

1 From Magma Chambers to Magma Oceans: A Unified  
2 Model for the Thermo-chemical-mechanical Evolution of  
3 Magma Bodies

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8 February 5, 2025

9 *This is a non-peer reviewed preprint submitted to EarthArXiv.*

## Abstract

Magma bodies play a critical role in Earth’s geological evolution, influencing volcanic activity, crustal differentiation, and planetary-scale processes. Understanding their thermo-chemical and mechanical evolution requires models that integrate fluid dynamics, phase changes, and chemical transport. This study presents a new numerical model that couples these processes using a multi-phase, multi-component formulation. The model simulates convection, phase segregation, and thermo-chemical evolution across a wide range of scales, from crustal magma chambers to planetary magma oceans. To ensure numerical stability and physical realism, adaptive regularisation schemes are implemented, including eddy diffusivity for higher-dimensional turbulent flows and convective mixing diffusivity for one-dimensional column models. Benchmark tests confirm the accuracy of the numerical scheme, and use cases demonstrate its applicability to scenarios such as fractional crystallisation, wall-rock assimilation, and magma recharge on crustal scales, and magma ocean solidification on planetary scales. By providing an open-source implementation, this work aims to advance our understanding of dynamic magmatic systems and their role in planetary evolution.

## 1 Introduction

Melt-rich magma chambers in Earth’s crust have long been recognised as sources of volcanic eruptions and sites of magma differentiation [e.g., [Marsh, 1989](#)]. These chambers host complex processes, including fractional crystallisation, crustal assimilation, magma recharge, and mingling or mixing. These end-member processes drive the differentiation trends and geochemical diversity observed in igneous rocks.

Similar processes occur in planetary-scale magma oceans [e.g., [Abe, 1997](#)], a critical stage of early planetary evolution when large portions of terrestrial bodies remain molten. Their crystallisation, driven by heat loss to space, induces simultaneous turbulent convection and phase segregation, forming mantle- and crust-like layers that set the initial conditions for long-term solid-state evolution.

All of these processes arise from the dynamic interplay of material transport, governed by multiphase fluid mechanics, and phase change and chemical exchange, dictated by multi-component chemical thermodynamics. While fluid mechanics [e.g., [Keller and Suckale, 2019](#)] and chemical thermodynamics [e.g., [Ghiorso and Sack, 1995](#)] are well-described individually, their non-linear interactions pose a significant challenge.

Addressing this requires numerical models that couple fluid mechanics with the thermo-chemical evolution of melt-rich magma bodies. Such models must simulate magma dynamics across a range of scales and compositions while accurately predicting major, trace, and isotopic magma compositions.

Active magma bodies are largely cryptic, with direct observations limited by their burial in the deep subsurface or loss in deep geological time. Our understanding of their dynamics and thermo-chemical evolution is derived from remote geophysical observations and the structural,

49 analytical, and experimental study of igneous rocks.

50 Geophysical data interpretation is constrained by limited spatial resolution relative to  
51 magma body size, brief observation windows compared to system lifespans, and an inherent  
52 non-uniqueness of interpretation. Structural, analytical, and experimental studies of volcanic  
53 and plutonic rocks, including phase transformations under varying temperature and pressure,  
54 provide valuable constraints on magma body dynamics. The density [Iacovino and Till, 2019],  
55 viscosity [Giordano et al., 2008], and melting behaviour [Holland et al., 2018] of many igneous  
56 materials are well understood.

57 However, interpreting major, trace, and isotopic compositions of igneous rocks remains  
58 challenging due to non-unique signatures inherited from mantle and crustal sources, as well  
59 as overprints from reaction-transport processes during magma ascent and storage. Magma  
60 oceans, being utterly inaccessible, are preserved only in lunar and meteorite records, where  
61 sparse samples complicate interpretation. Closing these knowledge gaps requires a method to  
62 resolve how petrological and geochemical signatures emerge from complex reaction-transport  
63 dynamics in magma bodies across crustal to planetary scales.

64 In this work, I present a comprehensive new model of melt-rich magma body dynamics and  
65 petrological and geochemical evolution. This contribution includes the formulation of governing  
66 equations, their numerical implementation, and demonstrations of key use cases. These include  
67 calibrating the petrological model to a specific petrogenetic context and simulating classical  
68 processes such as fractional crystallisation, host rock assimilation, magma recharge followed by  
69 mingling and mixing, and magma ocean solidification.

70 The model applies to both crustal-scale magma bodies and planetary-scale magma oceans.  
71 This broad applicability is enabled by an adaptive regularisation scheme that accounts for en-  
72 hanced mixing by sub-grid turbulent eddies. Additionally, reduced-dimensionality modes allow  
73 for rapid and efficient zero-dimensional box models of equilibrium and fractionating system evo-  
74 lution paths, as well as one-dimensional column models incorporating parameterised convective  
75 mixing.

76 Previous models of crustal magma chamber evolution fall into two categories, each address-  
77 ing complementary but incomplete aspects of these systems. The first category treats magma  
78 chambers as radially symmetrical, isotropic bodies, where temperature, phase proportions, in-  
79 ternal pressure, and chamber volume evolve in response to continuous magma recharge, expo-  
80 sure to cool visco-elastic wall rock, and periodic evacuation by eruption [Jellinek and DePaolo,  
81 2003, Karlstrom et al., 2010, Degruyter and Huber, 2014].

82 These models are useful for studying magma chamber growth, thermal stability, and erup-  
83 tion potential under varying conditions. However, they do not resolve internal convection or  
84 phase segregation, making them incapable of predicting the geochemical consequences of inter-  
85 nal dynamics or the generation and destruction of chemical diversity in magmas.

86 The second category of models represents magma chambers by coupling thermodynamic  
87 phase equilibria with mass balance calculations of diverse chemical components. These evolve  
88 through algorithmic recipes representing fractional crystallisation, crustal assimilation via remelt-

89 ing and stoping (ingestion of crustal blocks from the roof), and recharge from deeper levels of  
90 an assumed transcrustal magma system [Bohrson et al., 2014, 2020, Heinonen et al., 2020].

91 While these models effectively reproduce differentiation trends and geochemical diversity  
92 observed in igneous rocks, they do not resolve internal magma chamber dynamics. Instead,  
93 they rely on idealised assumptions for fractionation, assimilation, and recharge rates, without  
94 accounting for how these processes are constrained by conservation of momentum and energy  
95 in natural systems.

96 Previous models of magma oceans generally follow two approaches, similar to those used for  
97 magma chambers. One class of models employs reduced dimensionality, often treating magma  
98 oceans as well-mixed reservoirs or layered convective systems with simplified phase change  
99 dynamics [e.g., Abe, 1993]. These models provide insight into large-scale thermal evolution,  
100 including heat loss to space, convective vigour, and the timescales of crystallisation. However,  
101 they do not fully resolve the interactions between phase change, convective flow, and phase  
102 segregation, limiting their ability to capture the development of compositional heterogeneity  
103 and its consequences for planetary differentiation.

104 A second class of models focuses on petrological evolution, often incorporating algorithmic  
105 prescriptions for the formation of cumulate stacks, flotation crusts, and residual melt layers.  
106 These approaches effectively reconstruct differentiation sequences and predict the final geochem-  
107 ical stratigraphy of solidified magma oceans. However, they rely on assumed phase separation  
108 efficiencies and mixing rates, rather than explicitly simulating the interplay of thermodynamics,  
109 fluid dynamics, and phase segregation. As a result, they may overlook the self-consistent feed-  
110 backs between crystallisation, melt migration, and convective redistribution, which are crucial  
111 for understanding the final structure of differentiated planetary interiors.

112 Few models of magma body evolution have integrated both multi-phase transport and multi-  
113 component reactions in one [Solano et al., 2012, Jackson et al., 2018] or two [Dufek and Bachmann,  
114 2010, Gutiérrez and Parada, 2010] spatial dimensions. While the latter studies represent the  
115 current state of the art, their methods and results have not been reproduced or widely applied  
116 in over a decade. Neither model has been made publicly available, raising questions about their  
117 implementation and reproducibility.

118 To advance beyond the *status quo*, this contribution introduces a new open-source numerical  
119 model for multi-phase, multi-component magma dynamics, enabling the study of system-scale  
120 thermo-chemical-mechanical evolution in crustal magma bodies. The model represents magma  
121 as a mixture of three material phases: silicate melt, crystals, and volatile fluid bubbles. These  
122 phases are composed of approximately half a dozen pseudo-components, calibrated to reflect a  
123 specific petrogenetic context.

124 The model follows the generalised framework of Keller and Suckale [2019] and is based on  
125 continuum mixture theory. This approach assumes that system-scale behaviour can be ef-  
126 fectively described by governing equations formulated through averaging over a large sample  
127 of local-scale phase topologies and their interactions. However, averaging small-scale inter-  
128 actions to derive large-scale dynamics is generally intractable. Consequently, the model re-

129 lies on strongly idealised phenomenological material coefficients to represent how local-scale  
130 phase topologies permit fluxes of mass, momentum, and entropy within and between phases  
131 [Keller and Suckale, 2019].

132 The model is formulated in the zero-segregation-compaction-length limit (ZSCL) [Wong and Keller,  
133 2023], where crystals and bubbles are treated as being suspended in melt, the carrier phase,  
134 while compaction effects in solid-rich layers are neglected.

135 The model is numerically implemented in Matlab using a staggered-grid finite-difference  
136 discretisation with a grid-based, non-oscillatory, conservative advection scheme for material  
137 transport and a second-order implicit time integration scheme. The numerical algorithm is  
138 validated through the Method of Manufactured Solutions and by verifying accurate conservation  
139 of mass and energy over time.

140 Phase equilibrium is determined using an idealised pseudo-phase diagram based on temper-  
141 ature, pressure, and bulk composition. This local phase equilibrium model is calibrated against  
142 a state-of-the-art thermodynamic equilibrium solver [Riel et al., 2022] using a Markov-Chain  
143 Monte Carlo (MCMC) parameter fitting routine.

144 The applicability of the model is demonstrated across zero-dimensional (0-D) box models,  
145 one-dimensional (1-D) column models, and two-dimensional (2-D) vertical cross-section models.  
146 0-D box models are used to generate equilibrium and fractional crystallisation sequences, while  
147 1-D column models highlight the role of gravity-driven phase segregation in magma differen-  
148 tiation. The effect of convective mixing on the equilibration of temperature and composition  
149 within convectively unstable layers is parameterised using an effective diffusivity approach.

150 In 2-D models, the system exhibits a range of convection styles, from whole-chamber mixing  
151 to layered convection, with asymmetrical evolution of convectively stable and unstable boundary  
152 layers controlling the thermo-chemical evolution. Scenarios approaching turbulent convection  
153 are regularised using an eddy viscosity approach, adaptively increasing momentum, thermal,  
154 and chemical diffusivities to limit grid-scale eddy development. This methodology enables  
155 simulations spanning from the 10-metre scale of crustal sills to the 1000-km scale of planetary  
156 magma oceans. The simulation code is released as an open-source software package.

## 157 **2 Methods**

### 158 **2.1 Model Overview**

159 The mathematical model and its numerical implementation are structured as follows: (i) the  
160 mixture model, defining material phases and chemical components representing the physical  
161 and chemical states of magma; (ii) the petrological model, describing how phase proportions  
162 and compositions depend on pressure, temperature, and bulk composition; (iii) the thermo-  
163 chemical model, governing the evolution of phase fractions, composition, and heat content over  
164 time via conservation of energy and mass; (iv) the fluid-mechanics model, based on bulk mass  
165 and momentum conservation, to compute magma mixture and phase segregation velocities as  
166 well as magma pressure; (v) the material model, providing closures for magma density, viscosity,

167 and phase segregation coefficients; and (vi) the geochemical model, tracking the evolution of  
168 geochemical tracers using mass conservation.

169 The section concludes with the numerical implementation of the governing equations using  
170 a finite-difference scheme on a regular, square, staggered grid, a flexible three-point (semi-  
171 )implicit time integration scheme, and regularisation techniques for representing eddy mixing  
172 in turbulent flows and convective layer mixing in 1-D column models.

173 The model is posed in a Cartesian coordinate system  $\mathbf{x}$  with its origin at the top of the  
174 magma body and the  $z$ -coordinate pointing vertically down in the direction of gravity  $\mathbf{g} = g\hat{\mathbf{z}}$ .  
175 For the sake of generality, the governing equations are given in full 3-D form, but the numerical  
176 implementation that follows is limited to 0-D, 1-D, and 2-D Cartesian cases.

177 All variables and parameters are generally functions of space,  $\mathbf{x}$ , and time,  $t$ , unless noted  
178 otherwise.

## 179 2.2 Mixture Model

### 180 2.2.1 Phases

181 The model is formulated at the system scale ( $\sim 10$ - $1000$  m) using a continuum mixture approach  
182 [Passman et al., 1984, Drew and Passman, 2006, Keller and Suckale, 2019]. Magma is treated  
183 as a three-phase mixture consisting of a liquid silicate melt suspending solid silicate crystals and  
184 volatile fluid bubbles. Each phase is characterised by its mass fractions,  $f^i$  [wt = kg/kg], with  
185  $i = m, x, f$  for melt, crystal, and fluid phases, mass densities,  $\rho^i$  [kg/m<sup>3</sup>], and average local-scale  
186 constituent sizes,  $d^i$  [m]. Local-scale ( $\mu$ m–m) interactions between melt, crystals, and bubbles  
187 are not explicitly resolved but instead parameterised through idealised assumptions regarding  
188 phase topology (proportions, constituent sizes, connectivity) and their influence on large-scale  
189 deformation and transport. Phase mass fractions are converted into volume fractions using:

$$\phi^i = \frac{\bar{\rho}}{\rho^i} f^i, \quad (1)$$

190 where  $\bar{\rho} = (\sum_i f^i / \rho^i)^{-1} = \sum_i \phi^i \rho^i$ . Overbars denote phase-averaged bulk properties of the  
191 multi-phase mixture.

192 For readability, the following notations will occasionally be used for phase-specific mass and  
193 volume fractions:  $m = f^m$ ,  $x = f^x$ ,  $f = f^f$ , and  $\mu = \phi^m$ ,  $\chi = \phi^x$ , and  $\phi = \phi^f$ .

### 194 2.2.2 Components

195 In natural systems, magma consists of a dozen or more major and minor element oxides (e.g.,  
196 SiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, MgO, FeO, CaO) along with a few volatiles (mostly H<sub>2</sub>O, CO<sub>2</sub>). These elements  
197 form multiple thermodynamic phases, including minerals such as quartz, solid-solution end-  
198 members like forsterite and fayalite (olivine) or anorthite and albite (plagioclase), silicate melt,  
199 and volatile fluid.

200 Tracking the full chemical composition of all relevant thermodynamic phases would result

201 in a highly complex and computationally expensive model. To reduce complexity, the model  
202 constrains chemical variability to a relatively small number ( $\sim 4-8$ ) of dimensions, termed  
203 *pseudo-components*. These are represented by their bulk concentrations  $\bar{c}_j = xc_j^x + mc_j^m$  ( $j =$   
204  $1, \dots, n_{\text{cmp}}$ ), assuming partitioning only between one solid and one melt phase.

205 A special case is the volatile component, which exists only in the melt and fluid phases  
206 and is represented by its bulk concentration  $\bar{c}_v = fc_v^f + mc_v^m$ . Consequently, the solid phase  
207 is considered free of dissolved volatiles, while the fluid phase contains no dissolved pseudo-  
208 components.

209 To map pseudo-component compositions onto petrologically meaningful representations,  
210 each pseudo-component is assigned a reference composition based on a set of mineral end-  
211 members and their major oxide compositions. By selecting appropriate mineral end-members  
212 and tuning their oxide compositions, the pseudo-component approach can be calibrated to a  
213 specific petrogenetic context (see calibration procedure below).

## 214 **2.3 Petrological Model**

### 215 **2.3.1 Local Phase Equilibrium**

216 Understanding magmatic petrogenesis requires determining the local phase equilibrium, i.e., the  
217 stable proportions and compositions of thermodynamic phases at a given temperature  $T$ , ther-  
218 modynamic pressure  $P_t$ , and bulk composition  $\bar{c}_j$ . Various computational tools exist for calcu-  
219 lating local phase equilibria by minimising Gibbs free energy (e.g., MELTS [Ghiorso and Sack,  
220 1995], MAGEMin [Riel et al., 2022]). However, none are computationally robust or efficient  
221 enough to be used *on-the-fly* in a dynamic model, where phase assemblages must be rapidly  
222 and reliably determined across the model domain, multiple times per time step, over thousands  
223 of time steps.

224 One alternative is to pre-compute look-up tables, requiring only relatively inexpensive inter-  
225 polation during a coupled model run [Rummel et al., 2020]. However, this either significantly  
226 increases the memory footprint, as tables must cover the entire relevant  $P, T, \bar{c}_j$  space, or ne-  
227 cessitates a complex algorithm for dynamically generating tables based on the specific portions  
228 of parameter space accessed during a simulation. Additionally, artefacts from discrete repre-  
229 sentation and interpolation can introduce robustness issues.

230 Another alternative is to use simplified two-component phase diagrams, such as linearised  
231 solidus-liquidus planes [Weatherley and Katz, 2012], a single-phase loop [Katz, 2008], or single-  
232 sided eutectic [Solano et al., 2014]. While computationally efficient and conceptually straight-  
233 forward, these approaches capture only the first principal component of magma compositional  
234 diversity.

235 The approach adopted here formulates an adaptable multi-component pseudo-phase dia-  
236 gram based on simplified thermodynamic relations [Keller and Katz, 2016]. This method is  
237 robust and efficient enough for *on-the-fly* application while preserving sufficient complexity to  
238 capture well over 90% of magma compositional variance. It can be meaningfully calibrated



239 against full thermodynamic models and experimental data, as demonstrated below with a cal-  
 240 ibrated model example.

### 241 2.3.2 Pseudo-phase Equilibrium Model

242 Following this approach, we formulate a multi-component pseudo-phase diagram as a simplified  
 243 model of local phase equilibrium. The model determines phase proportions  $f^i$  and phase com-  
 244 positions  $c_j^i$  (for components  $j = 1, \dots, n_{\text{cmp}}, v$  in phase  $i = m, x, f$ ) at given  $P_t, T, \bar{c}_j$ . The phase  
 245 diagram forms an  $n_{\text{cmp}}$ -dimensional phase loop in  $T, \bar{c}_j$  space, shifting upward with increasing  
 246 pressure and downward with increasing melt volatile content.

247 Note that we assume local thermal and mechanical equilibrium, meaning the model uses a  
 248 single absolute temperature  $T \equiv T^i \geq 0$  and a single thermodynamic pressure  $P_t \equiv P_t^i$  for all  
 249 phases.

250 To incorporate volatile effects, we extend the method of Keller and Katz [2016] to account  
 251 for both the depression of melting temperatures due to dissolved volatiles and the exsolution  
 252 of fluid bubbles upon volatile saturation. While this approach can be generalised for multiple  
 253 volatiles, we limit the model to H<sub>2</sub>O as the sole volatile component here. Assuming no major  
 254 elements dissolve into the fluid phase, its composition is taken as constant and uniform:  $c_v^f \equiv$   
 255  $c_{\text{H}_2\text{O}}^f \equiv 1$  and  $c_j^f \equiv 0$  for all non-volatile components.

256 The following section summarises the multi-component pseudo-phase equilibrium model  
 257 of Keller and Katz [2016], highlighting its extension to a volatile-bearing, three-phase magma  
 258 system.

259 The model of Keller and Katz [2016] defines partition coefficients between solid and melt  
 260 phases for a set of pseudo-components, expressed as calibrated functions of pressure and tem-  
 261 perature. The partition coefficients  $K_j \equiv c_j^x/c_j^m$  follow a simplified relationship derived from  
 262 ideal solution thermodynamics:

$$K_j = \exp \left[ \frac{\Delta s}{r_j} \left( 1 - \frac{T}{T_{m,j}} \right) \right], \quad (2)$$

263 where  $\Delta s$  is the entropy jump of fusion (assumed constant and uniform for all components),  
 264  $T_{m,j}$  are pressure- and volatile-dependent pure-component melting temperatures, and  $r_j$  are  
 265 shape factors that adjust the phase diagrams to more open or closed phase loop topology.

266 The pressure dependence of all components follows a non-linear Simon's law [Rudge et al.,  
 267 2011], while the water dependence of melting temperatures is described by a power-law rela-  
 268 tionship [Katz et al., 2003]. The pure-component melting points are given by:

$$T_{m,j} = (T_{0,j} - D_j c_{\text{H}_2\text{O}}^m{}^p) \times \left( 1 + \frac{P_t}{A} \right)^{1/B}. \quad (3)$$

269 The parameters in (3) include the reference melting temperature at zero pressure and anhydrous  
 270 composition,  $T_{0,j}$ , as well as the component-specific prefactors  $D_j$  and power-law coefficient  
 271  $p = 0.75$  governing water dependence.



272 The melt water content  $c_{\text{H}_2\text{O}}^m$  at a given bulk water content  $\bar{c}_{\text{H}_2\text{O}}$  increases with crystallinity  
 273 (assuming solids are anhydrous) but is limited by the saturation point  $c_{\text{H}_2\text{O}}^{m,\text{sat}}$ :

$$c_{\text{H}_2\text{O}}^m = \min\left(\frac{\bar{c}_{\text{H}_2\text{O}}}{m}, c_{\text{H}_2\text{O}}^{\text{sat},m}\right). \quad (4)$$

274 Here, the empirical parameterisation of Moore et al. [1998] is used to calculate  $c_{\text{H}_2\text{O}}^{m,\text{sat}}$  as a  
 275 function of  $P_t, T, c_j^m$ .

276 With (2)–(4), local phase equilibrium is determined using the three-phase lever rule:

$$\bar{c}_j = mc_j^m + xc_j^x + fc_j^f, \quad (5)$$

277 along with unity sum constraints on phase and component fractions:

$$\sum_i f^i = 1, \quad (6a)$$

$$\sum_j c_j^i = 1. \quad (6b)$$

278 Solving (5) for  $c_j^m$  and  $c_j^x$ , while substituting the other phase composition using partition  
 279 coefficients and the given fluid composition, leads to an implicit equation for the melt fraction  
 280 at local phase equilibrium:

$$\sum_j \frac{\bar{c}_j - fc_j^f}{m/K_j + (1 - m - f)} - \sum_j \frac{\bar{c}_j - fc_j^f}{m + (1 - m - f)K_j} = 0, \quad (7a)$$

$$\bar{c}_{\text{H}_2\text{O}} - mc_{\text{H}_2\text{O}}^m - f = 0, \quad (7b)$$

281 which, together with (5) for  $j = v = \text{H}_2\text{O}$  solved for  $f$ , forms a system of equations for  $m, f$ .  
 282 This system can be solved using a root-finding method such as Newton’s method.

283 Once equilibrium phase proportions are obtained, phase component fractions are given by:

$$c_j^m = \frac{\bar{c}_j - fc_j^f}{m/K_j + (1 - m - f)}, \quad (8a)$$

$$c_j^x = \frac{\bar{c}_j - fc_j^f}{m + (1 - m - f)K_j}. \quad (8b)$$

284 Solidus and liquidus temperatures at a given bulk composition, pressure, and melt water  
 285 content are found by substituting  $m = 0$  and  $x = 0$  into (7a), along with partition coefficients  
 286 as a function of temperature (2), and solving for  $T$  using a suitable root-finding method.

### 287 2.3.3 Phase Equilibrium Calibration

288 While the above algorithm ensures a robust and efficient *on-the-fly* solution for local phase  
 289 equilibrium, the challenge lies in defining pseudo-components and calibrating their melting  
 290 parameters to approximate a given petrogenetic context. Keller and Katz [2016] calibrated

291 the model for mid-ocean ridge-style mantle decompression melting qualitatively by comparison  
292 with experimental constraints.

293 Here, we introduce a more quantitative approach using machine learning techniques. The  
294 following section provides a high-level summary of the procedure, with a detailed demonstration  
295 for an example petrological use case following further below.

296 Ground-truthing the calibration requires phase equilibrium data obtained from either petro-  
297 logical experiments or energy-minimising thermodynamic models. Since our focus is on solidi-  
298 fication and differentiation of melt-rich magma bodies, the dataset should ideally span temper-  
299 atures from the liquidus to near-solidus, covering a broad range of bulk compositions along a  
300 relevant liquid line of descent to capture a typical differentiation trend from primitive melt to  
301 the relevant eutectic minimum.

302 For simplicity, we currently restrict our analysis to dominantly anhydrous mineral assem-  
303 blages. However, this constraint could be relaxed in future work to incorporate volatile-bearing  
304 systems.

305 Given suitable ground-truth data, the calibration procedure consists of the following steps:

- 306 i. **Data Preparation:** Merge or discard minor or accessory phases (e.g., merge spinel +  
307 ilmenite, discard minor biotite near the solidus), remove minor elements (e.g., discard Ca  
308 in olivine, K in clinopyroxene), and normalise phase and mineral compositions to unity  
309 sum.
- 310 ii. **Mineral End-members:** Apply principal component analysis (PCA) and end-member  
311 estimation (EME) to simplify compositional trends and determine suitable end-members  
312 for each major mineral system (e.g., olivine, plagioclase, clinopyroxene).
- 313 iii. **Data Projection:** Use regularised least squares to project melt and solid phase com-  
314 positions onto the reduced compositional space of selected mineral end-members. Apply  
315 PCA and EME to determine the optimal number of pseudo-components, and extract an  
316 initial estimate of their compositions.
- 317 iv. **Final Calibration:** Refine pseudo-component compositions in terms of mineral end-  
318 member fractions and determine  $P_t, T$ -dependent melting parameters in (2)-(3) via an  
319 MCMC parameter fitting routine, minimising misfit between model predictions and ground-  
320 truth data for phase fractions, phase oxide compositions, and  $P$ -dependent solidus-liquidus  
321 constraints.

322 This procedure generalises across various petrological systems. Tested use cases include  
323 (shallow) fractional crystallisation following a tholeiitic trend for dry, reduced MORB-type  
324 basalt (demonstrated below), a calc-alkaline trend for wet, oxidised arc-type basalt, and an  
325 anhydrous lunar magma ocean composition (latter two not shown here).

326 Additionally, the calibration process helps judiciously limit complexity compared to the  
327 ground-truth dataset, which can be advantageous when formulating idealised petrogenetic hy-  
328 potheses for coupled modelling. Despite reducing compositional variability to a limited set of

329 mineral end-members forming a few pseudo-components, this approach still captures the evo-  
 330 lution of a comprehensive set of major mineral and melt phases and their oxide compositions  
 331 across model space and time. This, in turn, enables the use of material models (e.g., density,  
 332 viscosity; see below) as functions of mineral stability and oxide composition, producing results  
 333 directly comparable to igneous mineral and whole-rock compositional analyses.

## 334 2.4 Thermo-chemical Evolution Model

### 335 2.4.1 Energy and Entropy

336 To model the dynamic evolution of a magma body, we must track the temporal changes in  
 337 compositional variables and temperature (i.e., heat content). The sensible and latent heat  
 338 content of the magma is expressed using specific phase entropies,  $s^i$  [J/kg] [Rudge et al., 2011,  
 339 Katz, 2022], which sum to the mixture entropy weighted by phase mass fractions:  $\bar{s} = \sum_i f^i s^i$ .

340 Using entropy for energy conservation, rather than internal energy or enthalpy, naturally  
 341 incorporates latent heat and adiabatic effects without requiring additional terms in the gov-  
 342 erning equation. The melt phase entropy serves as the reference point for phase change  
 343 latent heat. The entropy jumps of crystallisation,  $\Delta s^x$ , and fluid exsolution,  $\Delta s^f$ , are as-  
 344 sumed uniform and constant, defining the crystal and fluid phase entropies relative to the melt:  
 345  $s^x = s^m + \Delta s^x$ ,  $s^f = s^m + \Delta s^f$ . Consequently, bulk entropy can be expressed as  $\bar{s} = s^m + \Delta \bar{s}$ ,  
 346 where  $\Delta \bar{s} = x \Delta s^x + f \Delta s^f$ .

### 347 2.4.2 Mass and Energy Conservation

348 The evolution of phase and component fractions and heat content follows the fundamental  
 349 principles of mass conservation and entropy production [Keller and Suckale, 2019]:

$$\frac{\partial F^i}{\partial t} + \nabla \cdot F^i \mathbf{v}^i = -\nabla \cdot \mathbf{q}_\phi^i + \Gamma^i, \quad (9a)$$

$$\frac{\partial C_j}{\partial t} + \nabla \cdot \sum_i F^i c_j^i \mathbf{v}^i = -\sum_i \nabla \cdot \mathbf{q}_j^i, \quad (9b)$$

$$\frac{\partial S}{\partial t} + \nabla \cdot \sum_i F^i s^i \mathbf{v}^i = -\nabla \cdot \mathbf{q}_s + \Upsilon_s. \quad (9c)$$

350 On the left-hand side, the equations describe rates of change (first term) and advective  
 351 fluxes carried by phase velocity fields  $\mathbf{v}^i$  (second term). On the right-hand side, they include  
 352 diffusive fluxes  $\mathbf{q}$ , phase change rates  $\Gamma^i$ , and the entropy production or heat dissipation rate  
 353  $\Upsilon_s$  (see below). We neglect heat production from radioactive decay and assume no external  
 354 sources or internal production of phase or component mass.

355 Equations (9) introduce quantity densities [ $\cdot/\text{m}^3$ ] as primary variables for phase, component,

356 and entropy evolution:

$$F^i = \bar{\rho} f^i, \quad (10a)$$

$$C_j = \bar{\rho} \bar{c}_j, \quad (10b)$$

$$S = \bar{\rho} \bar{s}. \quad (10c)$$

357 Several summation constraints apply. Since  $\sum_i f^i = 1$  (saturated mixture), we require  
 358  $\sum_i \mathbf{q}_\phi^i = 0$  and  $\sum_i \Gamma^i = 0$ . Summing (9a) over all phases yields bulk mass conservation:

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot \bar{\rho} \mathbf{v} = 0. \quad (11)$$

359 Similarly, since  $\sum_j c_j^i = 1$  (complete composition), we require  $\sum_j \mathbf{q}_j^i = 0$ . Summing (9b)  
 360 over all components again recovers bulk mass conservation (2.4.2).

### 361 2.4.3 Diffusive fluxes

362 The diffusive fluxes on the right-hand side of (9) include the heat flux  $\mathbf{q}_s$  driven by temperature  
 363 gradients, phase-wise component fluxes  $\mathbf{q}_j^i$  driven by gradients in phase component concentra-  
 364 tions, and phase volume fluxes  $\mathbf{q}_\phi^i$  driven by gradients in phase volume fractions  $\phi^i$  ( $i = m, x, f$ ):

365

$$\mathbf{q}_s = -k_s \nabla T, \quad (12a)$$

$$\mathbf{q}_j^i = -k_c \nabla c_j^i, \quad (12b)$$

$$\mathbf{q}_\phi^i = -k_\phi^i \Delta (\nabla \phi)^{i*}. \quad (12c)$$

366 The entropy diffusion parameter,  $k_s = \bar{k}_T/T$ , is the bulk thermal conductivity  $\bar{k}_T$  divided  
 367 by temperature. The component diffusion coefficient  $k_c$  does not represent molecular diffusion  
 368 of major elements, which is negligible at system scale, but instead captures the system-scale  
 369 effects of local fluctuations in phase segregation speeds and unresolved convective mixing in  
 370 turbulent flows and one-dimensional column models. The phase diffusion coefficient  $k_\phi^i$  serves  
 371 a similar role.

372 The operator  $\Delta(\cdot)^{i*}$  applied to phase fraction gradients in (12c) enforces the zero-sum con-  
 373 straint on phase volume fluxes. This method, along with the definitions of  $k_c$  and  $k_\phi^i$ , will be  
 374 further detailed in the section on model regularisations below.

### 375 2.4.4 Entropy and Temperature

376 While we represent the system's heat content in terms of entropy, it is often more convenient  
 377 to specify temperature directly. Temperature is required as input for the phase equilibrium  
 378 model introduced above and for several material models discussed below. Following standard  
 379 thermodynamic relations, changes in phase entropies can be expressed as functions of changes

380 to absolute temperature  $T$  and thermodynamic pressure  $P_t$ :

$$Tds^i = c_P^i dT - \frac{T\alpha_T^i}{\rho^i} dP_t, \quad (13)$$

381 where  $c_P^i$  is the specific heat capacity,  $\alpha_T^i$  the thermal expansivity, and  $\rho^i$  the mass density of  
382 phase  $i$ .

383 Multiplying all terms in (13) by partial phase densities  $\rho^i \phi^i$  and taking the sum over all  
384 phases  $\sum_i$  we find an expression for changes in temperature as a function of changes in phase  
385 entropies and pressure,

$$dT = \frac{\bar{\rho}T}{\bar{\rho}c_P} ds^m + \frac{\bar{\alpha}_T T}{\bar{\rho}c_P} dP_t. \quad (14)$$

386 Note that  $ds^i \equiv ds^m$  due to the simplifying assumption of uniform and constant entropy jumps  
387 of phase change made above. Other parameters are the phase-averaged heat capacity density  
388  $\bar{\rho}c_P$  and the phase-averaged thermal expansivity  $\bar{\alpha}_T$ . The evolution of potential temperature  $T_p$   
389 (the temperature a parcel of mass would have if brought to zero pressure without heat exchange  
390 with its environment) is given by a similar relationship,

$$dT_p = \frac{\bar{\rho}T}{\bar{\rho}c_P} ds^m. \quad (15)$$

### 391 2.4.5 Phase Closures

392 To solve eqs. (9) for the bulk densities  $S, C_j$ , we require closures for phase entropies  $s^i$  and  
393 phase compositions  $c_j^i$ . The latter are given by the phase equilibrium model in (8), while the  
394 former are extracted from the solution variable  $S$  as:

$$s^m = \frac{S}{\bar{\rho}} - \Delta \bar{s}_0, \quad (16a)$$

$$s^x = s^m + \Delta s_0^x, \quad (16b)$$

$$s^f = s^m + \Delta s_0^f. \quad (16c)$$

### 395 2.4.6 Pseudo-equilibrium Approach

396 Magma dynamics models coupling fluid mechanics to phase change have traditionally employed  
397 either equilibrium [Katz, 2008] or disequilibrium [Rudge et al., 2011] approaches. The equilib-  
398 rium approach directly imposes phase fractions and compositions from a phase diagram at each  
399 time step, eliminating the need for explicit phase and component mass conservation or reaction  
400 rate prescriptions. This simplifies the governing equations to energy and bulk composition  
401 conservation, as phase fractions and compositions remain constrained by the phase diagram.

402 However, achieving non-linear convergence in coupled heat and phase fraction evolution  
403 can be challenging, especially where minor temperature variations cause abrupt phase fraction  
404 changes, such as near cotectic or eutectic points. Stability often requires iterative lagging  
405 schemes. Additionally, the absence of explicit phase change rates complicates quantitative

406 diagnostics of phase change dynamics. While phase change rates can be reconstructed in post-  
 407 processing, this requires precise numerical reconstruction of phase advection, which can be  
 408 challenging.

409 The disequilibrium approach treats equilibrium phase properties as targets for reaction rate  
 410 terms in a full set of phase and component mass conservation equations. This allows phase  
 411 proportions and component concentrations to evolve dynamically while being nudged toward  
 412 equilibrium, capturing transient disequilibrium effects. Additionally, reaction rates provide key  
 413 diagnostic insights into reaction-transport coupling.

414 However, solving additional conservation equations increases computational cost, and ki-  
 415 netic models for reaction rates are often poorly constrained. Earlier studies [Keller and Katz,  
 416 2016] demonstrated that rapid reaction rates (relative to advective transport) recover behaviour  
 417 converging towards the equilibrium approach but exacerbate non-linear convergence challenges,  
 418 while slow reaction rates permit disequilibrium build-up that can destabilise solutions. Reac-  
 419 tion rates optimal for model stability and robustness must therefore constrain reaction rates to  
 420 drive equilibration on timescales similar to advective transport, effectively acting as a physics-  
 421 informed lagging scheme that maintains proximity to phase equilibrium while improving non-  
 422 linear convergence.

423 Here, I propose a hybrid pseudo-equilibrium approach that balances the conceptual appeal  
 424 and computational efficiency of equilibrium models with the diagnostic utility and numerical  
 425 robustness of disequilibrium methods. This approach defines linear kinetic reaction rates as:

$$\Gamma^i = \frac{\bar{\rho}}{\tau_r} (f_{\text{eq}}^i - f^i), \quad (17a)$$

426 where  $\Gamma^i$  represents mass transfer rates to phase  $i$  (melting  $\Gamma^m$ , crystallization  $\Gamma^x$ , fluid exso-  
 427 lution  $\Gamma^f$ ), subject to the zero-sum constraint  $\sum_i \Gamma^i = 0$ . These rates act as source terms in  
 428 phase mass conservation (9a).

429 The kinetic timescale  $\tau_r$  is adaptively set to a small multiple of the system's fastest transport  
 430 timescale (typically advection, occasionally diffusion). In the discretised system (see below),  
 431 the reaction time is set to  $\tau_r \equiv 10\Delta t$ , where  $\Delta t$  is the stable discrete time step, ensuring  
 432 equilibration lags slightly behind transport-driven disequilibrium.

433 By solving only bulk component concentrations (as in the equilibrium approach) rather  
 434 than individual phase compositions, computational costs remain low, and component-specific  
 435 phase change and chemical exchange reactions need not be explicitly defined [Rudge et al., 2011,  
 436 Keller and Katz, 2016]. Phase fractions evolve to closely track—but not fully match—equilibrium  
 437 states from the phase diagram. This minor deviation from the lever rule (5) necessitates adjust-  
 438 ing phase compositions to maintain consistency with slight disequilibrium in phase fractions.  
 439 A simple iterative procedure ensures that disequilibrium phase compositions conform to both  
 440 the lever rule as well as the unity sum constraint on complete compositions,  $\sum_j c_j^i = 1$ .

## 2.5 Fluid-mechanics Model

### 2.5.1 Mixture Flow

The fluid mechanics of the magma mixture are governed by the compressible Navier-Stokes equations:

$$\frac{\partial \bar{\rho} \mathbf{v}}{\partial t} + \nabla \cdot (\bar{\rho} \mathbf{v} \otimes \mathbf{v}) = \nabla \cdot \eta_\phi \underline{\mathbf{D}}(\mathbf{v}) - \nabla P + \Delta \bar{\rho} \mathbf{g}, \quad (18a)$$

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \mathbf{v}) = 0, \quad (18b)$$

where  $P$  is the mixture dynamic (non-lithostatic) pressure, and  $\mathbf{v}$  the mixture velocity. The mixture mass flux is given by  $\bar{\rho} \mathbf{v} = \bar{\rho}(\mathbf{v} + \sum_i f \Delta \mathbf{v}^i)$ , where  $\Delta \mathbf{v}^i = \mathbf{v}^i - \mathbf{v}$  represents the phase-to-mixture velocity differences.

In the ZSCL limit [Keller and Suckale, 2019, Wong and Keller, 2023], phase pressure differences are assumed negligible ( $P \equiv P^i$ ). The term  $\underline{\mathbf{D}}(\mathbf{v})$  denotes the deviatoric strain rate tensor, and  $\eta_\phi$  is the effective mixture viscosity;  $\partial/\partial t$  is the partial time derivative, and  $\nabla = \partial/\partial \mathbf{x}$  represents spatial derivatives.

Convective magma flow is driven by horizontal mixture density contrasts:

$$\Delta \bar{\rho} = \bar{\rho} - \langle \bar{\rho} \rangle_x, \quad (19)$$

where  $\langle \bar{\rho} \rangle_x$  is the horizontal average of the mixture density. This is used to integrate the corresponding lithostatic pressure:

$$P_{\text{lith}} = P_0 + \int \langle \bar{\rho} \rangle_x g dz, \quad (20)$$

with  $g$  as the gravitational acceleration and  $P_0$  as the surface pressure at  $z = 0$ .

### 2.5.2 Phase Segregation

Each phase is transported by the magma mixture flow but can segregate based on its relative buoyancy,  $\Delta \rho^i = \rho^i - \langle \bar{\rho} \rangle_x$ , and phase segregation mobility,  $K^i$ . In the ZSCL limit, phase segregation occurs purely due to buoyancy across suspension, mush, and porous flow regimes, with lateral segregation driven by compaction pressures assumed negligible [Wong and Keller, 2023]:

$$\Delta \mathbf{v}^i = \mathbf{v}^i - \mathbf{v} = K^i \Delta \rho^i \mathbf{g}. \quad (21a)$$

The phase segregation coefficients  $K^i$  are detailed below.

With the reference velocity of the magma mixture,  $\mathbf{v}$ , the phase segregation velocity differences,  $\Delta \mathbf{v}^i$ , and the phase diffusion fluxes,  $q_\phi^i$ , the effective phase velocities are given by:



$$\mathbf{v}^i = \mathbf{v} + \Delta \mathbf{v}^i + \mathbf{q}_\phi^i / \phi^i. \quad (22a)$$

### 466 2.5.3 Entropy Production

467 The entropy production rate,  $\Upsilon_s$ , accounts for heat dissipation due to magma convection, phase  
468 segregation, and heat diffusion:

$$\Upsilon_s = \frac{1}{T} \left( \check{\eta} [\underline{\mathbf{D}}(\mathbf{v})]^2 + \sum_i \frac{\phi^i}{K^i} [\Delta \mathbf{v}^i]^2 + k_s [\nabla T]^2 \right). \quad (23)$$

469 Here,  $[\mathbf{a}]^2 = \mathbf{a} \cdot \mathbf{a}$  and  $[\underline{\mathbf{a}}]^2 = \underline{\mathbf{a}} : \underline{\mathbf{a}}$  denote dot products of vectors and tensors with themselves.  
470 Contributions from chemical and phase volume diffusion, as well as phase change reactions, are  
471 assumed negligible and are omitted.

### 472 2.5.4 Net Volume Change and Pressure

473 As the model allows for compressible materials, flow problems generally exhibit some net volume  
474 change across the domain. To accommodate this, a uniform expanding or contracting velocity  
475 field is applied at the domain boundaries. For all tested scenarios, the amplitude of this volume-  
476 compensating boundary flow is negligible compared to internal convection and segregation  
477 speeds.

478 The model includes a simplified visco-elastic response of the wall rock to net volume  
479 change, calculating the resulting chamber overpressure relative to the surrounding wall rock  
480 [Degruyter and Huber, 2014]:

$$\frac{\partial P_{\text{chmb}}}{\partial t} = E_{\text{wall}} \dot{V}_{\text{chmb}} - \frac{E_{\text{wall}}}{\eta_{\text{wall}}} P_{\text{chmb}}, \quad (24)$$

481 where  $P_{\text{chmb}}$  is the chamber overpressure,  $E_{\text{wall}}$  the Young's modulus, and  $\eta_{\text{wall}}$  the shear viscosity  
482 of the wall rock. This calculation is only applicable where the model setup represents a magma  
483 body enclosed by wall rock.

484 The thermodynamic pressure  $P_t$  used in phase equilibrium calculations must be related to  
485 the mechanical pressure  $P$  from the fluid mechanics equations (18). Since the model does not  
486 account for bulk viscosity or elasticity, we assume that  $P_t$  corresponds to the full mechanical  
487 pressure, i.e., the sum of lithostatic pressure, dynamic pressures, and chamber overpressure:

$$P_t \equiv P + P_{\text{lith}} + P_{\text{chmb}}. \quad (25)$$

488 However, including dynamic and chamber pressure components can introduce nonlinear conver-  
489 gence issues between phase change and mechanical solutions. Thus, in practice, the coupling  
490 can be relaxed by approximating thermodynamic pressure as the lithostatic pressure alone:  
491  $P_t \approx P_{\text{lith}}$ .

## 2.6 Material Closures Model

### 2.6.1 Density

Applying the fluid mechanics model to melt-rich magma bodies requires suitable closures for phase densities, segregation coefficients, and effective mixture viscosity. Phase densities are computed using a linearised equation of state as a function of temperature and pressure:

$$\rho^i = \rho_0^i(c_j^i) \left( 1 - \alpha_T^i(T - T_0) + \beta_P^i(P_t - P_0) \right), \quad (26)$$

where  $\rho_0^i(c_j^i)$  is the composition-dependent reference phase density at reference conditions  $T_0, P_0$ ,  $\alpha_T^i$  is the phase thermal expansivity, and  $\beta_P^i$  is the phase compressibility, both assumed uniform and constant for each phase.

The compositional dependence of reference densities is determined using the melt oxide composition, following the DensityX model [Iacovino and Till, 2019] for melt density, and by averaging mineral end-member densities according to their mass fractions for solid density. Since the fluid phase consists only of water, its reference density is taken as a constant.

### 2.6.2 Phase Segregation Mobility

The phase segregation coefficients and effective mixture viscosity are computed based on the multi-phase material closures model of Keller and Suckale [2019]. These closures assume that shear stress within the mixture and momentum transfer between phases are mediated by local-scale momentum diffusion between phase constituents. The coefficients are derived from weighted geometric means of phase viscosity contrasts, with weights representing a phenomenological measure of local-scale phase connectivity. These are calibrated against theoretical models as detailed in Keller and Suckale [2019] and Wong and Keller [2023], with the three-phase calibration of Wong and Keller [2023] applied here.

One modification from previous work is that local-scale phase constituent sizes are not taken as constant but instead decrease as a function of their corresponding phase fraction:

$$d^i = d_0^i(1 - \phi^i)^{1/2}. \quad (27)$$

This reduces phase segregation mobility as a phase becomes dominant or forms the matrix. For example, in dilute suspensions, the segregation mobility of melt as the continuous phase is suppressed, while crystal settling and bubble flotation mobilities remain largely unaffected. Figure XXX illustrates how the resulting segregation coefficients and effective mixture viscosity vary with phase fractions for given reference phase viscosities  $\eta_0^i$  and constituent sizes  $d_0^i$ .

### 2.6.3 Viscosity

The effective mixture viscosity  $\eta_\phi$  is the volume average of effective phase viscosities [Keller and Suckale, 2019], which are in turn depend on composition and temperature. The reference melt viscosity is calculated as a function of melt oxide composition and temperature using the model of

524 [Giordano et al. \[2008\]](#). The reference solid viscosity is obtained from a geometric average of  
 525 mineral end-member viscosities, weighted by their relative volume fractions in the solid phase,  
 526 with an Arrhenius-type temperature dependence characterized by an activation energy  $E_a^x$ . The  
 527 potential pressure-dependence of viscosity is neglected.

## 528 2.7 Geochemical Evolution

529 In addition to the major and volatile components introduced above, trace elements and isotope  
 530 ratios are common tools used for detecting signatures of melt sources or dynamic transport  
 531 processes in igneous rock samples. As the geochemical variables do not affect the material  
 532 properties or phase equilibrium in the model system, they present a relatively inexpensive  
 533 model addition. Here, a group of geochemical concentrations,  $\bar{\theta}_k = \sum_i f^i \theta_k^i$  ( $k = 1, \dots, n_{\text{gch}}$ ) is  
 534 introduced to represent trace element concentrations or stable isotope ratios as elaborated in  
 535 the following paragraph. Geochemical concentrations are assumed to only partition between  
 536 the melt and crystal phases ( $\theta_k^f \equiv 0$ ) and are understood as dimensionless relative concentra-  
 537 tion normalised to some background concentration. The latter need not be specified unless  
 538 comparison to a specific data set is desired.

539 Trace elements partition between the melt and solid phases according to their partition  
 540 coefficients,  $K_k = \theta_k^m / \theta_k^x$ , such that  $K_k \gg 1$  represents an incompatible, and  $K_{tr} \ll 1$  a com-  
 541 patible trace element. Partition coefficients are defined as bulk averages of mineral end-member  
 542 partition coefficients such that mineral-specific trace element behaviour can be captured. For  
 543 stable isotope ratios,  $\theta_k$ , is assumed not to preferential partition between phases (i.e.,  $K_k \equiv 1$ ,  
 544  $\theta_k^x = \theta_k^m = \bar{\theta}_k$ ), hence providing a passive, non-fractionating tracer for the transport of melt  
 545 and crystal phases.

546 The geochemical evolution follows similar mass conservation laws as pseudo-components  
 547 above,

$$\frac{\partial \Theta_k}{\partial t} + \nabla \cdot \sum_i \theta_k^i \mathbf{v}^i = \nabla \cdot \sum_i \mathbf{q}_k^i . \quad (28)$$

548 The geochemical equations use the conserved trace element densities,

$$\Theta_k = \bar{\rho} \bar{\theta}^k , \quad (29)$$

549 as solution variables. Trace element densities evolve as a consequence of phase mass fluxes  
 550 carried on phase velocities  $\mathbf{v}^i$  and phase diffusive fluxes  $\mathbf{q}_k^i$  down trace element concentration  
 551 gradients,

$$\mathbf{q}_k^i = -k_c \nabla \theta_k^i , \quad (30)$$

552 using the same effective chemical diffusivity as major components to represent system-scale  
 553 mixing from regularising sub-grid scale turbulent eddies in 2-D models or convective mixing in  
 554 general in 1-D column models (see below). As trace element concentrations are interpreted as  
 555 normalised to some very small reference concentration no summation constraint over all trace  
 556 element is required in contrast to the major element component model above.

557 The phase trace element concentrations are found from the bulk concentration using the  
 558 partition coefficients and phase fractions,

$$\theta_k^m = \frac{\bar{\theta}_k}{m + xK_k}, \quad (31a)$$

$$\theta_k^x = \frac{\bar{\theta}_k}{m/K_k + x}. \quad (31b)$$

$$(31c)$$

559 Note that here it is assumed that trace elements are in instantaneous equilibrium with given  
 560 phase fractions..

## 561 2.8 Numerical Implementation and Model Setup

### 562 2.8.1 Spatial and Temporal Discretisation

563 The governing equations for fluid mechanics (18), thermo-chemical evolution (9), and geochemi-  
 564 cal evolution (28) are discretised using a staggered-grid finite-difference approach [Keller and Katz,  
 565 2016, Gerya, 2019, Katz, 2022, Wong and Keller, 2023]. Solution variables and material pa-  
 566 rameters are defined on a uniform grid of square cells with spacing  $h$ . Scalars are positioned  
 567 at cell centres, while vector components are placed on cell faces normal to their direction.  
 568 Diagonal tensor components are located at cell centres, and off-diagonal components at cell  
 569 corners. This arrangement enables second-order accurate central differencing for spatial deriva-  
 570 tives. Scalar parameters required at vector or tensor locations are averaged from adjacent cell  
 571 centres, using arithmetic means for most cases and geometric means for mixture viscosity and  
 572 phase segregation coefficients.

573 Mass flux divergence terms are discretised using higher-order, upwind-biased, flux-conservative  
 574 schemes, including the 2nd order Fromm scheme [Trompert and Hansen, 1996], the 3rd order  
 575 QUICK scheme [Leonard, 1995], the Total-Variation-Diminishing (TVD) scheme [Harten, 1997],  
 576 and 3rd and 5th order Weighted-Essentially-Non-Oscillating (WENO) schemes [Jiang and Shu,  
 577 1996].

578 Accurate and conservative advection schemes are crucial for modelling thermo-chemically  
 579 coupled magma dynamics. Keller et al. [2017] noted that advection-induced mass conserva-  
 580 tion errors are amplified in strongly partitioning chemical components, roughly proportional  
 581 to the magnitude of their partitioning coefficient. Comparisons indicate that the WENO-5  
 582 scheme best preserves mass conservation while minimising numerical diffusion and dispersion  
 583 [Dominguez et al., 2024]. Consequently, WENO-5 is recommended for advection-dominated 2-  
 584 D models, whereas lower-order schemes may suffice for numerically efficient 1-D column models.

585 The time-derivatives in thermo-chemical equations (9) are discretised using a generalised  
 586 time integration approach on a three-point stencil:

$$\frac{\partial Q}{\partial t} \approx \frac{a_1 Q^p - a_2 Q^{p-1} - a_3 Q^{p-2}}{\Delta t} = b_1 R(Q^p) + b_2 R(Q^{p-1}) + b_3 R(Q^{p-2}). \quad (32)$$

587 where  $Q$  represents the conserved quantity density,  $R(Q)$  its total rate of change,  $\Delta t$  the discrete  
588 time step, and  $p$  the time step counter. By selecting the time integration coefficients  $a_{1-3}$   
589 and  $b_{1-3}$ , this scheme can implement first-order Backward Euler Implicit, second-order Crank-  
590 Nicolson Semi-implicit, and second-order Three-point Backward Implicit and Semi-implicit  
591 schemes (see Table XX). Extensive testing has revealed that the Three-point Backward Implicit  
592 scheme performs best.

593 The stable discrete time step  $\Delta t$  is constrained by the Courant-Friedrich-Lewy (CFL) con-  
594 dition. The advective step must satisfy  $\Delta t \leq (h/2)/u_{\max}$ , where  $u_{\max}$  is the highest phase  
595 volume flux magnitude, while the diffusive step must satisfy  $\Delta t \leq (h/2)^2/\kappa_{\max}$ , where  $\kappa_{\max}$  is  
596 the maximum diffusivity.

## 597 2.8.2 Numerical Solution

598 The fluid mechanics equations (18) are solved using an implicit direct solver via Matlab's  
599 `mldivide` function, which efficiently approximates matrix inversion. Solver efficiency is en-  
600 hanced by vectorising the coefficient matrix assembly, precomputing block matrices for the  
601 pressure gradient, velocity divergence, and pressure diagonal once per simulation, and scaling  
602 the assembled matrix to ensure diagonal values remain of order one [Keller et al., 2013]. The  
603 momentum advection term is treated as a source term on the right-hand side, enabling the use  
604 of higher-order advection schemes.

605 The mixture mass conservation equation (18b) is implemented in the form,

$$\nabla \cdot \mathbf{v} = \dot{V}, \quad (33)$$

606 with the volume source term  $\dot{V} = -(\partial\bar{\rho}/\partial t + \nabla \cdot \sum_i f^i \Delta \mathbf{v}^i)$  including volume changes due to  
607 variable density and phase segregation effects.

608 Time integration is implemented as an explicit update using the residual of the time-  
609 dependent equations:

$$Q^q = Q^{q-1} - \alpha r^q \Delta t / a_1 + \beta (Q^{q-1} - Q^{q-2}), \quad (34a)$$

$$r^q = (a_1 Q^k - a_2 Q^{k-1} - a_2 Q^{k-2}) / \Delta t - (b_1 R(Q^k) + b_2 R(Q^{k-1}) + b_3 R(Q^{k-2})), \quad (34b)$$

610 where  $q$  is the iteration counter. The iterative update procedure can be tuned for robustness  
611 using the update step size parameter  $0 \leq \alpha \leq 1$  and the update damping parameter  $0 \leq \beta \leq 1$ .  
612 As the solution guess for the newest time step  $Q^p$  and its corresponding rate of change  $R(Q^p)$   
613 improves, the iterative scheme converges toward a semi- or fully implicit solution.

614 Although the iterative method converges toward a (semi-)implicit solution, achieving sig-  
615 nificantly larger time steps than the stable explicit limit is less straightforward compared to a  
616 direct solver. The iterative step size parameter  $\alpha$  must be adjusted to maintain stability. For  
617 instance, to use a time step 10 times the CFL limit,  $\alpha \leq 0.1$  is required, necessitating more  
618 iterations. The trade-off between time step size and non-linear iteration count generally favours  
619 taking smaller steps to minimise time discretisation errors.

620 The phase diagram calculation introduces additional non-linearity in hydrous systems com-  
621 pared to the original method in Keller and Katz [2016], as phase fractions depend on the solidus  
622 and liquidus curves, which are depressed by the water content in the melt. However, water is  
623 excluded from the solid phase, making the melt water content itself dependent on the phase frac-  
624 tions. This interdependence is resolved using an iterative scheme based on Newton’s method,  
625 typically converging to near machine precision within a few tens of iterations.

626 To adjust equilibrium phase compositions in response to the slight disequilibrium introduced  
627 by the pseudo-equilibrium approach, a numerically simple and lightweight predictor-corrector  
628 method is employed, usually achieving convergence within a dozen iterations.

### 629 2.8.3 Non-linear Iterations

630 The global system of fluid-mechanics and thermo-chemical governing equations, along with  
631 material closure and phase equilibrium models, contains multiple non-linearities. These are  
632 resolved using a fixed-point iterative scheme.

633 First, the thermo-chemical variables  $S$  and  $C_j$  are updated based on entropy production  
634 and component mass conservation. These are then converted to the petrological variables  $T$   
635 and  $\bar{c}_j$ , which determine the local equilibrium phase fractions  $f_{\text{eq}}^i$  and phase compositions  $c_j^i$   
636 by solving the phase diagram. The phase equilibrium is used to update phase change rates  $\Gamma^i$ ,  
637 which in turn are used to update disequilibrium phase fractions  $f^i$  according to phase mass  
638 conservation.

639 Next, updated phase fractions are used to reconstruct disequilibrium phase compositions  
640  $c_j^i$  and phase entropies  $s^i$ . All non-linear model parameters—including densities, viscosities,  
641 segregation coefficients, regularised diffusivities, and auxiliary fields such as lithostatic pressure,  
642 stresses, strain rates, and dissipation rates—are then recalculated. These updated parameters  
643 are used to solve the fluid-mechanics equations, yielding  $\mathbf{v}$  and  $P$ .

644 Phase segregation speeds are then updated to close phase velocities  $\mathbf{v}^i$ , which are used in  
645 the advection of thermo-chemical variables. Finally, geochemical variables are updated, and  
646 the non-linear residual norm is calculated to monitor convergence.

647 The residual norm is defined as the 2-norm of the iterative update, normalised by the 2-  
648 norm of the solution. Convergence criteria can be set based on absolute or relative residual  
649 norms, or a maximum iteration count, though the latter is primarily useful for rapid testing.  
650 Typically, reducing the relative residual by three orders of magnitude requires about a dozen  
651 iterations.

### 652 2.8.4 Numerical Efficiency

653 With the thermo-chemical solution updated explicitly and the coefficient matrix assembly for  
654 fluid mechanics efficiently vectorised, the primary computational bottleneck is the direct solve  
655 for the velocity-pressure system. While more efficient solvers, such as those leveraging external  
656 packages like SuiteSparse in MATLAB [Räss et al., 2017], have been demonstrated, the present  
657 approach prioritises computational efficiency while keeping algorithmic complexity minimal.

658 For a grid size of  $200 \times 200$  cells, computing one time step takes approximately 10-20  
659 seconds on a standard personal computer or a single node of a supercomputer cluster (tested  
660 on a MacBook laptop, Mac Studio desktop, and the Petrarch supercomputer at the University  
661 of Glasgow).

### 662 2.8.5 Reduced-dimensionality Modes

663 In 1D models or low-resolution 2D models, the Newton solver used for computing local phase  
664 equilibrium can occasionally become the rate-limiting step.

665 The numerical implementation is designed for two spatial dimensions but can be adapted  
666 at runtime based on the number of grid points. In a 0-D box model ( $N_x = N_z = 1$ ), there is no  
667 transport by flow, only isotropic deformation to accommodate volume changes caused by phase  
668 change or compressibility. In a 1-D vertical column model ( $N_x = 1$ ), there is no horizontal  
669 variability or flow.

670 The box model mode is useful for tracking the thermo-chemical and pressure evolution  
671 of an isotropic magma chamber under imposed cooling and/or assimilation rates. The column  
672 model mode highlights phase segregation in the absence of convection or with convective mixing  
673 parameterised as enhanced diffusivity. The full 2-D mode is useful for resolving how whole-  
674 chamber or layered convection interacts with phase change and segregation processes. Use cases  
675 for each mode are presented in the following sections.

676 In the column model mode the fluid mechanics equations reduce to a form where matrix  
677 assembly and direct solve by approximate matrix inversion are not required. Instead, the  
678 solution can be found by numerically integrating the vertical velocity  $W$  and dynamic pressure  
679  $P$  along the column given the appropriate momentum and volume source terms.

### 680 2.8.6 Initial and Boundary Conditions

681 The initial conditions for time-dependent solution variables  $S, C_j, \Theta_k$  are set to match the  
682 chosen fields for  $T, \bar{c}_j, \bar{\theta}_k$ . These fields can be initialised as a uniform value, representing a  
683 homogeneous magma chamber, as two horizontal layers for a simple layered chamber, or as a  
684 linear gradient from top to base.

685 Additionally, a smooth random perturbation field of specified amplitude can be introduced  
686 to add initial heterogeneity, facilitating the onset of flow dynamics.

687 By default, domain boundaries are treated as the magma-wall rock contact. Alternatively,  
688 the chamber walls can be placed inside the domain, with wall rock defined by  $T_{\text{wall}}, \bar{c}_{j,\text{wall}}, \bar{\theta}_{k,\text{wall}}$ .  
689 The rectangular domain can represent either the full chamber extent or a horizontal segment  
690 of a sill, in which case wall rock interaction is applied only at the top and base, with periodic  
691 side boundaries.

692 Wall rock interaction is simulated using a two-part approach. First, thermo-chemical vari-  
693 ables obey zero-flux boundary conditions ( $\partial[T, \bar{c}_j, \bar{\theta}_k]/\partial\mathbf{n} = 0$ ), while velocity-pressure variables  
694 follow no-slip conditions ( $\mathbf{v} = \mathbf{0}, \partial P/\partial\mathbf{n} = 0$ ). Second, volumetric cooling and/or assimilation



695 rates  $B_{\text{wall}}^a$  are applied in a boundary layer decaying exponentially away from the boundary:

$$B_{\text{wall}}^a = \frac{\bar{\rho}}{\tau_a} (a_{\text{wall}} - a) \exp(-d/\delta), \quad (35)$$

696 where  $a = [T, \bar{c}_j, \bar{\theta}_k]$ ,  $d$  is the distance from the boundary, and  $\delta$  is the imposed boundary layer  
 697 thickness. This approach, similar to Birnbaum et al. [2020], ensures stable boundary conditions  
 698 while avoiding numerical artefacts from sharp temperature and composition contrasts.

699 The cooling timescale  $\tau_a$  depends on an assumed external thermal boundary layer thick-  
 700 ness  $D_0$  (i.e., assumed thermal aureole) and wall rock diffusivity  $\kappa_0$ , approximated by  $\tau_a \approx$   
 701  $D_0^2/\kappa_0$ . For  $\kappa_0 = 10^{-6} \text{ m}^2/\text{s}$  and  $D_0 = [0.1, 1, 10] \text{ m}$ , this results in  $\tau_a = [10^4, 10^6, 10^8] \text{ s}$ , or  
 702  $\sim [3 \text{ hours}, 12 \text{ days}, 3 \text{ years}]$ .

703 Component assimilation timescales are harder to constrain. Purely diffusive assimilation is  
 704 much slower than thermal effects, but meso-scale processes such as wall rock disaggregation and  
 705 mechanical mingling may enhance assimilation rates. For simplicity, we assume assimilation  
 706 follows thermal timescales. Using internal wall rock boundaries can mitigate uncertainties,  
 707 though interactions remain limited to grid-resolved advection diffusion as well as additional  
 708 mixing by regularisation as discussed in the following section.

709 The boundary algorithm can also model scenarios where a more evolved, cooler magma is  
 710 underplated by hotter, more primitive recharge magma. In this case, boundary interactions are  
 711 applied only at the base, while the sides and top remain no-contact (zero-flux, free-slip). Instead  
 712 of setting the base condition to sub-solidus rock properties,  $T_{\text{wall}}, \bar{c}_{j,\text{wall}}, \bar{\theta}_{k,\text{wall}}$  are specified to  
 713 represent a hot and melt-rich recharge magma. The recharge setup can be initialised with the  
 714 recharge magma directly at the domain boundary or positioned as an internal layer within the  
 715 domain.

## 716 2.9 Model Regularisation by Diffusion

717 Diffusion, understood as the system-scale effect of local-scale fluctuating motion, is used in  
 718 four distinct ways in this model to represent sub-grid scale processes and regularise the model  
 719 for numerical stability in a physics-inspired manner. The four ways diffusion is used include  
 720 classical heat diffusion, phase fraction diffusion, turbulent mixing, and convective layer mixing  
 721 in one-dimensional models. The first does not require further discussion.

### 722 2.9.1 Phase Fraction Diffusion

723 Phase segregation at the granular scale is subject to local fluctuations around a meso-scale  
 724 mean segregation velocity [Segre et al., 2001, Keller and Suckale, 2019]. These fluctuations are  
 725 modelled by introducing a phase diffusivity:

$$\kappa_\phi^i = u_\phi^i \ell_\phi^i, \quad (36)$$

726 where  $u_\phi \approx |\Delta \mathbf{v}^i|$  is the characteristic magnitude of speed fluctuations of phase constituents  
727 (e.g., crystals, bubbles) around their mean segregation velocity, proportional to and of the same  
728 order of magnitude as the absolute segregation speed itself [Segre et al., 2001].  $\ell_\phi^i \approx 10 \times d^i$  is  
729 the characteristic correlation length linked to the local-scale phase constituent size [Segre et al.,  
730 2001]. This formulation ensures smooth phase fraction fields without artificially suppressing  
731 segregation processes.

732 To ensure a zero sum over all phase diffusion fluxes,  $\sum_i \mathbf{q}_\phi^i$  the flux in (12c) is not directed  
733 down gradients in phase fractions but rather down deviations in phase fraction gradients from  
734 a reference gradient [Keller and Suckale, 2019],

$$\Delta(\nabla \phi)^{i*} = \nabla \phi^i - \nabla \phi^* , \quad (37a)$$

$$\nabla \phi^* = \sum_i \frac{k_\phi^i}{\sum_l k_\phi^l} \nabla \phi^i , \quad (37b)$$

735 where the reference gradient is found from a weighted sum of phase gradients by relative weights  
736 of phase diffusion coefficients.

737 The diffusive transport of phase fractions affects the evolution of other properties carried  
738 along by phase transport, including heat, momentum, major, and trace composition. To ensure  
739 consistency in material transport through phase diffusion we include the phase diffusion flux  
740 as a component of phase velocities as described in (22). This effect is generally small and most  
741 relevant in dilute suspensions.

## 742 2.9.2 Eddy Diffusivity for Sub-grid Scale Mixing

743 In two-dimensional simulations which achieve a high Reynolds number ( $\text{Re} > 10$ ), turbulent  
744 eddies can cascade down to smaller and smaller spatial scales. Numerically, eddies can only  
745 be resolved robustly at scales well above the grid spacing. Increasing the effective viscosity  
746 (i.e., momentum diffusivity) has the effect of dampening out small-scale eddies. However,  
747 the additional mixing effected by sub-grid scale turbulent eddies on momentum, heat, and  
748 compositional transport are important to consider when regularising turbulent flows. This  
749 adaptive diffusivity enhances numerical stability in simulations approaching turbulence while  
750 preserving physically meaningful mixing dynamics.

751 These effects are parameterised through an eddy diffusivity approach [e.g., Gatski and Rumsey,  
752 2002]:

$$\kappa_{\text{trb}} = (C_{\text{trb}} h)^2 |\underline{\mathbf{D}}(\mathbf{v})| , \quad (38)$$

753 where  $\kappa_{\text{trb}}$  is the effective eddy diffusivity,  $0.5 \leq C_{\text{trb}} \leq 1$  is a dimensionless calibration constant,  
754  $h$  the grid spacing, and  $|\underline{\mathbf{D}}(\mathbf{v})|$  the magnitude of the strain rate tensor relating to the system-  
755 scale flow field. The eddy diffusivity is applied to momentum diffusion by multiplying to the  
756 magma density and adding the regularisation term to the effective viscosity of the magma  
757 mixture,

$$\check{\eta}_\phi = \eta_\phi + \kappa_{\text{trb}} \bar{\rho} , \quad (39)$$

758 where  $\eta_\phi$  is the non-regularised effective mixture viscosity.

759 The turbulent Prandtl and Schmidt numbers,  $\text{Pr}_t$  and  $\text{Sc}_t$ , the ratio of momentum diffusivity  
 760 (viscosity) to thermal and chemical diffusivities in turbulent flows, approach values of order  
 761 unity with increasingly turbulent dynamics [Reynolds, 1975, Gatski and Rumsey, 2002]. Hence,  
 762 the turbulent eddy diffusivity is used to enhance thermal and chemical diffusion coefficients as  
 763 a function of increasing Reynolds number,

$$\check{k}_s = \frac{\kappa_{\text{trb}}}{\text{Pr}} \frac{\rho C_P}{T} , \quad (40a)$$

$$k_c = \frac{\kappa_{\text{trb}}}{\text{Sc}} , \quad (40b)$$

$$[\text{Pr}, \text{Sc}] = [\text{Pr}_t, \text{Sc}_t] (1 - \exp(-\text{Re}/10))^{-1} . \quad (40c)$$

764 These relations prescribe effective eddy mixing diffusivities for thermal and chemical fields  
 765 which gradually approach the eddy diffusivity for Reynolds numbers above 10–100. Whereas  
 766 the eddy-enhanced chemical diffusivity  $k_c$  is the only diffusion process implemented for major  
 767 and trace components, the eddy-enhance thermal conductivity  $\check{k}_s$  is applied in addition to  
 768 the classical thermal conductivity  $k_s$ . An important distinction, however, is that eddy mixing  
 769 should move temperature towards an adiabatic profile and hence the regularised eddy diffusion  
 770 flux goes down gradients in potential temperature  $T_p$ , not full temperature  $T$ . The regularised  
 771 heat flux hence becomes,

$$\check{\mathbf{q}}_s = -k_s \nabla T - \check{k}_s \nabla T_p , \quad (41)$$

772 The eddy diffusivity is also added to all phase diffusion coefficients, scaled by the respective  
 773 phase volume fraction,

$$\check{\mathbf{q}}_\phi^i = \mathbf{q}_\phi^i + \kappa_{\text{trb}} \phi^i . \quad (42)$$

774 It is the regularised phase diffusion coefficient,  $\check{\mathbf{q}}_\phi^i$ , which is used to determine the reference  
 775 phase gradient  $\nabla \phi^*$  required to calculate phase diffusion fluxes as shown in (12c) and (37).

### 776 2.9.3 Convective Mixing in 1D Column Models

777 Convective mixing cannot be resolved in one-dimensional models. To approximate the effect  
 778 of convective mixing, an enhanced diffusivity is introduced for heat and composition in regions  
 779 diagnosed as convective [Abe, 1993, 1997]:

$$\kappa_{\text{cnv}} = |\mathbf{v}_{\text{cnv}}| \Delta_{\text{cnv}} , \quad (43)$$

780 where  $|\mathbf{v}_{\text{cnv}}|$  is the estimated magnitude of convective velocity, and  $\Delta_{\text{cnv}}$  is the convective mixing  
 781 length. The convective mixing speed is estimated using a Stokes law scaling relation on the  
 782 length scale of half the convective mixing length,

$$|\mathbf{v}_{\text{cnv}}| = \frac{2}{9} \frac{\max(-\partial \rho_{\text{np}} / \partial z, 0) g \Delta_{\text{cnv}}^2}{\check{\eta}} . \quad (44)$$

783  $\max(-\partial\rho_{\text{nP}}/\partial z, 0)$  diagnoses where unstable density stratification is present by taking the ver-  
784 tical gradient of the density calculated in the absence of any  $P$ -dependence. The gradient  
785 is taken by centred differencing over a depth interval corresponding to the convective mixing  
786 length.

787 According to Prandtl’s Mixing Length Hypothesis [Prandtl, 1925, Pirozzoli, 2014], the mix-  
788 ing length should be proportional to the distance from the convective layer boundary [Abe,  
789 1993], as convective cells and turbulent eddies are constrained by this distance. In our ap-  
790 proach, the mixing length is defined as the distance to the nearest convective layer boundary,  
791 capped at a maximum value, typically around 10-20% of the domain depth. Since magma  
792 bodies can contain multiple stably stratified convective layers, a peak-detection algorithm is  
793 employed to identify peaks in  $(\partial\rho_{\text{nP}}/\partial z)$ , which mark the boundaries of stable stratification.  
794 The mixing length is then computed as the shortest distance to any detected stratification  
795 boundary, including the top and bottom domain boundaries as well as any internal stable  
796 layers.

797 The resulting convective mixing diffusivity  $\kappa_{\text{cnv}}$  is used to enhance thermal, chemical, and  
798 phase diffusion in 1-D column models similarly to how the eddy viscosity  $\kappa_{\text{trb}}$  is employed in 2-D  
799 models. The only difference is that the Prandtl and Schmidt numbers are applied indepent on  
800 any scaling with Reynolds number (cf., (40)). This formulation ensures convectively unstable  
801 regions experience enhanced mixing, mimicking large-scale overturn processes in magma bodies  
802 such as large basaltic intrusions or planetary magma oceans.

### 803 **3 Acknowledgements**

804 The author acknowledges extensive code testing by P. Aellig, E. Machi, S. Swan, V. Perez, and  
805 L. Rey.

### 806 **4 Code availability**

807 The simulation code is open source under a Gnu General Public License Version 3 and available  
808 for download at <https://github.com/kellertobs/nakhla>.

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