current interface of rhyolite-MELTS, while flexible, can be somewhat cumbersome for the novice. We present a new interface that uses web services consumed by a VBA backend in Microsoft Excel©. The interface is contained within a macro-enabled workbook, where the user can insert the model input information and initiate computations that are executed on a central server at OFM Research. Results of simple calculations are shown immediately within the interface itself. It is also possible to combine a sequence of calculations into an evolutionary path; the user can input starting and ending temperatures and pressures, temperature and pressure steps, and the prevailing oxidation conditions. The program shows partial updates at every step of the computations; at the conclusion of the calculations, a series of data sheets and diagrams are created in a separate workbook, which can be saved independently of the interface. Additionally, the user can specify a grid of temperatures and pressures and calculate a phase diagram showing the conditions at which different phases are present. The interface can be used to apply the rhyolite-MELTS geobarometer. We demonstrate applications of the interface using an example early-erupted Bishop Tuff composition. The interface is simple to use and flexible, but it requires an internet connection. The interface is distributed for free from melts.ofm-research.org.

Index terms

1011, 3611, 8411, 1009, 3610, 8410, 3618, 3619, 1065

Keywords

Rhyolite-MELTS, thermodynamics, phase equilibria, software

1. Introduction

The thermodynamic modeling software MELTS [*Ghiorso and Sack*, 1995; *Asimow and Ghiorso*, 1998] and its derivatives [e.g. pMELTS, *Ghiorso et al.*, 2002] comprise a powerful and much utilized set of tools for investigating crystallization and melting in natural magmatic systems [e.g. *Ghiorso*, 1997; *Ghiorso and Gualda*, 2015]. Rhyolite-MELTS [*Gualda et al.*, 2012a] is a recent recalibration of MELTS aimed at better capturing the evolution of silicic magmas present in upper crustal systems (up to ~400 MPa pressure), while maintaining the fidelity of the original calibration to mafic and alkalic systems. Rhyolite-MELTS also includes many algorithmic modifications that improve computational performance when compared to MELTS [*Ghiorso*, 2013].

Currently, most users of MELTS, pMELTS, and rhyolite-MELTS rely on a graphical user interface (GUI) that runs on UNIX/LINUX-based systems, primarily Intel-based Mac OS X computers. One of the difficulties with deployment of the GUI is that it has to be built for each of the several existing computer architectures and operating systems. Also, while the GUI provides a powerful and flexible interface, the many options available in the GUI lead to a relatively steep learning curve for the novice user. Finally, there is currently no graphical output of the simulation results, and the output from the GUI is in the form of text files that need to be processed offline. For all these reasons, while MELTS and its derivatives are widely used for research purposes, there is substantial interest in the community for a version of MELTS for other operating systems and computer architectures. Further, these characteristics are probably the main reason why MELTS – despite great potential – has not been used more frequently for teaching purposes. The program PhasePlot (http://www.phaseplot.org/) is a modern graphic interface that allows quick visualization of computations performed using rhyolite-MELTS and pMELTS [see *Ghiorso and Gualda*, 2015], which makes it an ideal tool for some teaching purposes. However, PhasePlot is not designed for output of quantitative data, and there are some limitations to the types of calculations possible, which limits its use for many types of applications.

In this paper we present a new interface for rhyolite-MELTS developed in Microsoft Excel©. We aim to create a more interactive tool, which is easy to use, available to a widespread audience, and useful for both research and teaching. We first introduce the new interface, and we then present some examples of applications that can be developed with this interface. Finally, we list some of the current limitations of the new interface.

2. The new interface

MELTS_Excel uses web services consumed by a VBA backend client; all calculations are performed on the servers at OFM Research and Excel is used as an interface to send, receive, and process data exchanged with the server. One key advantage of this approach is that, with calculations being performed on servers, the only requirement for the end-user machine is for it to be able to run a version of Excel compatible with REST protocol web services (currently, Excel 2010 and 2013 for Microsoft Windows operating systems). The interface requires no installation, allowing use on machines regardless of the administrative privileges of the user; and there is no need for upgrades in the computation engine, given that all calculations are performed in a centrally maintained server. Further, the spreadsheet and graphic capabilities of Excel can be used to create formatted output, including both data and diagrams. The main disadvantage of the approach is that the interface requires an active internet connection to communicate with the OFM Research server that performs computations.

The interface is contained within a macro-enabled workbook where composition and conditions are set, which includes several sheets: (1) one sheet for simple calculations and display of live results, where the user can insert the model input information and trigger simple calculations, and where a summary of results for any given condition is given; (2) one sheet listing properties of all phases present at any given condition; (3) one sheet where the user can select phases to include or exclude in the calculations; and (4) one sheet where the user can specify sequences of calculations (variable T, P, or both, plus f_{O2}).

For calculations at one given condition, the results are immediately displayed within prespecified fields within the interface. For instance, a user can very rapidly determine the temperature at which a magma of a given composition is completely molten (i.e. find the liquidus); or determine which phases are present, in what abundances, their compositions, and their physical properties (e.g. density, viscosity) at any given combination of temperature, pressure and oxygen fugacity.

It is also possible to combine a sequence of calculations into an evolutionary path. The user can input starting and ending temperatures and pressures, temperature and pressure steps, and the prevailing oxidation conditions. Additionally, the user can specify a grid of temperatures and pressures and calculate a phase diagram in temperature-pressure space. At the conclusion of the calculations, a series of data sheets and diagrams are created in a separate workbook,

which can be saved independently of the interface. This way, the user can save the results separately from the interface, and the interface can be used repeatedly. The results workbook includes several sheets, including: (a) sheets with data for each phase (equivalent to [phase name].tbl files from the GUI); (b) one sheet with data for the whole system (previously included in melts-liquid.tbl); (c) one sheet with data for total solids (previously included in melts-liquid.tbl); (d) one sheet including mass, volume, density evolution of each phase, solids, and whole system as a function of temperature, pressure, f_{O2}; (e) charts with evolution of mass, volume, density as a function of temperature; (f) charts with compositional evolution of each phase as a function of temperature; (g) one sheet with affinities for all phases at all temperatures (useful for calculation of activities relative to mineral saturation); and (h) one sheet with initial conditions, a reference of the conditions employed in the calculation that can be used for easy reproduction of the simulation. The routines used to create the output can also be used to process tbl files returned by the GUI to create equivalent output in Excel.

3. Some examples

We present below a few examples that illustrate some of the capabilities of the interface. We start with examples that reproduce capabilities available in the GUI, and then present examples of applications facilitated by the new interface.

3.1. A simple calculation

We first present the case of a calculation performed at a single set of conditions (pressure, temperature, oxygen fugacity) for a given bulk composition. After entering the bulk composition of interest, the user has a number of options:

(1) *Equilibrate*: For the bulk composition and set of conditions specified, MELTS calculates the phases present, their compositions and abundances, as well as the thermodynamic properties of each phase present;
(2) *Find liquidus*: For the bulk composition, pressure and oxygen fugacity specified, MELTS calculates the temperature at which the only remaining phase is liquid; note that MELTS will try to dissolve all excess water by simply adjusting the temperature, such that unexpected results may occur for water-oversaturated systems;
(3) *Find wet liquidus*: Similar to "Find liquidus", except that it allows for excess water to be present with liquid at the calculated liquidus temperature; the results of both "Find

liquidus" and "Find wet liquidus" will be the same if the system does not contain free water at the liquidus;

(4) *Compute redox*: This option will partition FeO and Fe_2O_3 based on the specified oxygen fugacity value; this option is only useful when performing unconstrained redox calculations, in which case MELTS will use the ratio of Fe^{2+}/Fe^{3+} to determine the oxidation state; for calculations in which f_{O2} is constrained, MELTS recalculates the Fe^{2+}/Fe^{3+} using total Fe, irrespective of how FeO and Fe_2O_3 are partitioned in the input values;

(5) *Normalize*: This recalculates the bulk composition so that the sum of the oxides is 100; this calculation is immaterial for MELTS, as it assumes that the quantities entered are grams of each oxide;

(6) *Normalize anhydrous*: Recalculates the bulk composition so that the sum of oxides, except water, is 100; this is also immaterial for MELTS and only for the convenience of the user;

(7) In the event that the user would like to exclude phases from the calculations, the sheet "Phases" should be selected, and the box next to each phase to be excluded should be unchecked.

After performing computations with "Equilibrate", "Find liquidus", or "Find wet liquidus", a summary of the resulting phase properties is displayed in the "Input" sheet, while more detailed results are displayed in the "Results" tab. Only phases calculated to be present are displayed in the "Results" sheet, while the affinities [for details, see *Ghiorso and Gualda*, 2013] of each phase included in the computation are also shown in the "Input" sheet.

In Figure 1, we show a screenshot illustrating the results of a calculation performed using "Equilibrate" for a composition representative of the early-erupted Bishop Tuff [from *Hildreth*, 1979], under water-saturated conditions, and fugacity constrained to the Ni-NiO buffer, at a temperature of 755 ºC and pressure of 175 MPa. Clicking on "Find wet liquidus" would lead to the temperature being reset to 760.3 ºC, with 4.34 g of water present. In this case, "Find liquidus" would give a physically implausible result given that a substantial amount of excess water is present at the liquidus. Readjusting H_2O to 4.00 would cause both "Find liquidus" and "Find wet liquidus" to calculate a liquidus temperature of 798.9 ºC.

We expect that using the interface in this mode will greatly facilitate building intuition about magmas and their properties. This mode will also be useful for selecting parameters for more complex calculations including sequences and grids described below.

3.2. An isobaric sequence of calculations

One of the most common uses of MELTS is to perform isobaric calculations that span a range of temperatures with a specified temperature step. One of the advantages of the new interface is that it is straightforward to use simple calculations like those presented above to constrain the temperature interval over which to perform a sequence of calculations. Using the same composition and pressure as the example above, we use the "wet liquidus" temperature as the starting point, and we find that a temperature range of only 10 ºC leads to substantial (>50 wt. %) crystallization [*Gualda et al.*, 2012a; *Gualda et al.*, 2012b]. We thus run a sequence of calculations by filling out the fields in the "Sequences" sheet:

(1) T1, T2, and ΔT are the starting temperature, ending temperature, and temperature step, respectively; we usually use T1 as the highest temperature, with positive ΔT representing a decrement, because a down-temperature calculation is more efficient computationally; but we emphasize that, at least for equilibrium calculations, the order in which the calculations are performed is immaterial to the final result, given that each calculation represents a thermodynamic equilibrium state that is thus independent of the path leading to that state [*Ghiorso and Gualda*, 2015]; for fractionation or assimilation calculations, the results are intrinsically dependent upon the sequence of the calculations;

(2) P1, P2, and ΔP are the pressure equivalents of the quantities above; for an isobaric calculation, both P1 and P2 should be set to the same values, while ΔP could have any value;

(3) f_{O2} represents the oxygen fugacity constraints to be used in the calculation; for constrained calculations ("Constrained" box checked) the user can enter the oxygen fugacity relative to a variety of buffers, while for unconstrained calculations the FeO and Fe_2O_3 values in the "Input" sheet are used to calculate the initial oxygen fugacity condition, and f_{O2} is allowed to vary as the calculations progress [*Ghiorso and Gualda*, 2015];

(4) The user would hit the "Run PT Sequence" button to trigger the sequence of calculations.

Using the same composition as the example above, we perform an isothermal calculation from 765 to 755 ºC in 0.5 ºC steps, at 175 MPa and f_{O2} constrained along the Ni-NiO buffer. The calculations take place over several seconds, with partial updates shown in the "Input" sheet as the calculation progresses. At the end of the calculation, Excel switches to the resulting workbook, which includes all the data generated during the calculations and a number of automatically generated diagrams (some of which are shown in Figure 2).

While the example focuses on an isobaric calculation, the interface also allows for isothermal calculations under variable pressure, as well as calculations in which both temperature and pressure vary simultaneously. In the latter, the number of steps is chosen between the temperature and pressure inputs as the one that leads to the larger number of steps, and both temperature and pressure are varied continuously from T1 and P1 to T2 and P2. In all cases, the output diagrams are constructed as a function of temperature, which will render them less useful for isothermal calculations.

One of new features of the Excel interface, which distinguishes it from the GUI, is that it includes in the output the affinities of all phases included in the calculation. The affinities can be useful in that they relate quite simply to the activities of the corresponding components [*Ghiorso and Gualda*, 2013], which can be helpful in the application of Ti-in-quartz, Ti-in-zircon, and Zr-in-titanite geobarometers [*Ferry and Watson*, 2007; *Hayden et al.*, 2008; *Thomas et al.*, 2010; *Wark and Watson*, 2006]. We demonstrate here the capabilities by calculating a_{TiO2} as a function of temperature from the calculation output. Because both T and a_{TiO2} are known, we can also compute the expected variation in Ti-in-zircon concentration as a function of temperature (Figure 3). Interestingly, the observed compositions of early-erupted zircon [*Reid et al.*, 2011] are consistent with crystallization primarily at temperatures below 758 ºC, which matches the temperature interval over which crystallization of early-erupted magmas should have taken place (see Figure 2).

3.3. A phase diagram calculation

Another new feature in comparison with the GUI is that phase diagram calculations can be easily performed with the new interface, with a graphic output being generated automatically. The calculation is also called using the "Sequences" sheet. In this case, the user sets both

temperature and pressure intervals and decrements, again with a choice of f_{O2} conditions. A grid of points in temperature-pressure space is created and a full calculation is performed for each grid point.

The main concern with this type of calculation is that the number of calculations increases very rapidly, and individual phase diagram calculations can take from several minutes to many hours. Simple calculations, as well as PhasePlot, can be used to constrain the range of parameters to be used. Phase diagram calculations are performed as a series of isobaric sequences. To avoid unnecessary calculations, for each sequence (i.e. pressure), calculations for temperatures greater than the wet liquidus are skipped; similarly, calculations are halted once the liquid abundance drops below 10 wt. %. This results in dramatic improvements in speed, and it allows the user to select a wide range of temperatures consistent with the range of liquidus and solidus temperatures observed for the pressure interval of interest. At the end of the calculations, the user is presented with a new workbook that includes all the data, and a diagram displaying the temperatures at which each phase saturates – a phase-in curve – is also generated; we note that phase-out curves, which would be present if a phase were to become unstable and completely disappear, are not currently displayed.

As an illustrative example, we use again the same early-erupted Bishop Tuff composition, and we calculate a phase diagram for the temperature range of 810-730 ºC, with 1 ºC steps, and the pressure range 250-100 MPa, with 25 MPa steps. Of the 567 points in this grid, only 87 calculations fall at temperatures between the wet liquidus and the 10 wt. % liquid threshold, so only a relatively small subset of the grid points actually require calculations to be performed. In the resulting phase diagram (Figure 4), the liquid-in curve represents the lowest superliquidus temperature on the grid for each pressure. This is also true for the water-in curve in this case, because we added enough water to the system for it to be water-saturated at the liquidus for all pressures. It can be seen from this example calculation the nearly invariant nature of the early-erupted Bishop Tuff compositions, which crystallize over a very narrow temperature interval [*Gualda and Ghiorso*, 2013; *Gualda et al.*, 2012a; *Gualda et al.*, 2012b].

3.4. A calculation using the rhyolite-MELTS geobarometer

The new interface also makes it possible to apply the rhyolite-MELTS geobarometer [*Gualda and Ghiorso*, 2014], which uses rhyolite-MELTS to calculate the pressure at which a given melt

composition can be in simultaneous equilibrium with the expected felsic assemblage (quartz and feldspars).

Parameters for the pressure calculations are set in the same way as for the phase diagram calculations and, in fact, the calculations are performed in the same way; the only difference is that an extra sheet is included in the output workbook where the pressure calculations are made. For proper functioning of the capabilities of this sheet, the user needs to check "Trust access to the VBA project object model" within the "Macro Settings" of Microsoft Excel "Trust Center").

The composition used in the examples above is representative of both early-erupted Bishop Tuff bulk rocks [*Hildreth*, 1979] and quartz-hosted glass inclusions [*Anderson et al.*, 2000]. Early-erupted magmas are characterized by the presence of quartz, sanidine, and plagioclase [*Anderson et al.*, 2000; *Gualda and Ghiorso*, 2013; *Hildreth*, 1979]. The pressure calculations (Figure 4) show that all three phases are in simultaneous equilibrium at pressures of ~170 MPa (Figure 4b). Even if melt inclusions were entrapped prior to saturation in both feldspars, the estimated saturation pressure would still be the same (Figure 4c) [for more details, see *Gualda and Ghiorso*, 2014].

4. Some current limitations

MELTS_Excel is in active development, and not all the envisioned functionality is implemented. As such, there are some current limitations:

(1) MELTS_Excel currently only works with rhyolite-MELTS, and there is no interface with pMELTS (rhyolite-MELTS effectively replace MELTS, given that the calibration for mafic systems is identical, and it takes advantage of the much improved calculation algorithms included in rhyolite-MELTS [*Ghiorso*, 2013]);

(2) Only equilibrium mode calculations are currently implemented; implementation of fractionation modes is planned for the near future;

(3) Only calculations using pressure and temperature (as opposed to entropy and volume) as independent variables (i.e. Gibbs free-energy minimization and related f_{O2}-constrained Korzhinskii potential minimization [*Ghiorso and Gualda*, 2015]) are currently implemented, which precludes isenthalpic or isochoric calculations available through the existing MELTS GUI; we intend to eventually implement such capabilities;

(4) No assimilation mode is currently implemented;

We envision that, for most users, the new interface will replace the existing GUI. However, one of the hallmarks of the GUI is its flexibility and the ability to simulate complex evolution histories. In many ways, the new Excel interface is currently less flexible, which may cause some advanced users to prefer the GUI for specific calculations. In these cases, the ability to import and process tbl files to generate equivalent output (under "Tools" tab) may be a useful functionality of MELTS_Excel.

5. Conclusions

In this paper we present MELTS_Excel, a new interface for rhyolite-MELTS based on Microsoft Excel. It utilizes web services to perform calculations on a remote server at OFM Research and deliver results to the user in an Excel workbook. It takes advantage of spreadsheet and graphic capabilities of Microsoft Excel to simplify both data input and output. Due to differences in capability of web services available in the various versions of Excel, MELTS_Excel currently only works on versions 2010 and 2013 of Microsoft Excel for Windows.

The interface is contained within a macro-enabled workbook, which includes editable cells where the user can insert the model input information. Results of simple calculations are shown immediately within the interface itself.

It is also possible to combine a sequence of calculations into an evolutionary path. The user can input starting and ending temperatures and pressures, temperature and pressure steps, and the prevailing oxidation conditions, and the program will perform the calculations showing the magma properties at every step; at the conclusion of the calculations, a series of data sheets and diagrams are created in a separate workbook, which can be saved independently of the interface.

Additionally, the user can specify a grid of temperatures and pressures and calculate a phase diagram showing the conditions at which different phases are present. Pressure estimation using the rhyolite-MELTS geobarometer is also possible using the interface.

The main advantages of this new interface are that it is simple to use and flexible. The interface is built on a popular platform and which is widely available. The interface requires no installation and it is distributed for free. The main drawback is that operation of the workbook requires an internet connection. The interface is actively being developed, so not all features of the GUI are currently implemented in MELTS_Excel.

We expect that the new interface will facilitate the use of rhyolite-MELTS, particularly for the novice user, but also for users performing a large number of simulations. We hope that MELTS_Excel will also facilitate the use of MELTS for teaching purposes.

6. Acknowledgements

MELTS_Excel can be downloaded for free from: http://melts.ofm-research.org. Financial support was provided by NSF (EAR-1321806, EAR-1151337, EAR-0948528 to Gualda and EAR-0948734, EAR-1321924 to Ghiorso) and by a Vanderbilt University Discovery Grant to Gualda.

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8. Figure captions

Figure 1. Screenshot showing the "Input" sheet of MELTS_Excel, where the system composition is defined, as well as temperature, pressure and oxygen fugacity conditions for simple calculations. Several buttons that trigger sample calculations can be seen. The result of an "Equilibrate" calculation at the conditions listed are displayed on the right portion, including the names, abundances and compositions of phases present, as well as the affinities of all phases that are not present but which are included in the calculation. More detailed results are presented in the "Results" sheet.

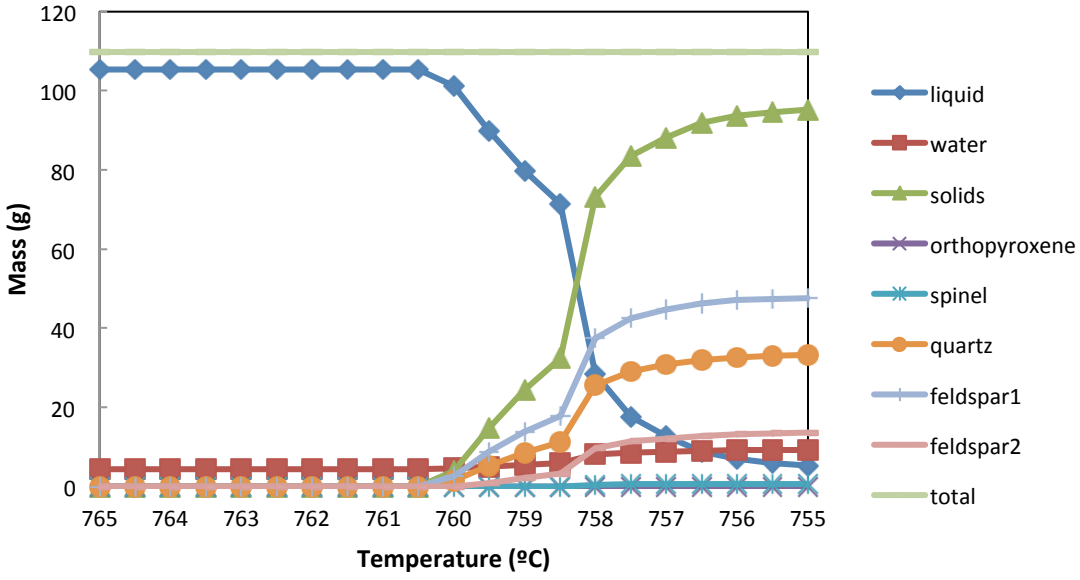
Figure 2. Graphics displaying some of the results of an isobaric sequence of calculations. The composition is the same as shown in **Figure 1**. The temperature range is 765-755 ºC, in 0.5 ºC steps, at 175 MPa, with f_{O2} constrained along the Ni-NiO buffer. *Top*: Variation in mass as a function of temperature for all phases present, for all solids, and for the whole system. *Middle*: Variation in liquid composition as a function of temperature; note that SiO_2 is shown on a different vertical scale (to the right) than the other oxides. *Bottom*: Variation in the composition of feldspars as a function of temperature; the highest temperature feldspar appears at 760 ºC, while a lower temperature feldspar saturates at 759.9 ºC; the zigzag lines demonstrate the coexistence of two feldspars within that temperature range.

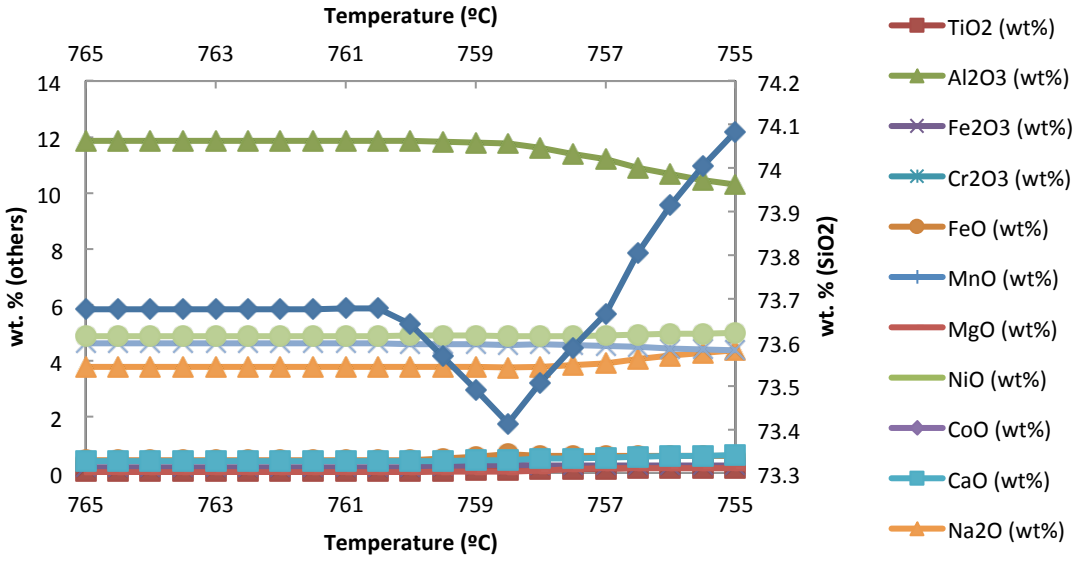
Figure 3. Example of the use of rhyolite-MELTS to calculate a_{TiO2} and Ti-in-zircon as a function of temperature using the variation in the affinity of rutile as a function of temperature. *Top*: Variation in a_{TiO2} as a function of temperature calculated using the relationship shown on the right panel [see *Ghiorso and Gualda*, 2013]. *Bottom*: Variation in Ti-in-zircon as a function of temperature calculated using the Ti-in-zircon calibration of Ferry & Watson [2007]; panel on the right shows histogram of Ti abundances in zircon from early-erupted Bishop Tuff [*Reid et al.*, 2011], on the same vertical scale as the plot on the left; the histogram shows that the vast majority of zircons are expected to have crystallized at temperatures below 758 ºC, consistent with the range of temperatures over which crystallization of early-erupted magmas should have taken place (see **Figure 2**).

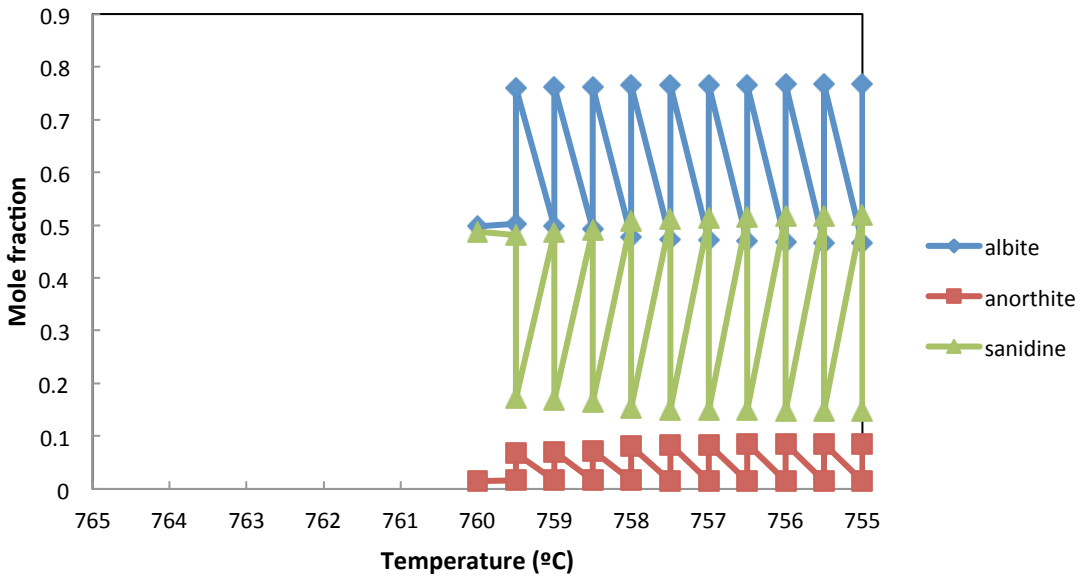
Figure 4. Example calculation of a phase diagram and application of the rhyolite-MELTS geobarometer. *Top*: Phase diagram calculated for the same composition as in the prior examples, over a temperature range of 810-730 ºC (1 ºC steps) and a pressure range of 250-100 MPa (25 MPa steps). *Bottom*: Diagrams showing the application of the rhyolite-MELTS

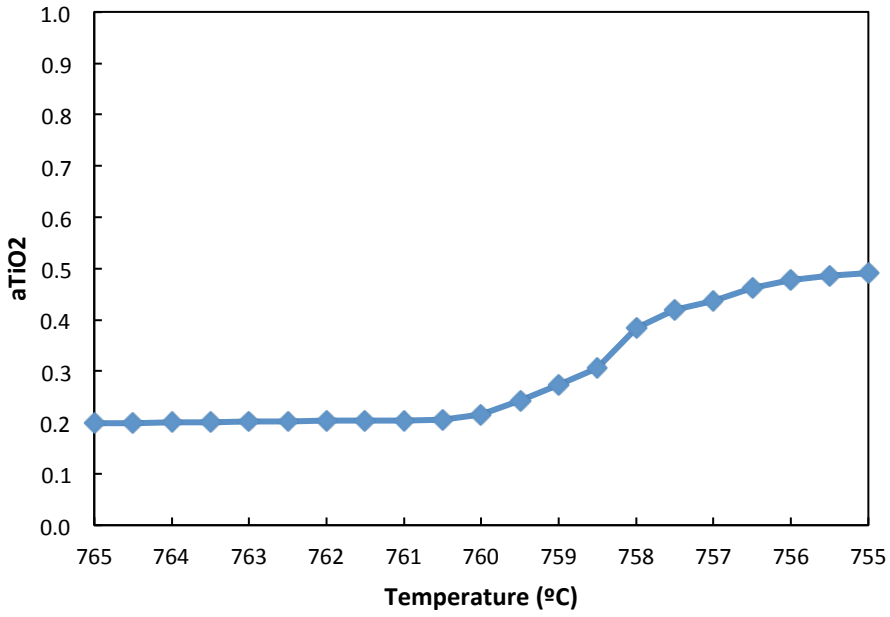
420 geobarometer; left panel shows calculation of the pressure at which quartz and two feldspars
421 are expected to be in equilibrium with the input glass composition; right panel shows calculation
422 of the pressure at which quartz and one feldspar are expected to be in equilibrium with the
423 input glass compositions [for further details, see *Gualda and Ghiorso*, 2014].

	A	B	C	D	E	F	G	H	I	J
1		***System***		***System***		***Unit***		***System***	***109.80***	
2	SiO_2	77.700		P	175	MPa		Liquid	12.66	
3	TiO_2	0.080		T	755.0	°C		Solids	97.15	
4	Al_2O_3	12.500		log fO2	0.00	ΔNNO				
5	Fe_2O_3	0.192		☑ fO2 constrained						
6	Cr_2O_3							***Phase***	***Mass***	***Formula***
7	FeO	0.487		Equilibrate				liquid	12.66	SiO_2 0.77 TiO_2 0.00 Al_2O_3 0.12 Fe_2O_3 0.00 FeO 0.01 MgO 0.00 CaO 0.01 Na_2O 0.04 K_2O 0.05 H_2O 0.05
8	MnO			Find Liquidus				feldspar	44.65	$K_{0.51}Na_{0.47}Ca_{0.01}Al_{1.02}Si_{2.98}O_8$
9	MgO	0.030		Find Wet Liquidus				quartz	30.77	SiO_2
10	NiO			Compute Redox				feldspar	12.19	$K_{0.15}Na_{0.77}Ca_{0.08}Al_{1.08}Si_{2.92}O_8$
11	CoO			Normalize				water	8.88	H_2O
12	CaO	0.430		Normalize Anhydrous				spinel	0.66	$Fe''_{1.19}Mg_{0.06}Fe'''_{1.42}Al_{0.07}Cr_{0.00}Ti_{0.26}O_4$
13	Na_2O	3.990								
14	K_2O	4.890						***Potential Phase***	***Affinity (kJ)***	***Formula***
15	P_2O_5							orthopyroxene	0.28	opx $Na_{0.00}Ca_{0.99}Fe''_{0.0}Mg_{0.51}Fe'''_{0.50}Ti_{0.01}Al_{0.52}Si_{1.48}O_6$
16	H_2O	9.500						rhm-oxide	0.95	$Mn_{0.05}Fe''_{0.00}Mg_{0.85}Fe'''_{0.24}Al_{0.00}Ti_{0.88}O_3$
17	CO_2							clinopyroxene	1.50	cpx $Na_{0.00}Ca_{0.99}Fe''_{0.0}Mg_{0.53}Fe'''_{0.48}Ti_{0.01}Al_{0.50}Si_{1.50}O_6$
18	SO_3							biotite	1.53	$K(Fe''_{1.00}Mg_{0.00})_3AlSi_3O_{10}(OH)_2$
19	Cl2O-1							tridymite	2.15	SiO_2
20	F2O-1							cristobalite	2.21	SiO_2
21				Success: Equilibrate				olivine	3.71	$(Ca_{0.0}Mg_{0.0}Fe''_{0.1}Mn_{0.38}Co_{0.38}Ni_{0.38})_2SiO_4$
22								cummingtonite	7.00	$(Fe''_{0.00}Mg_{1.00})_7Si_8O_{22}(OH)_2$
23								rutile	7.10	TiO_2
24								fayalite	8.33	Fe_2SiO_4
25								garnet	11.68	$(Ca_{0.11}Fe''_{0.89}Mg_{0.00})_3Al_2Si_3O_{12}$
26								sillimanite	15.20	Al_2SiO_5
27								sphene	15.36	$CaTiSiO_5$
28								corundum	15.59	Al_2O_3
29								ortho-oxide	18.34	$Fe''_{0.03}Mg_{0.00}Fe'''_{1.94}Ti_{1.03}O_5$
30								muscovite	25.83	$KAl_2Si_3AlO_{10}(OH)_2$
31								perovskite	29.83	$CaTiO_3$
32								hornblende	34.65	$NaCa_2Mg_{3.98}Fe_2{}^+{}_{0.02}Al_{1.00}Fe_3{}^+{}_{0.00}Al_2Si_6O_{22}(OH)_2$
33								nepheline	43.62	neph $Na_{0.07}K_{3.92}Ca_{0.00}[]_{0.02}Al_{3.98}Si_{4.02}O_{16}$
34								melilite	44.78	$Na_{0.00}Ca_{2.00}Al_{0.59}Mg_{0.06}Fe_{0.65}Si_{1.71}O_7$
35								aenigmatite	45.80	$Na_2Fe_5TiSi_6O_{20}$
36								alloy-solid	65.90	solid $Fe_{1.00}Ni_{0.00}$
37								alloy-liquid	70.50	liquid $Fe_{1.00}Ni_{0.00}$
38								aegirine	141.08	$NaFeSi_2O_6$


Mass (g)
120
100
80
60
40
20
0
765 764 763 762 761 760 759 758 757 756 755
Temperature (ºC)
liquid
water
solids
orthopyroxene
spinel
quartz
feldspar1
feldspar2
total


Temperature (ºC)
765 763 761 759 757 755
wt. % (others)
14
12
10
8
6
4
2
0
wt. % (SiO2)
74.2
74.1
74
73.9
73.8
73.7
73.6
73.5
73.4
73.3
Temperature (ºC)
TiO2 (wt%)
Al2O3 (wt%)
Fe2O3 (wt%)
Cr2O3 (wt%)
FeO (wt%)
MnO (wt%)
MgO (wt%)
NiO (wt%)
CoO (wt%)
CaO (wt%)
Na2O (wt%)


Mole fraction
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
765 764 763 762 761 760 759 758 757 756 755
Temperature (ºC)
albite
anorthite
sanidine

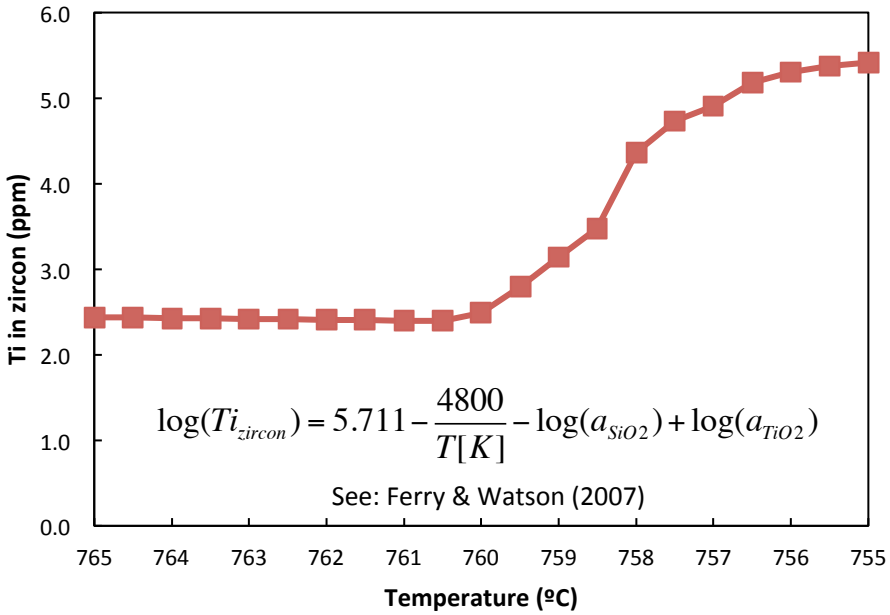


Chemical affinity for rutile saturation

$$a_{TiO2}^{liquid-rutile} = \exp\left(-\frac{A_{rutile}}{RT}\right)$$

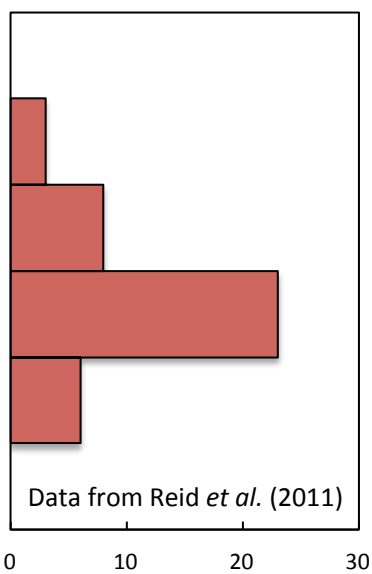
Activity of TiO_2 referenced to rutile saturation

See: Ghiorso & Gualda (2013)

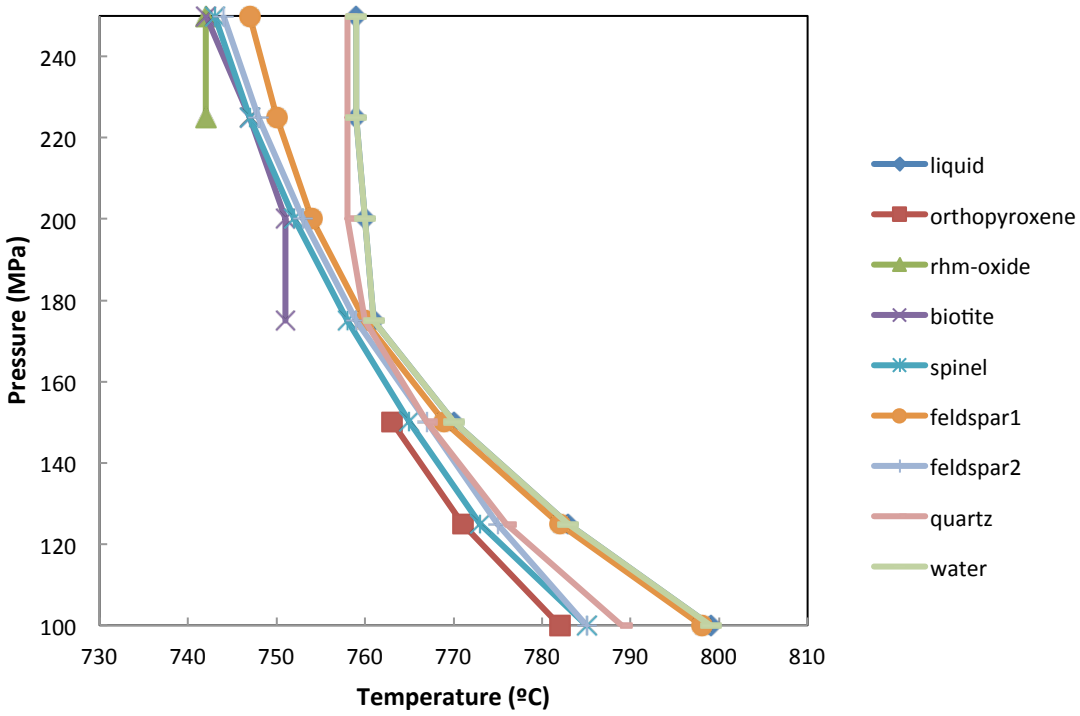


$$\log(Ti_{zircon}) = 5.711 - \frac{4800}{T[K]} - \log(a_{SiO2}) + \log(a_{TiO2})$$

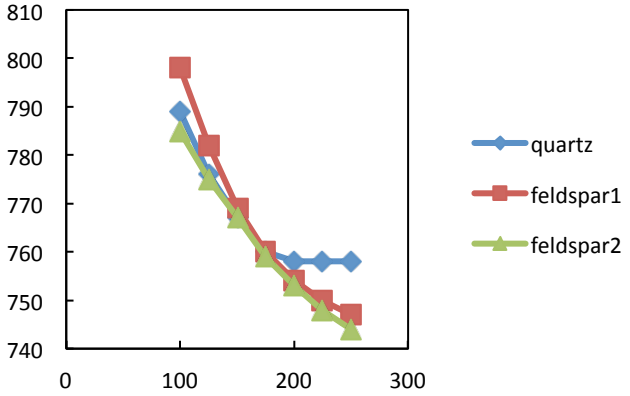
See: Ferry & Watson (2007)

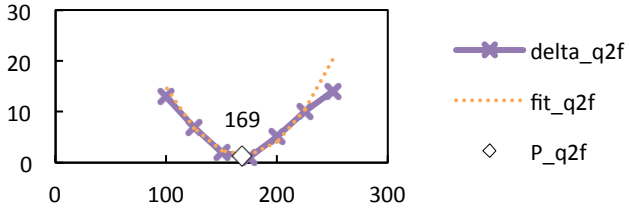


Data from Reid *et al.* (2011)



Quartz+2 Feldspars





Quartz+1 Feldspar