Thermodynamic limits for assimilation of silicate crust in primitive magmas

Jussi S. Heinonen1*, Frank J. Spera2 and Wendy A. Bohrson3

1Department of Geosciences and Geography, University of Helsinki, P.O. Box 64, 00014 Helsinki, Finland
2Department of Earth Science and Institute for Crustal Studies, University of California, Santa Barbara, California 93106, USA
3Department of Geology and Geological Engineering, Colorado School of Mines, Golden, Colorado 80401, USA

ABSTRACT

Some geochemical models for basaltic and more primitive rocks suggest that their parental magmas have assimilated tens of weight percent of crustal silicate wall rock. But what are the thermodynamic limits for assimilation in primitive magmas? We pursue this question quantitatively using a freely available thermodynamic tool for phase equilibria modeling of open magmatic systems—the Magma Chamber Simulator (https://mcs.geol.ucsb.edu)—and focus on modeling assimilation of wall-rock partial melts, which is thermodynamically more efficient compared to bulk assimilation of stumped wall-rock blocks in primitive igneous systems. In the simulations, diverse komatiitic, picritic, and basaltic parental magmas assimilate progressive partial melts of preheated average lower, middle, and upper crust in amounts allowed by thermodynamics. Our results indicate that it is difficult for any subalkaline primitive magma to assimilate more than 20–30 wt% of upper or middle crust before evolving to compositions with higher SiO2 than a basaltic magma (52 wt%). On the other hand, typical komatiitic magmas have thermodynamic potential to assimilate as much as their own mass (59–102 wt%) of lower crust and retain a basaltic composition. The compositions of the parental melt and the assimilant heavily influence both how much assimilation is energetically possible in primitive magmas and the final magma composition given typical temperatures. These findings have important implications for the role of assimilation in the generation and evolution of, e.g., ultramafic to mafic trans-Moho magmatic systems, siliceous high-Mg basalts, and massif-type anorthosites.

INTRODUCTION

Magmatic assimilation of crustal materials has important consequences for magma differentiation and crustal growth. Assimilation induces the formation of ore deposits (e.g., Dallai et al., 2011; Rivera et al., 2017). It is also effective in masking incompatible trace element and isotopic signatures of mantle-derived magmas (e.g., Carlson et al., 1981; Lightfoot et al., 1990; Moore et al., 2020). Studying mantle sources and mantle versus crustal contributions of magmatic systems therefore requires an understanding of assimilation processes.

Much of the modeling of assimilation has been based on binary mixing and assimilation–fractional crystallization (AFC) equations (e.g., DePaolo, 1981) that rely solely on trace element and isotopic data. These methods may be useful in providing tentative information, but they do not inform the modeler about the associated changes in phase equilibrium or whether the results are reasonable in terms of energy conservation. Incompatible and compatible trace element concentrations in bulk assimilant may be magnitudes lower or higher, respectively, than in associated partial melts. Accordingly, amounts of crustal assimilation in excess of 30 wt% (relative to the initial magma) have been implied for basaltic or more primitive magmas by such models (e.g., Carlson et al., 1981; Lightfoot et al., 1990; Larsen and Pedersen, 2009). Is it possible for primitive magmas to assimilate such high amounts of silicate crust or its partial melts? Would the contaminated magmas remain basaltic?

In this study, we quantitatively test thermodynamic limits for assimilation in primitive magmas using the Magma Chamber Simulator (MCS, https://mcs.geol.ucsb.edu; Bohrson et al., 2014, 2020). MCS is a freely available open-system thermodynamic model that computes the thermal, mass, and compositional evolution of a multicomponent-multiphase composite system using a selected MELTS (http://melts.fsm-research.org) engine (here rhyolite-MELTS version 1.2.0; Gualda et al., 2012; Ghiorso and Gualda, 2015). The rhyolite-MELTS algorithms are suitable for modeling phase equilibria in multicomponent magmatic systems, and they generally provide reasonable first-order results when compared to natural and experimental data not used in their calibration (e.g., Hirschmann et al., 1998; Panukcu et al., 2015; Pichavant et al., 2019). In the thermodynamically constrained AFC simulations presented here, komatiitic, picritic, and basaltic magmas assimilate progressive partial melts of average lower crust (LC), middle crust (MC), and upper crust (UC). This approach builds on earlier, more rudimentary models (e.g., Sparks, 1986; Thompson et al., 2002) and enables direct thermodynamic evaluation of how much assimilation of silicate-crust partial melt is possible by primitive crystallizing magmas before they evolve to intermediate to felsic compositions.

MODELING WITH MAGMA CHAMBER SIMULATOR

In MCS, assimilation can be modeled as assimilation of wall-rock partial melts–fractional crystallization (MCS-AFC) or assimilation of stumped blocks–fractional crystallization (MCS-SFC), or their combination (Bohrson et al., 2020). For the purpose of searching for thermodynamic limits of assimilation, attention is focused on MCS-AFC because MCS-SFC results in higher amounts of crystallization in the parent magma. This is because the added crystalline mass is of lower specific enthalpy.
Figure 1. Results of Magma Chamber Simulator (https://mcs.geol.ucsb.edu) simulations of assimilation of wall-rock partial melts–fractional crystallization (MCS-AFC) shown in SiO$_2$ versus Na$_2$O + K$_2$O (total alkalis–silica, TAS) diagrams (Le Bas et al., 1986; basalt field highlighted in yellow). (A,D,G) Komatiitic and meimechitic parental melts (MgO $> 18$ wt%; SiO$_2$ $< 52$ wt%; alkalis not considered). (B,E,H) Picritic parental melts (MgO $\approx 12$–$18$ wt%; SiO$_2$ $< 52$ wt%; alkalis not considered). (C,F,I) Basaltic and picrobasaltic parental melts (MgO $< 12$ wt%; SiO$_2$ $< 52$ wt%; Na$_2$O + K$_2$O $< 5$ wt%) (Le Bas et al., 1986; Le Bas, 2000). Parental melt locations and sources are given in Table S1 (see footnote 1). Each open symbol represents assimilation step where wall-rock partial melt above percolation threshold of 10 wt% is homogenized with resident melt. Dark and light gray trendlines highlight high-Mg compositions (komatiitic or meimechitic and picritic in terms of MgO, respectively) outside of TAS classification (see Fig. 2). Only results with $< 50$ wt% crystallinity of resident magma are shown. Stippled lines and numbers in italics in C and F indicate total amount of assimilation (in weight percent relative to initial parental melt) in end of simulations using arc parental melts 1, 2, 3, and 8. UC, MC, LC—upper, middle, and lower crust, respectively; Subalk.—subalkaline; LIP—large igneous province; GB—greenstone belt; MORB—mid-oceanic ridge basalt; CFB—continental flood basalt; MEI—meimechitic; FP—ferropicritic.
compared to partial melt of the same composition and temperature (see the Discussion section, and the Supplemental Material).

Input for MCS-AFC scenarios includes pressure, initial temperature, wall-rock melt percolation threshold, and the relative mass of the magma and the wall rock and their respective major element compositions. Additionally, thermal input parameters for modeling the behavior and phase equilibria of the wall rock at near-solidus conditions are required. For a thorough explanation of the model input, see Bohrsen et al. (2020). In an MCS-AFC model, the sensible and latent heat released by crystallizing magma heats and partially melts the wall rock. After the amount of partial melt in the wall rock exceeds a percolation threshold, portions of wall-rock melt above this threshold are assimilated by the magma. The simulation proceeds until the magma and wall rock reach thermal equilibrium.

Full listings of the compositional input as well as discussion and sources for the model parameters can be found in the Supplemental Material. The 30 selected parental komatiitic or meimechitic, picritic, and picrobasaltic or basaltic parental melts represent different ages and tectonic settings (Fig. 1). The more magnesian parental melts are relevant to high-temperature Archean and large-igneous-province settings, whereas less magnesian parental melts are relevant to modern arc and other settings not related to mantle plumes. Water has been added to some of the compositions reported as dry, and initial FeO/FeO has been estimated based on constraints relevant to each set and composition. The wall-rock compositions represent the average modern LC (basaltic andesitic; SiO2 = 53 wt%), MC (dacitic; SiO2 = 63 wt%), and UC (dacitic; SiO2 = 66 wt%) of Rudnick and Gao (2003). The mass of wall rock in the simulations is set at twice that of the initially pristine primitive magmas. To maximize assimilation, the initial temperature of the wall rock is slightly hypersolidus such that wall rock contained melt but was below the approximated percolation threshold of 10 wt% melt (LC: 9.4 wt% melt at 1060 °C and 0.8 GPa; MC: 9.7 wt% melt at 880 °C and 0.5 GPa; UC: 6.9 wt% melt at 700 °C and 0.2 GPa). Such conditions would approximate tabular chambers and high magma input having caused earlier crustal heating and steep geotherms prior to the intrusion of the modeled magma batch.

RESULTS OF THE MODELING

The results of the 90 (30 parental melts at 3 crustal settings) MCS-AFC simulations are illustrated in total alkalis–silica diagrams in Figure 1 and in histograms in Figure 2. The full output with additional preliminary models can be found in the Supplemental Material. Simulations using LC and UC assimilants present end-member scenarios among the presented simulations—simulations using a MC assimilant show transitional characteristics but are very much reminiscent of the UC cases in general.

It is unlikely for any primitive parental melt to assimilate more than 20–30 wt% (relative to the mass of the parental melt) of MC or UC before evolving to compositions with higher SiO2 than basalts (52 wt%) (Fig. 2). Basaltic parental melts also cannot assimilate LC in excess of 20–30 wt% and remain basaltic. On the other hand, komatiitic parental melts have thermodynamic potential to assimilate as much as their own mass of LC (range of 59–102 wt%) and remain basaltic. Even picritic parental melts, relevant to Phanerozoic intraplate settings, can assimilate 28–49 wt% of LC before surpassing the SiO2 content of basalts. Assimilation of LC partial melts can also increase the alkalinity of the magma series, which is more unlikely to be realized by assimilation of relatively more Si-rich MC or UC melts (Fig. 1).

DISCUSSION

A rather clear energetic limit exists for assimilation of anatectic melts of granitic crust by basaltic or more MgO-rich and SiO2-poor magmas. Traditional binary mixing or AFC models that rely on trace elements and radiogenic

![Figure 2. Results of Magma Chamber Simulator (https://mcs.geol.ucsb.edu) simulations of assimilation of wall-rock parental melts–fractional crystallization (MCS-AFC) shown in histograms. (A,D,G) Komatiitic and meimechitic parental melts. (B,E,H) Picritic parental melts. (C,F,I) Basaltic and picrobasaltic parental melts. See Figure 1 for more details and numbering of parental melts on horizontal axis. Vertical axes denote amount of assimilation relative to mass of parental melt. Amounts of assimilation in models are shown for three categories, where modeled resident melt composition can be considered komatiitic or meimechitic, picritic, or basaltic (see Fig. 1) and is below <5 wt% of crystallinity of resident magma. Numerical data used to construct this figure are tabulated in Table S2 (see footnote 1). UC, MC, LC—upper, middle, and lower crust, respectively.](https://mcs.geol.ucsb.edu)
isotopes and suggest more than ~20–30 wt% assimilation of granitoid crust in primitive komatiitic, picritic, or basaltic systems are not broadly supported by the modeling (Figs. 1 and 2). For example, compositions produced by notable amounts of assimilation of felsic crust by komatiitic magmas correspond to siliceous high-Mg basalts and not komatites or picrites (Fig. 3; see also Sparks, 1986; Pearce and Reagan, 2019). Our results underline the importance of considering thermodynamics and phase equilibria before attempting to model trace elements and isotopes in magmatic systems.

In contrast to the UC cases, the thermodynamic potential of komatiitic and picritic magmas to partially melt and assimilate LC and still retain primitive Si-poor compositions is considerable. This may have fundamental importance for how trans-Moho magmatic systems evolve. Examples include mineralization related to large-scale melting-infiltration fronts (e.g., Barnes et al., 2020) and generation of massif-type anorthosites and associated mafic rocks with geochemical evidence of considerable element input from (lower) crustal sources (e.g., Sparks, 1986; Heinonen et al., 2010; Bybee and Ashwal, 2015). Such magmatic systems may be easier to explain with a more dominant role for LC and its partial melts in their evolution than previously realized, and we encourage future thermodynamically constrained studies on these issues.

The presented modeling is also directly linked to fundamental research questions concerning the growth versus reworking of continental crust through time and in various geological settings (e.g., Hawkesworth et al., 2019). For example, modern arc basalts cannot assimilate more than 10–20 wt% of crustal materials and remain basaltic (basaltic parental melts 1, 2, 3, and 8 in Fig. 2). For LC assimilation scenarios, basaltic parental melts cannot even evolve to considerably more SiO₂-rich compositions before assimilation halts due to thermal equilibrium reached with the mafic LC wall rock (Fig. 1I). Subsequent differentiation in such lower-crustal chambers would thus take place via fractional crystalization. For MC and UC assimilation scenarios, however, the magmas evolve to andesitic-dacitic compositions while assimilating >40 wt% of crustal materials (Figs. 1C and 1F). These constraints may be relevant for studies that concentrate on the differentiation of arc magmas, e.g., within the framework of melting-assimilation-storage-homogenization (MASH; Hildreth and Moorbath, 1988) scenarios. We encourage the future use of MCS to place thermodynamic constraints on assimilation also in more evolved systems.

The prerequisites for maximum degrees of assimilation are that the crust has been preheated by earlier magma pulses (or the geotherm is otherwise anomalously steep) and that the partial melts are effectively transported and mixed with the resident melt. It is well known that dynamic factors such as boundary-layer fractionation (e.g., Trip and Spera, 1990; Kuritani et al., 2005) may significantly inhibit the latter. In alternative models of bulk assimilation (e.g., reactive bulk assimilation; Beard et al., 2005), the crystallinity in the magma more readily reaches ~50 wt% due to the "enthalpy deficit" induced by incorporation of solid rather than partial melt, thus raising magma viscosity and potentially transforming magma to a semi-rigid crystal network rheologically incapable of subsequent large-scale differentiation (see Glazner, 2007). This feature is also shown by our comparative MCS-SFC simulations (see the Supplemental Material) that otherwise show similar results to the MCS-AFC simulations. In all the MCS-AFC results discussed here, the crystallinity of the resident magma stays <50 wt%.

Although reactive bulk assimilation may play an important role in the evolution of some low-temperature intermediate-felsic magmas (Beard et al., 2005), the considerable thermodynamic potential of ultramafic-mafic magmas to partially melt crustal materials (Figs. 1 and 2) suggests that the latter may dominate the style of assimilation in primitive magmatic systems (see also Kvsassnes and Grove, 2008; Borisova et al., 2017). We nevertheless consider the amounts of partial-melt assimilation suggested by our simulations to represent absolute maximum values for natural settings—it is indeed very likely that other physical factors, not considered in our thermodynamic modeling, prevent assimilation in magma systems before the full thermodynamic potential of the intruding magmas has been harnessed. Thermodynamic models, as presented here, provide a framework into which additional kinetic and dynamic constraints can be placed to study natural systems in more detail.

It is also noteworthy that the computations presented in this study, especially in terms of the crustal assimilants, represent common and average compositions—these results are thus not directly applicable to scenarios involving rarer magma types or wall rock (e.g., ultrapotassic or carbonate compositions) or involving magma-wall rock interaction dominated by processes other than assimilation of wall-rock partial melts (e.g., selective metasomatism; Dyer et al., 2011). In spite of these shortcomings, we believe that...