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PyMelt: An extensible Python engine for mantle melting calculations

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Abstract

Modelling the melting of Earth's mantle is crucial for understanding the distribution of volcanic activity on Earth and for testing models of mantle convection and mantle lithological heterogeneity. PyMelt is a new open-source Python library for calculating the melting behaviour of multi-lithology mantle and can be used to predict a number of geophysical and petrological observations, including melt productivity, spreading centre crustal thickness, lava trace element concentrations, and olivine crystallisation temperatures. The library is designed to be easily extensible, allowing melting models to be added, different methods for calculating lava chemistry to be applied, and new melting dynamics and properties to be incorporated.

1 Introduction

Models for melting the Earth's mantle have been used widely in studies of Earth's convecting mantle, often to provide quantitative constraints on mantle temperature variability [e.g., Ball et al., 2021], mantle compositional variability [e.g., Brown and Lesher, 2014; Gleeson et al., 2021], or as a means of estimating primary melt compositions [e.g., Jennings et al., 2016]. These melting models calculate mantle melting behaviour either by minimising thermodynamic potentials at each calculation step [e.g., Smith and Asimow, 2005], or by using expressions parameterised directly from melting experiments [e.g., Lambart et al., 2016]. The parameterised approach is particularly useful for calculations requiring many runs of a melting model, for example when inverting for mantle properties from geochemical or geophysical observations [e.g., McKenzie and O'Nions, 1991; Matthews et al., 2021].

PyMelt is an open-source extensible Python library that employs the parameterised approach, providing a powerful and flexible tool for calculating the melting behaviour of lithologically heterogeneous mantle. The library incorporates existing melting parameterisations (Section 3), in addition to methods for estimating igneous crustal thickness, magmatic productivity, lava trace element concentrations, and olivine crystallisation temperatures. The library is designed to be extensible: new models can be added to the library very simply, in addition to new functions for predicting geochemical and geophysical observations.

A number of software tools are available that can perform similar, though more limited, calculations, including INVMEL [McKenzie and O'Nions, 1991], REEBOX-PRO [Brown and Lesher, 2016], MELTPX [Lambart et al., 2016], and BDD21 [Ball et al., 2022]. While these packages have been used extensively in studies of mantle melting, pyMelt offers a number of advantages. PyMelt is the only package that is simultaneously open-source, incorporates mantle lithological heterogeneity, and can be easily integrated with other Python libraries (e.g., Monte-Carlo inversion tools). Open-source software is an essential part of open, transparent, and reproducible science, and it provides the basis for the development of more advanced codes and integration with other libraries. The importance of modelling the effects of lithological heterogeneity on mantle melting behaviour for accurately predicting magmatic productivity, melt compositions, and magmatic teperatures is becoming increasingly clear [Phipps Morgan, 2001; Pertermann and Hirschmann, 2003; Shorttle et al., 2014; Matthews et al., 2021]. PyMelt therefore occupies an important niche in mantle melting calculations

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and will provide the basis for solving new problems related to melt generation and magmatism for many years to come.

In this manuscript we review the main features of pyMelt, the library structure, the underlying mathematical formulation, and the computational approaches it takes. Users are directed to the pyMelt documentation (pyMelt.readthedocs.io) for a comprehensive guide to using the library, and to the interactive tutorials available on myBinder. The pyMelt repository is hosted on GitHub (github.com/simonwmatthews/pyMelt), where the code can be obtained, bugs reported, new features requested, and new contributions made. PyMelt can also be installed directly using the pip package manager.

2 PyMelt structure

Figure 1 summarises the modular structure of the pyMelt library and its workflow. The melting behaviours of individual lithologies (e.g., lherzolite or pyroxenite) are contained with `lithology` classes (Section 3), which can be combined in specified mass fractions ϕ to form a `Mantle` class (Section 4). Any `lithology` class in pyMelt can be converted to a `hydrousLithology` class where the effect of water on its solidus and melt productivity is estimated (Section 5). An adiabatic decompression calculation can then be performed on a `Mantle` class instance at a specified mantle potential temperature T_p (the temperature a parcel of mantle would have following decompression to 0 bar while undergoing no chemical changes) using its `adiabaticMelt` method (Section 4) which returns a `meltingColumn` instance. If desired, the trace element concentrations in these melts can be calculated by calling the `calculateChemistry` method of the `meltingColumn` class (Section 6). To calculate geological setting specific properties, such as crustal thickness t_c at a mid-ocean ridge, a `geoSetting` class can be created using the `meltingColumn` class instance (Section 7). The results can then be extracted from the `geoSetting` class instance and plotted, used in further calculations, or saved (see the tutorial notebooks).

3 Mantle lithologies

The experiments that are used to parameterise melting models are performed on particular bulk compositions, or lithologies. This means that each melting model, unless parameterised also for bulk composition [e.g., Lambart et al., 2016], represents a particular lithology, with its own melting behaviour. At a minimum, the `lithology` class has methods defined for the solidus and liquidus temperatures as a function of pressure P (`TSolidus` and `TLiquidus`), and for the melt fraction F as a function of P and

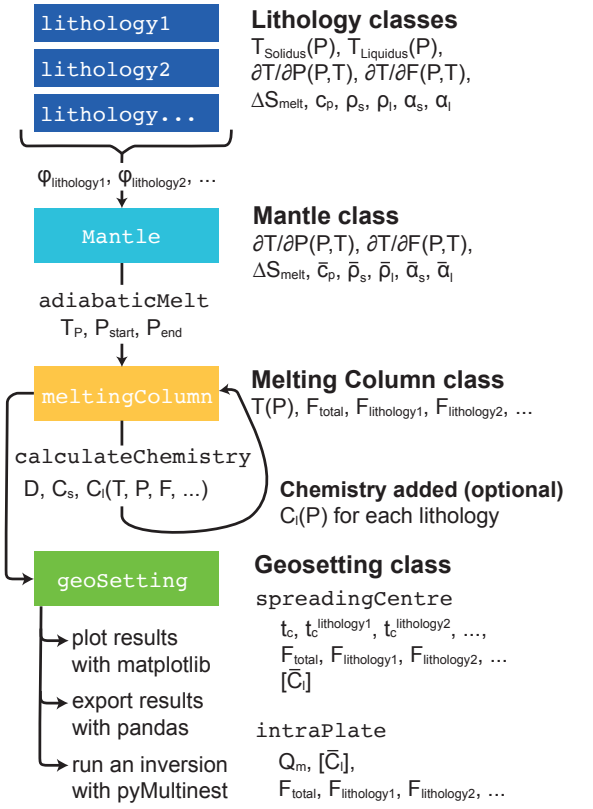

Figure 1: Summary of the structure of pyMelt. Each box represents an instance of a pyMelt class, either created directly by the user (with variables as specified on the arrows) or returned by a method call. The properties and methods of each class are shown on the right hand side (symbols as defined in the text).

temperature T (`F`). The models contained within pyMelt already have methods for $\left(\frac{\partial T}{\partial F}\right)_P$ (`dTdF`) and $\left(\frac{\partial T}{\partial P}\right)_F$ (`dTdP`), but pyMelt can also calculate their values numerically from the `TSolidus`, `TLiquidus`, and `F` methods. Additionally, each lithology has values associated with it for the density of the solid lithology ρ_s and its melt ρ_l,their thermal expansivities α_s and α_l, the heat capacity C_p, and the entropy change on melting ΔS.

Table 1 lists the melting models for which `lithology` classes are defined in pyMelt. The pyroxenitic lithologies are categorised as having a relative excess or deficit in silica, with the silica-excess models in pyMelt representing a mid-ocean ridge basalt like composition, and the silica-deficient pyroxenites representing a mixture of basalt and lherzolite.

4 Mantle melting

Before melting calculations can be performed, the `lithology` class instances must be assembled in a `Mantle` class, with their relative mass fractions spec-

Table 1: The pure lithology melting models built into pyMelt. See Lambart et al. [2016] for a description of the pyroxenite classification.

Reference	Class name	Lithology type
McKenzie and Bickle [1988]	`mckenzie.lherzolite`	Lherzolite
Pertermann and Hirschmann [2003]	`pertermann.g2`	Pyroxenite (silica-excess)
Katz et al. [2003]	`katz.lherzolite`	Lherzolite
Shorttle et al. [2014]	`shorttle.kg1`	Pyroxenite (silica-deficient)
	`shorttle.harzburgite`	Harzburgite (non-melting)
Matthews et al. [2021]	`matthews.klb1`	Lherzolite
	`matthews.kg1`	Pyroxenite (silica-deficient)
	`matthews.eclogite`	Pyroxenite (silica-excess)
Ball et al. [2022]	`ball.depleted`	Lherzolite
	`ball.primitive`	Lherzolite
	`ball.mixed`	Lherzolite

ified. pyMelt does not limit the number of lithologies that can be assembled in a `Mantle` class, though in most situations one each of a lherzolite, pyroxenite, and harzburgite lithology are sufficient. The `Mantle` class replicates many of the properties of the `lithology class` (Figure 1), with methods returning either the mass-weighted average properties, or an array with each lithology's value. Implicit in our treatment of the lithology objects, and our application of the melting formulation by Phipps Morgan [2001], is an assumption of complete thermal equilibrium but complete chemical disequilibrium between lithologies.

Adiabatic decompression melting calculations are performed by the `adiabaticMelt` method of the `Mantle` class, requiring only that a value for T_p is specified. By default the calculation will begin at the solidus and end at 0.01 GPa with a pressure decrement of 0.004 GPa at each decompression step; though all of these parameters can be modified.

The calculation proceeds by simultaneously integrating $\frac{dF}{dP}$ for each lithology i, and $\frac{dT}{dP}$ for the melting assemblage, to obtain the melt fractions (F_i) of each lithology and the mantle temperature (T) at each step. The value of $\frac{dF}{dP}$ is determined for each melting lithology using Eq. 29 of Phipps Morgan [2001] (the mass-weighted average values of c_p, α, and density ρ are indicated with a bar):

$$\frac{dF_i}{dP} = -\frac{\frac{\overline{c_p}}{T}\frac{\partial T_i}{\partial P} - \frac{\overline{\alpha}}{\overline{\rho}}\sum_{n\neq i}\left[\phi_n \Delta S_n^m \frac{\frac{\partial T_i}{\partial P} - \frac{\partial T_n}{\partial P}}{\frac{\partial T_n}{\partial F_n}}\right]}{\phi_i \Delta S_i^m + \sum_{n\neq i}\left[\phi_n \Delta S_n^m \frac{\frac{\partial T_i}{\partial F_i}}{\frac{\partial T_n}{\partial F_n}}\right] + \frac{\overline{c_p}}{T}\frac{\partial T_i}{\partial F_i}} \quad (1)$$

The value of $\frac{dT}{dP}$ is then obtained from Eq. 28 of Phipps Morgan [2001] using the values for one lithology j (arbitrarily, the one with the most negative $\frac{dF}{dP}$ in pyMelt):

$$\frac{dT}{dP} = \frac{dT_j}{dP} + \frac{dT_j}{dF_j}\frac{dF_j}{dP} \quad (2)$$

The integration is performed using a fourth-order Runge-Kutta routine. The results of the melting calculation are returned as a `meltingColumn` class, which records the melt fractions of each lithology, in addition to the aggregate melt fraction and the temperature at each pressure step.

When the calculation is started at a specified pressure, high mantle T_p may mean the mantle has already exceeded its solidus. In this case an interval of isobaric melting will occur before decompression starts, such that entropy is conserved. The computational method for this isobaric step is described in the supporting information of Matthews et al. [2021]. Decompression melting then proceeds, as described above.

Since the Phipps Morgan [2001] melting formulation assumes batch melting (whereby the melt is not separated from the solid residue), when performing calculations where one lithology is more fusible than another lithology j, the heat extracted by melting of the more fusible lithology can cause $dF_j/dP > 0$ (i.e., refreezing) in the other lithology. By default pyMelt will prevent freezing from occurring by setting $dF_j/dP = 0$, thereby more closely representing continual melt extraction. This is set as the default behaviour because the `chemistry` module requires monotonically increasing melt fractions.

5 Hydrous melting

Any lithology in pyMelt can be turned into a hydrous lithology using the `hydrousLithology` class. To approximate the effect of hydrous melting a similar formulation to that developed by Katz et al. [2003] is used. In this formulation the solidus temperature is depressed according to their Eq. 16:

$$T_{\text{solidus}}^{\text{hydrous}} = T_{\text{solidus}} - K X_{\text{H}_2\text{O}}^{\gamma} \quad (3)$$

where K and γ are constants and $X_{\text{H}_2\text{O}}$ is the water concentration in the melt in wt%. This differs slightly from the equations developed by Katz et al. [2003] as they did not apply the $-KX_{\text{H}_2\text{O}}^{\gamma}$ term to every instance of T_{solidus} in their expressions (e.g., their Eq. 19). The amount of water that can be

dissolved in magmas is limited, but increases with pressure. Katz et al. [2003] model this effect using (their Eq. 17):

$$X^{\text{sat}}_{H_2O} = \chi_1 P^{\lambda} + \chi_2 P, \quad 0 < \lambda < 1 \tag{4}$$

which is also implemented in pyMelt.

The concentration of H_2O present in the melt decreases as melting proceeds, owing to H_2O partitioning favourably into the melt and being continually diluted by new additions of magma. Katz et al. [2003] modelled this change by using the batch melting equation:

$$X_{H_2O} = \frac{X^{\text{bulk}}_{H_2O}}{D_{H_2O} + F(1 - D_{H_2O})} \tag{5}$$

where D_{H_2O} is the partition coefficient during melting. We extend this formulation to consider also the removal of H_2O from the system by near-fractional melting, as modelled previously by Asimow et al. [2003]; however, since the melting models in pyMelt are implicitly expressions of batch (or equilibrium) melting, modelling the effect of H_2O extraction by fractional melting cannot be done entirely self-consistently. The effect is approximated in pyMelt by replacing Eq. 5 with an expression for near-fractional melting:

$$X_{H_2O} = \frac{X^{\text{bulk}}_{H_2O}}{(1-\phi)D + \phi}(1-F)^{\frac{(1-\phi)(1-D)}{(1-\phi)D}} \tag{6}$$

where ϕ is the porosity during melting.

When a `hydrousLithology` class is created, the supporting methods from the original `lithology` class are copied, along with the `TLiquidus` method (which is not changed by the hydrous melting extension). A new method for `TSolidus` is defined, which applies Eq. 3 to the original `TSolidus` method. Since the value of F depends on X_{H_2O}, which itself depends on F, a new `F` method is created, which solves the equation:

$$F_{\text{calc}}(P, T, F_{\text{guess}}) - F_{\text{guess}} = 0 \tag{7}$$

where $F_{\text{calc}}()$ is the original `F` method (which will provide the hydrous melt fraction as it calls the modified `TSolidus` method) and F_{guess} is the value changed by the root finding method. pyMelt uses the `brentq` algorithm implemented in the `SciPy.optimize.root_scalar` method [Virtanen et al., 2020]. New methods for $\left(\frac{\partial T}{\partial F}\right)_P$ and $\left(\frac{\partial T}{\partial P}\right)_F$ are created, which calculate the values numerically using `SciPy.misc.differentiate`, alongside `SciPy.optimize.root_scalar` to find the T-P curve at constant F.

The default values for K, γ, χ_1, χ_2, λ, and D_{H_2O} are taken from Katz et al. [2003] who calibrated them for hydrous-lherzolite melting. While pyMelt provides the opportunity to model hydrous-pyroxenite melting in the same way, the user must choose appropriate constant values for pyroxenite.

6 Trace elements

Following the creation of a `meltingColumn` class by the `mantle.adiabaticMelt` method, the pyMelt `chemistry` module can be used to calculate the trace element contents of the melts $C_{i,l}$ (Figure 1). The calculation is performed by the `meltingColumn.calculateChemistry` method and requires the concentration of each trace element in each lithology $C_{i,s}$, in addition to the parameters required by the chemical model (e.g., the partition coefficients D_i). There are four built in chemical models: batch melting, near-fractional melting (instantaneous and accumulated melts), and the INVMEL forward model [McKenzie and O'Nions, 1991]. For the batch and near-fractional melting models the partition coefficient can either be a constant, or a user defined function of F, P, and T.

Each element (in each lithology) to be included in the calculation is defined as a `species` class instance that contains its solid concentration c_0 and a `composition` method for calculating the melt composition as a function of F (and possibly P and T). Defining each element separately permits the incorporation of more complex partitioning behaviour for some elements alongside simpler models for other elements. Generally, users will be unaware of the `species` class: the `meltingColumn.calculateChemistry` method can assemble them automatically.

The INVMEL model incorporates the effects of phase changes and phase exhaustion on the partioning of trace elements, in particular the effects of garnet- and clinopyroxene-present melting, but requires many more parameters to be defined. The partition coefficients used by default are those compiled by Gibson and Geist [2010], and other parameters are set to the values used by Ball et al. [2021].

For convenience, the `chemistry` module has a number of estimates for partition coefficients and mantle trace element concentrations built in (see the documentation for more details).

7 Geological settings

In many cases the information provided by the `meltingColumn` object is sufficient; in other cases a user may be interested in derived properties for a particular geological setting, aggregate melt compositions for example. The pyMelt `geoSetting` classes (`spreadingCentre` and `intraPlate`) provide this facility, taking a `meltingColumn` instance as an input (Figure 1).

When calculating aggregate properties of the melting region we must consider how each melt in the melting column should be weighted to account for mantle flow. For example, active upwelling in a mantle plume causes more mantle ma-

terial to pass through the melting region at its base [Maclennan et al., 2001], meaning deeper melts should have a greater weighting in plume models. User defined weighting functions may be specified for each calculation, but how they are implemented varies between `geoSetting` classes. An example weighting function built into pyMelt (`geosettings.weighting_expdecay`) has the form:

$$w(P) = \mu \exp\left(-\frac{1}{\lambda}\frac{P_{\max} - P}{P_{\max} - P_{\min}}\right) \tag{8}$$

where λ and μ are constants, and $P_{\max}$ and $P_{\min}$ are the maximum and minimum pressures from which melts are formed at the geological setting.

7.1 Spreading centres

When an instance of the `spreadingCentre` class is initialised, the crustal thickness will be calculated, assuming passive corner-flow mantle upwelling [Plank and Langmuir, 1992]. To account for the triangular melting region, the total melt fraction is integrated over the melting column, until the pressure exerted by the crust (calculated by stepwise integration with the trapezium rule) is equal to the pressure of the melting step:

$$t_c = \frac{1}{g\rho_c}\int_{P_{\text{start}}}^{P_{\text{crust}}} (1+w)\frac{\sum \phi_i F_i}{1-\sum \phi_i F_i} dP \tag{9}$$

where g is the acceleration due to gravity on Earth, and ρ_c is the density of the crust. The term w is the optional user-defined weighting function, which takes $w = 0$ by default. Using the form $1 + w$ allows separation of the passive upwelling component and the active upwelling component. The $(1 - \sum \phi_i F_i)$ term in the denominator accounts for compaction, i.e., mantle material will continuously replace the volume lost due to melt extraction [White et al., 1992]. The contributions of each lithology to the aggregate crust is calculated similarly:

$$t_c^n = \frac{1}{g\rho_c}\int_{P_{\text{start}}}^{P_{\text{crust}}} (1+w)\frac{\phi_n F_n}{1-\sum \phi_i F_i} dP \tag{10}$$

When modelling continental rifts, the pressure exerted by the lithosphere can be imposed and the thickness of igneous crust calculated.

If the `meltingColumn` class used to generate the `spreadingCentre` class has chemistry, upon initialisation of the `spreadingCentre` class, the composition of the homogenised melt is calculated. Similarly to the crustal thickness calculations, homogenisation of chemistry takes into account the triangular melting region, compaction and any additional weighting function. The equation is modified from McKenzie and O'Nions [1991]:

$$\overline{C} = \frac{\int_{P_{\text{start}}}^{P_{\text{end}}} (1+w)\frac{\sum \phi_i F_i C_{l,i}}{1-\sum \phi_i F_i} dP}{\int_{P_{\text{start}}}^{P_{\text{end}}} (1+w)\frac{\sum \phi_i F_i}{1-\sum \phi_i F_i} dP} \tag{11}$$

and is evaluated using the trapezium rule. If the calculated melt compositions represent instantaneous and not batch melts, each column is first homogenised, with each melt weighted according to its lithology fraction and melt fraction, as above. The weighting function $w(P)$ is not applied in this step.

The crystallisation temperature of melts extracted from the top and base of the melting region can be calculated, using the method described by Matthews et al. [2016]. The olivine saturation temperature at the pressure of magma storage is found using the pressure dependence of the olivine saturation surface [$39.16\,\text{K}\,\text{GPa}^{-1}$, Putirka, 2008]. This method is available also in the `intraPlate geoSetting` class.

7.2 Intra-Plate settings

To initialise an instance of the `intraPlate geoSetting` class, the pressure at the base of the lithosphere must be provided. The calculation results stored in the `meltingColumn` will be truncated at that pressure. If the relative density of the mantle is provided ($\Delta\rho = \rho_{\text{ambient-mantle}} - \rho_{\text{plume-mantle}}$), the melt flux Q_m is calculated during initialisation using the equation:

$$Q_m = \frac{\pi}{8}\frac{\Delta\rho g r^4}{\mu}\sum \phi_i \int_0^{F_{i(\max)}} w\, dF_i \tag{12}$$

which is modified from the equation for volume flux through a deformable conduit [Turcotte and Schubert, 2002]. $F_{i(\max)}$ is the melt fraction of lithology i at the top of the conduit, r is the conduit radius (default: 100 km), and μ is the viscosity of the plume (default: 10^{19} Pa s), with the default values taken from Shorttle et al. [2014].

If the `meltingColumn` class used to initialise the `intraPlate` class has chemistry and the melt compositions represent instantaneous melts, they will be homogenised during initialisation according to:

$$\overline{C} = \frac{\sum \phi_i \int_0^{F_{i(\max)}} w\, C_i\, dF_i}{\sum \phi_i \int_0^{F_{i(\max)}} w\, dF_i} \tag{13}$$

If the melt compositions represent accumulated melts and there is a weighting function applied, no result will be returned.

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Author contributions

SM conceived the idea of a modular mantle melting engine built in Python, and designed the over-

arching structure of the library. SM and KW wrote the code for the melting models, developed the documentation, and drafted the manuscript. KW led the development of the INVMEL chemistry code and many of the features in the chemistry module. MG developed the hydrous melting code, which was generalised by SM. All authors contributed to editing the manuscript.

Data availability

The latest version of pyMelt can be obtained from github.com/simonwmatthews/pyMelt and the pip package manager. pyMelt version v1.960 is archived in a Zenodo repository with DOI 10.5281/zenodo.6013925.

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