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² Diagnosing open-system magmatic processes using the Magma

- ³ Chamber Simulator (MCS): part I—major elements and phase
- 4 equilibria

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9 Abstract

10 The Magma Chamber Simulator (MCS) is a thermodynamic tool for modeling the evolution of magmatic systems that are 11 open with respect to assimilation of partial melts or stoped blocks, magma recharge + mixing, and fractional crystallization. 12 MCS is available for both PC and Mac. In the MCS, the thermal, mass, and compositional evolution of a multicomponent-13 multiphase composite system of resident magma, wallrock, and recharge reservoirs is tracked by rigorous self-consistent 14 thermodynamic modeling. A Recharge-Assimilation (Assimilated partial melt or Stoped blocks)-Fractional Crystallization 15 $(R_nAS_nFC; n_{tot} \le 30)$ scenario is computed by minimization or maximization of appropriate thermodynamic potentials using 16 the family of rhyolite- and pMELTS engines coupled to an Excel Visual Basic interface. In MCS, during isobaric cooling and 17 crystallization, resident magma thermally interacts with wallrock that is in internal thermodynamic equilibrium. Wallrock 18 partial melt above a user-defined percolation threshold is homogenized (i.e., brought in to chemical potential equilibrium) 19 with resident magma. Crystals that form become part of a cumulate reservoir that remains thermally connected but chemi-20 cally isolated from resident melt. Up to 30 instances ($n \le 30$) of magma mixing by recharge and/or bulk assimilation of stoped 21 wallrock blocks can occur in a single simulation; each recharge magma or stoped block has a unique user-defined composi-22 tion and thermal state. Recharge magmas and stoped blocks hybridize (equilibrate) with resident melt, yielding a single new 23 melt composition and temperature. MCS output includes major and trace element concentrations and isotopic ratios (Sr, 24 Nd, Hf, Pb, Os, and O as defaults) of wallrock, recharge magma/stoped blocks, resident magma melt, and cumulates. The 25 chemical formulae of equilibrium crystalline phases in the cumulate reservoir, wallrock, and recharge magmas/stoped blocks 26 are also output. Depending on the selected rhyolite-MELTS engine, the composition and properties of a possible supercriti-27 cal fluid phase (H_2O and/or CO_2) are also tracked. Forward modeling of theoretical magma systems and suites of igneous 28 rocks provides quantitative insight into key questions in igneous petrology such as mantle versus crustal contributions to 29 terrestrial magmas, the record of magmatism preserved in cumulates and exsolved fluids, and the chronology of RASFC 30 processes that may be recorded by crystal populations, melt inclusions, and whole rocks. Here, we describe the design of the 31 MCS software that focuses on major element compositions and phase equilibria (MCS-PhaseEQ). Case studies that involve 32 fractional crystallization, magma recharge + mixing, and crustal contamination of a depleted basalt that resides in average 33 upper crust illustrate the major element and phase equilibria consequences of these processes and highlight the rich array of 34 data produced by MCS. The cases presented here, which represent an infinitesimal fraction of possible RASFC processes 35 and bulk compositions, show that the records of recharge and/or crustal contamination may be subtle and are not necessarily 36 those that would be predicted using conventional intuition and simple mass balance arguments. Mass and energy constrained 37 thermodynamic tools like the MCS quantify the open-system evolution of magmas and provide a systematic understanding

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38 of the petrology and geochemistry of open system magmatic processes. The trace element and isotope MCS computational 39 tool (MCS-Traces) is described in a separate contribution (part II).

40 Keywords Magma Chamber Simulator · Open-system magma processes · Modeling · Magma differentiation ·

41 Thermodynamics

Introduction 42

Studies of igneous rocks provide evidence that magmas 43 evolve as open systems where exchange of matter and energy 44 occurs at a range of spatial and temporal scales. Since the 45 1950s, improvements in geochemical instrumentation have 46 enabled high precision analyses of igneous products (e.g., 47 melts and fluid inclusions, single crystals, populations of 48 crystals) at increasingly smaller spatial and temporal scales. 49 These analytical advancements have led to many new 50 insights into the complexities of how magmas evolve and 51 aggregate. To fully utilize the enormous potential afforded 52 by such data sets, a parallel advancement in computational 53 modeling is a logical complement. 54

Trace element and isotopic models of open system magma 55 processes have evolved from earlier studies that focused on 56 mass balance (e.g., Taylor 1980; DePaolo 1981 and others) 57 to those that incorporated mass and energy balance in the 58 context of open system evolution (e.g., Spera and Bohrson 59 2001; Bohrson and Spera 2001, and references therein). 60 Thermodynamic modeling has also progressed in impor-61 tant ways, and present-day models such as the family of 62 rhyolite-MELTS models (Ghiorso and Sack 1995; Asimow 63 and Ghiorso 1998; Gualda et al. 2012; Ghiorso and Gualda 64 2015), pMELTS (Ghiorso et al. 2002) and THERMOCALC 65 (e.g., Powell and Holland 1988, 1994; Powell et al. 1998) 66 provide tools for documenting mineral-melt-fluid phase 67 equilibria in differentiating magmatic systems. In this con-68 tribution, we present the Magma Chamber Simulator (MCS; 69 Bohrson et al. 2014) as a versatile computational tool for the 70 igneous petrologist/geochemist. MCS utilizes the MELTS 71 family of models to combine thermodynamic constraints on 72 melt-solid-fluid equilibria with mass and energy conserva-73 tion for a composite open magma undergoing magma mixing 74 via recharge, crustal assimilation via wallrock partial melt-75 ing and stoping, and fractional crystallization. Model output 76 includes compositional, isotopic, mass, and thermal data on 77 all melts, solids, and fluid in each subsystem. 78

MCS is a forward modeling tool (discussion of both for-79 ward and inverse modeling in geochemistry may be found 80 in Albarede 1995) that can serve in several ways to elu-81 cidate the evolution of magmatic systems. Forward mod-82 eling helps to understand how variations in the values of 83 specific parameters (e.g., pressure, parental magma com-84 position, wallrock initial temperature, number and mass 85 of recharge events) affect the course of magmatic system 86

evolution. This approach enables one to obtain an intuitive 87 understanding of open system magmatic processes, includ-88 ing a basis for concluding which variables have the largest 89 effect. Forward modeling is also useful when attempting 90 to model a particular natural system. In this case, one can 91 adjust input parameters to best reproduce petrological and 92 geochemical data from a particular suite of igneous rocks. 93 Understanding the sensitivity of the solution to input param-94 eters is especially important when modeling natural systems, 95 because the investigator is often confronted with significant 96 uncertainties. 97

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The use of MCS to both build intuition and to model data from individual volcanic or plutonic systems addresses a range of goals in the study of igneous rocks. Among the 100 questions that can be addressed by MCS are how does the 101 balance of mantle and crust change with time in a particular 102 magmatic system; are there systematic differences in mantle 103 versus crustal input in different tectonic settings (e.g., Cox 104 and Hawkesworth 1984; Asmerom et al. 1991; Moore et al. 105 2018); what influences where magma storage zones form 106 (shallow versus middle versus deep crust, e.g., Walker et al. 107 1993; Mangiacapra et al. 2008; Becerril et al. 2013; Weber 108 and Castro 2017); what conditions favor large versus small 109 magma bodies; and what processes and/or conditions mod-110 eled by MCS influence magma bodies to erupt (e.g., Tepley 111 et al. 2000, 2013; Wark et al. 2007; Scruggs and Putirka 112 2018; Ubide and Kamber 2018)? 113

In this contribution, we provide an overview of the 114 design of the major element and phase equilibria part of the 115 code (MCS-PhaseEQ); the trace element and isotope part 116 of MCS (MCS-Traces) will be discussed in a companion 117 paper (Heinonen et al. 2020). We also highlight the utility 118 of forward modeling by providing a comparison of cases 119 that illustrate the petrologic and geochemical consequences 120 of five recharge, assimilation, stoping, fractional crystal-121 lization (RASFC) scenarios (FC, R₂FC, AFC, S₂FC, and 122 R₂AFC where the subscript defines the number of "events"). 123 The results of these models provide perspective on how 124 melt + crystals + fluid in a crustal magma system may evolve 125 in response to different combinations of open-system pro-126 cesses. Presentation of these models also serves to illustrate 127 the rich array of results that MCS produces and how these 128 results may be used to distinguish different open system sce-129 narios (e.g., presence or absence or magma recharge, stop-130 ing versus assimilation of anatectic melt). In the companion 131 paper, trace element and isotopic characteristics for these 132

same five cases are presented along with the theory and code
logistics for MCS-Traces. Examples of the use of MCS in
studies of natural systems are given elsewhere (e.g., Borisova et al. 2017; Takach 2018, Heinonen et al. 2019).

137 Design of the Magma Chamber Simulator

138 What is the Magma Chamber Simulator?

The Magma Chamber Simulator is a thermodynamic 139 model that quantifies the evolution of an open composite 140 magmatic system composed of four subsystems: resident 141 magma, cumulate reservoir, wallrock, and distinct recharge 142 reservoirs. These subsystems interact by exchange of mat-143 ter and energy following the constraints imposed by local 144 thermodynamic equilibrium, as described below. MCS mod-145 els simultaneous fractional crystallization, contamination 146 by partial melt assimilation (AFC in the MCS jargon) and 147 stoping (S, SFC in the MCS jargon), and magma mixing by 148 recharge (RFC in the MCS jargon). 149

In MCS, the resident Magma subsystem (M), initially, a 150 finite mass of melt in a well-defined thermodynamic state, is 151 coupled to its host Wallrock (WR) via a diabatic and semi-152 permeable boundary. During AFC processes, sensible (melt 153 cooling) and latent heat (formation of cumulates by frac-154 tional crystallization, FC) flows across the M-WR bound-155 ary, heating up and potentially partially melting wallrock. If 156 partial melt forms and the melt fraction in wallrock exceeds 157 a rheologically determined, user-specified critical threshold 158 $(f_m^0 \text{ or fmZero})$, this anatectic melt thoroughly mixes and 159 equilibrates with melt in the M subsystem (called M melt 160 for brevity). Crystals that form in response to AFC become 161 part of a cumulate reservoir that is thermally connected to 162 but chemically isolated from M melt. The extent of matter 163 transfer between WR and M is governed by key parameters 164 connected to ambient geological conditions and initial bulk 165 compositions (Tables 1, 2, e.g., is WR cold or warm, wet or 166 dry, gabbroic or granitic)? In addition to contamination of 167 M melt by wallrock partial melt, contamination can occur by 168 the process of stoping (S). In MCS, stoped wallrock is added 169 en masse to M melt, and the contaminated system comes 170 to a new equilibrium state at a new thermodynamically 171

Table 1 System variables and compositions of parent magma, recharge magmas, wallrock and stoped blocks for five MCS simulations

System variables		
Pressure (GPa)	0.1	
Percolation threshold	0.1	
fO2 (during simulation)	None/absent	
Compositions		
Oxide in wt.%	Parental (resident) and recharge magma composi- tion	Wallrock and stoped block composition
SiO ₂	49.38	64.53
TiO ₂	1.73	0.62
Al ₂ O ₃	13.79	14.92
Fe ₂ O ₃	1.83 ^a	1.30 ^b
Cr ₂ O ₃	0	0
FeO	8.73	3.71
MnO	0.18	0.1
MgO	7.82	2.4
NiO	0	0
CoO	0	0
CaO	12.09	3.48
Na ₂ O	2.12	3.17
K ₂ O	0.23	2.71
P ₂ O ₅	0.15	0.15
H ₂ O	1.96	1.94
CO ₂	0.00	0.97

^aFor the parent magma, Fe⁺²/Fe⁺³ was calculated at FMQ at 1129 °C and at 0.1 GPa after adding ~2 wt.% of H₂O. Following this fO_2 calculation, the magma composition was normalized to 100%. See text for additional discussion

^bFor the WR, Fe^{+2}/Fe^{+3} was calculated at FMQ at 740° C and at 0.1 GPa after adding ~2 wt.% of H₂O and ~1 wt.% of CO₂; following this fO_2 calculation, the WR composition was normalized to 100%. See text for additional discussion

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Table 2 Initial conditions for five MCS simulations

	FC	R ₂ FC	AFC	S_2FC	R ₂ AFC
Magma liquidus temperature (°C)	1129	1129	1129	1129	1129
Temperature decrement (°C)	5	5	5	5	5
Magma initial mass (expressed as mass units, m.u.)		100	100	100	100
Hard stop temperature (°C) ^a		900	800	900	800
Wallrock find solidus start temperature (°C) ^b	880	880	880	880	880
Wallrock find solidus end temperature (°C) ^b	700	700	700	700	700
Wallrock find solidus temperature decrement (°C) ^b		5	5	5	5
Wallrock initial temperature (°C)		100	700	100	700
Wallrock initial mass (m.u.)		200	200	200	200
Recharge/stope event 1: mass (m.u.)		75		17	75
Recharge/stope event 1: temperature of recharge/stoped block when recharge/stoping occurs ($^{\circ}C$) ^c		1130		760	1130
Recharge/stoping occurs (°C) ^d		1050		1015	1050
Recharge/stope event 2: mass (m.u.)		75		38	75
Recharge/stope event 2: temperature of recharge/stoped block when recharge/stoping occurs (°C) ^c		1080		795	1080
Recharge/stope event 2: temperature of magma when recharge/stoping occurs $(^{\circ}C)^{d}$		1000		908	1000

^aHard stop temperature is temperature at which simulation ends, if this temperature is achieved prior to wallrock and magma reaching thermal equilibrium

^bThese parameters represent the starting and ending temperatures and the temperature decrement that are used in the wallrock find solidus routine of MCS. See https://mcs.geol.ucsb.edu for more information

^cThis represents the temperature of the recharge magma/stoped block when it enters the M melt

^dThis represents the temperature of the resident magma (*M* melt and cumulates) when the recharge/stoping event occurs. Note that the temperature at which recharge actually occurs (e.g., ~1049 °C for R1 in R₂FC case) differs slightly from that reported in the input (1050 °C), because the recharge event occurs in the step after that target temperature is reached

controlled temperature. The stoping event may cause crys-172 talline solids or a fluid to precipitate, and naturally, the con-173 taminated M melt assumes a different bulk composition. A 174 final process that MCS accounts for is magma mixing by 175 recharge (R). During R, a finite mass of internally equili-176 brated recharge magma, in a well-defined thermodynamic 177 state, is added to M melt, and the new mixture attains chemi-178 cal potential equilibrium. This operation is computationally 179 identical to the stoping operation. The user-defined condi-180 tion that triggers an R or S event is either a specified M melt 181 temperature or a temperature decrement from the last S or 182

R event. The current version of MCS allows a total of up to 183 30 distinct events of the S or R type. For more information 184 185 about the theoretical underpinnings of MCS, the reader is directed to Bohrson et al. (2014). 186

187 How does the Magma Chamber Simulator computer code work? 188

The MCS calculations are undertaken in two parts: (1) MCS-189 PhaseEQ: the major element and phase equilibria computa-190 tion of the RASFC evolution, and (2) MCS-Traces: the trace 191 192 element and isotopic (Sr, Nd, Hf, Pb, Os, and O) consequences of the RASFC scenario from output of MCS-Pha-193 seEQ. This bipartite structure recognizes that robust trace 194 element/isotopic calculations are necessarily built upon an 195

accurate major element solution that quantifies phase abundances, compositions, and temperatures. A researcher may 197 iterate in step (1) by comparing observables with predicted 198 results before investing effort into trace element and isotopic 199 modeling. Conversely, because of the bipartite structure, a 200 researcher can run multiple trace element and isotopic ratio 201 calculations using, for example, different initial trace ele-202 ment compositions and/or mineral-melt, mineral-fluid par-203 tition coefficients for M, WR, S and R utilizing the same 204 part (1) RASFC solution. Feedback to MCS-PhaseEQ for 205 different trace element concentrations and isotopic ratios is 206 not required, because major phase stability is not typically 207 sensitive to trace elements. The bipartite approach maintains 208 maximal flexibility in the pursuit of a 'best-fit' model and 209 aids in understanding the sensitivity of a full solution (phase 210 equilibria, trace elements and isotope) to the initial condi-211 tions and parameters. 212

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MCS-PhaseEQ is the union between a computational 213 thermodynamic engine and an executive brain (Bohrson 214 et al., 2014). The executive brain is built with Microsoft's 215 Visual Basic programming language; a snapshot of the 216 user interface of the current version is presented in Fig. 1. 217 The brain is responsible for implementing the particular 218 R_nAS_nFC scenario specified by the user by (1) sending 219 instructions to the chosen rhyolite- or pMELTS engine, (2) 220 performing additional internal calculations based on values 221

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Fig. 1 Command functions in the phase equilibria/major element interface of MCS-PhaseEQ. Step 1 initiates MCS communication with rhyolite- or pMELTS. Step 2 involves choosing an output file name and input MES file from those available. Step 3 is a preliminary calculation that prepares the WR subsystem by computing a solidus or near solidus thermodynamic state for wallrock for eventual coupling with the M subsystem, a requirement for AFC scenarios. Step 4 launches and runs the MCS-PhaseEQ simulation. Step 5 involves exporting the simulation results to an Excel workbook (see Online Resource 6). The other steps provide enhanced capability for running MCS, and these are detailed on the MCS website

returned from rhyolite- or pMELTS, (3) making the conditional and complex sequential executive decisions required to carry out the user-defined R_nAS_nFC petrological scenario, (4) producing a variety of real-time and archived graphical and numerical output, and (5) archiving input and output in
a systematic manner enabling a synoptic view of the results.226Several separate tools are available from the MCS website to
mine and utilize the output for various purposes.228

The thermodynamic engine implemented in the MCS-230 PhaseEQ is one of the rhyolite- or pMELTS codes currently 231 available. These are enumerated as pMELTS, and rhyolite-232 MELTS versions 1.0.2, 1.1.0, or 1.2.0 (Ghiorso and Sack 233 1995; Asimow and Ghiorso 1998; Ghiorso et al. 2002; 234 Gualda et al. 2012; Ghiorso and Gualda 2015; https://melts 235 .ofm-research.org/). A centerpiece of rhyolite- or pMELTS 236 is a thermodynamic model for the dependence of Gibbs free 237 energy of silicate liquids as a function of melt composition, 238 temperature (roughly 1000–2000 K), and pressure (roughly 239 0-3 GPa). For numerical calculations, the laws of thermody-240 namics, which are adhered to in rhyolite- and pMELTS are 241 not sufficient, and must be adjoined with the thermodynamic 242 properties of the materials composing the composite system. 243

More about critical design features of Magma Chamber Simulator

MCS was designed as a thermodynamic model that has 246 built-in assumptions about the ways in which the subsystems 247 interact. Like all models, the design of MCS leads to limita-248 tions in its application to natural systems and to developing 249 a framework for understanding how RASFC processes, in all 250 their complexity. In this section, we enumerate key aspects 251 of the design features of MCS and highlight limitations in 252 its use. 253

First and perhaps foremost, as noted, MCS is a thermo-254 dynamic model that, while allowing for open system behav-255 ior, assumes local thermodynamic equilibrium. There are 256 no compositional, pressure, temperature or other gradients 257 within wallrock, magma or recharge reservoirs. Because 258 MCS is a thermodynamic and not a transport model, thor-259 ough and complete homogenization is assumed when mag-260 mas mix, blocks are stoped, or partial melts are assimilated. 261 Heat and matter are instantaneously exchanged between 262 wallrock, magma (melt + cumulates) and recharge/stoping 263 subsystems, and each subsystem is, therefore, characterized 264 by a uniform temperature in each "step" of a simulation. 265 Enthalpy is conserved, and thus the temperature of the M 266 melt and cumulate subsystems is affected not only by tem-267 perature decrements imposed by user-defined cooling (see 268 below), but also by adjustments required by addition of hot-269 ter or colder recharge magma or wallrock stoped blocks or 270 anatectic melt. 271

In MCS, no absolute timescale is defined. However, an MCS 'arrow of time' (i.e., sequence of events) is defined by a user-specified RASFC scenario. Output archives an evolutionary record of melt composition, cumulate petrology, anatectic melt composition, wallrock residual mineralogy, 276

and pre-mixing state of stoped blocks and recharge mag-277 mas. Quantification of timescales can be approximated 278 using simple scaling arguments based on observed features 279 such as mineral zoning and magma mixing times (e.g., Old-280 enburg et al. 1989; Costa et al. 2008; Spera et al. 2016) 281 in consort with MCS results. A critic might object to the 282 purely thermodynamic approach noting that many irrevers-283 ible processes with concomitant entropy production (heat 284 conduction and convection, chemical diffusion, transport 285 of momentum by the action of viscosity) surely come into 286 play during the evolution of magmatic systems. We would 287 not argue against this vantage. However, experience shows 288 that local equilibrium is indeed often attained in high-tem-289 perature petrologic systems. Both the existence of a host of 290 useful geothermometers, geobarometers, and geohygrom-291 eters (e.g., Putirka 2008, 2017; Wade et al. 2008; Coogan 292 et al. 2014; Neave and Putirka 2017) and the consistency 293 of laboratory experiments with observed features in natu-294 ral magmatic systems (e.g., Bowen 1928; Yoder and Tilley 295 1962; Grove et al. 1992; Villiger et al. 2007) support the 296 notion that a thermodynamic approach has validity and can 297 be used to provide a useful 'reference frame' with which 298 transport considerations can be contemplated. Development 299 of an open system magmatic system model that simulta-300 neously incorporates transport phenomena at macroscopic 301 to molecular scales and embraces the assumption of local 302 thermodynamic equilibrium, when appropriate and valid for 303 three-dimensional representations, lies in the future. 304

The thermodynamic solutions provided by MCS are 305 dependent on the quality of the thermodynamic data that 306 underpins rhyolite- or pMELTS. These data include the 307 standard state properties of all phases, activity-composi-308 tion relations for all crystalline solutions defined by end-300 members with known standard state properties, the mixing 310 properties of H₂O-CO₂ supercritical fluids, the form of the 311 equation of state, and the Gibbs excess free energy model 312 for silicate liquids. The latter gives the excess Gibbs energy 313 of silicate melt as a function of composition, temperature, 314 and pressure for multicomponent silicate melt. Any thermo-315 dynamic model is no better than the data and basic assump-316 tions upon which it is based. The MELTS thermodynamic 317 database, while robust, has its limitations. For example, the 318 activity-composition relations for garnet, trioctahedral mica, 319 and amphibole family phases are reasonable but imperfect. 320 Hence, in volcanic and plutonic rocks where these phases 321 are modally abundant, the predictions of system evolu-322 tion are more uncertain. The coverage in p-T space for 323 which the rhyolite- and pMELTS engines are optimized is 324 roughly 1000-2000 K and 0-3 GPa, limiting modeling to 325 the outer ~ 100 km of Earth and deeper on smaller bodies 326 such as the Moon, Mars, Venus, Mercury and the asteroids. 327 Fortunately, this coverage is sufficient for a great variety of 328 igneous environments that may be modeled with MCS. 329

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Finally, we list additional design features that are criti-330 cal for the MCS user to appreciate: (1) MCS is an isobaric 331 model, and therefore, the composite system is defined by 332 a single pressure (e.g., Table 1); (2) during assimilation, 333 anatectic melt is transferred between wallrock and M melt. 334 A fluid phase and solids are not; they remain as a part of 335 the wallrock subsystem; (3) the criterion that a threshold 336 fraction of melt be attained in wallrock before partial melt 337 is added to and equilibrated with resident melt is informed 338 by the rheological properties of crystal-liquid mixtures 339 (Lesher and Spera 2015); however, the mass of partial melt 340 added from wallrock is simply the difference between the 341 evolving local melt fraction in wallrock and this user-defined 342 threshold value. There is no Darcy percolation per se. Trans-343 port details justifying melt extraction dynamics are given 344 elsewhere (Spera and Bohrson 2001; Bohrson et al. 2014); 345 (4) wallrock temperature is uniform throughout the entire 346 wallrock mass; (5) the output of MCS includes mass, ther-347 mal, and compositional information for melt, solids and fluid 348 phase for all subsystems; the user must be astute when com-349 paring (e.g.,) melt compositions in MCS with whole-rock 350 compositions from an igneous suite, as magmas (and their 351 solidified equivalents) can be complex combinations of melt, 352 crystals and fluid phase. 353

A complete description of the MCS along with the code 354 (both PC and Mac versions), examples, tutorials, and related 355 tools may be found at https://mcs.geol.ucsb.edu, the MCS 356 website. One of the related tools, the MCS Visualizer, oper-357 ates on the output produced by the MCS-PhaseEQ code 358 to generate an animated portrayal of a simulation, and the 359 Cumulate Calculator compiles the compositional informa-360 tion of the incremental and bulk cumulate and residual 361 wallrock composition for any MCS simulation; the Cumu-362 late Calculator is particularly useful to track compositional 363 model data relevant to intrusive environments. The Visual-364 izer and Cumulate Calculator are not described here; details 365 may be found on the MCS website. The MCS is continu-366 ously being developed so the reader is referred to the website 367 for news and the most up-to-date version available. 368

Comparison of closed (fractional crystallization) and open-system magma evolution illustrated by MCS

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We present five MCS-PhaseEQ simulations that compare 372 the melt composition and phase equilibria evolution of a 373 magma body undergoing fractional crystallization (FC), 374 recharge (two events)-fractional crystallization (R₂FC), 375 assimilation-fractional crystallization (AFC), fractional 376 crystallization accompanied by assimilation through stop-377 ing (two events) (S₂FC), and recharge (two events)-assimila-378 tion-fractional crystallization (R₂AFC). We provide detailed 379

comparisons of temperatures, masses, and compositions 380 of the results, and we acknowledge that these models are 381 illustrative; they are not intended to represent a particular 382 magmatic system, and different parameters and starting 383 bulk compositions will, indeed, yield different results. By 384 presenting these cases, our intent is, first, to highlight the 385 rich data sets that can be generated by MCS. Second, by 386 describing the results in some detail, we hope to provide 387 a roadmap for how MCS results can be used to unravel the 388 RASFC evolution of a particular magmatic system. Table 3 389 lists MCS variables and typical ranges used in modeling of 390 crustal systems. It also provides examples of petrological 391 and geochemical data that can be used to both inform choice 392 of input and to evaluate how MCS output can be utilized 393 to determine 'best-fit' results. Finally, via these specific 394 models, we elucidate characteristics of magma systems that 395 may-or may not-allow identification of a specific pro-396 cess like crustal assimilation or magma recharge/mixing. A 397 related longer term goal is to use MCS, in a vastly expanded 398 way, to develop a systematic framework for identifying and 399 distinguishing magma processes such as recharge, crustal 400 assimilation, and crystallization. 401

For each simulation, the fixed composite system pressure 402 is 0.1 GPa, which corresponds to the shallow crust at circa 403 3 km depth. The percolation threshold (fmZero) is 0.1 (mass 404 fraction), which means that before anatectic melt can be 405 transferred from wallrock to M melt, 10 wt.% melt must be 406 present in wallrock; any mass above this threshold is trans-407 ferred and equilibrated with M melt. For all simulations, the 408 mass of wallrock involved is twice (200 mass units, m.u.) 409 that of the initial magma (100 m.u.), yielding a wallrock/ini-410 tial resident magma mass ratio of two. This choice of mass 411 ratio implies that the heat available from the cooling and 412 crystallization of M magma is allowed to thermally interact 413 with country rock mass twice that of the original magma. 414 Because the enthalpy generated by the crystallization of fer-415 romagnesian phases (olivine, clinopyroxene, spinel) in mafic 416 magma is higher by about a factor of two than the fusion 417 enthalpy of the salic phases in the wallrock and because 418 the specific isobaric heat capacity increases with increas-419 ing temperature, a mass ratio of two is justified. However, 420 it is important to note that in MCS, the ratio of wallrock to 421 magma is an initial parameter of the calculation. The MCS 422 is not a heat transport model. All simulations discussed here 423 utilized rhyolite-MELTS v1.2.0. Tables 1, 2 list composi-424 tions and other initial conditions for the five simulations. 425

The parental magma for the five simulations is depleted mantle-derived continental tholeiite from the ~ 180 Ma Karoo Large Igneous Province (sample P27-AVL, Luttinen and Furnes 2000) (Table 1). Initial H₂O was set at ~ 2 wt.%, and the Fe²⁺ to Fe³⁺ ratio was initially calculated at FMQ (at liquidus temperature of 1129 °C and pressure of 0.1 GPa); each simulation was then run under fO_2 -buffer absent 450

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conditions. This means that the system is closed with respect 433 to the addition or subtraction of oxygen, and thus, during 434 the run, the fugacity of oxygen will rise or fall according 435 to the dictates of Gibbs energy minimization of the com-436 posite system. Each simulation has a user-chosen magma 437 temperature decrement of 5 °C, which means that the state 438 of the system (magma and wallrock melt, minerals, fluid 439 phase) is determined and archived at 5 °C temperature dec-440 rements for the FC case (Table 2). Within these 5-degree 441 decrements, the M subsystem can be envisaged to evolve by 442 equilibrium crystallization after which the formed minerals 443 are fractionated to the cumulate pile before the next step. 444 MCS-PhaseEO internally adjusts the M melt and cumulate 445 temperature to values other than those defined by the user-446 defined decrement in response to the homogenization of 447 recharge magma(s), stoped block(s), or anatectic melt with 448 M melt. 449

For the cases involving recharge (i.e., R_2FC , R_2AFC), the recharge magma compositions (including initial H_2O wt.% and fO_2) are identical to parent (resident) magma. Wallrock bulk composition is average upper continental crust from Rudnick and Gao (2003), with initial fO_2 calculated at FMQ (at 740 °C and 0.1 GPa), initial H_2O of ~2 wt.%, and initial CO_2 of ~1 wt.% (Table 1).

The models are discussed and compared in detail below. 457 Online Resource 1 provides input for the cases (similar to 458 Table 1 but in Excel format), and Online Resources 2-5 459 present detailed comparison data for mass and temperature 460 outcomes, mineral assemblage, fluid saturation, and selected 461 melt compositional parameters for resident magma, wall-462 rock, and recharge magmas for each case. Figure 2 shows the 463 model outcomes in illustrations that are annotated snapshots 464 from the MCS Visualizer tool and Figs. 3, 4, 5, 6, 7, 8 illus-465 trate selected mass, thermal, and compositional data for melt 466 and minerals for resident magma and wallrock. 467

All model input and output are presented in Online 468 Resource 6, and we recommend viewing the output files 469 (concentrating on the RunSummary tab) simultaneously 470 when reading the following sections. The structure of the 471 output files is uniform across all cases and, hence, time 472 invested in learning the structure of the output makes the 473 digestion of data relatively easy after an investment of effort. 474 By way of introduction, the different tabs of the output that 475 store the relevant information are specifically named in the 476 discussion of the FC case. In addition, the MES input files 477 are included in Online Resource 7; this means that all the 478 cases discussed here can be replicated. It should be noted 479 that there can be small differences at the part per thousand 480 level when MCS is run in different computing environments. 481 These differences are well below levels that have an impact 482 on interpretation of results in cases where we have studied 483 this phenomenon. Finally, case-specific animations that help 484 to follow the changes in the bulk system and which were 485

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MCS parameter	Typical range employed in MCS for crustal magmatic systems	Constraints provided by data from plutonic and volcanic systems	Best-fit decision making: how do I evaluate the model parameter?
Pressure of crustal magma systems	< 0.1 to ~ 1.0 GPa	Pressure-dependent phase assemblage, inde- pendent geobarometry	Different pressure runs may yield different major and trace element trends, cumulate assemblages, cumulate mineral composi- tions, sequence ('arrow of time') of cumulate mineral compositions
Oxygen fugacity of system	Unconstrained, IW, COH, QFM, NNO HM	Mineral equilibria. For many systems without such constraints QFM or NNO buffer is appropriate; otherwise setting at QFM to determine ferrous/ferric in M parent melt and then running unconstrained is also appropriate	Different buffers may show different major and trace element trends; typically, FeO, Fe ₂ O ₃ , TiO ₂ are most distinctive; different cumulate mineral assemblages may result from different fO_2 as well
fmZero (residual melt fraction held in wall- rock)	0.04 to> 0.12	Melt inclusions may provide composition of partial melt. Melt wets silicate and oxide grain boundaries to form interconnected net- work at low melt fractions; values at larger end of range for more silicic wallrock	Different fmZero will lead to different anatectic melt compositions, may yield different major and trace element trends, cumulate assem- blages, cumulate mineral compositions. Melt inclusions may represent anatectic melt, comparison between model output and these data may help constrain fmZero
Parent magma composition	Basalt to rhyolite	Most primitive of exposed suite of related rocks, estimate of parent magma based on melt inclusions, reconstruction of parental from mineral data	Comparison of most primitive sample with initial composition of MCS run
Wallrock composition	Peridotite to granite	Outcrops, drill cores, xenoliths, melt inclu- sions, seismic data	Different wallrock compositions may yield different major/trace element/isotope trends, cumulate assemblages, cumulate mineral compositions, sequence ('arrow of time') of cumulate mineral compositions, in situ isotopic record
Initial wallrock temperature	0 to~750 °C	Pressure estimates coupled with estimates of geothermal gradient, evidence of thermal priming	Different wallrock temperatures may yield different major/trace element/isotope trends, cumulate assemblages, cumulate mineral compositions, sequence ('arrow of time') of cumulate mineral compositions/isotopes. Will also change temperature of magma at which assimilation begins; this record may be detected in compositional and isotopic data in cumulate crystals, and via changes in isotopes in samples where absolute or relative ages are documented

constraints provided by plutonic and volcanic data, and suidelines for evaluating model results
 Table 3
 Typical input ranges of MCS parameters.

Table 3 (continued)			
MCS parameter	Typical range employed in MCS for crustal magmatic systems	Constraints provided by data from plutonic and volcanic systems	Best-fit decision making: how do I evaluate the model parameter?
Ratio of initial wallrock mass to initial magma mass	>0 to~3	Upper limit from enthalpy balance. For natural systems, the value depends on many transport and thermophysical properties as well as the state of stress in wallrock (both 'tectonic' stress and thermal stress); each natural system requires unique characteriza- tion	Different ratio may yield different major/trace element/isotope trends, cumulate assemblages, cumulate mineral compositions, sequence ('arrow of time') of cumulate mineral compo- sitions/isotopes. Will also change temperature of magma at which assimilation begins; this record may be detected in compositional and isotopic data in cumulate crystals, and via changes in isotopes in samples where absolute or relative ages are documented
Recharge magma composition	Basalt to rhyolite	Reconstructions based on compositional zoning of crystals in solidified products, composition of enclaves, end-member composition of distinct members of mingled rocks, composition of melt inclusions	Different compositions may yield different major/trace element/isotope trends, cumulate assemblages, cumulate mineral composi- tions, sequence ('arrow of time') of cumulate mineral compositions/isotopes
Temperature of magma when recharge/stoping event occurs ('trigger temperature')	Liquidus temperature to near solidus tempera- ture	Geothermometry applied to zoned crystals, to melt inclusions, and to mingled rocks, erup- tion temperature	Different compositions may yield different major/trace element/isotope trends, cumulate assemblages, cumulate mineral composi- tions, sequence ('arrow of time') of cumulate mineral compositions/isotopes. First evidence of recharge also dependent on 'trigger' tem- perature. Record may be detected via in situ compositional and isotopic data in cumulate crystals, and may also be detected through changes in isotopes in samples where absolute or relative ages are documented
Temperature and crystallinity ("state") of recharge magma at recharge event	Liquidus temperature to below solidus tem- perature, 100% melt to solid	Character of enclaves (i.e., crystal versus glass/groundmass), crystal populations in solidified products that might inform state of recharge magma	Different 'state' may yield different major/trace element/isotope trends, cumulate assemblages, cumulate mineral compositions, sequence ('arrow of time') of cumulate mineral compo- sitions/isotopes. 'State' also impacts M melt temperature change when recharge occurs; this may be documented via geothermometry of cumulate crystals
Ratio of recharge mass to initial magma mass	<0.1 to > 2	Compositional contrasts documented in rock suites that have relative or absolute age information (e.g., dacitic eruption fol- lowed by basaltic eruption), composition of enclaves, melt inclusions	Different ratio may yield different major/trace element/isotope trends, cumulate assemblages, cumulate mineral compositions, sequence ('arrow of time') of cumulate mineral compo- sitions/isotopes

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MCS parameter	Typical range employed in MCS for crustal magmatic systems	Constraints provided by data from plutonic and volcanic systems	Best-fit decision making: how do I evaluate the model parameter?
Temperature and crystallinity ('state') of stoped wallrock at stoping event	Near to below solidus temperature	Xenoliths or xenocrysts of crustal origin, melt inclusions	Different 'state' may yield different major/trace element/isotope trends, cumulate assemblages, cumulate mineral compositions, sequence ('arrow of time') of cumulate mineral compo- sitions/isotopes. 'State' also impacts <i>M</i> melt temperature change when stoping occurs; this may be documented via geothermometry of cumulate crystals
Ratio of stoped block(s) mass to initial magma mass		Compositional and isotopic contrasts docu- mented in rock suites that have relative or absolute age information	Different ratio may yield different major/trace element/isotope trends, cumulate assemblages, cumulate mineral compositions, sequence ('arrow of time') of cumulate mineral compo- sitions/isotopes

Table 3 (continued)

built with the MCS Visualizer are given in Online Resource 486 8. 487

Case 1: fractional crystallization (FC) 488

The output of the FC case is stored in "MCS-FC output 489 PhaseEQ.xlsx" file in Online Resource 6. The parent basalt 490 specified above has a liquidus temperature of ~1129 °C at 491 0.1 GPa, and the FC simulation ends at a user-chosen tem-492 perature of ~900 °C. Via fractional crystallization, the melt 493 composition evolves from tholeiitic basalt to dacite, with 494 the dacitic melt forming through ~76 wt.% fractional crys-495 tallization (Figs. 2a and 3, see ChartTAS tab in the output). 496 Magma melt becomes H₂O-saturated at ~ 1029 °C. At the 497 end-temperature (~900 °C), the H₂O-fluid phase consti-498 tutes ~1 wt.% of the magma system, with melt composing 499 the remaining ~ 23 wt.% (Fig. 3) as noted by examination of 500 columns I through L on row 52 of the RunSummary tab in 501 the output. Major oxide trends behave as anticipated for a 502 basaltic system undergoing fractional crystallization (Fig. 4). 503

Olivine is the first liquidus phase (see column Z of the 504 RunSummary tab), and its composition is Fo₈₂ (line 269, 505 SolidFormulas tab, color code darker blue). It is followed 506 closely by clinopyroxene (first appearance at ~1119 °C) and 507 plagioclase (first appearance at ~ 1084 °C, An₈₄). Additional 508 phases include spinel (first appearance at ~ 1069 °C) and 509 rhombohedral oxide (first appearance at~984 °C). By the 510 end of crystallization, the cumulate is dominated by clino-511 pyroxene and plagioclase, each of which composes ~40 wt.% 512 of the bulk cumulate mass; olivine constitutes ~ 15 wt.%, 513 spinel ~ 6 wt.% and rhombohedral oxide < 1 wt.% (Fig. 5). 514 This information is graphically portrayed on the output tabs 515 ChartMassFrac, ChartPPD, and ChartPMD. The composi-516 tional range of minerals is large (see output SolidFormulas 517 tab and Online Resource 3), as anticipated for a parental 518 basaltic melt that evolves to dacitic after significant frac-519 tional crystallization. 520

The initial wallrock temperature for this simulation is 521 100 °C. Enthalpy transferred from magma due to cooling and crystallization yields a final wallrock temperature of ~ 329 °C (Fig. 2a), too low for any partial melting 524 to occur. Thus, although the wallrock heats up, it remains 525 below its solidus temperature, and no mass transfer occurs. 526

Case 2: recharge–fractional crystallization (R₂FC) 527

The output of the R2FC case is stored in "MCS-R2FC_out-
put_PhaseEQ.xlsx" file in Online Resource 6. Two recharge
events simulate intrusion of mantle-derived magma into resi-
dent magma melt as it evolves by fractional crystallization in
an upper crustal (0.1 GPa) magma storage system. The first
recharge event involves a recharge magma/initial magma
mass ratio of 0.75 (that is, for an initial parent melt mass of
534528
529



Fig. 2 Results of MCS-PhaseEQ simulations for five cases (FC, AFC, R_2FC , S_2FC , R_2AFC) shown in annotated MCS Visualizer snapshots that depict the situation after the final magma crystallization step (AFC and R_2AFC include one additional step of wallrock equilibration before the simulation ends). Completions of R and S events and beginning of A are indicated in the cumulate pile where applicable. Note that the phase proportions are based on mass fractions not vol-

ume fractions and that the wt.% of the subsystems are relative to the whole magma-wallrock system; M melt, M fluid, and M cumulate comprise the total magma chamber mass. See Online Resource 8 for full animations. Mineral abbreviations: *ol* olivine, *opx* orthopyroxene, *cpx* clinopyroxene (FC and S_2FC include two separately output cpx solid-solution phases, see the respective outputs in Online Resource 6), *plag* plagioclase, *qtz* quartz, *spl* spinel, *rhm* rhombohedral oxide



Fig. 3 Results of MCS-PhaseEQ simulations for five cases (FC, AFC, R_2FC , S_2FC , R_2AFC) shown in magma temperature (°C) versus **a** absolute and **b** relative *M* magma liquid (melt) mass, **c** absolute and **d** relative total cumulative mass of crystals removed to the cumulate reservoir, and **e** absolute and **f** relative total cumulative mass of fluid phase. Each simulation runs from parent magma liquidus tempera-

ture to the end of the simulation. For cases involving assimilation, the simulation ends when magma and wallrock are at or close to thermal equilibrium. For cases that do not involve assimilation, the simulation ends at a user-defined "hard stop" temperature. Completions of R and S events and beginning of A are indicated for the relevant runs in a. See text, tables and Online Resources for additional details

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Fig. 4 Results of MCS simulations for five cases (FC, AFC, R₂FC, S₂FC, R₂AFC) shown in magma melt SiO₂ (wt.%) versus **a** TiO₂, **b** Al₂O₃, **c** Fe₂O₃, **d** FeO, **e** MgO, **f** CaO, **g** Na₂O, **h** K₂O, **i** P₂O₅, and **j** H₂O (wt.%)

100 m.u., 75 m.u. of recharge magma is added (Table 2)).
This recharge magma at ~ 1130 °C (100 wt.% melt) intrudes
into and fully hybridizes with resident melt at ~ 1049 °C

(Tables 1, 2, Online Resource 2). Note that the temperature at which recharge actually occurs differs slightly from that reported in the input (Table 2, 1050 °C), because the 540





Fig. 4 (continued)

recharge event occurs in the step after the target tempera-541 ture is reached. Prior to the first recharge event, the resi-542 dent magma had been crystallizing a mineral assemblage 543 of olivine (Fo_{70}) + clinopyroxene $(Mg\#_{77})$ + plagioclase 544 (An_{81}) + spinel. Immediately following the recharge event, 545 the new, equilibrated state of hybridized M melt yields a 546 547 new temperature of 1093 °C due to addition of enthalpy from recharge magma, and crystallization of clinopyroxene, 548 plagioclase, and spinel is suppressed. Thus, in response to 549 mixing, resident magma (melt+cumulates) temperature 550 increases by almost 50 °C and the hybridized magma crys-551 tallizes only olivine that is more magnesian (Fo78) than oli-552 vine crystallizing just prior to the recharge event. With 5 °C 553 of additional post-recharge cooling, clinopyroxene (Mg $\#_{82}$) 554 returns to the M crystallizing assemblage, and with an addi-555 556 tional~25-30 °C of cooling, plagioclase (An₈₂) and spinel also returns to the crystallizing assemblage. For most major 557 oxides, the first recharge event has only a subtle effect on 558 resident melt composition: the most pronounced changes are 559

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an increase in MgO from ~4.4 to 6.2 wt.%, and a decrease in SiO_2 from 52.6 to 50.9 wt.% (Fig. 4).

560

561

The second recharge event is compositionally identical 562 to and has the same mass constraints as the first (75 m.u.), 563 but for this recharge event, the temperature of the recharge 564 magma is ~ 1080 °C; thus the magma is 21 wt.% crys-565 talline [mode of the assemblage is ~ 12 wt.% is olivine 566 (Fo₇₆), ~82 wt.% is clinopyroxene (Mg $\#_{81}$), and ~6 wt.% is 567 plagioclase (An_{83})] at the time recharge is triggered (Online 568 Resource 5). This second "event" yields a new M tempera-569 ture of ~1040 °C, an increase of ~40 °C. Plagioclase and 570 spinel crystallization is suppressed for only ~5 °C. The com-571 positions of the minerals change in response to recharge: oli-572 vine $(Fo_{55} \rightarrow Fo_{68})$ + clinopyroxene $(Mg\#_{70} \rightarrow Mg\#_{77})$ + pla-573 gioclase $(An_{71} \rightarrow An_{77})$. At 985 °C, orthopyroxene joins 574 the mineral assemblage, followed by rhombohedral oxide 575 at ~980 °C; orthopyroxene crystallization ceases at 955 °C. 576 Importantly, some of the major oxide changes pre- and post-577 recharge are more profound compared to the first recharge 578



Fig. 5 Magma temperature ($^{\circ}$ C) versus wt.% of minerals in the bulk cumulate in the five MCS simulations. **a** olivine, **b** clinopyroxene (cpx), **c** plagioclase, **d** spinel, **e** rhombohedral oxide, and **f** orthopyroxene (opx)

event, because the contrast between resident melt and
recharge magma is greater. For example, from pre- to postrecharge, SiO₂ decreases from ~58 to 54.5 wt.% (as opposed

to a decrease of < 2 wt.% SiO₂ in *M* following Recharge 582 event 1; see also Fig. 4). 583

The final temperature of the R_2FC simulation is ~900 °C, 584 and the final melt composition is dacitic. The final R_2FC 585

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Fig. 6 Wallrock temperature (°C) versus wt.% of **a** alkali feldspar, **b** plagioclase, and **c** quartz in wallrock solids (restite after partial melt is transferred to magma) for two MCS cases involving assimilation of wallrock anatectic melt (AFC, R_2AFC). Wallrock initial temperature

is 700 °C, and assimilation starts at wallrock temperature of 747 °C when the percolation threshold has been exceeded. Wallrock heats up to the end of the simulation, where magma and wallrock temperature are at or close to thermal equilibrium

melt major oxide compositions are similar to those of the 586 FC case; that is, the record of the increases in MgO and 587 decreases in SiO₂ is not preserved in the final melt composi-588 tion (Fig. 4), although a record is preserved in the compo-589 sitional record of the cumulate phases. The proportion of 590 crystals, melt, and fluid phase at the final simulation tem-591 perature is similar between R₂FC and FC (~77 wt.% crys-592 tals, 22 wt.% melt, 1 wt.% fluid for R₂FC versus ~ 76 wt.% 593 crystals, 23 wt.% melt, 1 wt.% fluid for FC, respectively; 594 Fig. 3). The proportions of phases in the final cumulate are 595 similar, with the obvious exception of orthopyroxene, which 596 makes up ~ 2 wt.% of the final cumulate in R_2FC (Fig. 5). 597 The general range of mineral compositions is also similar 598 (Online Resource 3). 599

What is distinctly different between FC and R_2FC is the overall mass of the system, which is ~ 2.5 times greater in

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 R_2FC , because the recharge events add 150 (2×75) m.u. 602 into the system. Thus, the total mass of the R₂FC sys-603 tem is 250 m.u., compared to 100 m.u. in the FC case. 604 The masses of melt, cumulates, and fluid are also propor-605 tionally larger, as anticipated (Fig. 3). Finally, the larger 606 magma system mass significantly affects the wallrock tem-607 perature, with a final wallrock temperature of ~ 656 °C, 608 compared to ~ 329 °C for FC alone (Fig. 2). The hotter 609 wallrock is due to the added enthalpy of recharge magma 610 intruding into resident melt. This suggests that recharge 611 systems are more prone to induce partial melting in their 612 host rocks due to this 'enthalpy-pumping' effect (all other 613 conditions remaining constant). 614

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Fig. 7 Magma temperature (°C) versus a absolute and b relative amount of cumulative anatectic melt assimilated into M melt once assimilation begins. Completions of the R events for the R2AFC case are indicated



Fig.8 Magma temperature (°C) versus a instantaneous "r", and b cumulative "r" shown for two MCS cases with assimilation of wallrock anatectic melt (AFC, R₂AFC). The definition of "r" is based on DePaolo (1981) and is the mass of anatectic melt assimilated/mass of crystals formed. Instantaneous refers to those masses for each individual temperature step where assimilation ± recharge occurs, and cumulative refers to the total mass of anatectic melt assimilated/total



mass of cumulates produced from the start of the simulation to the magma temperature shown. The value of "r" is zero before assimilation begins, and for simplicity, this part of the AFC or R₂AFC is not shown. Instantaneous and cumulative "r" after completion of recharge events 1 and 2 labeled, as are the values at which anatectic melt productivity decreases due to complete reaction of alkali feldspar. See text for discussion

Case 3: assimilation of wallrock anatectic 615 melts-fractional crystallization (AFC) 616

The output of the AFC case is stored in "MCS-AFC_out-617 put PhaseEQ.xlsx" file in Online Resource 6. This case 618 reflects assimilation of upper continental crust by a depleted 619 continental tholeiite evolving in an upper crustal (0.1 GPa) 620 magma storage system. All other parameters being identical, 621 the initial conditions of the AFC simulation contrast with 622

those of the FC case with regard to the initial temperature 623 of wallrock; it is 700 °C compared to 100 °C. The elevated 624 wallrock temperature is intended to maximize the assimila-625 tion signature and simulates assimilation in crust that has 626 been thermally primed by previous episodes of magmatism 627 (e.g., Moore et al. 2018). 628

As resident melt cools from its liquidus, it first evolves 629 like in the FC case. For a wallrock/initial magma mass 630 ratio of two, anatectic (wallrock) partial melt begins 631

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Cumulative "r" 9.0 9.0 70 8.0

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to contaminate magma melt at a M melt temperature 632 of ~1069 °C (Fig. 3a). At this point, the wallrock is ~747 °C 633 and its percolation threshold (10 wt.%) for anatectic melt 634 has been exceeded. Anatectic melt above this limit is trans-635 ferred into, and thoroughly hybridized and equilibrated with 636 *M* melt. Note that because incoming anatectic melt is at a 637 lower temperature and different specific enthalpy than M 638 melt, the assimilation of wallrock partial melts drives M 639 melt to a slightly lower temperature. This is a consequence 640 of the isenthalpic AFC process. That is, the energy for par-641 tial melting of wallrock is derived by the cooling and crystal-642 lization of the M subsystem. The new, lower magma tem-643 perature following assimilation can catalyze crystallization 644 of the contaminated melt. These crystals, like all crystals 645 in MCS-PhaseEQ, become part of the cumulate reservoir, 646 where they remain in thermal contact with M melt. 647

At the onset of assimilation, the assemblage that crys-648 tallizes continues to be olivine + clinopyroxene + plagio-649 clase + spinel, albeit in slightly smaller proportions than 650 before AFC onset. Contaminated melt becomes fluid satu-651 rated at ~985 °C, which is ~44 °C lower than the FC case; 652 this is most likely due to the design feature in MCS that 653 does not (currently) permit fluid phase transfer with anatec-654 tic melt, although H₂O does enter into M magma, because 655 anatectic melt is H₂O-saturated. This effect is mediated by 656 pressure. At the low pressure of the simulation, the water-657 content of anatectic melt is low since the solubility of water 658 in anatectic melt is small. At higher pressure, more H₂O 659 component would be delivered to M magma by partial 660 melt assimilation. At magma temperature ~ 1000 °C, oli-661 vine becomes unstable, and is replaced by orthopyroxene. 662 At~952 °C, rhombohedral oxide joins the stable mineral 663 assemblage and clinopyroxene crystallization effectively 664 ceases (Fig. 5). 665

By the terminus of the run (M-WR equilibration tem-666 perature of ~852 °C), contaminated M melt has evolved to a 667 dacitic composition; at that temperature, the final wt.% SiO₂ 668 produced by the FC and AFC runs are within 1 wt.% (69 ver-669 sus 70 wt. %, Fig. 4) of each other. Once assimilation begins, 670 at the same SiO₂ compared to FC, AFC Al₂O₃ and K₂O have 671 distinctly higher concentrations, whereas Na₂O, H₂O, and 672 FeO are lower. CaO, MgO, Fe₂O₃, and TiO₂ are similar, and 673 P_2O_5 behavior is more complicated: it is initially a bit higher 674 and then distinctly lower at the same SiO_2 (Fig. 4). 675

The effect of assimilation on crystallization is marked; 676 the proportion of crystals in the cumulate reservoir of the 677 AFC magma system (~43 wt.%) is much smaller than 678 that associated with FC (76 wt.%); the proportion of fluid 679 phase in AFC is an order of magnitude smaller (0.1 versus 680 1 wt.%) (Fig. 3). The final AFC cumulate is different than 681 the FC one; there is slightly less olivine and clinopyrox-682 ene, very similar percentage of plagioclase, and in AFC, 683 orthopyroxene makes up ~ 12 wt.% of the final cumulate 684

(Fig. 5). In addition, the total ranges in olivine and plagio-685 clase compositions are different (Online Resource 3). The 686 last olivine to crystallize in AFC is Fo₆₂ (compared to Fo₂₃ 687 in FC) and the final plagioclase to crystallize is slightly 688 more anorthitic (An_{54}) compared to FC (An_{47}) . Thus, addi-689 tion of anatectic melt changes not only the crystallizing 690 assemblage (e.g., orthopyroxene precipitates, and olivine 691 and clinopyroxene disappear as cumulus phases) but also 692 changes the balance of melt versus cumulate (Fig. 3). AFC 693 also delays the onset of fluid saturation by tens of degrees, 694 and the total proportion of the magma system that is an 695 exsolved fluid phase is much smaller (Fig. 2c). 696

The mineral abundances of wallrock at its solidus are 697 plagioclase >> quartz > alkali feldspar > orthopyroxene; 698 spinel + rhombohedral oxide + biotite + apatite are acces-699 sory phases (Online Resource 4). Note also that wallrock 700 is fluid saturated. Wallrock reaches its percolation thresh-701 old temperature at ~747 °C; in the first instance of partial 702 melting above the percolation threshold, apatite reacts and 703 ceases to be a part of the wallrock residual mineral assem-704 blage; the same is true of biotite. The restite assemblage 705 of plagioclase + quartz + alkali feldspar + orthopyroxene. 706 with accessory spinel + rhombohedral oxide, persists until 707 wallrock temperature ~ 782 °C, at which point, alkali feld-708 spar is totally consumed (Fig. 6a). The remaining minerals 709 persist in wallrock restite to the equilibration temperature. 710

For each step of anatectic melt transfer into M melt 711 (except the first one), the size of anatectic melt incre-712 ment is $\sim 2-3$ wt.% of the initial mass of the wallrock 713 system (i.e., mass transfer involves ~ 4-6 m.u. of the ini-714 tial 200 m.u. of wallrock). This mass rate of melt trans-715 fer changes when alkali feldspar completely dissolves. 716 After this (wallrock T ~ 782 °C, Fig. 6a), wallrock melt 717 productivity decreases, and the size of the increments 718 transferred goes down to < 1 wt.% of the initial wallrock 719 mass (<2 mass units) (Fig. 7, magma T~920 °C where 720 slope changes slightly). Anatectic melt that is transferred 721 and homogenized with resident magma melt is mostly rhy-722 olitic, varying in SiO₂ between ~ 70 (at onset of assimila-723 tion) and 76 wt.% (at the equilibration temperature). The 724 cumulative percent anatectic melt added to the magma 725 system can be viewed in two different ways. The total 726 proportion of the wallrock system that was assimilated 727 into resident magma is ~ 35 wt.% (~71 m.u. of the initial 728 200 m.u., Fig. 7). When assessed as a part of the resident 729 magma, this assimilated mass represents about 41 wt.% 730 of the final resident magma (melt + crystals + fluid phase 731 body mass: ~71 m.u. of the final 171 m.u. system). By 732 the time thermal equilibrium is attained, the wallrock 733 has melted ~ 42 wt.%; this value is different than the total 734 amount of wallrock assimilated, because 10 wt.% anatec-735 tic melt remains within the wallrock system. See Online 736 Resource 2 for details of these mass relations. 737

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In the current available version of MCS, fluid phase pre-738 sent in WR is not permitted to transfer from WR to M. There 739 may be circumstances that favor fluid phase bulk transfer 740 with partial melt as it percolates into M magma. For exam-741 ple, fluid bubbles of low viscosity may be swept into M melt 742 by the same Darcian percolative flow that transports partial 743 melt. The likelihood of such transport depends on many fac-744 tors including the bulk H₂O content of wallrock as well as 745 the stability of possible hydrous phases such as amphibole 746 or biotite. Work to provide the user with the ability to trans-747 fer fluid phase, when it exists in wallrock, is ongoing and 748 will be presented in an updated version of MCS. To assess 749 the effects of possible fluid transfer on the results presented 750 here, four comparisons were run in which the M melt com-751 positions at two temperatures (1061 °C and 861 °C) were 752 adjusted by arbitrarily adding 20 wt.% and 40 wt.% of the 753 mixed $(H_2O + CO_2)$ fluid present in wallrock at the relevant 754 temperatures (i.e., the temperature of WR in the AFC run 755 at the M temperatures of 1061 and 861 °C) of 747 °C and 756 845.°C, respectively. These new, "fluid-enhanced" magmas 757 were examined in rhyolite-MELTS v 1.2.0 at 1055 °C and 758 855 °C using the equilibrium crystallization function. (i.e., 759 5 °C below the temperature of fluid enhancement). The 760 phase assemblages between the MCS results and the rhyo-761 lite-MELTS results are virtually identical, as are the M melt 762 compositions. The only significant difference is the mass/ 763 proportion of fluid phase in the melt. The likelihood that M 764 magma fluid saturates is obviously higher when fluid phase 765 is allowed to migrate across the wallrock-magma subsystem 766 boundary. See Online Resource 9 for the outcomes of this 767 comparison. 768

Case 4: assimilation of stoped wallrock blocks-fractional crystallization (S₂FC)

The output of the S₂FC case is stored in "MCS-S2FC_out-771 put_PhaseEQ.xlsx" file in Online Resource 6. Stoping in 772 MCS is considered as a process whereby crustal contami-773 nation (synonymous with crustal assimilation) occurs via 774 reaction of a block (or a set of multiple small blocks with a 775 combined mass equal to the respective S event) of wallrock 776 incorporated wholesale into magma melt. The pre-stoping 777 temperature of the stoped block dictates its thermodynamic 778 state; that is, the block can be stoped with different pro-779 portions of crystals, melt, and fluid phase. The S₂FC case 780 presented here involves two stoping events, with all other 781 parameters being identical to those of the FC case. 782

In MCS, stoped blocks are incorporated into M melt
using the recharge function since the thermodynamics of
stoping are identical to those of magma recharge and mixing. The initial (bulk) composition of the stoped blocks,
however, is the same as initial wallrock in the AFC case
(Table 1). Stoped block temperatures and masses were

chosen, where possible, to provide relevant comparison with 789 the AFC case. For stoping event 1, the mass of the stoped 790 block was chosen to reflect the cumulative mass of anatectic 791 melt assimilated by M by ~ 1015 °C (~ 17 m.u.; the ratio of 792 stoped block to initial magma mass is 0.17); the tempera-793 ture of the stoped block was chosen to reflect the wallrock 794 temperature at that point as well (~760 °C). At 760 °C, the 795 (mushy) block is composed of ~78 wt.% crystals, 20 wt.% 796 melt and 2 wt.% fluid phase, and its mineral assemblage is 797 plagioclase > quartz > orthopyroxene > alkali feldspar, with798 spinel and rhombohedral oxide as accessory phases. The co-799 existing melt is rhyolitic and fluid saturated. We note that in 800 contrast to the current version of MCS in which fluid phase 801 is not able to transfer into M melt during partial melt assim-802 ilation, stoping allows the fluid phase to be incorporated 803 into M melt. Prior to the first stoping event, resident magma 804 temperature was ~ 1014 °C, and M melt was crystallizing 805 olivine + clinopyroxene + plagioclase + spinel. Following 806 complete homogenization of the stoped block (including its 807 fluid phase), the resident magma temperature decreased to 808 967 °C, and orthopyroxene becomes stable in the cumu-809 late assemblage over the range 967–947 °C. Rhombohedral 810 oxide is the final phase to join the crystallizing assemblage 811 at a magma temperature of 942 °C. Upon stoping, resident 812 magma melt SiO₂ increases from ~ 56 to ~ 62 wt.% (Fig. 4). 813

The second stoped block reflects the conditions of the 814 wallrock in the AFC run at M temperature ~ 908 °C; at this 815 temperature, the wallrock is ~795 °C and cumulative ana-816 tectic melt assimilated is ~ 55 m.u. (ratio to initial magma 817 mass is ~ 0.55). Stoped block 2, therefore, has a tempera-818 ture of ~795 °C and its mass is 38 m.u. (55-17 that was 819 assimilated in the first stoping event). Stoped block 2 is hot-820 ter than stoped block 1, and therefore, it has proportionally 821 more melt: crystal, melt, fluid phase proportions are 60, 38, 822 and ~2 wt.%, respectively. Its mineral composition is plagio-823 clase >> orthopyroxene > quartz, with accessory spinel and 824 rhombohedral oxide. Like stoped block 1, the co-existing 825 melt is rhyolitic and fluid saturated. For stoping event 2, 826 the magma temperature before stoping is ~907 °C and after 827 stoping is 862 °C. Prior to the second stoping event, resi-828 dent magma was crystallizing olivine + clinopyroxene + pla-829 gioclase + spinel + rhombohedral oxide. Following assimila-830 tion of the second stoped block, olivine and clinopyroxene 831 cease to crystallize, and orthopyroxene becomes a part of 832 the cumulate assemblage. Upon the second stoping event, 833 SiO₂ increases from ~ 67 to ~ 73 wt.% (Fig. 4). 834

This simulation ends at ~856 °C, which is a similar end temperature to that of the AFC case. Compared to assimilation of anatectic melt ('classical' AFC), stoping favors crystallization, as the resultant proportion of crystals in the magma system is higher in S₂FC (68 wt.%) than AFC (43 wt.%; Fig. 3d). The percent fluid phase is also higher in S₂FC (Fig. 3e). The final cumulate shares some 841

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characteristics with those of the AFC case: similar percent-842 ages of olivine, spinel, and orthopyroxene, slightly less 843 clinopyroxene and less rhombohedral oxide, and slightly 844 more plagioclase (Fig. 5). The range of olivine composition 845 is more similar to the FC case. Interestingly, plagioclase 846 in S_2FC is the most albitic of all the simulations (Online 847 Resource 3). The final melt at ~856 °C is rhyolitic. Oxide 848 concentrations are more similar to the FC case than the AFC 849 case (Fig. 4). For example, the distinct enrichment in Al_2O_3 850 seen in the AFC case is absent in the stoping case. K₂O is 851 enriched compared to FC, but less so than AFC. 852

The final temperature of wallrock is 296 °C. This is the 853 lowest final wallrock temperature of the five simulations. 854 Adding cooler stoped bocks impacts the amount of enthalpy 855 available for wallrock heating. In addition, upon stoping, 856 in the new equilibrium M melt, quartz and alkali feldspar 857 (where present in the stoped block) are not stable. Hence, 858 there is an enthalpy cost to resorbing/reacting these phases, 859 which decreases enthalpy available for transfer into the 860 wallrock. 861

⁸⁶² Case 5: recharge–assimilation of wallrock anatectic ⁸⁶³ melts–fractional crystallization (R₂AFC)

The output of the R₂AFC case is stored in "MCS-R2AFC 864 output PhaseEQ.xlsx" file in Online Resource 6. The two 865 recharge events from the R₂FC case were imposed on the 866 AFC case; recall that the wallrock initial temperature is high 867 (700 °C) and reflects an assumption that previous magma 868 intrusion raised the wallrock temperature compared to an 869 ambient geotherm. For the two recharge events, like R₂FC, 870 the recharge magma/initial magma mass ratio is 0.75, and 871 the temperatures of the recharge magmas at the instance of 872 recharge are 1130 °C and 1080 °C for recharge events 1 873 and 2, respectively. Also, like R₂FC, recharge magma 1 is 874 100 wt.% melt, and recharge magma 2 is 21 wt.% crystalline. 875 Assimilation begins at magma temperature of ~1069 °C as 876 in the AFC run (Fig. 3a), and by recharge event 1, M has 877 assimilated ~ 8 wt.% anatectic melt (where percent is cal-878 culated based on the initial mass of resident magma-i.e., 879 cumulative addition of 8 m.u. of anatectic melt). Immedi-880 ately preceding recharge event 1, the magma temperature 881 is ~ 1041 °C, with a crystallizing mineral assemblage of oli-882 vine + clinopyroxene + plagioclase + spinel. In response to 883 recharge event 1, the resident magma temperature increases 884 to~1087 °C, and plagioclase and spinel stop crystallizing. 885 SiO₂ decreases from ~ 54 to 52 wt.% and MgO increases 886 from 3.9 to 5.8 wt.% (Fig. 4). 887

After the first recharge event, AFC continues; at ~1050 °C, spinel rejoins the crystallizing assemblage, and at magma temperature ~1020 °C, orthopyroxene starts to crystallize and at ~1014 °C, plagioclase rejoins the crystallizing assemblage. Recharge event 2 is triggered when the resident magma is 998 °C; the addition of enthalpy via 893 recharge heats the resident magma to ~ 1026 °C. Olivine 894 begins to crystallize again for a small temperature interval, 895 and plagioclase and orthopyroxene briefly stop crystalliz-896 ing. After ~ 10 °C of cooling, the mineral assemblage returns 897 to its pre-recharge assemblage of clinopyroxene + plagio-898 clase + spinel + orthopyroxene. At 991 °C, clinopyroxene 899 ceases to crystallize, and magma melt reaches fluid satura-900 tion (with a mixed $H_2O + CO_2$ fluid), but the proportion of 901 fluid phase in the magma system is quite small (~0.001 m.u.; 902 Fig. 3e). At 979 °C, rhombohedral oxide joins the assem-903 blage. A modest change in melt composition is noted; 904 upon recharge, SiO_2 again decreases, this time from ~ 60 to 905 57.5 wt.% and MgO increases from 2.3 to 3.2 wt.% (Fig. 4). 906

The equilibration temperature for R_2AFC is ~965 °C. 907 The final magma melt composition is distinctly lower in 908 SiO₂ compared to the other four simulations and plots at 909 the low SiO₂ end of the dacitic field. R₂AFC manifests a 910 similar enrichment in Al₂O₃ and K₂O compared to AFC; 911 likewise, the depletions in FeO, H₂O and Na₂O are similar 912 to AFC (Fig. 4). P_2O_5 is the least enriched among all cases. 913 Like AFC, R₂AFC suppresses crystallization. Regardless 914 of their high absolute mass of 133 m.u., crystals make up 915 only ~ 38 wt.% of the magma body in the R₂AFC run, com-916 pared to ~76 wt.% in FC, and R₂AFC expresses the smallest 917 degree of fluid saturation (Fig. 3). The range of olivine and 918 plagioclase compositions is most similar to AFC, with the 919 most Fe-rich olivine being Fo₆₆ and the most Na-rich pla-920 gioclase being An₇₀ (Online Resource 3). 921

For each step of anatectic melt transfer into magma melt, 922 the size of anatectic melt increment is $\sim 2-5$ wt.% of the ini-923 tial wallrock system (i.e., 4-10 m.u.) and generally increases 924 as wallrock heats up. This changes after alkali feldspar com-925 pletely reacts and ceases to be part of the wallrock solid 926 assemblage. After this (wallrock temperature of ~788 °C, 927 magma temperature ~ 1015 °C, Fig. 7), wallrock melt pro-928 ductivity decreases and the size of the increments trans-929 ferred decreases to 1-2 wt.% of the initial wallrock mass 930 (3–4 m.u.). Melt productivity increases again at wallrock 931 temperature of ~845 °C. Like the wallrock melt in AFC, 932 the anatectic melt that is transferred and homogenized with 933 resident magma melt is mostly rhyolitic ($\sim 70-76 \text{ SiO}_2$). 934

At the equilibration temperature of ~965 °C, ~51 wt.% 935 of the wallrock system has been assimilated into the res-936 ident magma (102 m.u. out of the original 200; Fig. 7a). 937 Thus, substantially more anatectic melt was assimilated 938 due to recharge, consistent with more enthalpy being 939 available from magma cooling and crystallization to heat 940 wallrock compared to AFC. However, when assessed as a 941 percentage of the resident magma system, this assimilated 942 mass represents only ~ 29 wt.% of the final magma body 943 (melt + crystals + fluid phase)—in contrast to 41 wt.% of the 944 final magma body in the AFC case (Fig. 7b); thus, although 945

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the mass assimilated is larger, the addition of recharge magma "dilutes" the crustal signature. Like the R_2FC case (compared to FC), the size of the magma body system (melt + cumulate + fluid phase, 352 m.u.) is substantially greater than AFC (Fig. 3).

951 Discussion

It is instructive to compare outcomes of the cases described 952 above (FC, R₂FC, AFC, S₂FC, R₂AFC) to illustrate how 953 fractional crystallization, recharge, and contamination (by 954 assimilation of wallrock partial melts or by assimilation of 955 stoped blocks) affect the evolution of the composite shallow 956 crustal magma system. We have purposely kept the com-957 positions of M, WR, and R magmas constant to focus upon 958 process and sequence rather than subsystem compositional 959 variations. These five cases reflect a very small fraction of 960 possible RASFC scenarios, but they underscore some of the 961 challenges petrologists face in trying to identify crustal pro-962 cesses that dictate magma compositions. 963

964 Comparison of thermal and mass characteristics

The final modeled wallrock temperature is related to the 965 overall size of the magma body, the mass of cumulates 966 formed, and the mass and thermodynamic state of the 967 recharge magma/anatectic melt/stoped blocks added to the 968 magma system. AFC and R₂AFC provide a contrast that 969 illustrates the impact of magma recharge; the final wallrock 970 temperature of R₂AFC (965 °C) is higher than that of AFC 971 (852 °C), reflecting the addition of recharge magma with its 972 attendant enthalpy (Fig. 6). All other parameters of these 973 simulations are the same, including the initial wallrock tem-974 perature of 700 °C. The added enthalpy from hotter recharge 975 magma into resident magma yields a larger increase in wall-976 rock temperature during resident magma cooling and crystal-977 lization. Not only is there more resident magma to cool (i.e., 978 more sensible heat), but also the mass of crystals formed in 979 R₂AFC is also greater, adding more latent heat of crystal-980 lization. The higher final wallrock temperature also means 981 that wallrock melts to a greater extent for R₂AFC than AFC 982 (56 wt.% versus 42 wt.%, respectively). More anatectic melt 983 is transferred into the magma body per decrement of magma 984 cooling (Fig. 7a), and thus, the cumulative amount of wall-985 rock partial melt transferred is larger in R₂AFC. However, 986 while the total mass of anatectic melt added to resident melt 987 is larger in R₂AFC than AFC (~102 versus 71 m.u.; Fig. 7a), 988 the percentage of the magma system mass that comes from 989 anatectic melt is smaller (29 wt.% in R₂AFC versus 41 wt.% 990 in AFC; Fig. 7b) due to the added recharge magma mass that 991 makes the R₂AFC total magma system mass larger (~352 992 versus 171 m.u. for R₂AFC versus AFC, respectively, Online 993

Resource 2). These collective differences, although perfectly 994 clear in hindsight, are neither trivial nor easily predicted. 995 They also bring into focus the difficulty of defining "rates" 996 or amounts of assimilation. Furthermore, the enhancement 997 of assimilation in systems with significant recharge might 998 not be obvious geochemically due to the effects of recharge 999 in diluting the geochemical signature of assimilated partial 1000 melt. Even in this simple comparison, one notes the com-1001 plex feedbacks that can take place. The magnitude of these 1002 non-linear compositional effects varies depending on most 1003 of the sensible parameters of a given simulation. Although 1004 it is difficult to make broad brush statements, appreciation 1005 of these complex feedbacks clearly emerges once the MCS 1006 RAFC models are computed. 1007

The final wallrock temperatures for FC, R₂FC and S₂FC 1008 are 329 °C, 656 °C, and 296 °C (Fig. 2), respectively. The 1009 lowest temperature of the stoping case is due to addition of 1010 cold blocks of wallrock. In addition, minerals in the blocks 1011 such as guartz and alkali feldspar are not stable after the 1012 blocks equilibrate with M melt. The energetic cost of resorb-1013 ing these is debited to the magma, and thus magma has less 1014 enthalpy available to transfer to wallrock. The higher final 1015 WR temperature of R₂FC of 656 °C (compared to FC and 1016 S₂FC) is a function of added enthalpy due to recharge and 1017 underscores the energy impact and thermal priming potential 1018 that recharge can have: with two recharge events of modest 1019 recharge to initial magma mass ratio (0.75), the wallrock 1020 temperature increases from its initial (100 °C) to a tempera-1021 ture that reflects a relatively high geothermal gradient akin to 1022 the assimilation cases presented here. While different param-1023 eters will yield different outcomes, these examples highlight 1024 the potential for thermal priming via recharge. 1025

The total mass of the magma system (which does not 1026 include the residual wallrock) is an obvious outcome of 1027 MCS, and one that is simple to contrast. FC, a "closed-sys-1028 tem" process, yields the smallest magma body size, where 1029 the magma body includes resident magma melt + cumu-1030 lates + fluid phase. The AFC and S_2FC cases are ~1.5 to 1031 $1.7 \times$ bigger than the FC magma body, R₂FC is ~ $2.5 \times$ big-1032 ger, and R₂AFC is the biggest at ~ $3.5 \times$ (Online Resource 1033 2; these comparisons relate masses upon completion of the 1034 simulations). These differences are obviously related to addi-1035 tion of recharge magma, anatectic melt and/or stoped crustal 1036 blocks and have implications for the sizes of potential erup-1037 tions, the growth of the crust (i.e., mass of magma added to 1038 the crust), its state of stress, and local geotherms. 1039

Another difference, not necessarily obvious, is the percent 1040 melt versus crystals among these different magma systems. 1041 AFC and R₂AFC suppress crystallization, compared to the 1042 other cases. In the AFC and R₂AFC cases, the cumulate 1043 reservoir composes about 38–43 wt.% of the resident magma 1044 system, whereas it is ~76 wt.% of the magma body mass in 1045 the FC and R₂FC cases; S₂FC yields approximately 67 wt.% 1046

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crystals (Fig. 3d). Suppression of crystallization is caused 1047 by addition of anatectic melt, which changes the tempera-1048 ture-composition relationships such that the mass of crys-1049 tals that form per decrement of cooling of M melt is lower 1050 when assimilation is ongoing (e.g., the slope of the magma 1051 temperature versus percent cumulative crystals is lower for 1052 AFC and for the assimilation-influenced parts of the R2AFC 1053 compared to FC and R₂FC, Fig. 3d). Thus, in the two cases 1054 that invoke assimilation, the magma system is dominated 1055 by melt: 57 wt.% for AFC and 62 wt.% for R₂FC (Fig. 3b). 1056 The higher equilibration temperature for R₂AFC plays a role 1057 in the high proportion of melt, but even if the slope of the 1058 R₂AFC magma temperature versus percent cumulative crys-1059 tals trend (Fig. 3d) is extrapolated to a higher final magma 1060 temperature, the percent crystals is still lower than the R₂FC 1061 and FC cases. Note that although the proportion of crystals 1062 in R₂AFC is smaller than in FC and S₂FC (Fig. 3d), the total 1063 mass of crystals is larger (Fig. 3c), as expected from the 1064 larger total system mass. This outcome leads to the predic-1065 tion that basaltic systems recharged with magmas similar 1066 to the initial parent magma will build large cumulate piles 1067 whereas basaltic systems that experience contamination by 1068 average upper crust may be melt dominated systems. 1069

Explicit tracking of instantaneous and cumulative masses 1070 of minerals crystallized and anatectic melt assimilated (ver-1071 sions of the DePaolo (1981) "r", which was defined in this 1072 paper as mass assimilation rate/mass fractional crystalliza-1073 tion rate) provides a platform by which to examine the ratio 1074 of mass of anatectic melt assimilated to the mass of cumu-1075 lates formed during AFC. Here, instantaneous refers to the 1076 ratio of the mass of anatectic melt assimilated divided by 1077 the mass of crystals formed in a single (circa 5 °C) AFC 1078 magma temperature decrement (i.e., crystallization fol-1079 lowed by assimilation); in the case when recharge occurs 1080 (R_2AFC) , the crystal mass includes crystals formed upon 1081 recharge added to those formed in a fractional crystalliza-1082 tion "event." Cumulative refers to the total mass of anatectic 1083 melt divided by the total mass of crystals from the first step 1084 in the simulation to the present temperature step. For AFC, 1085 instantaneous and cumulative "r" values vary from 0.71 to 1086 2.6 and 0.13 to 0.99, and for R₂AFC from 0.16 to 2.0 and 1087 0.13 to 0.83, respectively (values reflect start of assimila-1088 tion to end of the simulation, Fig. 8). For the first part of 1089 the AFC instantaneous and cumulative trends (from M melt 1090 temperate of ~ 1055-930 °C), the productivity of melt in 1091 wallrock systematically increases as magma temperature 1092 goes down. The marked change (decrease) in instantaneous 1093 "r" between ~ 930 and 922 °C reflects decreased anatectic 1094 melt productivity because alkali feldspar is no longer part 1095 of the wallrock assemblage; this change is reflected in the 1096 change in slope of the cumulative plot as well (Fig. 8). The 1097 subsequent increase in instantaneous "r" is due to a decrease 1098 in the mass of crystals produced with each AFC "event." 1099

For the R_2AFC case, instantaneous and cumulate "r" are 1100 the same as AFC until the first recharge event. Upon recharge 1101 (event 1, R₂AFC, Fig. 8a), instantaneous "r" increases sys-1102 tematically (offset to a higher temperature due to the effects 1103 of recharge), because the mass of anatectic melt transferred 1104 from wallrock after the recharge events is higher than before; 1105 this leads to an increase in instantaneous "r". The decrease 1106 in R_2AFC instantaneous "r" at temperatures between ~ 1020 1107 and 998 °C (before recharge event 2) occurs because alkali 1108 feldspar in the wallrock is fully reacted, and anatectic melt 1109 productivity decreases as a result. A consequence of the sec-1110 ond recharge event (that brings the magma temperature up 1111 to ~1026 °C) is a short-lived pulse of crystallization that 1112 yields a decrease in both instantaneous and cumulative "r" 1113 (Fig. 8). Following this, the somewhat complex trend seen 1114 in the instantaneous "r" is the result of changes in crystal-1115 lization as the magma system responds to being heated by 1116 recharge as well as the changing restitic mineral composition 1117 of wallrock and the associated consequences on wallrock 1118 melt production. 1119

Three outcomes of the analysis above are that (1) crystal-1120 lization and assimilation "rates" are difficult if not impos-1121 sible to predict in the absence of thermodynamic treatment, 1122 and thus, (2) quantitative thermodynamic treatment of 1123 RAFC processes is absolutely essential to characterize these 1124 rates. Furthermore, (3) these rates are, therefore, neither pre-1125 dictable nor constant, and models that use constant "r" val-1126 ues as defined, for example, by DePaolo (1981) do not reflect 1127 the phase equilibria or energetic consequences of these pro-1128 cesses. Given the availability of computational tools that 1129 provide thermodynamic estimations of magma systems, 1130 we suggest that tools that lack phase equilibria treatment of 1131 igneous systems may, at best, provide only rough estimates 1132 of natural processes and, therefore, should be used with 1133 considerable caution. In addition, one should be wary of 1134 conventional arguments and inferences often applied when 1135 analyzing petrological and geochemical data. Many of these 1136 notions are based on closed system behavior and/or bulk 1137 assimilation without inclusion of phase equilibria. 1138

Geochemical and petrological indicators of open-system processes

The major oxide signatures of open-system magmatic pro-1141 cesses manifest in ways that may not be obvious or intui-1142 tive. Among the best indicators of open-system processes 1143 are radiogenic and stable isotopes, assuming that there is iso-1144 topic contrast between resident magma, crust, and recharge 1145 magma. Why then toil to identify or quantify fingerprints of 1146 RASFC using major element data? The first reason is prac-1147 tical; typically, many more samples are analyzed for major 1148 elements than for isotopes and some trace elements. Second, 1149 careful reconstruction of major element characteristics as 1150

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well as the crystallizing mineral assemblage is required for 1151 accurate calculation of trace element and isotopic signatures 1152 of an open-system magma via the use of mineral/melt and 1153 mineral/fluid distribution coefficients. Thus, to document 1154 trace element and isotopic open system signatures, one 1155 must know the open-system history of melt, minerals, and 1156 fluid. The third reason is that a higher number of constraints 1157 (major oxides, trace elements, isotopes) leads to better mod-1158 els, and better models can lead to more refined interpreta-1159 tions. For example, determining whether a magma storage 1160 system is more likely located in the shallow versus deep 1161 crust has implications for volcanic eruption monitoring and 1162 hazard mitigation. All such models should naturally always 1163 be assessed in relation to MCS-independent evidence such 1164 as geophysical constraints. Fourth, as has been shown in 1165 numerous studies, in some cases isotopic contrast between 1166 magma and wallrock, for example, is lacking (e.g., Stern 1167 and Johnson 2010), and thus pursuit of open-system major 1168 element and phase equilibria models is an absolute necessity. 1169 Below, we highlight major element and phase equilib-1170 ria comparisons that illustrate the complexity of identify-1171

ing open-system processes and that emphasize the value of thermodynamic modeling.

1174 Identifying the fingerprint of magma mixing from melt1175 and mineral data

Classic linear trajectories often ascribed to binary mixing 1176 are not present in many of the R₂FC major element plots 1177 (e.g., SiO₂ versus MgO, Na₂O, TiO₂; Fig. 4). This is because 1178 homogenization is followed by crystal removal through frac-1179 tional crystallization. The inverse is also true: there are seg-1180 ments of some of the FC oxide arrays that are approximately 1181 linear (e.g., K_2O , P_2O_5 , H_2O , Al_2O_3 at $SiO_2 > \sim 55$ wt.%), 1182 and thus may resemble mixing trends. Thus, the assumption 1183 that mixing can be diagnosed by linear trends is misleading. 1184 The similarity of many oxide trends for FC and R₂FC 1185 (Fig. 4) underscores the difficulty of diagnosing process 1186 using such data. But some oxides can show distinctive 1187 behavior with recharge. In the simulations highlighted here, 1188 MgO is the most telling. Its concentration changes beyond 1189 analytical uncertainty when recharge with a more primitive 1190 magma occurs, but the difference between FC and R₂FC is 1191 subtle and might be difficult to detect in a suite of samples 1192

As recognized in numerous studies, crystal cargo (e.g., 1194 Davidson et al. 2007; Streck 2008, and references therein; 1195 Edwards et al. 2019, Ubide et al. 2019; Ubide and Kramer 1196 2018; Streck et al. 2008; Ginibre et al. 2007; Davidson et al. 1197 1997) can provide a rich inventory of mixing histories. Are 1198 MCS results applicable to such data? The answer is yes, 1199 with careful consideration of the design features of MCS. 1200 The current version of MCS immediately fractionates all 1201

that lack stratigraphic control.

1193

crystals, and thus zoned crystals are technically not pro-1202 duced and no resorption of cumulates is permitted. What 1203 is produced is a sequential record of crystallization. The 1204 crystals that are fractionated into a separate cumulate res-1205 ervoir during progressive RFC "events" can be reimagined 1206 as growing, zoned crystals that remain in the M melt and 1207 interact thermally but not chemically with host magma; the 1208 mass and energy balance for such zoned crystals is the same 1209 as it is for crystals fractionated to the cumulate reservoir. 1210 By using the sequential record and carefully applying it to 1211 crystal cargo data (subject to the limitation in the current 1212 version of MCS that crystals do not chemically interact with 1213 M melt), one can utilize MCS results to better understand 1214 possible crystal behavior that results from RASFC. 1215

Envisioning crystals as growing in this way, the R₂FC 1216 modeling results indicate that in some cases, the record of 1217 recharge may be selective. In R₂FC, the complete record 1218 of mixing is not preserved in plagioclase, which is not 1219 stable upon mixing, but returns to the stable assemblage 1220 within ~ 25 °C of cooling after the first recharge event 1221 and ~5 °C of cooling after the second. Its compositional 1222 change is small after the first event (An_{81} to An_{82}) but larger 1223 and detectable after the second (An_{71} to An_{77}). In stark con-1224 trast to plagioclase behavior, olivine crystallizes both before 1225 and after mixing, thus recording a complete phase equilibria 1226 record of the effects of mixing. The mineral changes com-1227 position abruptly from Fo70 to Fo78 after the first recharge/ 1228 mixing event, and from Fo₅₅ to Fo₆₈ after the second event. 1229 These changes are easily detected by electron microprobe 1230 analysis, provided the zoning is preserved. 1231

Crystals produced during mixing may also preserve a 1232 record of temperature changes. For R₂FC, the temperature of 1233 the magma increases 40-50 degrees after each mixing event. 1234 That record may be preserved in mineral geothermometry. 1235 In R₂FC, olivine and clinopyroxene would be the best indi-1236 cators of the temperature change, as they preserve the most 1237 complete record of mixing. In contrast, plagioclase would 1238 not likely record heating associated with the first recharge 1239 event for the reasons discussed in the previous paragraph. 1240 The takeaway lesson from this single example is that to fully 1241 document temperature excursions associated with recharge 1242 that are recorded in minerals, one needs a complete picture 1243 of the phase equilibria changes that occur in response to 1244 the mixing event. Even with such data, documenting tem-1245 perature changes may be challenging given the equilibrium 1246 requirements and uncertainties of many geothermometers 1247 (e.g., Putirka 2017). 1248

The presence or absence of distinctive recharge signatures is a function of the magma mixing scenario. In the cases highlighted here, the same parent magma is mixed into its evolving counterpart. Different scenarios will lead to different mixing fingerprints. For example, the mass of the recharge event compared to the resident magma/melt mass 1250

will influence the extent to which pre- and post-recharge 1255 magmas change composition, and a substantial composi-1256 tional contrast between resident melt and recharge magma 1257 may yield recharge signatures that are more obvious than 1258 those presented here. Myriad forward modeling case stud-1259 ies can be done in MCS to examine the temperature, com-1260 position, and mass landscape of mixing and crystallization 1261 processes. 1262

1263 Identifying the fingerprint of crustal assimilation from melt1264 and mineral data

Similar to the FC versus R₂FC comparison, some major 1265 oxides do not show evidence of crustal assimilation. For 1266 example, AFC and R₂AFC are generally similar to FC and 1267 R₂FC in SiO₂ versus MgO (with the exception of the notable 1268 change immediately after the recharge events for R2AFC and 1269 R_2FC) and CaO (Fig. 4). This is an interesting result given 1270 the anatectic melt and recharge magma have very different 1271 concentrations of these oxides, and yet, the SiO₂ versus CaO 1272 and MgO trends are indistinguishable for these four cases 1273 at > 55 wt.% SiO₂. 1274

In contrast, three major elements that show quite dis-1275 tinct differences are K₂O, Na₂O, and Al₂O₃ (Fig. 4). Once 1276 assimilation begins, Al₂O₃ is more concentrated in AFC 1277 and R₂AFC than in their non-assimilation equivalents (at 1278 the same SiO₂). Because these cases contrast with respect 1279 to not just the bulk composition of the added anatectic melt, 1280 but also in the mass and identity of cumulus phases, there 1281 could be a number of explanations for these differences. 1282 The total final percentage of cumulus plagioclase in FC and 1283 AFC is similar (~39 wt.%), whereas for R_2 AFC, it is smaller 1284 (~26 wt.%) (Fig. 5c). Thus, for FC and AFC, about the same 1285 final proportional amount of plagioclase was removed as a 1286 fractionating phase, but that final tally obscures differences 1287 as the systems evolve. Reference to Fig. 5c shows that plagi-1288 oclase makes up a smaller proportion of the cumulate assem-1289 blage in AFC, compared to FC, for most of the simulation. 1290 The reason the final proportions are similar is because the 1291 end temperature of AFC (~856 °C) is lower than that for FC 1292 (~899 °C), which provides a slightly longer crystallization 1293 temperature interval for plagioclase in the AFC case. For 1294 most of the AFC simulation, for each cooling step, less pla-1295 gioclase forms, and thus the resident melt is not debited in 1296 Al₂O₃ as extensively as in the FC case (Fig. 4b). In the case 1297 of R₂AFC, Al₂O₃ is slightly higher at the same wt.% SiO₂ 1298 than in the AFC case and reflects the lower cumulate pla-1299 gioclase proportion, compared to AFC (Fig. 5c). Thus, less 1300 Al₂O₃ is removed from resident melt. R₂AFC and AFC have 1301 distinctly lower Na₂O at the same SiO₂ (once assimilation 1302 begins), whereas K₂O is distinctly higher than FC and R₂FC 1303 (Fig. 4g, h). The bulk composition of wallrock and the way 1304 it melts are responsible for these differences. Alkali feldspar 1305

melts disproportionately into anatectic melt, enriching the melt in K_2O . Plagioclase (~ An_{37-35}), on the other hand, disproportionately increases in abundance in wallrock restite, and thus, anatectic melt addition dilutes Na_2O in resident magma melt. All these changes are recorded in the respective output files in the Online Resource 6. 1300

Resident melt H₂O is less concentrated in AFC and 1312 R_2AFC compared to FC and R_2FC (Fig. 4j) due to an 1313 assumption imposed on the current version of MCS. As 1314 discussed in the Section entitled "Case 3: assimilation-frac-1315 tional crystallization (AFC)", while wallrock is fluid-sat-1316 urated upon initiation of melting, the fluid phase is not 1317 incorporated into magma melt although H₂O dissolved in 1318 anatectic melt is. Once assimilation begins, dilution due to 1319 anatectic melt addition is evident, and lower rates of crys-1320 tallization (i.e., mass of crystals fractionated per decrement 1321 of cooling in resident magma) of anhydrous minerals in the 1322 AFC case lessens the amount of H₂O enrichment. R₂AFC 1323 parallels the AFC trend until the first recharge event, which 1324 dilutes H₂O. The second causes additional dilution. The 1325 combination of recharge and lower rates of crystallization 1326 vields the lowest magma melt H₂O contents of all the cases 1327 by the termination of the simulation. The remaining oxides 1328 also show differences, but these are less pronounced and 1329 are due to differences in anatectic melt versus magma melt 1330 compositions and the associated phase equilibria differences 1331 between the FC and AFC cases. 1332

Based on the analysis above, for the AFC and R₂AFC 1333 cases presented here in which a depleted basalt is being con-1334 taminated by anatectic melt from average upper continental 1335 crust, the only major element and phase equilibria indicators 1336 that are likely to be diagnostic are the resident melt K_2O_1 , 1337 which is enriched by $\sim 5 \times$ by the end of the AFC versus FC 1338 simulation (Fig. 4h). An expectation that crustal assimilation 1339 would lead to more profound and obvious changes in other 1340 oxides might yield a misinterpretation of these data that 1341 attributes the geochemical signals to mantle heterogeneity. 1342 Likewise, depletion of Na₂O might be easily misinterpreted 1343 as representative of mantle heterogeneity and/or alteration. 1344 While the AFC/R₂AFC Al₂O₃ versus SiO₂ trends are distinct 1345 from those of FC, Al₂O₃ may be difficult to interpret as its 1346 concentration is partly a function of the amount of plagio-1347 clase crystallization, which may vary according to crystal-1348 lization conditions. While we recognize that these results 1349 are case specific, they underscore the importance of open-1350 system models that evaluate phase equilibria. 1351

Mineral fingerprints of assimilation are potentially preserved in the cumulate assemblage. The most obvious is the presence of orthopyroxene, which is not stable in FC and is in much smaller proportion in R_2FC (~1 wt.%) compared to > 10 wt.% for AFC and R_2AFC (Fig. 5f). Orthopyroxene is stabilized by SiO₂ added by anatectic melt; on the other hand, fractionation of orthopyroxene enriches *M* melt 1359 ¹³⁵⁹ in SiO₂ less than crystallization of olivine so the effect of ¹³⁶⁰ adding SiO₂ into the system by assimilation is counteracted ¹³⁶¹ (Fig. 4). Other wt.% differences for the cumulate assem-¹³⁶² blages are evident. For example, olivine and clinopyroxene ¹³⁶³ do not crystallize for the full AFC simulation whereas they ¹³⁶⁴ do in FC.

Similar to predictions about the effects of magma 1365 recharge and mixing, the case studies involving assimila-1366 tion bring into focus the difficulty of postulating a priori the 1367 patterns expected on element and oxide variation diagrams 1368 and in mineral compositions and identities. Major element 1369 and mineralogical responses to these processes may not be 1370 easily predicted or distinguished. The overarching conclu-1371 sion of the recharge and assimilation case studies is that 1372 using closed system reasoning may produce misleading and 1373 spurious conclusions, because the effects of open-system 1374 processes are non-linear and, in many cases, non-intuitive. 1375

1376 Distinguishing the mode of crustal contamination: crustal1377 assimilation versus stoping

1378Here, we compare and contrast AFC and S_2FC to illustrate a1379possible range of effects from different mechanisms of crus-1380tal contamination. As anticipated, evidence of bulk assimila-1381tion of stoped blocks compared to assimilation of anatectic1382melt is preserved in some oxide trends, but not in others.

In the S₂FC scenario, SiO₂ versus MgO and CaO are 1383 quite similar to AFC, and TiO₂, Fe₂O₃, and P₂O₅ show 1384 only subtle differences (Fig. 4). In contrast, Al₂O₃, FeO, 1385 K₂O, Na₂O, and H₂O are markedly different for AFC ver-1386 sus S₂FC. For the first stoping event, Al₂O₃ versus SiO₂ 1387 has a slope that is rather similar to FC and R₂FC trends, 1388 and thus is much lower in concentration (at the same 1389 SiO_2) compared to AFC. While the Al_2O_3 content of the 1390 stoped block is slightly higher than M melt, addition of 1391 the stoped block (with its Al_2O_3) is apparently offset by 1392 a "pulse" of plagioclase crystallization (described in the 1393 next paragraph) that removes Al₂O₃. While intuition may 1394 dictate that adding an Al-rich stoped block would lead to 1395 increased Al₂O₃ in M melt, this will not always be the case 1396 and this example again illustrates how simplistic reasoning 1397 can be misleading (e.g., polyphase mixing is not identical 1398 to melt-melt mixing). Likewise, Al₂O₃ remains at lower 1399 concentrations compared to AFC during and after the sec-1400 ond stoping event for the same reason. Spinel also experi-1401 ences a pulse of crystallization with both stoping events, 1402 and likely contributes to the lower Al₂O₃ in the S₂FC case. 1403 S₂FC Na₂O is higher than AFC (Fig. 4g); by the first stop-1404 ing event, Na₂O in the stoped block is much higher than 1405 in the equivalent anatectic melt (i.e., at approximately, the 1406 same wallrock temperature), and thus Na₂O in the S₂FC 1407 case is higher than in the AFC case. K₂O is the opposite 1408 (Fig. 4h). S₂FC K₂O is not as enriched as in the AFC case, 1409

because the stoped block K₂O concentration is lower than 1410 that of anatectic melts. These differences are both a direct 1411 result of the difference in style of contamination. Through 1412 assimilation by stoping, bulk wallrock contaminates M 1413 melt, whereas the process of partial melting during AFC 1414 enriches K₂O content and depletes Na₂O in anatectic melt. 1415 H_2O is more enriched at a given SiO₂ in S₂FC than in 1416 AFC, because, in the current version of MCS, all of the 1417 fluid phase is transferred into resident melt via stoping, as 1418 opposed to remaining in wallrock restite in the AFC case. 1419

Assimilation by stoping also has an effect on the cumu-1420 late assemblage. Upon homogenization of the first stoped 1421 block, all of the quartz and alkali feldspar react away. As 1422 noted above, a "burst" (i.e., large mass) of plagioclase 1423 crystallizes (Fig. 5c; $7.5 \times$ more than had been crystalliz-1424 ing in prior magma temperature decrements) in response 1425 to assimilation of the stoped block. Spinel also experiences 1426 a crystallization burst (Fig. 5d; increase by $7 \times$), but the 1427 total mass is much smaller than plagioclase. Similar to 1428 stoping event 1, during homogenization of stoped block 1429 2, quartz completely reacts, and, plagioclase and spinel 1430 crystallization bursts occur, and these are proportionally 1431 much larger than after stoping event 1 (Fig. 5; e.g., for 1432 plagioclase, ~ 30 × more than had been crystallizing in 1433 prior magma temperature decrements). While plagioclase 1434 continuously crystallizes in both AFC and S₂FC, the mass, 1435 thermal and compositional records are quite different. In 1436 AFC, each set of fractional crystallization-assimilation 1437 "events" yields about the same mass of plagioclase, and its 1438 composition varies smoothly from An₈₃ when assimilation 1439 begins to An₅₄ at the simulation's termination. The tem-1440 perature record is also smoothly varying with decreases 1441 of ~15 °C per fractional crystallization-assimilation 1442 "event". For stoping events 1 and 2, there is a dramatic 1443 increase in the mass rate of plagioclase crystallization and 1444 an abrupt change in plagioclase Na content (from An₇₅ 1445 to An_{65} for event 1, and from An_{51} to An_{38} for event 2), 1446 and the melt temperature decreases are ~47 $^{\circ}$ C and 45 $^{\circ}$ C, 1447 respectively. Both of these changes would be detectable 1448 by modern analytical methods and geothermometers. By 1449 the end of the simulation, plagioclase in S₂FC is distinctly 1450 more albitic than that in AFC (An_{37} versus An_{54}), consist-1451 ent with the addition of Na₂O from stoped blocks com-1452 pared to the "dilution" effect seen in AFC due to partial 1453 melting of wallrock. The difference in plagioclase compo-1454 sition highlights the difference in bulk addition of a stoped 1455 block versus addition of partial melt from wallrock. Par-1456 tial melting favors reaction of alkali feldspar over plagio-1457 clase, and thus the resulting anatectic melts substantially 1458 enriches resident melt in K and depletes it in Na. These 1459 elemental differences influence the M melt phase equilibria 1460 response. 1461

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1462 Quantifying mantle versus crustal contributions1463 to magma systems

A key goal in petrology and geochemistry-to distinguish 1464 and quantify how mantle versus crustal contributions to a 1465 magma system change in space and time-informs models 1466 of crustal growth and evolution, models of mantle evolu-1467 tion, and mass and thermal fluxes between these reservoirs. 1468 The literature abounds with studies of magmatic systems 1469 in which geochemical and petrologic signatures are quan-1470 titatively or qualitatively attributed to mantle versus crust 1471 (e.g., Hildreth and Moorbath 1988; Asmerom et al. 1991; 1472 Arndt et al. 1993; Wooden et al. 1993; Baker et al. 2000). 1473 Modeling results presented here illustrate the complexity 1474 associated with this enterprise and some potential pitfalls. 1475 The FC case assumes that mantle-derived magma intrudes 1476 the crust and undergoes fractional crystallization without 1477 involvement of any crust. Thus, the entire compositional sig-1478 1479 nal derives from the mantle mediated by low-pressure crystal fractionation. Magmas that have undergone only fractional 1480 crystallization without interaction with crust and/or without 1481 magma mixing are probably uncommon given the realities 1482 of moving low-viscosity materials through large sections 1483 of crust of contrasting composition as well as the episodic 1484 nature of magma intrusion. The case of FC only is, therefore, 1485 admittedly a simplification but serves as a point of com-1486 parison. Discussion of how the mass of mantle versus crust 1487 is portrayed, as discussed in the Section "Comparison of 1488 thermal and mass characteristics" underscores the challenges 1489 with quantifying crust versus mantle. 1490

Based on many thousands of MCS models, we have 1491 collectively run over the past several years, we suggest a 1492 top-down approach to distinguishing crust versus mantle 1493 contributions. That is, we recommend characterizing and 1494 quantifying possible open system crustal processes first. 1495 Once plausible and potential RASFC scenarios are fully 1496 explored (i.e., running many MCS models), remaining dis-1497 crepancies between model results and data from a natural 1498 system might then be postulated to be caused by mantle het-1499 erogeneity of the M subsystem magma. 1500

1501 Magma Chamber Simulator: ongoing developments

The MCS has undergone continuous development and
improvement since its first incarnation, and we continue to
expand its functionality. Here, we review four major extensions presently under development.

A critical enhancement of MCS is to free it from its dependence on Excel, which is a temperamental platform on which to build and sustain development. A high priority for MCS is to port the code to a new platform with an accessible web user interface. The second enhancement addresses the limitation that cumulate crystals cannot react with M

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melt. It is well established in the rock record that crystal 1512 (cumulate)-melt interaction occurs. As one example, the 1513 concept of crystal resorption has been part of the petrologi-1514 cal literature for a long time (e.g., Fries 1939; Wiebe 1968; 1515 Couch et al. 2001; Ginibre et al. 2007; Erdmann et al. 2012); 1516 orthopyroxene rims on olivine-cored crystals is perhaps the 1517 type example (e.g., Ambler and Ashley 1977). MCS will be 1518 modified to allow some fraction of earlier formed cumulates 1519 to react with M melt. A third MCS future development, as 1520 noted, is to allow transfer of some proportion of the fluid 1521 phase in wallrock to transfer into M melt. Finally, planning is 1522 underway to implement a Monte Carlo version of the MCS. 1523 To run a single R₂AFC simulation like the one illustrated 1524 here, circa 80 parameters should be specified in the MES 1525 input file (including all the oxides for magma, wallrock, and 1526 recharge magmas). In attempting to model a natural system, 1527 one recognizes that there are inherent uncertainties in these 1528 parameters. Therefore, the MCS algorithm will be extended 1529 by adoption of a Monte Carlo approach by allowing each 1530 input parameter to be specified as a possible range of values 1531 (e.g., SiO₂ of the wallrock lies between 67 and 69 wt.% etc.). 1532 Once ranges for all input parameters have been defined, the 1533 algorithm will select randomly or by Bayesian methods a 1534 particular set of initial conditions. In this manner, thousands 1535 or even tens of thousands of MCS models can be run, each 1536 with a unique set of input parameters and associated output. 1537 Once archived in a searchable database, the user can then 1538 ask questions such as: Of the thousands of simulations run, 1539 which ones compare best to the data from the particular nat-1540 ural system under study? Using this Monte Carlo approach, 1541 solutions can be filtered to find the best fit to observables 1542 using some objective criterion such as the residuals of the 1543 squared differences between the model and the observations. 1544

Conclusions

Analysis of attributes of igneous systems suggests that 1546 open system behavior is dominated by crystal fractionation, 1547 magma mixing, and the interaction of magmas with their 1548 host environments via partial melting and stoping of wall-1549 rock. An important task for the petrologist/geochemist is to 1550 unravel the most important RASFC processes by quantifica-1551 tion and temporal ordering. Establishing a magmatic 'arrow 1552 of time' is intrinsically a complex task due to the vast range 1553 of temporal and spatial scales involved-from microns to 1554 kilometers and from hours to several million years. Deci-1555 phering such records demands a variety of approaches. 1556

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As precision and spatial resolution of analyses of magmatic products have improved, so has the petrologist's ability to quantify the magmatic processes that generate compositional diversity. Forty years of progress have seen improvements in modeling, from those that focused exclusively on 1561

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mass balance, to mass and enthalpy balance, to those that 1562 are underpinned by a thermodynamic database. The Magma 1563 Chamber Simulator is a mass- and energy-balanced, ther-1564 modynamic tool that addresses open-system magmatic pro-1565 cesses that govern the evolution of a multicomponent-mul-1566 tiphase composite system of wallrock, resident magma, 1567 and recharge/stoping reservoirs. MCS-PhaseEQ models 1568 the major element and phase equilibria consequences of 1569 RASFC, and MCS-Traces, the subject of a companion paper, 1570 models trace elements and isotopes. MCS-PhaseEO relies 1571 on rhyolite- and pMELTS as its thermodynamic engine and 1572 Visual Basic as its executive brain. MCS provides signifi-1573 cant insight into crustal magma processes and the origin 1574 of compositional diversity via modeling how variations in 1575 specific input (e.g., pressure, parental magma composition, 1576 wallrock initial temperature, number and mass of recharge 1577 events) contribute to magma diversity and eruptability. Sys-1578 tematic modeling of this sort affords the development of a 1579 framework for systematizing potentially distinctive charac-1580 teristics of RASFC processes. MCS forward modeling also 1581 abounds with potential for describing the evolution of par-1582 ticular volcanic and plutonic rock suites, thus providing a 1583 quantitative framework for interpreting the remarkable and 1584 abundant compositional and isotopic data sets that are now 1585 routinely generated for igneous rocks. The five case studies 1586 we discuss (FC, R₂FC, AFC, S₂FC, and R₂AFC) illustrate 1587 the rich data set that MCS produces and elucidate both the 1588 challenges of identifying open system processes from major 1589 element and phase equilibria data and the utility of using 1590 open-system thermodynamic models such as MCS to docu-1591 ment open magma systems. 1592

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