Arc Basalt Simulator Version 5.00 Tutorial

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Updated from Arc Basalt Simulator Ver. 3.10 Tutorial, Nov. 28, 2011 version by J.-I. Kimura (JAMSTEC) and R.J. Stern (U. Texas, Dallas) (Kimura, 2012)

INTRODUCTION

Arc Basalt Simulator (ABS) is a petrologic and geochemical simulation program for basalt, high-Mg andesite, and adakitic dacite genesis in a subduction zone. ABS consists of two different calculation modules: (a) slab dehydration and melting along an appropriate subduction zone $P$–$T$ path, and (b) melting of mantle wedge peridotite due to fluxing by slab-derived liquid (Fig. 1; Note: “slab” refers to the subducted oceanic plate lithosphere, igneous crust, sediment, and part of the mantle wedge that are dragged down with the oceanic plate slab). ABS is intended to be easy to use, requiring only a PC or Mac that can run Microsoft® Excel®. This tutorial is intended to introduce the interested geoscientist to ABS5, and to help them use it in their own research. The present version is ABS5 (November 2016) but this is updated from time to time.

Fig. 1 Schematic cross-section of a subduction zone and the Arc Basalt Simulator version 5 model (Kimura, 2017). MwP: mantle wedge peridotite; SED: sediment; AOC: altered oceanic crust; LBAS: lower basalt; DIKE: dike; UGAB: upper gabbro; LGAB: lower gabbro; SlbP: slab peridotite.
The first half of this tutorial explains the fundamental parameters, assumptions, and calculations of the model. First, the general calculation scheme is presented, then each of the principal ABS5 calculation steps are outlined as follows: 1.1. Slab dehydration and melting simulation (comprising 1.1.1. Petrology of the slab in prograde metamorphism and 1.1.2. Trace element and isotope compositions of slab liquid); 1.2. Zone refining reaction between slab liquid and mantle (currently not frequently used); 1.3. Liquid-fluxed melting calculations for mantle peridotite (comprising 1.3.1. Mode and melt compositions for fluxed melting and 1.3.2. Trace element calculations for liquid-fluxed open system melting); and 1.4. Use of forward model for inversion calculations.

The second part of this tutorial explains how to use the ABS5 Excel spreadsheet. The third part describes the data structure and the roles of the worksheets. For further background, please read Kimura et al. (2009) for ABS2, Kimura et al. (2010) for ABS3, Kimura et al. (2014) for ABS4, Kimura and Nakajima (2014) for the relation to geophysical observations, and Kimura (2017) for ABS5 results (Kimura, 2017; Kimura et al., 2010; Kimura et al., 2003; Kimura and Nakajima, 2014; Kimura et al., 2009). These papers describe in full the concept and the calculation scheme and provide examples of how ABS is used to quantitatively address arc magmagenetic problems. Appropriate paper(s) should be cited in publications where ABS is used.

**Fig. 2** Flow diagram indicating the calculation modules used in the ABS5 model; follow processes counter clockwise from upper left. Large gray box shows the source compositions of eight slab layers: slab peridotite (SlbP), lower gabbro (LGAB), upper gabbro (UGAB), dike (DIKE), lower basalt (LBAS), altered oceanic crust (UBAS = AOC), and sediment (SED), plus metasomatized peridotite in the mantle wedge sole (Mwp). Blue box shows the chromatographic reactions in the slab. Thin black vertical arrows show downgoing solids. The white horizontal arrows show upwelling slab liquids. Slab liquids are taken up from the slab as a mixture of AOC, SED, and Mwp liquids (see panel c). Large yellow box shows the interaction of the slab liquids with subsolidus mantle modeled by zone refining. Large orange box shows fluxed mantle melting by addition of the slab liquid to the mantle wedge (Kimura et al., 2014).
1. GENERAL CALCULATION SCHEME

The following sections describe the calculation scheme used in Arc Basalt Simulator version 5 (ABS5) (Fig. 2).

1.1. Petrological Model for Slab Dehydration and Melting

1.1.1. Petrology of the Slab in Prograde Metamorphism

The slab dehydration calculations are based on the Perple_X version 5 thermodynamic model (Connolly and Kerrick, 1987; Connolly and Petrini, 2002). The model provides the amount of water dehydration and the residual mineralogic mode. This slab model was first established for ABS2 (Kimura et al., 2009) and later extended to the melting regime in ABS3 (Kimura et al., 2010). The modifications include slab melting, which uses experimental datasets for pelagic sediment (SED), igneous oceanic crust with mid-ocean ridge basalt (MORB) composition, and peridotite with depleted MORB-source mantle (DMM) composition (Grove et al., 2006; Moyen, 2009; Moyen and Stevens, 2006; Schmidt et al., 2004). Source compositions of the slab layers for Perple_X calculations are water-saturated. Three source compositions apply (Hacker, 2008): DMM for SlbP and MwP; MORB for LGAB, UGAB, DIKE, LBAS, and AOC; and pelagic sediment for SED (see Figs. 1 and 2 for slab layers). Chemical compositions of the GAB layers in the oceanic plates are MORB-melt component dominant (Adachi and Miyashita, 2003; Gillis et al., 2014); use of MORB composition for GAB is supported. The phase relations in Fig. 3 are from the ABS5 slab model for SED, AOC, and DMM. Typical siliceous sediments (chert, terrigenous sediment, and clay) differ only in the abundance of quartz relative to other minerals (e.g., chlorite, amphibole, garnet, clino.pyroxene, lawsonite). Although this affects the bulk partition coefficients between slab liquid and SED, the effects are limited due to extremely low partition coefficients in quartz for all incompatible trace elements (Kimura et al., 2010). Carbonate sediments are not considered.

![Phase relations and maximum bound water content in igneous oceanic crust, sediment, and depleted peridotite. Example P–T paths are shown by rainbow-colored lines for MwP: mantle wedge peridotite; SED: sediment; AOC: altered oceanic crust; LBAS: lower basalt; DIKE: dike; UGAB: upper gabbro; LGAB: lower gabbro; and SlbP: slab peridotite (Kimura, 2017).](image-url)
Fig. 4-1 Modal composition in pressure–temperature (P–T) space for a subducted slab. Slab materials are igneous oceanic crust (IOC), gabbro (GAB), sediment (SED), and depleted peridotite (PERID). Color maps indicate the modal compositions, with the gray field indicating the absence of phases. Thin lines indicate the slab P–T paths of eight slab layers calculated using the geodynamic model for the Nankai (SW Japan) subduction zone. The modal compositions are given by weight. Gt: garnet; Cpx: clinopyroxene; Ol: olivine; Opx: orthopyroxene; SiO₂: silica minerals; Plag: plagioclase; Chl: chlorite; Bio: biotite; Phen: phengite; Amp: amphibole (Kimura, 2017).
Fig. 4-2 Slab modes calculated for NE Japan (NEJ) and SW Japan (SWJ) slab geotherms. The slab layers are MwP: mantle wedge peridotite; SED: sediment; AOC: altered oceanic crust (UBAS); DIKE: dike (LBAS); UGAB: upper gabbro; LGAB: lower gabbro; and SlbP: slab peridotite (oceanic lithosphere mantle). The mineral phases are given in the key (Kimura, 2017).

Modal compositions of metamorphic minerals, H_2O, and melt fractions in the slab are given in individual lookup tables for the $P$–$T$ range 0.15–6 GPa, 100–1200°C in ABS5 (Figs. 4-1 and 4-2). $P$–$T$ paths of the slab layers are taken from a geodynamic model for 56 subduction zones worldwide (Syracuse et al., 2010; van Keken et al., 2011) (Figs. 4-1 and 4-2); using the lookup tables, the modal compositions and released water and melt
fractions are obtained along the designated $P$–$T$ paths (Fig. 4-2).

1.1.2. Trace Element and Isotope Compositions of Slab Liquid

In ABS2–3, interactions between the released slab liquids and the overlying slab layers were only considered for the MwP layer using zone refining calculations. With the increase in number of slab layers to eight (ABS4–5), there is more interaction within a 1-D vertical column (Fig. 2). In ABS5, all of the dehydration/melting reactions are treated as incremental batch calculations (Shaw, 2000) (Fig. 5).

In the calculations, the fraction of melt or dehydrated fluid in any cell (area in $P$–$T$ space in Fig. 5) is treated as $F$, and the additional fluid or melt fraction that is lost from the underlying cell in the 1-D column ($F_{x-1}$) is incrementally added to the overlying cell. Precipitation of minerals or increase in $F$ due to the additional liquids is not considered either in the phase changes of the solids or changes in $F$ in the cells. However, the composition of the liquid and solid in each cell changes because of the liquid addition, which results in considerable changes in both the trace element and isotopic abundances. Isotopic compositions are calculated using a computational solution that calculates isotopic abundances based on the isotope abundance ratios. H$_2$O is treated as an incompatible element using $D$(H$_2$O) = $D$(Ce) = 0.01 (Dixon et al., 2002). This is also applied to slab melting and H$_2$O contents in the slab melts are calculated by $X_{H_2O}/X_{slab melt}$, assuming 100% solubility of water in slab liquid (Hermann et al., 2006).

The interaction between ascending slab liquids and their surroundings depends not only on the degree of dehydration or melting, but also on the nature of fluid flow, such as porous flow or fracture flow (Bebout, 2007). The differences in flow type cause different degrees of element redistribution. We model this by using the $\%R_{slab}$ factor to
modify the $F$ parameter in the batch dehydration/melting/reaction calculations. This factor alters all $F$ values used in the calculation matrix as $F' = F \times \%R_{slab}/100$. It can be varied from 0 (no slab liquid movement) to several hundred. When $\%R_{slab} = 100$, $F' = F \times \%R_{slab}/100$. That is, all liquid released from one cell moves to the cell above it. When $\%R_{slab} < 100$, $F'$ is smaller, which results in more effective extraction of elements from the solids. This simulates a reactive porous flow regime. The reverse is true for $\%R_{slab} > 100$, which simulates fracture (crack) flow. This particularly affects isotope ratios because it enhances or dilutes differences between source materials. Therefore, the match for isotope ratios can be improved without much change in element concentrations just by varying the $\%R_{slab}$ factor. Different $\%R_{slab}$ factors can be applied to the different slab layers, but we applied the same $\%R_{slab}$ factor to all layers. This function is available in ABS4–5 (Kimura et al., 2014).

Using the mineralogical mode and dehydration of the subducted slab, it is possible to calculate the slab-derived liquid composition (Figs. 4 and 5). Partition coefficients for slab liquids/minerals are similar to those used in ABS2. Due to the wide temperature range of 100–1200°C in the slab, temperature-dependent $D_{mineral/liquid}$ values need to be used whenever available. These are available for garnet and clinopyroxene from experimental data (Kessel et al., 2005). Formulation of $T$–$D_{mineral/liquid}$ relationships has been made as $D_{mineral/liquid} = a \times \exp^{bT}$, where “$a$” and “$b$” are constants for garnet and clinopyroxene (Kimura et al., 2009) (Table 1). ABS5 applies this simple extrapolation for the $T$-dependence of $D_{mineral/liquid}$ to most of the elements, with some approximations for K, Pr, Tb, and Ho, which were not determined by Kessel et al. (2005). High field strength elements (HFSEs), such as Nb, are buffered by residual rutile due to an extremely high partition coefficient (Green, 1995).

At low $P$–$T$ conditions the element behavior in oceanic basalt is affected by numerous metamorphic minerals. ABS5 applies $D_{mineral/liquid}$ for lawsonite, chloritoid, phengite (Green and Adam, 2002), and zoisite (Feineman et al., 2007) from experiments, and for lawsonite (Usui et al., 2007) from field studies. The values for olivine and rutile were taken from Ayers et al. (1997) and Ayers and Watson (1993) without consideration of temperature-dependence. We also use mineral/mineral partitioning for orthopyroxene $D_{opx/cpx}$ (Spandler et al., 2004), amphibole $D_{amphibole/cpx}$ (Ionov and Hofmann, 1995), and chlorite $D_{chlorite/opx}$ (Garrioto et al., 2005). Partition coefficients ($D$s) for amphibole, orthopyroxene, and chlorite were inferred from $T$-dependent $D$s in clinopyroxene or garnet. The $D$ values for silica minerals (quartz, coesite, stishovite) or aluminous minerals (such as sapphire) are treated as $D_{mineral/liquid} = 0$. There are no data for serpentine minerals, such as talc and antigorite, available for the multiple element examination used in this study, which are also treated as $D_{mineral/liquid} = 0$ (Kimura et al., 2009) (Table 1). In addition, partition coefficients for melts are assumed to be 3-times those for aqueous fluids (Hermann et al., 2006). Comparison of these $D$ values to the compiled $D_{bulk}$ experimental data (Moyen and Stevens, 2006) shows the above assumptions to be valid.

Examples of bulk partition coefficients for representative incompatible elements in representative slab layers are shown in Fig. 6. The change in $D$s during prograde metamorphism depends both on the mineralogic modes in the residual slab layer and the temperature.
Table 1 Temperature-dependent partition coefficients, mineral/mineral partitioning ratios, and fixed partition coefficients used for slab minerals.

<table>
<thead>
<tr>
<th>Mineral</th>
<th>$D_{\text{Gar}} = a \times x^{b}$</th>
<th>$D_{\text{Cpx}} = a \times x^{b}$</th>
<th>$D_{\text{Min(min)}}$</th>
<th>$D_{\text{MgSiO}_3}$</th>
<th>$D_{\text{Cpx(Cpx)}}$</th>
<th>$D_{\text{MgSiO}_3(Cpx)}$</th>
<th>$D_{\text{Cpx(Cpx)}}$</th>
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<td>0.0000051</td>
<td>0.0105 Rb</td>
<td>0.850</td>
<td>0.00016</td>
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<td>Ba</td>
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<td>0.059122</td>
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<td>Th</td>
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<td>0.000015 Th</td>
<td>0.059145</td>
<td>0.000264 Th</td>
<td>0.00014</td>
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<td>0.079</td>
</tr>
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<td>0.000015</td>
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To assess the behavior of HFSE-bearing minerals (including rutile and zircon), the residual modes of these minerals are treated as variable (manually adjusted for wt.% in slab SED) when slab melting occurs. This is because these minerals are highly soluble in melts and insoluble in aqueous fluids and thus largely $T$-dependent. Source composition also affects their modal composition. Therefore, the effects on bulk $Ds$ for these minerals are difficult to constrain using the fixed slab composition in ABS. The important role and behaviors of these minerals are well-described by the solubility model for these minerals (Kimura et al., 2016; Xiong et al., 2011), making it difficult to model HFSE abundances and isotopes such as Hf (Tollstrup and Gill, 2005) without manual adjustment. This function is incorporated in ABS5.
Fig. 6 Examples of bulk partition coefficients of representative elements in slab layers. Partition coefficients are dependent on both temperature and residual mineralogy. Rapid bulk $D$ changes at ~700 °C are associated with dry eclogite transformation in the SED and AOC layers. $P$–$T$ paths of the slab layers are shown in the bottom right panel. The example is for the NE Japan Arc (Kimura, 2017).

Fig. 7 Examples of slab liquid compositions released from the slab during prograde metamorphism calculated by ABS5 for SW Japan and NE Japan slab geotherms (Kimura, 2017). Normalization values from Sun and McDonough (1989). Slab liquid compositions are similar at a given slab temperature, irrespective of $P$–$T$ path (see overlap between high-$P$ NE Japan liquids (blue) with those of low-$P$ slab liquids from SW Japan (red)).
Examples of calculated slab liquid compositions are shown in Fig. 7. It is notable that the slab liquid compositions are similar at similar slab temperatures, irrespective of the previous P–T path. This is due to a small loss of slab mass by dehydration/melting, confining the nearly-original bulk composition to depths greater than those of subduction zones (Kimura et al., 2016).

1.2. Zone Refining Reaction Between Slab Liquid and Mantle

ABS5 uses zone refining (ZR). In ABS5, the reaction degree (n factor) of ZR is simulated by the contribution of MwP fluid to pristine mantle peridotite (DMM). The calculation equations used for ZR are shown below.

$$X'_{FLUID} = X'_{PERID} - \frac{X_{PERID}}{D_{PERID/FLUID}} \times \exp \left( -n \times D_{PERID/FLUID} \right)$$

where

- $X'_{FLUID}$: reacted liquid composition of an element
- $X'_{PERID}$: metasomatized mantle peridotite composition of an element
- $X_{FLUID}$: slab liquid composition of an element derived from Eq(1)
- $D_{PERID/FLUID}$: partition coefficient of an element between mantle peridotite and liquid

A zone-refining reaction is useful for modeling the mantle wedge sole because it can simulate slab liquid–PERID interactions, ranging from no reaction ($n = 0$) to full reaction ($n = \infty$). This function, however, is found not to be useful, suggesting almost no contribution of the subsolidus mantle to the slab liquids in the sole of the wedge beneath the partially molten mantle core (Fig. 1). This would suggest fissure (crack) flow liquid transportation rather than porous flow in this region.

1.3. Liquid-Fluxed Melting Calculations for Mantle Peridotite

1.3.1 Mode and Melt Compositions for Fluxed Melting

Parameterizations of melting mode and melt composition are performed using the pMELTS thermodynamic model (Ghiorso et al., 2002) for fluid-fluxed melting with DMM source mantle (Workman and Hart, 2005). Using the results, lookup tables are generated as a function of pressure ($P_{perid}$) and melt fraction ($F_{perid}$). Modal and melt compositions for melt-fluxed melting at different melt flux fractions ($X_{melt}$) are also calculated after additions of averaged felsic slab melt (Moyen and Stevens, 2006) in steps of 5 wt.% from 0 wt.% to 25 wt.% (Kimura et al., 2010). Since there are systematic discrepancies between experimental results for both residual mode and melt compositions (Lambart et al., 2012), adjustments of the pMELTS results are made using empirical equations. The discrepancies in mode are adjusted by applying the correction factor,
\[ X_{\text{ol, corrected}} = X_{\text{ol}} \times 0.99 \times \exp[(–0.002 \times P^2 + 0.0135 \times P – 0.0115) \times F], \]

and renormalization of the total sum of the modal composition.

Experimental adjustment is also needed for the SiO\(_2\) and MgO contents of the melts, owing to the overestimation of olivine stability in pMELTS at >1.0 GPa. Corrections are made by

\[ \text{SiO}_2_{\text{correct}} = \text{SiO}_2 \times [0.05229 \times P + 0.967133] \text{ and} \]
\[ \text{MgO}_{\text{correct}} = \text{MgO} \times [-0.11458 \times P + 1.113095] \]

with renormalization of the total sum of major elements (Kimura, 2017). The adjusted results are shown in Fig. 8 for an enriched mantle (primitive mantle: PM). The same adjustments are applied for slab melt-fluxed mantle. The results reproduce well the experimental results for melt-fluxed mantle melting of Mallik et al. (2016) (not shown; see {Kimura, 2017 #969}). Note that Na\(_2\)O and K\(_2\)O are not used for calculations of melt compositions. ABS5 treats K\(_2\)O as an incompatible element. ABS5 does not calculate Na\(_2\)O and uses the value in the primary magma examined.

ABS5 treats the role of H\(_2\)O in partial melting using the parameterization of Katz et al. (2003) based on experimental data rather than the results from pMELTS (Kimura et al., 2010). The degree of partial melting (\(F_{\text{perid}}\)) at given \(P–T–X_{H_2O}\) is calculated from the parameterization (Fig. 9) and replaces \(F\) in the lookup tables for simulating modes and melt compositions in both liquid- and melt-fluxed melting (Figs. 10 and 11). \(X_{H_2O}\) in the mantle peridotite is calculated based on the water content in the slab liquid and its flux fraction in the partially molten mantle (\(X_{\text{slab liquid}}\)).

![Fig. 8 Comparisons between model and experimental results of mantle melting. (a) Residual mode compositions of modified pMELTS and experimental results. (b) Melt compositions of modified pMELTS and experimental results. Experimental data from the literature (Baker and Stolper, 1994; Falloon et al., 1999; Walter, 1998). Figure adopted from (Kimura, 2017).](image)
Fig. 9 Relations between $P$ (vertical axis) – $T$ (abscissa) and degree of partial melting $F$ (color contours) at given $X_{H_2O}$ (wt.% in five panels) in DMM. Calculations are from Katz et al. (2003). The same subsets are given for variously depleted mantle ranging from DMM (modal cpx = 0.15) to PM (modal cpx = 0.18).

Fig. 10 Melting relation and residual mineralogic mode of DMM and DMM fluxed by slab melt at 0, 5, 10, 15, and 20 wt.% of the mantle at given $P$–$F$ conditions. Once the mantle $P$–$T$ and $F$ are given, the modal compositions ($X_a$) are obtained. The degree of melting ($F = 0$–56 wt.%) and modal compositions (0–1 fraction) are shown by color maps; the gray field indicates the absence of phases. Ol: olivine; Cpx: clinopyroxene; Opx: orthopyroxene; Gar: garnet; Sp: spinel (Kimura, 2017).
Fig. 11 Melting relation and generated melt composition of depleted mantle. The five columns show melt compositions for SiO₂, Al₂O₃, FeO, MgO, and CaO. Degree of melting (0–56 wt.%) and magma compositions (0–60 wt.%) are shown by color maps; gray fields indicate the absence of phases (Kimura, 2017).

Addition of H₂O or felsic slab melt changes the modal composition of the residual mantle, particularly the proportions of olivine and orthopyroxene (Fig. 10). This does not strongly affect the bulk $D_s$ of trace elements due to extremely low $D_s$ in these minerals. However, calculated major element compositions are strongly affected by the decomposition of olivine and stabilization of orthopyroxene, which results in an increase in SiO₂ in the primary magma. ABS5 uses a fixed slab melt composition (average of experimental melts), so the calculated major element composition in the primary basalt should have strong model dependence. However, the major element melt composition does indicate whether silica is over-saturated or under-saturated at the mantle melting conditions examined. This is an important factor for examinations of high-Mg andesite and adakitic dacite, and even for silica-deficient alkali basalts. The major element data are therefore particularly useful, as shown by examples from SW Japan using ABS4.
\( \) (Kimura et al., 2014) and boninite from Izu using ABS5 (Kimura, 2017).

### 1.3.2 Trace Element Calculations for Liquid-Fluxed Open System Melting

Finally, the calculated modal composition of the mantle \( (X_a) \), the degree of partial melting \( (F_{\text{perid}}) \), and the composition of the mantle and the slab liquid are input into an open system melting equation along with partition coefficients from the hydrous melting experimental results of Green et al. (2000) (Table 2) (Kimura et al., 2009). The liquid fraction added to the mantle melting region is calculated using \( F_{\text{liq}} = \beta F \) (Ozawa and Shimizu, 1995). The ABS5 model can deal with any primary high-Mg basalts, high-Mg andesites, and adakitic dacites formed by slab fluid-fluxed melting and slab melt-fluxed melting of up to 25% of the mantle mass and at \( P = 0.8–3.0 \) GPa (Kimura et al., 2014).

**Table 2** Partition coefficients of minerals and melt used for fluxed melting of a hydrous mantle.

<table>
<thead>
<tr>
<th>Ds</th>
<th>D(ol)</th>
<th>D(opx)</th>
<th>D(cpx)</th>
<th>D(Gar)</th>
<th>D(Sp)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rb</td>
<td>0.0098</td>
<td>0.0001</td>
<td>0.0018</td>
<td>0.0001</td>
<td>0.000</td>
</tr>
<tr>
<td>Ba</td>
<td>0.0099</td>
<td>0.0001</td>
<td>0.0018</td>
<td>0.0002</td>
<td>0.000</td>
</tr>
<tr>
<td>Th</td>
<td>0.00835</td>
<td>0.0001</td>
<td>0.0002</td>
<td>0.001</td>
<td>0.000</td>
</tr>
<tr>
<td>U</td>
<td>0.00835</td>
<td>0.0002</td>
<td>0.0005</td>
<td>0.002</td>
<td>0.000</td>
</tr>
<tr>
<td>Nb</td>
<td>0.01</td>
<td>0.0113</td>
<td>0.0058</td>
<td>0.0005</td>
<td>0.010</td>
</tr>
<tr>
<td>Ta</td>
<td>0.01</td>
<td>0.0025</td>
<td>0.0019</td>
<td>0.0025</td>
<td>0.010</td>
</tr>
<tr>
<td>K</td>
<td>0.0068</td>
<td>0.0006</td>
<td>0.016</td>
<td>0.015</td>
<td>0.000</td>
</tr>
<tr>
<td>La</td>
<td>0.0067</td>
<td>0.0008</td>
<td>0.029</td>
<td>0.029</td>
<td>0.000</td>
</tr>
<tr>
<td>Ce</td>
<td>0.0069</td>
<td>0.0016</td>
<td>0.055</td>
<td>0.055</td>
<td>0.000</td>
</tr>
<tr>
<td>Pb</td>
<td>0.0075</td>
<td>0.0024</td>
<td>0.072</td>
<td>0.072</td>
<td>0.000</td>
</tr>
<tr>
<td>Pr</td>
<td>0.0066</td>
<td>0.0032</td>
<td>0.089</td>
<td>0.089</td>
<td>0.000</td>
</tr>
<tr>
<td>Sr</td>
<td>0.008</td>
<td>0.0012</td>
<td>0.11</td>
<td>0.0023</td>
<td>0.000</td>
</tr>
<tr>
<td>Nd</td>
<td>0.0066</td>
<td>0.0006</td>
<td>0.14</td>
<td>0.08</td>
<td>0.000</td>
</tr>
<tr>
<td>Sm</td>
<td>0.0066</td>
<td>0.0015</td>
<td>0.18</td>
<td>0.18</td>
<td>0.000</td>
</tr>
<tr>
<td>Zr</td>
<td>0.012</td>
<td>0.032</td>
<td>0.23</td>
<td>0.043</td>
<td>0.010</td>
</tr>
<tr>
<td>Hf</td>
<td>0.013</td>
<td>0.06</td>
<td>0.25</td>
<td>0.073</td>
<td>0.010</td>
</tr>
<tr>
<td>Eu</td>
<td>0.0068</td>
<td>0.03</td>
<td>0.23</td>
<td>0.33</td>
<td>0.000</td>
</tr>
<tr>
<td>Gd</td>
<td>0.0077</td>
<td>0.034</td>
<td>0.27</td>
<td>0.75</td>
<td>0.000</td>
</tr>
<tr>
<td>Tb</td>
<td>0.008</td>
<td>0.054</td>
<td>0.27</td>
<td>1.5</td>
<td>0.000</td>
</tr>
<tr>
<td>Dy</td>
<td>0.0096</td>
<td>0.077</td>
<td>0.3</td>
<td>2.4</td>
<td>0.000</td>
</tr>
<tr>
<td>Y</td>
<td>0.01</td>
<td>0.095</td>
<td>0.24</td>
<td>3.9</td>
<td>0.000</td>
</tr>
<tr>
<td>Ho</td>
<td>0.01</td>
<td>0.1</td>
<td>0.25</td>
<td>3.7</td>
<td>0.000</td>
</tr>
<tr>
<td>Er</td>
<td>0.011</td>
<td>0.12</td>
<td>0.24</td>
<td>4.4</td>
<td>0.000</td>
</tr>
<tr>
<td>Tm</td>
<td>0.0125</td>
<td>0.17</td>
<td>0.23</td>
<td>5.45</td>
<td>0.000</td>
</tr>
<tr>
<td>Yb</td>
<td>0.014</td>
<td>0.22</td>
<td>0.22</td>
<td>6.5</td>
<td>0.000</td>
</tr>
<tr>
<td>Lu</td>
<td>0.016</td>
<td>0.22</td>
<td>0.18</td>
<td>6.7</td>
<td>0.000</td>
</tr>
</tbody>
</table>

\( \) Ol: olivine; Opx: orthopyroxene; Cpx: clinopyroxene; Gar: garnet; Sp: spinel. Values from ABS5 (Kimura, 2017).

The calculation scheme assumes that open system melt-fluxed melting is identical to fluid-fluxed melting apart from the effect of slab-melt on residual mantle mineralogy (Ozawa and Shimizu, 1995; Shaw, 2000). The equation, after Zou (1998, 1999), is as follows:
$$X_{BAS} = \frac{1}{F - Fc} \cdot \frac{1}{P - \beta - 1} \times$$

$$X_{slabliq} \cdot \beta \cdot (Fc - F) +$$

$$\left\{X_{slab} \cdot \beta \cdot D + X_{PERID} \cdot (P - \beta - 1) \right\} \left[ D + \alpha - Fc \cdot (\alpha + P) \right]$$

$$\left[ D + Fc \cdot (1 + \beta - P) \right] \cdot (\alpha + \beta + 1)$$

$$\left[ D + \alpha - Fc \cdot (\alpha + P) \right]$$

$$\left[ (1 + \beta - P)/(\alpha + P) \right]^{t}$$

where

$$X_{BAS}$$: basalt melt composition of an element

$$X_{PERID}$$: source peridotite composition

$$D$$: bulk melt distribution coefficient of an element determined by

$$D = \sum_{1}^{n} Xa \times Da \quad \sum_{1}^{n} Xa = 1$$

$$Xa$$: modal composition of a residual mineral phase

$$Da$$: melt distribution coefficient of a mineral

$$P$$: contribution of consumed mineral

$$Pa$$: modal composition of a consumed mineral

$$\alpha$$: melt distribution coefficient of a mineral

$$\phi$$: porosity of melting system or residual melt mass fraction after melting

$$\beta$$: mass fraction of fluid in generated melt (when fluid influx is constant)

$$F$$: degree of partial melting

$$Fc$$: defined by $$\alpha/(\alpha+\beta+1)$$

$$X_{slabliq}$$: slab liquid composition

Porosity is set at $$\phi = 0.01$$ throughout the calculation. Isotopic abundance ratios are also calculated with the same equation using each isotope as an element. These include slab liquids and mantle peridotite. The isotopes are subsequently ratioed to generate the isotopic composition in a primary magma. With this treatment, any complex calculation equations are applicable (Kimura et al., 2014; Kimura et al., 2009). The primary basalt compositions obtained are Rb, Ba, Th, U, Nb, Ta, K, La, Ce, Pb, Pr, Sr, Nd, Sm, Zr, Hf, Eu, Gd, Tb, Dy, Y, Ho, Er, Tm, Yb, Lu, and $^{87}$Sr/$^{86}$Sr, $^{143}$Nd/$^{144}$Nd, $^{176}$Hf/$^{177}$Hf, $^{206}$Pb/$^{204}$Pb, $^{207}$Pb/$^{204}$Pb, $^{208}$Pb/$^{204}$Pb. Major elements SiO$_2$, TiO$_2$, Al$_2$O$_3$, FeO, MgO, CaO, K$_2$O, and H$_2$O are obtained separately from the lookup tables in section 1.3.1 (Fig. 11).

### 1.4. Use of Forward Model for Inversion Calculations

Since ABS5 is a petrological and geochemical forward model to simulate slab dehydration/melting and liquid-fluxed mantle melting and calculates the compositions of
a primary arc magma, this model is useful to estimate the slab and mantle conditions. Estimation is accomplished by fitting the calculated magma composition to the observed composition. Necessary geochemical input data in ABS5 are the source compositions of the slab layers (MwP, LGAB, UGAB, DIKE, LBAS, AOC, SED, and MwP) and the mantle wedge (PERID). These should include 26 trace elements (Rb, Ba, Th, U, Nb, Ta, K, La, Ce, Pb, Pr, Sr, Nd, Sm, Zr, Hf, Eu, Gd, Tb, Dy, Y, Ho, Er, Tm, Yb, Lu) and $^{87}\text{Sr}/^{86}\text{Sr}$, $^{143}\text{Nd}/^{144}\text{Nd}$, $^{176}\text{Hf}/^{177}\text{Hf}$, $^{206}\text{Pb}/^{204}\text{Pb}$, $^{207}\text{Pb}/^{204}\text{Pb}$, $^{208}\text{Pb}/^{204}\text{Pb}$ isotopes. Major elements are unnecessary because fixed compositions are used in the ABS5 model. Instead, the primary magma composition should include SiO$_2$, TiO$_2$, Al$_2$O$_3$, FeO, MgO, CaO, K$_2$O, H$_2$O, Rb, Ba, Th, U, Nb, Ta, (K), La, Ce, Pb, Pr, Sr, Nd, Sm, Zr, Hf, Eu, Gd, Tb, Dy, Y, Ho, Er, Tm, Yb, Lu, and $^{87}\text{Sr}/^{86}\text{Sr}$, $^{143}\text{Nd}/^{144}\text{Nd}$, $^{176}\text{Hf}/^{177}\text{Hf}$, $^{206}\text{Pb}/^{204}\text{Pb}$, $^{207}\text{Pb}/^{204}\text{Pb}$, $^{208}\text{Pb}/^{204}\text{Pb}$.

Primary magma compositions can be estimated using models for fractional crystallization in a crustal magma chamber. Useful models are PRIMACALC2 (Kimura and Ariskin, 2014) and PRIMELT3 (Herzberg and Asimow, 2015). In particular, the former model is tuned for arc basalts, including crystal fractionation in a magma chamber under a pressure range of 0–0.1 GPa using a thermodynamic model for water-bearing systems. Estimation of mantle equilibrium for the calculated primary basalt is also made using experimental phase equilibrium data, which are tuned for water-bearing peridotite systems. Estimations of primary magmas for high-Mg andesite and adakitic dacite are more difficult. These are not discussed here and readers should refer to the relevant paper (Kimura et al., 2014).

Table 3 ABS5 parameters that control primary magma composition and are used as fitting parameters in inversion calculations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{slab}$</td>
<td>Slab surface temperature in °C</td>
</tr>
<tr>
<td>$P_{sc}$</td>
<td>Slab surface depth in GPa</td>
</tr>
<tr>
<td>$T_{slab}$</td>
<td>Slab temperature in °C</td>
</tr>
<tr>
<td>$P_{max}$</td>
<td>Slab depth in GPa</td>
</tr>
<tr>
<td>$F_{pm}$</td>
<td>Degree of partial melting of slab layer either by fraction or by % as noted</td>
</tr>
<tr>
<td>$T_{pm}$</td>
<td>Mantle peridotite temperature in °C</td>
</tr>
<tr>
<td>$P_{pm}$</td>
<td>Mantle peridotite depth in GPa</td>
</tr>
<tr>
<td>$F_{pm}$</td>
<td>Degree of partial melting of peridotite either by fraction or by % as noted</td>
</tr>
<tr>
<td>$X_{H_2O}$</td>
<td>H$_2$O content (fraction)</td>
</tr>
<tr>
<td>Flq(AOC)</td>
<td>Fraction of AOC liquid</td>
</tr>
<tr>
<td>Flq(SED)</td>
<td>Fraction of SED liquid</td>
</tr>
<tr>
<td>Flq(MwP)</td>
<td>Fraction of MwP liquid</td>
</tr>
<tr>
<td>$F_{slab}$</td>
<td>Fraction of slab liquid in the mantle wedge</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Open system melting parameter given by $\beta = b/(a + b)$ where $a$ and $b$ are slab liquid and mantle melt</td>
</tr>
</tbody>
</table>

Once a primary magma composition is available, ABS5 can simulate the magma compositions. The major parameters that control magma composition are listed in Table 3. Some examples of fitting results are shown in Fig. 12. Fitting is explored by two methods. The parameters in Table 3 are altered manually by input or automatically using Monte Carlo calculations in ABS5. The entire magma chemistry, including major elements, trace elements, and isotope ratios, is explored simultaneously. Obtained parameters that result in a reasonable fit are considered to represent slab and mantle conditions. The parameters include geophysical intensive and extensive variables; therefore, this inversion approach provides unique implications for geodynamics using the geochemical mass balance model, namely Chemical Geodynamics.
**Fig. 12** ABS5 calculation results and comparisons with target magmas. (a)–(e) show trace elements. Black solid lines indicate target magmas; red lines with open circles indicate ABS5 calculation results; and thin red lines indicate minimum and maximum values. The values are normalized to the primitive mantle composition results of Sun and McDonough (1989). (f)–(i) show isotopes. Solid symbols represent observed values, and open symbols represent those calculated by ABS5. Error bars are two standard deviations. Min: minimum; Max: maximum; Avg: average; OBS: observed; CALC: calculated; LKTH: low-K tholeiite; MKCA: medium-K calc–alkaline; HMA: high-Mg andesite; ADK: adakitic dacite; BON: boninite (Kimura, 2017).

ABS5 does not facilitate sophisticated Monte Carlo calculations, such as MCMC (Markov Chain Monte Carlo) calculations. This is partly because of the very narrow range of the fitting results. The relatively rigid (fixed) ABS5 petrological model reduces the dimension and parameters explored to only 8 for 32 elements/isotope data. In many cases, simple Gaussian distributions are obtained with the fitting windows. In some cases, bimodal solutions are obtained for some parameters, such as $F_{\text{perid}}$. Further refinement is available using the results recorded in the [SUMMARY] worksheet. Once users obtain
result values in the [SUMMARY] worksheet, one can narrow the statistical conditions by examining the % relative deviation (%RD) values recorded for all the trace elements. Filtering is accomplished by using the **SORT** function in the Excel spreadsheet applied to each %RD value.

Tighter windows for LREEs (e.g., La, Ce), MREEs (Nd, Sm), and HREEs (Yb, Lu) are the first priority because REEs are critical for constraining the melting depth, degree of partial melting, slab liquid fraction, and degree of depletion in the source mantle peridotite. This treatment improves significantly the fitting results from Monte Carlo calculations.

Second priority is given to HFSEs, such as Nb-Ta. Larger errors are expected for LILEs, and sometimes for HFSEs, due to large variations in source compositions for LILEs and uncertainties in residual slab minerals (i.e., zircon or rutile) for HFSEs. The recommended “good fit” is usually <10%RD for HREEs, <15%RD for MREEs, and <20%RD for LREEs. U and Th should be <10%RD but sometimes larger. LILs, such as Rb, Ba, K, Sr, and Pb, can be >50%RD or more.

Then, SiO₂ should be examined to determine whether the result satisfies the major element constraints. SiO₂ should be within ±3 wt.% of the target composition. Isotope ratios are usually consistent with the target when the trace element mass balance is satisfactorily established and the assumed source material compositions are sound (Fig. 12). Other major element compositions of Al₂O₃, TiO₂, FeO, MgO, and CaO are usually consistent with the target when the mass balance of trace elements plus SiO₂ is reasonably established (Kimura, 2017; Kimura et al., 2014).

Isotopic compositions are also useful for further narrowing of the fitting results. However, when a reasonable fit is made using the trace elements and major elements, the isotopes are naturally within a reasonable range, which is no surprise due to the role of %R_{slab}.

Histograms of the fitting parameters are also useful to evaluate their statistical distribution. Narrow unimodal distributions are the preferred solutions. When bimodal results appear, one can further narrow the results by removing the least important fitting results, if the selection criteria are met with reasonable statistics and petrological criteria.

The ABS5 model derives fairly narrow fitting results (e.g., <10%RD and <3 wt.% SiO₂) showing relatively rigid behavioral features. This is understandable due to the strong reduction in dimension by applying the tightly confined (fixed) petrological model. Introduction of more variables is possible but may lead to diffused solutions.
2. OPERATING ABS5

The basic function of the ABS5 model is to fit a magma composition using sequential calculations to match the major and trace elements and Sr–Nd–Hf–Pb isotope compositions of a target primary arc magma. This is achieved by altering intensive and extensive variables in the [CONTROL PANEL] worksheet (Fig. 13). Pre-defined and adjustable parameters are separated in order to save calculation steps and thus time. Color-coded yellow cells with red characters are input values that can be adjusted by the user. Each of these parameters is explained below. New users may notice that there are 14 different worksheets in the ABS5 Excel workbook, but most of these are used for calculations and should not be changed. Only yellow cells with red characters in the [CONTROL PANEL] and [DATA INPUT] worksheets should be changed. Users are encouraged to examine all of the spreadsheets but be sure to keep a back-up copy of ABS5 in case of inadvertently changing one of the parameters in other worksheets!

Fig. 13 Screenshot of the [CONTROL PANEL] worksheet in Arc Basalt Simulator version 5.00 (ABS5) (Kimura, 2017).

2.1. How to Adjust Parameters for ABS5 Forward Modeling

Five Pre-Defined Model Conditions (denominator, sample composition, slab solidus model, peridotite model, slab $P–T$ Model) and nine Fitting Parameters (Slab $P$, liquid fraction from SED $F_{\text{liq}(\text{SED})}$, liquid fraction from MwP $F_{\text{liq}(\text{MwP})}$, slab reaction parameter $R_{\text{slab}}$, target factor of zone refining, source mantle depletion $\%\text{MORB}_{\text{ext}}$, melting pressure of mantle $P_{\text{perid}}$, melting temperature of mantle $T_{\text{perid}}$, and fraction of slab liquid in the mantle $F_{\text{slblq}}$%) are required for ABS modeling. These are discussed further below.
2.1.1 Pre-defined Model Conditions

The inputs are found in the large green box in the [CONTROL PANEL] worksheet. At the top left, **DENOMIN** is the denominator composition in multielement plots. Users can choose MORB, primitive mantle (PM), or depleted MORB-source mantle (DMM) compositions by typing **M**, **P**, or **D**, respectively. Secondly, users can choose one of five primary magma compositions to model. Primary magma compositions are found in the [DATA INPUT] worksheet. The present spreadsheet (ABS5 Software DR1 in Kimura et al., 2017) contains five samples: IWT (Iwate) and SAN (Sannomegata) from the NE Japan Arc, ADK (Daisen adakite) and HMA (Setouchi high-Mg andesite) from the SW Japan Arc, and BON (boninite) from the Izu–Bonin–Mariana (IBM) Arc (Kimura, 2017). The user must then choose one **SAMPLE** from these by typing the number corresponding to that sample column from the [DATA INPUT] worksheet. The user must choose a SLAB SOLIDUS MODEL; either **W**et solidus or **D**ehydration solidus. Solidus curves from Herman and Spandler (2008), for wet solidus, and Schmidt et al. (2004), for dehydration solidus, are used. “W” is recommended for most arc magmas. The “D” model may be important for some arcs, such as the Izu volcanic front, where very high H2O (>5 wt.%) is expected in the primary basalt. The user should also choose one of four model peridotite compositions (PERID) by typing **W** (Workman and Hart, 2005), **S** (Salters et al., 2011), **PM** (Sun and McDonough, 1989), or **U** for “user-defined” composition. These trace element compositions are found in the [Per_Dep] worksheet and are changeable by the user. SLAB P–T MODEL defines the P–T paths of eight slab layers for the slabs in 56 subduction zones worldwide (Syracuse et al., 2010; van Keken et al., 2011), which are denoted by separate numbers in the [Slb_PT(PvK2011)] worksheet. Users must choose the most appropriate of these by typing the corresponding number in the **Model** cell (e.g., inputting **48** chooses the

![Fig. 14 Pre-defined conditions in ABS5 shown in the [CONTROL_PANEL] (Kimura, 2017).](image-url)
Other predefined parameters are the **SLAB LAYER MODEL**, which defines the thickness of each slab layer. The thickness (T km) assigned to each layer does not make a significant change in the calculations, so those used are the default. Only the SED layer thickness is from the geophysical database, linked with the choice of slab $P–T$ model (Syracuse et al., 2010). $%R_{\text{slab}}$ is shown for each layer but these are uniform reflecting the fitting parameter (see below). $%\text{mlt}$ shows the degree of melting of the slab layer obtained from the slab $P–T$ model and the slab solidus model (Fig. 14). The **GABBRO COMPOSITION** defines the trace element composition in the LGAB and UGAB layers as times X(DIKE), where the X(DIKE) composition represents normal (N)-MORB in the [DATA_INPUT] worksheet. In some cases, a better fit is obtained by using a hotter/colder slab $P–T$. The **SLAB T-FACTOR** (cell $I$15) lets the user adjust the slab $P–T$ by simple multiplication at all depths (1 is the default value). The **SLAB D FACTOR** manually alters the solid/melt partition coefficients of the slab minerals. The $\text{XD}($fluid/mlt$)$ parameter alters the solid/melt partition coefficients of large ion lithophile elements (LILEs), rare earth elements (REEs), and U and Th between dehydration and melting modes (0.3 times is default), and the $\text{XD}_{\text{HSFE}}($fluid/mlt$)$ parameter is for HFSEs (0.2 times is default); these values are approximated by experiments (Hermann and Spandler, 2008). The Xres Rutile, Xres Allanite, and Xres Zircon parameters artificially add residual minerals in modal wt.% in the slab SED using the fixed $D_s$ in Table 1. These last three factors are for evaluation of residual accessory minerals in the slab and are usually set at default values of 0. The **H$_2$O FRACTION IN FLUID** artificially alters the water content in the slab liquid to observe the effect of water flux on mantle melting (1 is default). The red–orange cells with red text here are the changeable boxes.

### 2.1.2 Fitting Parameters

The second set of inputs concerns the dark blue box **FITTING PARAMETERS** in the [CONTROL PANEL] worksheet (Fig. 15). This includes the **SLAB FLUX P–T CONDITION**, inputting the pressure of the slab where the slab liquid is derived, defined by Slab $P(GPa)$ correlating to the depth of the slab surface. This is an important ABS5 model parameter used to explore the depth of slab defluxing required to generate the designated arc magma examined. Pressure is related to depth by the following relationship: $P \ (\text{GPa}) \sim \text{depth (km)}/33 \ \text{(cell}$ $D$16$)$; the user needs an independent way to estimate depth, for example by referring to compilations of the slab depth ($h$) beneath volcanic arcs (Syracuse and Abers, 2006), or alternatively can freely alter the value with full trust in the geochemical mass balance model. ABS5 simulates the composition of either fluid or melt derived from the slab at $P$ between 0.5 GPa (~17 km deep) and 6.0 GPa (~200 km deep) at 0.1 GPa steps. Reasonable values are always between 2.8 (~90 km) and 6.0 GPa. Inputting the chosen depth produces a slab surface temperature (SST) at this point, determined from the **SLAB P–T Model** and the **SLAB T-factor**. This depth is shown graphically by the diamond in the subduction zone graphic to the immediate right (Fig. 15).

The **SLAB LIQ FRACTION/REACTIVITY** box, shown in Fig. 15, also determines the chemistry of the slab liquid. Liquid fractions of slab AOC, SED, and MwP are used to simulate a mixed slab liquid composition with fractions $F_{\text{liq}}(\text{AOC}) + F_{\text{liq}}(\text{SED}) + F_{\text{liq}}(\text{MwP}) = 1$ (Fig. 2). The top three slab layers are thought to comprise the region of slab liquid release via crack flow (Kimura and Nakajima, 2014) because of the dominant
intra-slab seismicity and low seismic velocity in the upper portion of the subducted slab beneath the volcanic front (Kita et al., 2006; Saita et al., 2015; Shiina et al., 2013). Inputs are made for $F_{liq}(SED)$ and $F_{liq}(MwP)$ only. Slab liquid reactivity controlled by porosity of the slab is defined by $\%R_{slab}$, as noted above (Fig. 5), and is defined here. The ZONE REFINING box defines the $n$ factor for the reaction of slab liquid and peridotite (see above). The DMM POROSITY defines the porosity $\phi$ (given in %) for the open system melting in the [OSM] worksheet, which is fixed as 1%. Another user-adjustable parameter is the degree of source mantle depletion, as in the DMM DEPLETION box. This is controlled by altering $\%MORB_{ext}$, which alters the percentage of MORB melt extraction from the mantle, from 0–25% in 0.1% steps. This parameter calculates the source mantle compositions that are more depleted than the model PERID chosen in cell $E7$ (Fig. 15). This adjustment is necessary for some arc magmas because sometimes the mantle source is more depleted than even the MORB source, perhaps as a result of earlier melting under a back-arc basin. Calculations are made in the [Per_Dep] worksheet. Due to the change in residual clinopyroxene caused by this depletion, the cpx mode in the depleted mantle is calculated in the cpx mode box below. This value originates from the [Per_Dep] worksheet and is used for calculations of the degree of peridotite melting in the [Katz+] worksheet.

The three parameters in the OPEN SYSTEM MELTING boxes (Fig. 15) relate to conditions in the melting mantle, which is modeled as open system liquid-fluxed mantle. This means that fluids and mantle are continuously flowing into the melting region at the same time as melt is flowing out of it (see Fig. 9 in Shaw (2000)). Parameters that can be adjusted are melting pressure $P$ (GPa) (cell $C27$), temperature of melting $T(\degree C)$ (cell $C28$), and percentage of phase $F$ (%) (cell $C29$).
and liquid fraction fluxing into the peridotite source $F_{\text{slb liq.}}$% (cell $C29$). Acceptable ranges are 1–3 GPa, 1000–1450°C, and 0–30 wt.% fraction, respectively. Users should have some independent idea about the depth of melt generation, for example from mantle tomography or inferences from REE patterns. Otherwise, ABS5 finds fitting results which are, in most cases, reasonable (Kimura, 2017; Kimura et al., 2014; Kimura and Nakajima, 2014). Note that the depth of mantle melting is shown graphically as a red dot in the panel immediately to the right (Fig. 15). Similarly, the user should use what they think is the mantle temperature at this depth, perhaps from their understanding of mantle potential temperatures or published thermal models for the mantle wedge. These parameters define the effect of H$_2$O and/or slab melt on the melting modes as well as the composition of the mantle source. The calculations also define the degree of partial melting $F_{\%}^{\text{PERID}}$, percent liquid fraction in the partially melted mantle $\beta$(%), H$_2$O in the slab liquid H$_2$O%$_{\text{slb liq.}}$, and H$_2$O in the generated magma H$_2$O%$_{\text{BAS}}$. Note that the H$_2$O content H$_2$O%$_{\text{slb liq.}}$ is always much less than 100%. This is because even low-$T$ hydrous fluid includes a lot of dissolved elements. H$_2$O content in slab melt is far less than this. There are two checkboxes (indicated by pink background and CHK) in the melting calculations. One is $F_{\%}^{\text{PERID}}$, which should be 30% by the limit of ABS5 model, and the other is H$_2$O%$_{\text{BAS}}$ indicating whether or not the primary magma is oversaturated with H$_2$O (Fig. 15).

**Fig. 16** Diagrams showing multielement plots, and Nd–Sr, Nd–Hf, and Pb–Pb isotope plots, plus a table showing major element composition and residual mantle mineralogy in ABS5 (Kimura, 2017).

### 2.1.3 Graphical and Numerical Evaluation of the Fitting Results

The fitting calculations are made by manually altering the input parameters. Model
outputs can be found in several tables and figures to the right of the [CONTROL PANEL]. To evaluate the fitting results, ABS5 modeled outputs include plots of trace element concentrations and Sr–Nd–Pb–Hf isotope compositions, and a table that shows the major element composition of the primary magma and the mineralogic mode of the residual mantle (Fig. 16). Users can observe changes in these diagrams and the values in the table to find the closest fit. The slab mode is shown at the depth where the slab liquid is defluxed, which is also in the lower portion of the [CONTROL PANEL] worksheet (Fig. 17).

Fig. 17 Table showing residual slab and mantle mineralogies and conditions (Kimura, 2017).

Important values that need to be worked with are found in the FITTING PARAMETERS, once the subduction setting is defined for a designated arc in the PRE-DEFINED MODEL CONDITIONS. In the case that the subduction conditions are not well known, such as an ancient arc, arc conditions that are expected for the target can be chosen (Kimura et al., 2016). Alternatively, all the typical arc conditions, such as hot SW Japan and cold NE Japan, are explored as extreme cases. A successful manual fitting process may begin with abundances of REEs, because REEs have the most well-constrained partition coefficients of the elements used. Moreover, the abundances and slopes of REEs in the multielement plot are the key to seeking the source conditions and compositions. Key factors are the degree of partial melting ($F_{perid}$) and amount of slab liquid ($F_{slab\ liq}$). These are controlled by the parameters $P_{perid}$, $T_{perid}$, and $F_{slab\ liq}$. An additional control is the depth of slab liquid defluxing ($P_{slab}$). This produces large variations in the slab-derived liquid (Fig. 7).

Relative depletion in HFSEs, such as Nb–Ta, is usually linked to HREE abundances (Kimura, 2017). Therefore, these are explored in terms of the degree of melting ($F_{perid}$) and of depletion in the source mantle (%MORBext). Detailed LILE profiles also depend on the depth of slab liquid release ($P_{slab}$), but the mixing rates of AOC, SED, and MwP liquids ($F_{slab\ (AOC)}$, $F_{slab\ (SED)}$, $F_{slab\ (MwP)}$) are additional factors. Isotope ratios are fundamentally controlled by the $F_{slab\ (AOC)} – F_{slab\ (SED)} – F_{slab\ (MwP)}$ mixing ratio, but are also significantly affected by slab liquid reactivity (%$R_{slab}$).
Finally, even if the above parameters are met for a reasonable fit, the major element composition may show a large discrepancy. Adjustment of the major element composition is often made in the final step. Usually, an increase in the slab melt fraction ($F_{slab\, liq.}$) decreases the degree of partial melting of the mantle ($F_{perid}$). Shallowing the mantle melting depth ($P_{perid}$) helps to increase SiO$_2$ in the primary magma (Kimura et al., 2014). These trends are suggested by the lookup table for major elements (Fig. 11). Each fitting parameter (Table 3, Fig. 14) can be explored independently with the other parameters set as fixed. Balancing the element mass balance for 30 elements and 4 isotope systems is not an easy task. However, a reasonable fit is eventually accomplished in most cases. Fine adjustment can be made by altering the SLAB FACTOR boxes after the overall fit is accomplished. This will particularly adjust the abundances of HFSEs (Nb, Ta, Zr, and Hf), and U and Th.

2.1.4 Automated Fitting and Statistical Evaluations of the Fitting Results

ABS5 allows the computer to automatically choose a best-fit model (Macintosh users need to install Windows OS to enable the use of Windows Excel including the original macro script). For automated fitting, the minimum (MIN) and maximum (MAX) values and the calculation step (STEP) of each parameter are set in the AUTO-FIT PARAMETERS boxes in the [CONTROL PANEL] worksheet (Fig. 18). The calculations use random numbers generated automatically by the computer based on the settings (Monte Carlo calculations). Calculations commence when the [ABS5 Macro] button is pressed. Results are saved in the [SUMMARY] worksheet when a reasonable fit is achieved. Tables in the [SUMMARY] worksheet are automatically erased at the beginning of autofitting for new samples. Therefore, users need to ensure that the previous results have been saved or copied to a different file before running the macro.

For automated fitting, users must set statistical filters. These are input as Limit values in the FITTING WINDOWS boxes, which delimit the maximum deviation (%) allowed from the target basalt composition. All trace elements are used and the Limit values need to be set in the boxes with red numbers and yellow background. Blue numbers with blue background below the input boxes are the calculated (Calc.) values for the current fitting conditions (Fig. 18). One can adjust the Limit values guided by the Calc. values. For SiO$_2$ and the five isotope ratios of $^{87}$Sr/$^{86}$Sr, $^{143}$Nd/$^{144}$Nd, $^{176}$Hf/$^{177}$Hf,
$^{207}\text{Pb}/^{204}\text{Pb}$, and $^{208}\text{Pb}/^{204}\text{Pb}$, minimum (Min) and maximum (Max) values should be given (Fig. 18). Target isotope compositions are shown below these input boxes as a guide (Fig. 18). It is recommended to obtain a “reasonable fit” manually before setting up these inputs in the AUTO-FIT PARAMETERS and FITTING WINDOWS. Alternatively, the full range of the auto-fit parameters, with wide ranges and coarse step intervals, can be used to explore the entire range of the eight control parameters, which is time consuming. Since the calculations are made using a Monte Carlo approach, users can finish the calculations whenever required. To do this, simply hit the [ESC] key on the keyboard. Users need to check the results in the [SUMMARY] worksheet and save.

Note: New users of ABS5 are strongly advised to change the parameters manually to better understand how changing the most important parameters listed in the [CONTROL PANEL], found in the large colored boxes “Pre-Defined Model Conditions” and “Fitting Parameters,” affects the model results.

**Fig. 19** Data input fields for target magma compositions and SlbP, DIKE, AOC, SED, and MwP compositions. Boxes with red/purple/green/blue text and yellow background are the areas for data input (Kimura, 2017).

### 2.2. Input Primitive Magma and Source AOC, SED, and PERID Compositions

To generate a model appropriate for samples, users must input primitive (or near-
primitive) magma compositions. Primary magma composition means the composition generated by melting of mantle peridotite. Primary magmas include high-Mg basalt and high-Mg andesite, and adakitic dacite melt. Once reasonably primitive arc magma compositions are obtained, the user should type the major, trace, and Sr, Nd, Pb, and Hf isotope data into the [DATA INPUT] worksheet (Fig. 19). Target primary magma compositions are from observed data with back calculations for mantle equilibrium. See relevant papers for a discussion of primary magma composition (Kimura and Ariskin, 2014; Kimura et al., 2014). The trace element compositions of the source materials are assumed from the geochemistry of the subducting materials, such as ocean sediment for SED (Plank and Langmuir, 1988), altered oceanic crust for AOC (Kelley et al., 2003), back-arc basin (BAB) mantle composition using BAB basalt chemistry for MwP (Hirahara et al., 2015), and non-altered MORB composition for the oceanic plate for SlbP (Class and Lehnert, 2012; Jenner and O’Neill, 2012). Isotopic compositions also vary for these materials (Fig. 19).

Local geochemical data are always useful for determining the source materials in a particular subduction system. This implies that ABS5 critically represents the mass balance of subduction zones (Kimura, 2017; Kimura et al., 2010; Li et al., 2013). Major element compositions and petrological models for the source materials are fixed in ABS5. This assumption may be an oversimplification. However, the element and isotope mass balance built on this simple model is still able to explain the geochemical variations in a wide range of subduction zones. Intensive and extensive variables obtained from the inversion calculations also provide reasonable results comparable with geophysical observations (Kimura, 2017; Kimura et al., 2010; Kimura et al., 2014; Kimura et al., 2016; Kimura and Nakajima, 2014; Li et al., 2013).

2.3. Data Output

Fig. 20 Data output fields for various intermediate and final liquid and melt compositions shown in the [RESULT_COMP] worksheet (Kimura, 2017).
Calculation results for the slab liquid composition at the depth of slab defluxing, the slab liquid composition after zone refining, and the calculated arc magma composition are shown in the [RESULT_COMP] worksheet (Fig. 20). One can copy the data from this worksheet. When an automated fit is performed, the fitted results are recorded in the [SUMMARY] worksheet along with statistical information.
3. DATA STRUCTURE AND CALCULATION WORKSHEETS

This section briefly describes the data structure and the roles and relationships of the worksheets in ABS5. This will help to understand the link between the calculation scheme (section 1) and data handling (section 2). Users who are interested to see the calculation details, and extract the intermediate data such as D values and mode in the lookup tables, are advised to go through this section.

3.1. CONTROL_PANEL

The [CONTROL_PANEL] worksheet (Fig. 21) is the main dashboard for ABS5 operation. All pre-defined and fitting parameters relevant to the ABS5 calculations are controlled from this worksheet. See section 2 for details of each parameter. In the green panel, the SLAB LAYER PROFILE diagram shows the subduction zone conditions including the locations of slab defluxing and mantle wedge melting. Slab layers in supersolidus condition are shown by small dots. In the yellow panel, the multielement plot shows the compositions of the target primary magma (thick black line), calculated primary magma (thick red line), slab liquid (thin blue line), and source mantle (MwP: thick yellow line). Compositional ranges of the fitting windows are also shown by black horizontal bars. Also in the yellow panel, three isotope plots show $^{87}\text{Sr}/^{86}\text{Sr}$ versus $^{143}\text{Nd}/^{144}\text{Nd}$, $^{143}\text{Nd}/^{144}\text{Nd}$ versus $^{176}\text{Hf}/^{177}\text{Hf}$, and $^{206}\text{Pb}/^{204}\text{Pb}$ versus $^{208}\text{Pb}/^{204}\text{Pb}$.

Compositions of MwP (DMM: large red dot), SED (large blue dot), and AOC (large green dot) indicate the sources. Subduction-modified MwP (small red dot), SED (small blue dot), AOC (small green dot), mixed slab liquid (small light blue dot), and primary magma (large open red dot) compositions are from ABS5. The target primary magma composition is shown by a large black open square. Ranges of isotope ratios determined in the fitting windows are shown by four black cross symbols. All of the symbols from the calculations move when the controlling parameters are altered. Users can immediately...
see the effects graphically. While the automated fit macro is running, the panel is frozen or even shows an irregular image. Users can confirm the progress from the indication in the bottom left outer frame, shown as “50 cycles done 2 fits / Total 5000000.”

Caveat: Do not alter the fields outside of the area and boxes shown in Fig. 21 other than those with red text with yellow and orange backgrounds.

3.2. DATA_INPUT
The function of the [DATA_INPUT] worksheet (Fig. 19) has been explained above and is not repeated here. This worksheet also provides a database of the source compositions for SED, AOC, DMM, and PM.

Caveat: Do not alter the colored cells other than data input fields with red text and yellow background.

3.3. RESULT_COMP
The function of the [RESULT_COMP] worksheet (Fig. 20) has been explained above.

Caveat: Do not alter any cells. Only data copy is allowed in this worksheet.

3.4. FIT_PARAM
The function of the [FIT_PARAM] worksheet is currently NOT used in ABS5.

Caveat: Do not alter any cells.

3.5. Slb_PT(PvK2011)
The [Slb_PT(PvK2011)] worksheet contains a database of slab $P$–$T$ paths for the eight slab layers in 56 subduction zones worldwide, used in van Keken et al. (2011) and modified from Syracuse et al. (2010) (Fig. 22). The left-hand vertical column shows the ID numbers of the subduction zones. Lookup table data on the right show slab $T$ (°C) at given pressure $P$ (GPa) for each 0.1 GPa step between 0.4 and 6.0 GPa.

Caveat: Do not alter any cells. Only data copy is allowed in this worksheet.
3.6. Slb_Mode
The [Slb_Mode] worksheet (Fig. 23) includes lookup tables of metamorphic minerals for DMM, MORB, and SED using the Perple_X thermodynamic model (Connolly and Kerrick, 1987; Connolly and Petrini, 2002) with replacement of the values between solidus–liquidus intervals organized based on experimental data. Dehydration solidus and vapor-saturated solidus modes are available. See Kimura et al. (2010) for details. Mineralogic modes are for Gt (garnet), Cpx (clinopyroxene), Ol (olivine), Opx (orthopyroxene), SiO₂ (silica minerals), Pl (plagioclase), Chl (chlorite), Bio (biotite), Phen (phengite), Amp (amphibole), Sheet (sheet silicates for SED and AOC; serpentine minerals, including antigorite, chrysotile, and lizardite, for MwP), PhA (phase A), Law (lawsonite), Zo (zoisite), and TiO₂ minerals (rutile, titanomagnetite, and ilmenite). H₂O and slab melt (including H₂O) fractions are also shown in the lookup tables below line 130. Modal compositions and slab fluid/melt and H₂O in the slab liquids are calculated along the given slab P–T paths for the eight layers. The calculations and results are shown in lines 71–128. The results are shown in the panels in lines 2–65 (Fig. 23).

Caveat: Do not alter any cells. Only data copy is allowed in this worksheet.

3.7. SDMS4.0
The [SDMS4.0] worksheet (Fig. 24) is the calculator of the slab dehydration/melting simulation for 26 trace elements Rb, Ba, Th, U, Nb, Ta, K, La, Ce, Pb, Pr, Sr, Nd, Sm, Zr, Hf, Eu, Gd, Tb, Dy, Y, Ho, Er, Tm, Yb, Lu, and H₂O, and Sr–Nd–Hf–Pb isotopes in the eight slab layers of MwP, SED, UBAS, LBAS, DIKE, UGAB, LGAB, and SlbP in descending order. Calculation matrices are divided into two areas: Area 1. Modal and elemental calculation area in columns A to BL; Area 2. Bulk partition coefficient calculation area in columns BK to IV.

Area 1 comprises the modal compositions of each slab layer (lines 62–215), dehydration rate (lines 217–227), melt fraction in each slab layer (lines 229–239), \(X_{H2O}\) in melt in each slab layer (lines 241–251), increment of melting degree (lines 253–263), increment of defluxing (lines 265–275), total sum of slab liquid (lines 277–287), bulk
partition coefficient by element in each slab layer (lines 289–499), source slab
composition including original Cs0 and modified Csx by element for each layer (lines
568–778), slab liquid composition C_Lx by element for each layer (lines 780–990), source
slab isotopic composition including original Cs0 and modified Csx by element for each
layer (lines 992–1174), and finally the calculation matrix for isotope ratios (lines 1076–1158). All of the above values are calculated along the P–T path of each slab layer
between 0.5 and 6.0 GPa at 0.1 GPa steps (columns E–BH).

Fig. 24 The [SDMS4.0] worksheet in ABS5 (Kimura, 2017).

Area 2 calculates the bulk partition coefficients for MwP (lines 62–124), SED
(lines 125–187), AOC (lines 188–250), LBAS (lines 251–313), DIKE (lines 314–376),
UGAB (lines 377–439), LGAB (lines 440–502), and SlbP (lines 503–565). All D values
are calculated along the P–T path of each slab layer between 0.5 and 6.0 GPa at 0.1 GPa
steps for the minerals (Gt, Cpx, and TiO2) available for temperature-dependent Ds (Table
1) and Amp, Opx, and Chl available indirectly with mineral/mineral Ds (Table 1)
(columns CF–EI, EL–GO, and GR–IU). Minerals with fixed Ds are tabulated in columns
BM–CC (Table 1). Partition coefficients are adjusted using different fluid/melt modes
given in the top line of each calculation matrix, corresponding to XD_{fluid/melt} in the
[CONTROL_PANEL]. Ds for accessory minerals are calculated manually with the given
modal composition in the [CONTROL_PANEL]. Other metamorphic mineral modes are
from the [Slb_Mode] worksheet; these are summarized in lines 62–215 in Area 1 of this
worksheet. The bulk Ds at each slab depth and in each slab layer are calculated by
integration of these Ds and X_a,s and are shown in lines 289–409 of Area 1. Area 1 also
calculates the solid and liquid composition in each prograde metamorphic step following
the chromatographic calculations (Fig. 5).

The final calculation result for the slab liquid is given in the top left corner of the
[SMDS4.0] worksheet along with graphical plots for the trace element compositions in
the slab liquids and in the residual solids (Fig. 24).

Caveat: Do not alter any cells. Only data copy is allowed in this worksheet.

### 3.8. ZRef

The [ZRef] worksheet calculates zone refining reactions in the subsolidus mantle between MwP and the mantle wedge (Fig. 25). The n factor and compositions of the slab liquid and depleted mantle are introduced from the [CONTROL_PANEL], and the [SDMS4.0] and [Peri_Dep] worksheets, respectively. Calculations are made according to the zone refining equation given in section 1.2.

**Caveat:** Do not alter any cells. Only data copy is allowed in this worksheet.

### 3.9. Per_Dep

The [Per_Dep] worksheet calculates depletion of a mantle peridotite by extraction of partial melts at a given degree of melting $F = \%MORB_{ext}$. The mantle composition is determined from the [CONTROL_PANEL] for “W” (Workman and Hart, 2005), “S” (Salters et al., 2011), “P” (Sun and McDonough, 1989), and “U”-ser. The melting calculations use equilibrium batch melting (Shaw, 2000) with melting mode calculated from pMELTS (Ghiorso et al., 2002). Calculations use parameterized values at each 0.1% melting step given in the [Per_Dep] worksheet (Fig. 26).

**Caveat:** Do not alter any cells. Only data copy is allowed in this worksheet.
Fig. 26 The [Per_Dep] worksheet in ABS5 (Kimura, 2017).

Fig. 27 The [Kaz+] worksheet in ABS5 (Kimura, 2017).
3.10. Kaz+

The [Kaz+] worksheet calculates the degree of partial melting of a mantle peridotite with various degrees of depletion (c.f., various modal cpx compositions) at given $P_{\text{perid}}$, $T_{\text{perid}}$, and $X_{H_2O,\text{perid}}$. $P_{\text{perid}}$ and $T_{\text{perid}}$ are obtained from the [CONTROL_PANEL], whereas $X_{H_2O,\text{perid}}$ is from [SDMS4.0]. The index of source mantle depletion given by the cpx mode is derived from the [Peri_Dep] worksheet and is input to the calculations in this worksheet via cell $C8$. The effect of an increase in $F_{\text{perid}}$ by addition of slab melt is considered (columns U–AF) and the difference in $F_{\text{perid}}$ is added to the results from Katz et al. (2003) (columns A–N). The dark gray field in columns H–N (Fig. 27) is the solver (minimum finder) matrix for solution of an equation in the calculations of Katz et al. (2003). Since the $P$–$T$ relations with $F$ in pMELTS calculations do not always follow those of the experimental results (Lambart et al., 2012), ABS5 uses the $P$–$T$–$F$ relation from the parameterization of Kats et al. (2013). Once $F_{\text{perid}}$ is determined for a given $P_{\text{perid}}$–$T_{\text{perid}}$–$X_{H_2O,\text{perid}}$ plus Cs (effect of slab melt addition), $F_{\text{perid}}$ is used for calculations of the trace element mass balance using an open system melting equation in the [OSM] and [IOSM] worksheets.

Caveat: Do not alter any cells. Only data copy is allowed in this worksheet.

3.11. Per_Mode_Melt

The [Per_Mode_Melt] worksheet is a new feature in ABS5. This worksheet calculates the modal composition of the residual mantle and melt compositions during flux melting. Calculations are made using pMELTS with DMM and PM mantle compositions with addition of 0–25% slab melts to the sources at each 5% step (Kimura, 2017). The calculated modal and melt compositions are then stored in lookup tables with given $P_{\text{perid}}$, $F_{\text{perid}}$, and $X_{\text{slab liq}}$ (Figs. 10 and 11). Tables are shown in the [Per_Mode_Melt] worksheet separately for DMM and PM with each dataset at different slab melt addition (0–25%, at each 5% step in columns B–EH), in the areas in lines 23–848 for modal compositions and lines 851–1698 for melt compositions (Fig. 28 lower panel). Integration of the lookup tables is made in cell fields $BS1$–$SW21$. The final calculation results at the given $P_{\text{perid}}$, $F_{\text{perid}}$, and $X_{\text{slab liq}}$ are shown in the [Peri Mode Melt] worksheet (Fig. 28).
F_{\text{perid}}$ and $X_{\text{slab liqu}}$ in cells $B$4, $D$4, and $G$4 are given in cell fields $YS2$–$ABS15$ (green box) of the [Per_Mode_Melt] worksheet (Fig. 28).

**Caveat:** Do not alter any cells. Only data copy is allowed in this worksheet.

![Fig. 29 The [OSM] (upper panel) and [IOSM] (lower panel) worksheets in ABS5 (Kimura, 2017).](image)

### 3.12. OSM

The [OSM] worksheet (Fig. 29) calculates the final step of the trace element calculations for Rb, Ba, Th, U, Nb, Ta, K, La, Ce, Pb, Pr, Sr, Nd, Sm, Zr, Hf, Eu, Gd, Tb, Dy, Y, Ho, Er, Tm, Yb, and Lu in the melt and residual mantle formed by flux melting of the mantle. $P_{\text{perid}}$, $T_{\text{perid}}$, and $X_{\text{slab liqu}}$ are from [CONTROL_PANEL] inputs, $F_{\text{perid}}$ is from the [Katz+] worksheet, and the mineralogic modes $X_a$ are from the [Per_Mode_Melt] worksheet. Mantle peridotite composition $C_s$ is from the [Peri_Dep] worksheet, and slab liquid compositions are from the [SDMS4.0] worksheets. The partition coefficients of the mantle minerals are from Table 2 (Kimura, 2017; Kimura et al., 2009). Calculations are made for each element in lines 69–48 using an open system melting equation (Zou, 1998, 1999). Porosity is assumed to be constant at $\varphi = 0.01$. The results are summarized in [RESULT_COMP] and graphically shown in [CONTROL_PANEL].

**Caveat:** Do not alter any cells. Only data copy is allowed in this worksheet.
3.13. IOSM

The [IOSM] worksheet (Fig. 29) does the same for the melt and residual mantle compositions of the $^{87}\text{Sr}/^{86}\text{Sr}$, $^{143}\text{Nd}/^{144}\text{Nd}$, $^{176}\text{Hf}/^{177}\text{Hf}$, $^{206}\text{Pb}/^{204}\text{Pb}$, $^{207}\text{Pb}/^{204}\text{Pb}$ isotope ratios.

Caveat: Do not alter any cells. Only data copy is allowed in this worksheet.

3.14. SUMMARY

Derivations of the calculated results in the [SUMMARY] worksheet (Fig. 30) are:
- Major element: [Per_Mode_Melt]
- Trace element: [OSM]
- Isotopes: [IOSM]

Those for residual mantle composition are:
- Trace element: [OSM]
- Isotopes: [IOSM]
- Mode: [Per_Mode_Melt]

Residual slab and slab liquid compositions are:
- Trace element: [SDMS4.0]
- Isotopes: [SDMS4.0]
- Mode: [Slb_Mode]

The [SUMMARY] worksheet consists of a large data table showing 1. Melting conditions, 2. Melt composition, 3. Fitting statistics (given by %RD), 4. Mantle mode, 5. Slab liquid composition, and 6. Residual mantle composition. These are as follows:

1. Melting conditions:
- $P_{\text{slab}}$ (GPa), $T_{\text{slab}}$ ($^\circ$C), $\%R_{\text{slab}}$, $F_{\text{liq}}$(AOC), $F_{\text{liq}}$(SED), $F_{\text{liq}}$(DMM), $n$(PERID), $P_{\text{perid}}$ (GPa), $T_{\text{perid}}$ ($^\circ$C), $\%\text{MORB}_{\text{ext}}$, $F_{\text{slbl liq}}$, $\%\text{H}_2\text{O}$ in slab liquid, $\%\text{H}_2\text{O}$ in PERID, $F_{\text{perid}}$(%), and $\beta$(%).

2. Melt compositions:
SiO₂, TiO₂, Al₂O₃, FeO, MgO, CaO, K₂O, H₂O, Rb, Ba, Th, U, Nb, Ta, K, La, Ce, Pb, Pr,
Sr, Nd, Sm, Zr, Hf, Eu, Gd, Tb, Dy, Y, Ho, Er, Tm, Yb, Lu, and ⁸⁷Sr/⁸⁶Sr, ¹⁴³Nd/¹⁴⁴Nd,
¹⁷⁶Hf/¹⁷⁷Hf, ²⁰⁶Pb/²⁰⁴Pb, ²⁰⁷Pb/²⁰⁴Pb, ²⁰⁸Pb/²⁰⁴Pb.

3. Fitting statistics %RD are given for:
Rb, Ba, Th, U, Nb, Ta, K, La, Ce, Pb, Pr, Sr, Nd, Sm, Zr, Hf, Eu, Gd, Tb, Dy, Y, Ho, Er,
Tm, Yb, and Lu.

4. Mantle modes:
Ol, Opx, Cpx, Gar, and Sp.

5. Slab liquid compositions:
SiO₂, TiO₂, Al₂O₃, FeO, MgO, CaO, K₂O, H₂O, Rb, Ba, Th, U, Nb, Ta, K, La, Ce, Pb, Pr,
Sr, Nd, Sm, Zr, Hf, Eu, Gd, Tb, Dy, Y, Ho, Er, Tm, Yb, Lu, and ⁸⁷Sr/⁸⁶Sr, ¹⁴³Nd/¹⁴⁴Nd,
¹⁷⁶Hf/¹⁷⁷Hf, ²⁰⁶Pb/²⁰⁴Pb, ²⁰⁷Pb/²⁰⁴Pb, ²⁰⁸Pb/²⁰⁴Pb.

6. Residual mantle compositions:
Rb, Ba, Th, U, Nb, Ta, K, La, Ce, Pb, Pr, Sr, Nd, Sm, Zr, Hf, Eu, Gd, Tb, Dy, Y, Ho, Er,
Tm, Yb, Lu, and ⁸⁷Sr/⁸⁶Sr, ¹⁴³Nd/¹⁴⁴Nd, ¹⁷⁶Hf/¹⁷⁷Hf, ²⁰⁶Pb/²⁰⁴Pb, ²⁰⁷Pb/²⁰⁴Pb, ²⁰⁸Pb/²⁰⁴Pb.

The “ease of use” provided by the Excel spreadsheet is an advantage for
improving access to the software for education purposes. Nevertheless, student users are
strongly recommended to read through the relevant papers and petrological/geochemical
textbooks for a critical understanding of the background to the calculations.

Caveat: Do not alter indications in lines 1–3. No data links in this worksheet.
REFERENCES

Adachi, Y., and Miyashita, S., 2003, Geology and petrology of the plutonic complexes in the Wadi Fizh area: Multiple magmatic events and segment structure in the northern Oman ophiolite: Geochemistry, Geophysics, Geosystems, v. 4, no. 9.


Green, T. H., 1995, Significance of Nb/Ta as an indicator of geochemical processes in the crust-mantle system: Chemical Geology, v. 120, p. 347-359.


pressure and ultra-high pressure rocks: Implications for element transfer in subduction zones:
Lithos, v. 92, no. 3–4, p. 399-417.


Herzberg, C., and Asimow, P. D., 2015, PRIMELT3 MEGA.XLSM software for primary magma calculation: Peridotite primary magma MgO contents from the liquidus to the solidus:
Geochimica, Geophysics, Geosystems, v. 16, no. 2, p. 563-578.


