

1 **Phase equilibria modeling of anatexis during ultra-high temperature**  
2 **metamorphism of the crust**

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11 Running title: Forward modeling of UHT metamorphism

12 **ABSTRACT**

13 Ultra-high temperature (UHT) granulite-facies metamorphism is commonly identified in Mg–  
14 Al-rich rocks. Many such lithologies are thought to be metasedimentary rocks based on the  
15 presence of detrital zircon. However, whether a metasedimentary protolith is required to form  
16 diagnostic mineral assemblages and how much melt is lost during burial and heating to reach  
17 UHT conditions varies significantly according to the prograde pressure–temperature path. In this  
18 study, integrated thermodynamic modeling, accessory mineral modeling, and trace element  
19 modeling has been conducted on an average metapelite composition and average mid-ocean  
20 ridge basalt (MORB) composition under open-system conditions. The results show at least three  
21 and two melt loss events occur before reaching UHT conditions in initially water-saturated  
22 pelitic and basaltic rocks, respectively. Around 22–27 vol. % S-type granite and 12–17 vol. %  
23 I-type granite would be produced during these evolutions, respectively. For pre-conditioned (dry)  
24 protoliths, however, melt loss is not required to reach UHT conditions. Melt extraction leads to  
25 an increase of Al and Mg in metapelite residua. Given a relatively Mg-rich protolith, mineral  
26 assemblage sapphirine + quartz is then allowed to form at higher grades; however, metabasalt  
27 does not form these UHT diagnostic assemblages, regardless of the amount of melt lost. During  
28 equilibrium melting, crustal differentiation induced by UHT metamorphism would significantly  
29 reduce the amount of heat-producing elements (HPEs) in the melt-depleted residuum, which  
30 progressively decreases a rock’s heat production capacity. In reality, however, new monazite  
31 grains likely form during peak metamorphism and some monazite grains would be shielded by  
32 porphyroblasts, resulting in an increase of Th in the residua during heating. Even so, we suggest  
33 the efficiency of heat production would still decrease, given the heat production rate of Th is  
34 much lower than U. Considering some granitic rocks with relatively high heat production are

35 emplaced into the granulite terrane, we suggest that radioactive heat production may be a  
36 contributing driving force for UHT metamorphism; however, it is not sufficient. Most heat  
37 required to generate UHT granulites must come from hybrid sources, such as advected heat from  
38 the mantle, conducted heat from nearby magmatic intrusions, radioactive heat production, and  
39 exothermic mineral reactions.

40 **Key words:** anatexis; crustal differentiation; forward modeling; open system; ultra-high  
41 temperature

## 42 **1 INTRODUCTION**

43 Ultra-high temperature (UHT) metamorphism ( $>900$  °C at 0.7–1.3 GPa) is the most  
44 thermally extreme condition that the continental crust may achieve (Harley, 1998, 2008), and  
45 several UHT localities have been identified throughout the geological record in rocks of Archean  
46 to Miocene age (Kelsey, 2008; Kelsey & Hand, 2015). Most UHT granulites have been  
47 recognized based on the diagnostic parageneses sapphirine + quartz, high-Al orthopyroxene +  
48 sillimanite, and osumilite-bearing mineral assemblages, which only stabilize in Mg–Al-rich bulk  
49 compositions; however, Mg–Al-rich granulites are volumetrically scarce in nature and have no  
50 geochemically equivalent sedimentary or igneous protolith (Chinner & Sweatman, 1968),  
51 making their origin controversial. Based on detrital zircon evidence and field relationships,  
52 Kelsey & Hand (2015) concluded that the most likely candidates were sedimentary rocks that  
53 had experienced significant partial melting (e.g. Drüppel, Elsäßer, Brandt, & Gerdes, 2013; Ellis,  
54 1980; Reinhardt, 1987; Sheraton, 1980; Sheraton, Tingey, Black, Offe, & Ellis, 1987), although  
55 this hypothesis has yet to be rigorously tested.

56 Crustal melting (anatexis) is ubiquitous in the middle and lower crust and plays an  
57 important role in crustal reworking and intracrustal differentiation (Sawyer, Cesare, & Brown,  
58 2011). Anatexis is a key process that generates voluminous granitic melt that forms a major  
59 component of Earth's upper continental crust, and melting may be induced by magmatic  
60 underplating, lithospheric extension, upwelling of asthenosphere, or an elevated concentration of  
61 heat-producing elements (Andreoli, Hart, Ashwal, & Coetzee, 2006; Clark, Fitzsimons, Healy, &  
62 Harley, 2011; Dewey, Robb, & Van Schalkwyk, 2006; McLaren, Sandiford, Powell, Neumann,  
63 & Woodhead, 2006; Yakymchuk, 2019).

64           If crustal anatexis and/or intracrustal differentiation is required to form Mg–Al-rich rocks  
65 that may then be metamorphosed and form UHT mineral assemblages (Baba, 2003; Brandt, Will,  
66 & Klemd, 2007; Clifford, Stumpfl, Burger, McCarthy, & Rex, 1981; Droop &  
67 Bucher-Nurminen, 1984; Lal, Ackermann, Seifert, & Haldar, 1978; Raith, Karmakar, & Brown,  
68 1997), systematic analysis of the fertility of likely precursor rocks should be able to identify the  
69 formation of these rare, but important, granulites, and also to provide key information about  
70 granite generation and the heat budget of the middle to lower crust. In this study, we briefly  
71 introduce the tectonic scenarios that can generate UHT metamorphism and their associated  
72 pressure–temperature ( $P$ – $T$ ) paths. Second, we use petrological forward modeling to quantify the  
73 amount of melt extraction required to generate UHT granulites along with the changing chemical  
74 composition of the melt and residua in each tectonic setting. These results are then coupled with  
75 geochemical trace element analysis and estimation of the heat budget of each lithology. These  
76 modeling results thus provide new understandings of the relationship between UHT  
77 metamorphism and crustal anatexis.

## 78 **2 TECTONIC ENVIRONMENTS CONDUCTIVE FOR UHT METAMORPHISM**

79           From an energetic point of view, heat produced in the lithosphere is redistributed by  
80 conduction and advection (Stüwe, 2007). Given the slow rates of thermal diffusion in silicate  
81 rocks, UHT metamorphism is difficult to induce purely via conductive heat transfer (Brown,  
82 2008; Jaeger, 1964; Sandiford & Hand, 1998; Stüwe, 2007; Whittington, Hofmeister, & Nabelek,  
83 2009). As such, several possible alternative heat sources have been proposed for raising the  
84 temperature of the crust at a regional scale, including advected heat from mafic magmatic  
85 intrusion, elevated concentrations of heat-producing elements coupled with slow erosion, and

86 ductile shearing (e.g. Clark *et al.*, 2011; Huang, Guo, Jiao, & Palin, 2019; Nabelek, Whittington,  
87 & Hofmeister, 2010; Vielzeuf, Clemens, Pin, & Minet, 1990).

88         Since melting is an endothermic process that buffers temperature increase (Stüwe, 1995),  
89 anatectic reactions will proceed until a reactant mineral is totally consumed, after which a rock  
90 may continue to heat up (Clemens, 2012; Schorn, Diener, Powell & Stüwe, 2018; Schorn &  
91 Diener, 2019). In such case, a previous episode of metamorphism may precondition the crust to  
92 allow it to reach the UHT condition. Beyond that, only a strong thermal anomaly combined with  
93 efficient melt extraction can drive rocks toward UHT conditions at a regional scale (Clark *et al.*,  
94 2011; Clemens, 2012). Several possible tectonic scenarios for generating UHT metamorphism  
95 can then be defined, including:

96 *Melt-bearing mantle upwellings or underplating of mafic magma beneath a continental arc.* This  
97 model has been proposed to explain extensive exposures of UHT granulites in Precambrian  
98 terranes. Owing to higher mantle potential temperatures during the Archean compared to today  
99 (Herzberg, Condie, & Korenaga, 2010), a weaker crust-mantle coupling on the early Earth would  
100 induce slab breakoff of subducted oceanic lithosphere at relatively shallow depths, followed by  
101 melt-bearing mantle upwelling and syn-rifting magmatic underplating. Rocks at the base of the  
102 overriding plate would then experience isobaric heating to UHT conditions (Sizova, Gerya, &  
103 Brown, 2014), as is noted from many Archean terranes worldwide. This model is broadly similar  
104 with ridge subduction and the back-arc model suggested by several researchers to explain some  
105 Phanerozoic UHT terranes (Kemp, Shimura, Hawkesworth, & EIMF, 2007; Pownall, Hall,  
106 Armstrong, & Forster, 2014).

107 *Orogen self-heating.* Owing to the paucity of basic intrusions in many UHT terranes, Clark *et al.*  
108 (2011) proposed an orogenic self-heating model to explain long-duration and extensive UHT

109 metamorphism. In this model, a long-lived overthickened hinterland with abundant  
110 heat-producing elements and low erosion rate would generate UHT granulites without any  
111 advective heat from magmatism. Rocks in this model would most likely experience heating  
112 during burial to peak pressure conditions, followed by decompression and heating to reach UHT  
113 conditions.

114 *Multi-period thermal anomaly.* Most granulites have experienced more than one period of  
115 heating (e.g. Kelsey & Hand, 2015). In some cases, they would experience a prolonged  
116 metamorphism, during which discrete episodes would sequentially heat up the granulite during  
117 residence in the lower crust. For example, metamorphic zircon in UHT granulites from the  
118 Khondalite Belt, North China Craton, record a continuous age range of formation from *c.* 1.96 to  
119 *c.* 1.88 Ga, with peaks at 1.95 Ga and 1.92 Ga (Huang *et al.*, 2019). Here, the older peak age of  
120 *c.* 1.95 Ga is interpreted as a precursor granulite-facies metamorphism event driven by the  
121 collision between two Archean blocks, leaving a pre-conditioned (dry) residual source rock that  
122 was then exhumed to the middle crust. Later mantle-derived mafic magmatism then heated the  
123 residual granulites to UHT conditions at *c.* 1.92 Ga. These rocks thus experienced a continuous  
124 *P–T* path showing compression and heating processes during prograde metamorphism,  
125 pseudo-isothermal decompression to shallower depths, and then isobaric second-stage heating to  
126 UHT conditions. In other cases, UHT granulites might experience polymetamorphism, which  
127 would not have a characteristic and continuous *P–T* path. We would not propose a possible *P–T*  
128 path in such case, but acknowledge the existence of this tectonic scenario. Nonetheless, it is  
129 important that all three of these tectonic scenarios are characterized by different *P–T* paths,  
130 which allow examination of the petrological evolution of different protoliths to be examined  
131 independently.

## 132 3 METHODS

### 133 3.1 Determination of initial bulk rock composition for modeling

134           When considering potential bulk-rock compositions for petrological modeling, it is key to  
135 consider the volume of melt that may be generated and lost from each lithology. Most crustal  
136 rocks may melt at temperatures as low as 650 °C in the presence of free H<sub>2</sub>O-rich fluid (Brown,  
137 2007; Palin and Dyck, 2020); however, fluid-present melting reactions have negative  $dP/dT$   
138 slopes and are accompanied by a bulk volume reduction, limiting the amount of melt that can  
139 form and escape from the local environment (Clemens & Droop, 1998). Upon consumption of all  
140 free fluid, hydrous minerals, such as muscovite and biotite in meta-sedimentary rocks, and  
141 hornblende in meta-basic rocks, may progressively break down to generate melt and peritectic  
142 anhydrous minerals (Palin *et al.*, 2016, White & Powell, 2002). Owing to positive  $dP/dT$  slopes  
143 and a net increase in volume over the course of each reaction, large amounts of melt can be  
144 generated by fluid-absent anatexis, and so escape once a critical threshold is breached (Clemens  
145 & Droop, 1998). Such processes are thought to be the primary mechanism for crustal  
146 differentiation (Brown, 2013; Clemens, 2012; Sawyer *et al.*, 2011; Yakymchuk, 2019). All micas  
147 are typically consumed upon reaching UHT conditions, and if most of the melt has already  
148 drained away, the fertility of the residuum is significantly reduced and the composition of any  
149 new melt produced via anhydrous mineral breakdown is no longer granitic (Sawyer *et al.*, 2011).

150           Based on this model, two bulk rock compositions were selected for phase equilibria  
151 modeling: an average amphibolite-facies pelite (Ague, 1991) and an average mid-ocean ridge  
152 basalt (MORB) glass (Albarède, 2005). The initial H<sub>2</sub>O contents in each were adjusted so that  
153 minimal (<0.1 mol. %) free H<sub>2</sub>O occurred at the intersect of solidus and each  $P$ - $T$  path, which  
154 applies a fluid-absent condition above the solidus (White, 2003; White, Pomroy, & Powell,

155 2005; White & Powell, 2002; Yakymchuk & Brown, 2014a, 2019; Yachymchuk, Kirkland, &  
156 Clark, 2018). This ensures that melt formation is not overestimated during early anatexis. The  
157 maximum melt proportion generated before drainage occurs – the melt connectivity transition  
158 (MCT) – was taken to be 7 vol. % for both lithologies (Rosenberg & Handy, 2005). Here, 6 vol.  
159 % was removed in each melt loss event (MLE) to simulate the common observation of small  
160 proportions (~1 vol. %) remaining on grain boundaries in rapidly chilled and drained migmatites  
161 (Yakymchuk & Brown, 2014a).

### 162 **3.2 $P$ – $T$ paths selection**

163 Three  $P$ – $T$  paths were used for phase equilibria modeling based on the possible tectonic  
164 scenarios for UHT metamorphism described above.  $P$ – $T$  path 1 involves isobaric heating at 0.8  
165 GPa, corresponding to a melt-bearing mantle upwelling or basic magma underplating at a  
166 convergent continental margin (Sizova *et al.*, 2014). The pressure of 0.8 GPa was chosen to  
167 represent rocks in the lower crust of extensional tectonic settings, and so are located close to the  
168 onset of UHT metamorphism as defined in  $P$ – $T$  space.  $P$ – $T$  path 2 represents the orogen  
169 self-heating model (Clark *et al.*, 2011), comprising compression-heating from 0.75 GPa at the  
170 solidus to 1.5 GPa at 850 °C followed by decompression-heating to 0.75 GPa at 1000 °C. The  
171 geothermal gradient of the peak condition (567 °C/GPa) represents typical intermediate  $dT/dP$   
172 type metamorphism, representing high-pressure granulite (Brown & Johnson, 2018).  $P$ – $T$  path 3  
173 represents a multi-period thermal anomaly model (Huang *et al.*, 2019). This  $P$ – $T$  path follows the  
174 same prograde evolution as  $P$ – $T$  path 2 up to peak pressure of 1.5 GPa at 850 °C, followed by  
175 isothermal decompression to 0.75 GPa at 850 °C, and a final period of heating to 1000 °C at 0.75  
176 GPa.

### 177 3.3 Phase equilibria modeling

178 Phase diagrams were calculated using THERMOCALC v. 3.40 (Powell & Holland, 1988)  
179 and the internally consistent data set (ds62) of Holland & Powell (2011). Both pelitic and  
180 basaltic bulk rock compositions were modeled in the Na<sub>2</sub>O–CaO–K<sub>2</sub>O–FeO–MgO–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub>–  
181 H<sub>2</sub>O–TiO<sub>2</sub>–O<sub>2</sub> (NCKFMASHTO) chemical system. Activity–composition (*a–x*) relations used  
182 for pelitic compositions were taken from White, Powell, Holland, Johnson, & Green (2014), and  
183 those for basaltic compositions comprised clinoamphibole, augite, and metabasite melt (Green *et*  
184 *al.*, 2016), orthopyroxene, garnet and biotite (White *et al.*, 2014), plagioclase and K-feldspar  
185 (Holland & Powell, 2003), ilmenite (White, Powell, Holland, & Worley, 2000) and magnetite  
186 (White, Powell, & Clarke, 2002). Quartz and rutile were considered as pure phases. Removal of  
187 six-sevenths of the melt present where each *P–T* path intersects the 7 mol. % melt isopleth was  
188 conducted by manipulating ‘rbi’ script in THERMOCALC, as described in Yakymchuk & Brown  
189 (2014a). The bulk compositions used for phase equilibria modeling and the compositions of  
190 extracted melt are listed in Table S1–2. The densities of the residua were calculated by using the  
191 ‘calc sv’ script in THERMOCALC.

### 192 3.4 Trace element modeling

193 Trace element modeling was carried out using the batch melting equation  $C_{\text{melt}}/C_{\text{source}} =$   
194  $1/[D + F \times (1 - D)]$  (Shaw, 1970), where  $C_{\text{source}}$  and  $C_{\text{melt}}$  represent concentrations of a trace  
195 element in the source rock and the resultant melt, respectively;  $D (= \sum Kd \times X)$  is the bulk  
196 partition coefficient, where  $Kd$  is mineral/melt partition coefficient and  $X$  is mol. % of the  
197 mineral; and  $F$  is the degree of melting. Initial bulk concentrations of 0.19 wt. % P<sub>2</sub>O<sub>5</sub>, 3.5 ppm  
198 U, 14 ppm Th, 150 ppm Zr, and 150 ppm LREE were used for the metapelite (Ague, 1991;  
199 Yakymchuk *et al.*, 2018), and 0.18 wt. % P<sub>2</sub>O<sub>5</sub>, 0.138 ppm U, 2.83 ppm Th, and 118 ppm Zr

200 were used for MORB (Albarède, 2005). The proportions of accessory minerals were calculated  
201 using the refined zircon solubility model from Boehnke, Watson, Trail, Harrison, & Schmitt  
202 (2013), the monazite solubility model from Stepanov, Hermann, Rubatto, & Rapp (2012), and  
203 the apatite solubility model from Harrison & Watson (1984). Values for Kd were taken from  
204 Bédard (2006) and Yakymchuk *et al.* (2018). The amounts of accessory minerals retained in the  
205 residuals are listed in Table S3, and the calculated U and Th concentrations in residua are listed  
206 in Table S4.

## 207 **4 PATH 1 – ISOBARIC HEATING AT 0.8 GPA**

### 208 **4.1 Closed system**

209 Closed-system pseudosections for pelite and MORB bulk compositions are shown in  
210 Figure 1 and Figure 2, respectively, and molar proportion of solid and melt phases along this  
211 isobaric heating segment are shown on temperature-phase proportion diagrams (“modeboxes”)  
212 below the  $P$ - $T$  diagrams.

213 For the metapelite, the closed-system phase diagram resembles that presented by  
214 Yakymchuk *et al.* (2018) and predicts that the rock experiences muscovite dehydration melting  
215 from the solidus up to 739 °C, producing 8 mol. % melt alongside peritectic K-feldspar via the  
216 reaction of  $Ms + Qz \rightarrow Kfs + Al_2SiO_5 + \text{melt}$ . Biotite content remains fixed at 27–28 mol. % at  
217 this stage. After muscovite is totally consumed, biotite starts to break down at 738–860 °C and  
218 generates up to 35 mol. % melt. The rate of melt production is low at the beginning of biotite  
219 consumption, but increases significantly after peritectic garnet stabilizes at 785 °C, marking the  
220 onset of the reaction of  $Bt + Sill + Qz \rightarrow Grt + Kfs + \text{melt}$ . After all hydrous minerals are  
221 consumed, anhydrous felsic minerals break down to generate melt. In this closed-system

222 environment, up to 70 mol. % of cumulative melt would be produced at 1000 °C. Notably, the  
223 diagnostic UHT mineral assemblage of Spr + Qz is not predicted, whereas Opx + Sil is predicted  
224 to occur at 1000–1020 °C. The calculated system density decreases continuously from 2.87  
225 g/cm<sup>3</sup> at subsolidus conditions to 2.68 g/cm<sup>3</sup> at UHT conditions, corresponding to an volume  
226 increase during fluid absent melting (Clemens & Droop, 1998).

227 For metabasalt, the modeled *P–T* path does not allow garnet to stabilize in this  
228 MnO-absent compositional system, although natural metabasites contain small amounts of MnO  
229 that should expand garnet’s calculated stability slightly on the phase diagrams shown here.  
230 Nonetheless, the mineralogy and topology of the phase diagram is relatively simpler than those  
231 for the metapelite, owing to MORB’s lower SiO<sub>2</sub> and K<sub>2</sub>O, leading to higher variance equilibria  
232 forming (Miyashiro, 1994; Huang, Brown, Guo, Piccoli, & Zhang, 2018). Anatexis begins at 660  
233 °C upon consumption of hornblende and quartz, corresponding to the reaction  $\text{Hbl} \pm \text{Qz} \rightarrow \text{Aug}$   
234  $+ \text{Pl} + \text{melt}$ . Orthopyroxene becomes stable at 855 °C, defining the beginning of granulite-facies  
235 metamorphism. At this point, 10 mol. % of cumulative melt would be generated. After that,  
236 hornblende breakdown would generate up to 35 mol. % of cumulative melt at 1000 °C. In this  
237 model, hornblende would remain stable up to at least 1000 °C, although in nature this is unlikely  
238 and may be a consequence of uncertainty in Al–Si partitioning between clinopyroxene and  
239 hornblende in the Green *et al.* (2016) *a–x* relation (cf. Forshaw, Waters, Pattison, Palin, &  
240 Gopon, 2019). Akin to the metapelite, the density of this closed system decreases continuously  
241 from subsolidus to UHT conditions, ranging between 3.04 and 2.89 g/cm<sup>3</sup>.

## 242 **4.2 Open system**

### 243 **4.2.1 Phase diagrams**

244 If melt can leave the local system when it reaches the MCT, bulk compositions must be  
245 continuously altered during metamorphism and melt loss. Here, pseudosection panels  
246 representing initial protolith composition and a sequence of progressively more residual bulk  
247 chemical compositions following MLEs are shown, and modebox diagrams are shown below  
248 each  $P$ - $T$  diagram.

249 For the metapelite, five MLEs produce six pseudosection panels along the isobaric  
250 heating path at 0.8 GPa, as shown in Figure 3. The lowest-temperature panel matches the  
251 low-temperature portion of the pseudosection in Figure 1 and the temperature of the ‘seam’  
252 between panels represents the condition of the first MLE. In this open-system environment, MLE  
253 1 occurs during muscovite dehydration melting at 738 °C, and MLEs 2–5 occur due to biotite  
254 dehydration melting at 800 °C, 823 °C, 843 °C and 863 °C. At 1000 °C, the rock has lost ~27  
255 mol. % of cumulative melt, which is clearly much less than the 70 mol. % cumulative melt  
256 predicted for a closed-system environment. Interestingly, Spr + Qz would form at 1038 °C at 0.8  
257 GPa in this open system, whereas Opx + Sil is not predicted. The density of the system shows a  
258 smooth decrease in each pseudosection panel, but an overall step-increase from 2.87 to 3.00  
259 g/cm<sup>3</sup> over the course of the metamorphic event.

260 For open system melting of metabasalt (Figure 4), four MLEs are predicted at 829 °C,  
261 864 °C, 924 °C, and 977 °C. When compared with a closed system scenario, the modeled  
262 isobaric heating to 1000 °C at 0.8 GPa would produce 22 mol. % of extracted melt, which is less  
263 than the closed system simulation (35 mol. %). In this open-system environment, orthopyroxene  
264 first stabilizes at 853 °C, which is almost identical to the closed system. This is likely a result of  
265 only one set of melt having been lost at that point, and so the bulk-rock compositions in both

266 cases remained fairly similar. Again, as seen in the metapelite, the density of the system shows a  
267 smooth decrease between MLEs, but an overall step-increase from 3.04 to 3.08 g/cm<sup>3</sup>.

#### 268 **4.2.2 Melt and residuum compositions**

269 Changes in the major oxide compositions of both protoliths along the modeled isobaric  
270 heating *P–T* paths at 0.8 GPa calculated by THERMOCALC are shown in Figs. 5–8. Equivalent  
271 compositions along other proposed *P–T* paths described below are also compiled in these  
272 diagrams and Table S1–2 for ease of comparison. Figures 5 and 6 show the bulk compositions of  
273 the metapelite used in *P–T* diagrams modeling and extracted melts, respectively. Figures 7 and 8  
274 present the bulk composition of the metabasalt and extracted melts, respectively. As a result of  
275 mass balance, extraction of melt that is depleted in any given component compared to the source  
276 will lead to an enrichment of the source, and vice versa (Rapp, Ryerson, & Miller, 1987). For the  
277 residua produced during metapelite anatexis, H<sub>2</sub>O, SiO<sub>2</sub>, K<sub>2</sub>O, and Na<sub>2</sub>O show step-like  
278 decreases, whereas Al<sub>2</sub>O<sub>3</sub>, CaO, MgO, FeO<sub>t</sub> and TiO<sub>2</sub> show increases. Associated melt extracted  
279 from the system becomes progressively depleted in H<sub>2</sub>O and Na<sub>2</sub>O, but increases in SiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>,  
280 CaO, MgO, and K<sub>2</sub>O. FeO<sub>t</sub> show an overall increase during metamorphism, but a slight decrease  
281 in the final extracted melt. For the metabasalt residuum, H<sub>2</sub>O, SiO<sub>2</sub>, K<sub>2</sub>O, and Na<sub>2</sub>O show  
282 step-like decreases up-grade, whereas CaO, MgO, and TiO<sub>2</sub> increase. Al<sub>2</sub>O<sub>3</sub> and FeO<sub>t</sub> are more  
283 complicated in their fine detail, but show an overall increase within the temperature interval of  
284 interest. Melt progressively lost from the system shows a progressive decrease in H<sub>2</sub>O, SiO<sub>2</sub> and  
285 K<sub>2</sub>O, but increase in CaO, MgO and FeO<sub>t</sub>. Al<sub>2</sub>O<sub>3</sub> and Na<sub>2</sub>O contents remain more or less  
286 constant. Calculated changes in trace element (U and Th) concentrations in the metapelite and  
287 metabasalt residua through five and four melt loss events are shown in Figure 9 and Figure 10,  
288 respectively. For the metapelite, U shows a step-like decrease, whereas Th shows a slight

289 increase after the first two MLEs, and then drops off to very low concentrations. For the  
290 metabasalt, U and Th contents both decrease during heating to 1000 °C.

### 291 **4.2.3 Heat production values**

292 The capacity for heat production within the residuum for each protolith was determined  
293 using its calculated concentrations of U, K, and Th, and density, using the equation originally  
294 proposed by Birch (1954) and modified after (Rybach, 1988):

$$295 \quad A = \rho \times (0.0952 \times C_U + 0.0348 \times C_K + 0.0256 \times C_{Th})$$

296 Where A is heat production in  $\mu\text{W}/\text{m}^3$ ,  $\rho$  is density in  $\text{g}/\text{cm}^3$ , and  $C_U$ ,  $C_K$ , and  $C_{Th}$  are  
297 concentrations of radioactive isotopes of U, K, and Th in ppm, wt. % and ppm, respectively. The  
298 calculated results are shown in Figs. 9–10 and Table S4. For a closed-system metapelite, the heat  
299 production would depend entirely on the change in density, given the inability for heat-producing  
300 radionuclides to leave when dissolved in a melt fraction. As such, this calculated value for A  
301 shows a continuous and smooth decrease from 2.32 to 2.17  $\mu\text{W}/\text{m}^3$ , although this is unrealistic  
302 based on the unrealistic assumption of wholesale melt retention just noted. In contrast, the heat  
303 production of a pelite residuum in a conditionally open system shows a step-like decrease from  
304 2.32 to 1.24  $\mu\text{W}/\text{m}^3$ . For metabasalt, the heat production shows an almost unchanged value of A  
305 = 0.08  $\mu\text{W}/\text{m}^3$  with temperature increase in a closed system, since the concentrations of  
306 radioactive isotopes are fixed, but shows a step decrease from 0.08 to 0.03  $\mu\text{W}/\text{m}^3$  in an open  
307 system.

## 308 **5 PATH 2 – CRUSTAL THICKENING FOLLOWED BY SLOW EROSION**

### 309 **5.1 Phase diagrams**

310 Figure 11 and Figure 12 shows mosaic pseudosection panels for the metapelite and  
311 metabasalt bulk compositions during crustal thickening followed by slow erosion ( $P$ - $T$  path 2).  
312 Modebox diagrams are shown below the  $P$ - $T$  diagrams.

313 For the metapelite, the pseudosection panel at the lowest temperature is very similar to  
314 that in  $P$ - $T$  path 1, except the bulk composition used for modeling contains a slighter lower  $H_2O$   
315 content to ensure the solidus is just saturated. During prograde metamorphism, the proposed  
316 compression-heating  $P$ - $T$  path closely follows contours for mol. % of melt, leading to little melt  
317 generation until muscovite dehydrates to form peritectic K-feldspar and melt. The first MLE  
318 occurs at 800 °C and 1.27 GPa, and MLE 2 occurs almost immediately afterwards at 802 °C and  
319 1.28 GPa. This supports other studies showing that muscovite dehydration melting can generate  
320 voluminous melt over a small temperature range. After muscovite is totally consumed, MLE 3 at  
321 824 °C and 1.38 GPa occurs due to biotite breakdown, which also produces peritectic garnet. No  
322 other melt event is calculated to happen before reaching peak  $P$ - $T$  conditions. During the  
323 decompression stage, the melt generation rate is extremely low, given the prior consumption of  
324 hydrous minerals in the residuum. The terminal MLE occurs at 938 °C and 1.06 GPa, leading to  
325 22 mol. % of melt extracted while following this  $P$ - $T$  path. Importantly, Spr + Qz would form at  
326 1000 °C at 0.75 GPa in this depleted bulk composition, whereas Opx + Qz is not predicted. The  
327 density of the system increases through each pseudosection panel between MLEs during  
328 prograde burial, with step increase at each melt loss event; however, bulk-rock density decreases  
329 during decompression until it increases sharply at the final MLE. The minimum and maximum  
330 density of the system during this evolution are 2.84 g/cm<sup>3</sup> at the solidus and 3.06 g/cm<sup>3</sup> at peak  
331 conditions.

332 For metabasalt, a total of four pseudosection panels are shown in Figure 12,  
333 corresponding to three MLEs. The pseudosection panel at the lowest temperature is the same as  
334 that for  $P$ - $T$  path 1, except it covers a larger  $P$ - $T$  range. MLE 1 occurs at 806 °C and 1.32 GPa,  
335 whereas MLE 2 occurs close to peak metamorphism at 847 °C at 1.48 GPa, with the mineralogy  
336 of the residuum representing high-pressure granulite. During decompression, the final MLE  
337 occurs at 906 °C at 1.22 GPa. Orthopyroxene stabilizes at 930 °C at 1.10 GPa, indicating a  
338 transition from high-pressure granulite to intermediate-pressure granulite facies, *sensu stricto*.  
339 The  $P$ - $T$  path crosses the elevated residuum solidus at 942 °C at 1.04 GPa, which would cause  
340 the rock to remelt at 989 °C at 0.81 GPa. The change of density of the residua shows a similar  
341 trend to that of the metapelite, with maximum of 3.27 g/cm<sup>3</sup> at peak condition and 3.03 g/cm<sup>3</sup> at  
342 initial solidus conditions.

## 343 **5.2 Melt and residuum compositions**

344 Changes in the major oxide compositions of the pelitic residua determined via phase  
345 diagram modeling show monotonic trends similar to those for  $P$ - $T$  path 1, even though the  
346 degree of melt loss is subdued (Figure 5). The extracted melts show irregular compositional  
347 characteristics as temperature increases: especially the final melt fraction (Figure 6). For  
348 metabasalt, the change in major oxide compositions resemble those documented for  $P$ - $T$  path 1,  
349 except that Al<sub>2</sub>O<sub>3</sub> decreases in a step-like fashion due to melt loss, instead of an overall increase  
350 (Figure 7). Compared with the extracted melts in  $P$ - $T$  path 1, the chemical compositions of  
351 extracted melts in  $P$ - $T$  path 2 also show irregular evolution as temperature increase.(Figure 8).

352 For trace element modeling, the concentration of U in the metapelite residuum shows a  
353 step-like decrease. By contrast, Th shows a slight increase after MLE 1 and a step-like decrease

354 thereafter (Figure 9). U and Th concentration in the metabasaltic residua both show stepping  
355 decreases as metamorphism progresses (Figure 10).

### 356 **5.3 Heat production values**

357 Using the heat production equation given above, the pelitic residuum shows an increase  
358 from  $A = 2.30 \mu\text{W}/\text{m}^3$  to  $A = 2.38 \mu\text{W}/\text{m}^3$  during prograde metamorphism before MLE 1. The  
359 heat production then decreases to  $1.18 \mu\text{W}/\text{m}^3$  during heating up to  $1000^\circ\text{C}$  (Figure 9), as  
360 heat-producing elements preferentially partition into the melt phase and leave the local  
361 environment. For metabasalt, the heat production shows a smooth increase from 0.08 to 0.09  
362  $\mu\text{W}/\text{m}^3$  before the first melt extraction, and decreases to  $0.04 \mu\text{W}/\text{m}^3$  thereafter (Figure 10).

## 363 **6 PATH 3 – MULTI-STAGE METAMORPHISM**

### 364 **6.1 Phase diagrams**

365 Figure 13 and Figure 14 show integrated pseudosections for the metapelite and  
366 metabasalt. Mineral proportion vs. temperature diagrams during prograde compression-heating  
367 and isobaric heating after isothermal decompression are shown below the  $P$ - $T$  diagram, and  
368 pressure vs. mineral proportion diagrams during isothermal decompression after peak conditions  
369 are shown next to the  $P$ - $T$  diagram.

370 Given that the prograde  $P$ - $T$  path considered here is the same as the prograde portion of  
371  $P$ - $T$  path 2, the melt loss events during this stage are identical in both situations. Thus, we  
372 discuss the evolution of both rocks during the latter (decompression) stages of this path. After  
373 reaching peak metamorphism, isothermal decompression would induce minor melt generation  
374 owing to the negative  $dP/dT$  slopes of melt production isopleths associated with phyllosilicate  
375 breakdown in the metapelite. The final MLE occurs during the isobaric heating segment at  $P$ - $T$

376 conditions of 881 °C and 0.75 GPa. The density of the residuum continues to decrease during  
377 isothermal decompression, and shows a smooth decrease during isobaric heating in each  
378 pseudosection panel. A sudden increase is noted at each MLE, and the maximum and minimum  
379 values within this range are the same as those for  $P$ - $T$  path 2.

380 For the metabasalt, the solidus is reached during isothermal decompression at 1.44 GPa  
381 and 850 °C owing to its negative  $dP/dT$  slope. Orthopyroxene is stabilized and marks the  
382 transition to intermediate-pressure granulite at 0.99 GPa and 850 °C, and garnet completely  
383 destabilizes at 0.89 GPa and 850 °C. The rock would begin to melt during isobaric heating at 860  
384 °C and 0.75 GPa, and two melt loss events would occur at 941 °C and 995 °C. The density of the  
385 system would continuously decrease during ITD, but shows a step-like increase during isobaric  
386 heating. The change of density of the residua is the same as those in  $P$ - $T$  path 2.

## 387 **6.2 Melt and residuum compositions**

388 Since the prograde  $P$ - $T$  segment in  $P$ - $T$  path 3 is the same as that for  $P$ - $T$  path 2,  
389 geochemical variation within the system for both protolith types would be identical to those  
390 discussed previously. After peak metamorphism, the major oxide bulk composition of the pelitic  
391 residuum shows a steady change following the first three melt loss events (Figure 5). The final  
392 melt extracted along  $P$ - $T$  path 3 has a higher  $\text{SiO}_2$ ,  $\text{MgO}$  but lower  $\text{Al}_2\text{O}_3$ ,  $\text{CaO}$  than the final  
393 melt extracted along  $P$ - $T$  path 2, whereas other elements are similar (Figure 6). The change in  
394 major element bulk composition of the basaltic residuum and melt are similar to those in  $P$ - $T$   
395 path 1 (Figure 7 and Figure 8). For the trace element contents, U and Th in both pelitic and  
396 basaltic residua show step-like decreases after the first melt loss events, but no change afterwards  
397 (Figure 9 and Figure 10).

### 398 **6.3 Heat production values**

399           The heat production capacities of the pelitic and basaltic melt-depleted residua before  
400 reaching peak metamorphism are identical to those calculated for  $P$ – $T$  path 2. After peak  
401 metamorphism, both show a step-like decrease to  $1.39 \mu\text{W}/\text{m}^3$  and  $0.03 \mu\text{W}/\text{m}^3$ , respectively, as  
402 a result of extensive melt loss (Figure 9 and Figure 10).

## 403 **7 DISCUSSION**

### 404 **7.1 Uncertainties associated with forward modeling**

405           Given that investigation of these tectonic models using practical techniques, such as  
406 high-temperature experimental petrology, is complicated by the geological necessity of repeated  
407 melt loss during burial and exhumation, we approach this problem using theoretical modeling  
408 techniques instead. However, it is well known that the modeling approach applied here carries  
409 various forms of uncertainty associated with (1) the bulk compositions selected for modeling; (2)  
410 the thermodynamic properties of end-members in the petrological data set; (3) the validity of  $a$ – $x$   
411 relations that describe mixing between end-members in a single phase; (4) the suitability of  
412 solubility models for accessory minerals; and (5) values for trace element partition coefficients.  
413 The magnitudes of each are themselves largely unconstrained (Powell & Holland, 2008),  
414 although many can be minimized to reduce overall uncertainty related to model results.

415           The initial compositions selected for phase equilibria modeling are a primary control on  
416 the topology of the phase diagram. As a result, the melt compositions generated during partial  
417 melting would be different if the protolith composition is different. In addition to major  
418 composition, the Zr, LREE, and  $\text{P}_2\text{O}_5$  would have a significant effect on the amount of accessory  
419 minerals in the residue (Kelsey et al., 2008; Yakymchuk et al., 2017). In this study, averaged

420 pelitic and basaltic bulk compositions were selected for modeling, which thus have implications  
421 for typical melt behavior and chemical composition evolution in the crust. Higher Zr and LREE  
422 concentrations in the protolith would allow more zircon and monazite to remain in the residue.  
423 Consequently, internal heat production might remain high, even at UHT conditions. It would also  
424 be reasonable that UHT granulites would have a higher heat production if the protolith had a  
425 higher initial U and Th content, although a recent evaluation of the geochemistry of global rocks  
426 types shows that the most post-Archean shales have similar values (e.g. Gard *et al.*, 2019).

427         The most up to date internally consistent dataset available to investigate phase equilibria  
428 in metamorphic rocks (ds62: Holland & Powell, 2011) was used in this study, as were the latest  
429 *a-x* relations for constraining subsolidus and suprasolidus metamorphism of metapelite and  
430 metabasalt (White *et al.*, 2014; Green *et al.*, 2016). While uncertainties (2) and (3) noted above  
431 represent the largest sources of error in any single phase diagram (Powell & Holland, 2008),  
432 using the same thermodynamic dataset reduces the relative uncertainty between models to  
433 around  $\pm 20$  °C and  $\pm 0.2$  kbar (e.g. Palin, Weller, Waters, & Dyck, 2016; Huang *et al.*, 2018).  
434 These values are sufficiently small to be disregarded as having a major influence on the  
435 calculated melt production and heat budget of each lithology.

436         For accessory mineral solubility modeling, we assumed that Zr, LREE, and P only reside  
437 in the accessory minerals zircon, monazite and apatite in metapelites, and zircon and apatite in  
438 metabasalts. In addition, no accessory minerals or major rock-forming mineral were considered  
439 to be carried away as entrained grains with extracted melt. This latter assumption is necessary to  
440 estimate the proportion of accessory minerals in the residuum. Here, we use the most commonly  
441 adopted zircon solubility model from Boehnke *et al.* (2013), which has been used in many such  
442 studies on zircon behavior during partial melting in the past decade (e.g. Yakymchuk & Brown,

443 2014b; Yakymchuk *et al.*, 2018). For monazite, we selected the solubility equation from  
444 Stepanov *et al* (2012) instead of Kelsey, Clark, & Hand (2008), as the former is more sensitive to  
445 temperature and the hydration state of the anatectic melt than the latter. Saturation equations for  
446 apatite have been defined by Harrison & Watson (1984) and Wolf & London (1994), although  
447 the latter was defined at low pressure (2 kbar) for peraluminous melt with ASI > 1.1, which  
448 would not be suitable for the modeling of metabasalt. In addition, the melt derived from  
449 metapelite partial melting at high pressure usually has compositions with ASI < 1.1  
450 (Yakymchuk, 2017; Yakymchuk *et al.*, 2018). Therefore, the apatite solubility model from  
451 Harrison & Watson (1984) was selected for the modeling in this study.

452         For modeling of U and Th concentrations, we did not consider potential U and Th host  
453 accessory minerals that are stable at subsolidus conditions, such as allanite and xenotime (e.g.  
454 Engi, 2017; Finger, Krenn, Schulz, Harlov, & Schiller, 2016; Spear & Pyle, 2010). Allanite is  
455 usually found in Ca-rich rocks at amphibolite-facies conditions in the crust, whereas it is not  
456 expected to coexist with melt at granulite-facies (or higher) metamorphic grades. As such, U and  
457 Th partition coefficients between mineral and melt – and their initial concentrations in the rock –  
458 are the major factors that affect the potential thermal capacity of the metamorphic products. The  
459 partition coefficients used in this study are constants typical for metapelite and metabasalt,  
460 except those between zircon and pelite-derived melt, which are functions of temperature  
461 (Kirkland, Smithies, Taylor, Evans, & McDonald, 2015). No partition coefficients for U and Th  
462 between muscovite and pelitic melt were assigned due to the lack of experimental data  
463 describing these relationships, which may potentially induce some errors, although muscovite is  
464 shown to destabilize very soon after partial melting begins. Thus, this is not expected to be an  
465 issue for values calculated for UHT conditions.

## 466 **7.2 Implications for partial melting in the crust**

467           Since fluid-absent dehydration melting plays a primary role in the generation of granite  
468 (e.g. Brown, 2013; Clemens, 2012; Sawyer *et al.*, 2011), rocks containing large volumes of  
469 hydrated minerals, such as muscovite, biotite, and hornblende, play significant roles in crustal  
470 differentiation during anatexis (Yakymchuk, 2019). Based on this assumption,  
471 amphibolite-facies metapelites, rich in mica, and metabasalts, rich in hornblende, were used to  
472 model the petrological evolution of a crustal column during metamorphism along various  $P$ - $T$   
473 paths.

474           Partial melting of a metapelite during isobaric heating at 0.8 GPa produces up to 70 vol.  
475 % of melt at 1000 °C in a closed system environment, but only 27 vol. % of cumulative melt in  
476 open system environment that allows sequential pulses of melt to leave the system once a critical  
477 threshold is reached. These results resemble anatexis in metabasalt, which generates 35 vol. % of  
478 melt up to 1000 °C during isobaric heating in a closed system, but only 22 vol. % of melt in an  
479 open system. Both results confirm the interpretations of previous models that progressive melt  
480 extraction significantly decreases the fertility of the remaining migmatite (Yakymchuk & Brown,  
481 2014a). In fact, melt extraction at an MCT of 7 vol. % is suggested to occur in the absence of  
482 syn-anatectic deformation (Rosenberg & Handy, 2005; Vigneresse, Barbey, & Cuney, 1996), and  
483 this threshold would likely to be lower in deforming rocks (Brown, 2010). Once a permeable  
484 network of partial melt is developed, the positive volume change of the system due to melt  
485 generation and viscosity difference between melt and solid residuum would promote melt  
486 exfiltration from the system and ascent to shallower crust driven by buoyancy (Clemens &  
487 Droop, 1998; Rutter & Mecklenburgh, 2006). Thus, modeling of partial melting in conditional  
488 open systems is most realistic for simulating natural tectonic processes.

489 Modeled  $P$ – $T$  path 1 corresponds to thermal metamorphism associated with mantle  
490 upwelling (Sizova *et al.*, 2014). In this scenario, all melt lost from the metapelite protolith is  
491 granitic and alkaline in composition, with systematic changes of elements as a function of  
492 temperature (Figure 15). All the melt compositions are peraluminous with ASI >1.1. As a result,  
493 a total of 27 vol. % of S-type granite would be generated. The compositions of extracted melts  
494 from metabasalt are all subalkaline and metaluminous, evolving from I-type granite to monzonite  
495 as temperature increases. Thus, 17 vol. % of I-type granite and 5 vol. % of monzonite would be  
496 produced at this tectonic setting.

497 In a tectonic setting involving crustal thickening followed by slow erosion (Clark *et al.*,  
498 2011), the metapelite-derived melts also have granitic and alkaline partial melts, but the ASI of  
499 the first two pulses are below 1.1. This produces 22 vol. % of S-type granite during partial  
500 melting of metapelite along this  $P$ – $T$  path. For metabasalt, three extracted melt fractions  
501 constitute 17 vol. % of the initial protolith and are all subalkaline granites with ASI values ~ 1.0.

502 For modeling of a multi-period thermal anomaly (Huang *et al.*, 2019), melts extracted  
503 during prograde metamorphism are the same as those documented for  $P$ – $T$  path 2. During  
504 subsequent isobaric heating at 0.75 GPa, the final extracted melt fraction from the metapelite is  
505 alkaline, granitic and peraluminous. In contrast, the final two extracted melt fractions from the  
506 metabasalt evolve from monzonitic to monzodioritic composition, with both being subalkaline  
507 and metaluminous. As a result, 22 vol. % of S-type granite would be formed from partial melting  
508 of metapelite, and 12 vol. % of I-type granite, 5 vol. % of monzonite, 5 vol. % of monzodiorite  
509 would be produced from partial melting of metabasalt in this tectonic setting.

510 As the densities of extracted melts are always lower than those of the residua, melt  
511 generated at this middle to lower crustal setting will ascend to shallower levels, driven by

512 buoyancy (Brown, 2013; Yakymchuk, 2019; Yakymchuk & Brown, 2014a). The emplacement  
513 and eruption of these granitic, dioritic, and gabbroic magma then drives inter-crustal  
514 differentiation, changing the composition of the upper continental crust through time and  
515 generally causing it to become more silica-rich (felsic), whereas silica-poor residua are left  
516 behind and drive the middle to lower crust to more basic compositions (Sawyer et al., 2011).  
517 Basalt-derived melts generated at high pressure and all pelite-derived melts are granitic, but  
518 basalt-derived melts generated from middle crust are much more mafic, especially at high  
519 temperature. It might be plausible that the volume fraction of mafic rocks in the middle crust  
520 would be important for determining the maficity of the upper crust. However, the modeling in  
521 this study only considers melt internally derived from granulite. In reality, magma mixing among  
522 melts derived from various sources is ubiquitous in granulite and UHT terranes. In a crustal  
523 thinning and mantle underplating scenario, some granite is usually generated by mixing of  
524 metamorphic melts and juvenile mafic magma, as well as significant amount of residua  
525 (Korhenon et al., 2015; Wang et al., 2018). Thus, we can only suggest the volume fraction of  
526 mafic rocks in the middle crust that might contribute to the maficity to the upper crust, but in  
527 reality magmatism would be much more complicated than our modeling. These data may  
528 therefore be considered as an ideal end-member scenario upon which more complex modeling  
529 studies may be built.

### 530 **7.3 Implications for identifying UHT metamorphism in the rock record**

531 As UHT granulites usually experienced extensive partial melting and melt loss, it is  
532 difficult to constrain the exact  $P$ - $T$  path, melt composition or melt volume that was lost during  
533 the prograde stage. In this study, we proposed several possible  $P$ - $T$  paths that UHT granulite  
534 might experience and used unconventional panel diagrams to investigate the melt behavior and

535 chemical composition evolution along these  $P$ – $T$  paths, which have some theoretical implications  
536 for the study of UHT metamorphism. Nonetheless, these assumed processes might be more  
537 complicated in natural systems.

538 Here, for a conventional (closed-system) phase diagram analysis, the diagnostic UHT  
539 mineral pairing Spr + Qz is not predicted to form in metapelitic rocks at high grade conditions  
540 (Figure 1), but high-Al orthopyroxene + sillimanite stabilizes in a restricted  $P$ – $T$  range of 1000–  
541 1020 °C, 0.69–0.72 GPa. This indicates that a protolith must already be Mg-rich to be able to  
542 generate this diagnostic UHT mineral assemblage, even though the  $P$ – $T$  range is narrow. In  
543 contrast, Spr + Qz does occur over a wide  $P$ – $T$  range under open-system conditions along several  
544  $P$ – $T$  paths (Figures 3, 11, and 13). However, other UHT diagnostic mineral assemblages, such as  
545 high-Al orthopyroxene + sillimanite, are not predicted to form under open-system conditions,  
546 which is a constraint of the effective bulk composition. We find a progressively increasing  
547 concentration of Al<sub>2</sub>O<sub>3</sub> and MgO in their respective residua: an effect that is more pronounced at  
548 low pressure, owing to more MLEs (Figure 5). The increase of Al<sub>2</sub>O<sub>3</sub> and MgO in the residue is  
549 due to relatively lower Al<sub>2</sub>O<sub>3</sub> and MgO in the melt than the original protolith, as shown by mass  
550 balance (Rapp, Ryerson, & Miller, 1987). Thus, whether or not a metapelite can form diagnostic  
551 UHT mineral assemblages is primarily controlled by protolith composition, and the degree of  
552 melt loss event being a subsidiary effect. In a relatively Mg-rich protolith, open-system  
553 metamorphism and melt loss is necessary to form Mg–Al rich domains from metasedimentary  
554 protoliths, as hypothesized previously (e.g. Baba, 2003; Brandt *et al.*, 2007; Clifford *et al.*, 1981;  
555 Droop & Bucher-Nurminen, 1984; Lal *et al.*, 1978; Raith *et al.*, 1997). If 7 vol. % melt is used as  
556 a threshold for accumulation before extraction in quartzo-feldspathic lithologies, at least three  
557 discrete melt loss events at high pressure (i.e. lower-crustal depth) or discrete four melt loss

558 events at lower pressure (i.e. middle-crustal depths) are necessary to create these diagnostic UHT  
559 assemblages. However, in actively deforming systems, where melt may exfiltrate at lower melt  
560 fractions, the same change in residuum composition may be achieved by a more continuous  
561 drainage as opposed to discrete pulses.

562 By contrast with metapelites, open-system vs. closed-system metamorphism and melt  
563 loss in metabasaltic compositions are more similar to one another, except for small variations in  
564 minor phase concentrations, such as ilmenite and rutile. At least two melt loss events occur prior  
565 to reaching UHT conditions along all considered  $P$ - $T$  paths. Even though some Mg-rich phases,  
566 such as orthopyroxene, are stable at UHT conditions, the overall stability of these minerals  
567 extends over a larger  $P$ - $T$  range both in closed-system and open-systems, leading to difficulty in  
568 identifying UHT conditions in mafic granulites. Compared with the evolution of  $Al_2O_3$  in a  
569 pelitic residue, the  $Al_2O_3$  in mafic residua shows a limited change along various  $P$ - $T$  paths. The  
570 evolution of other elements in the residua usually change consistently up-temperature. Although  
571 feldspar may begin to take on characteristics of ternary compositions, this may be lost upon  
572 cooling due to retrograde cation equilibration. Thus, in line with the results of previous studies,  
573 we find that UHT metamorphism is very difficult to identify in meta-basic rocks, regardless of  
574 the degree of melt loss, as the mineral assemblages that occur at lower-granulite facies  
575 conditions largely resemble those that stabilize above 900 °C. This result is problematic given  
576 the abundance of evidence showing that the lower crust is largely mafic in composition,  
577 equivalent to a basaltic andesite. Although the upper and middle crust is more felsic  
578 (granitic/pelitic), UHT conditions are significantly more difficult to achieve at these depths,  
579 except for unusual circumstances that may lead to temperatures locally exceeding 900 °C around  
580 hot and dry magmatic intrusions.

581 This modeling also provides new insight into the thermal energy budget of partially  
582 melted rocks in the lower crust. Some researchers have proposed a high content of heat  
583 producing elements at such depths, which could generate  $>3.5 \mu\text{W}/\text{m}^3$  and so possibly induce  
584 UHT conditions in regions with low erosion rates ( $<0.05 \text{ mm}/\text{y}$ ) (e.g. Clark *et al.*, 2011).  
585 However, the heat production values calculated in this study show an overall decrease with  
586 temperature in various tectonic settings, even though volume reduction during burial due to melt  
587 loss acts to slightly increase heat production owing to an increase in density (Figure 9 and Figure  
588 10). These calculated results show similar trends in metapelitic and metabasaltic lithologies,  
589 although heat production values for the latter are extremely low ( $<1.0 \mu\text{W}/\text{m}^3$ ) regardless, such  
590 that they would make no realistic contribution to increasing or sustaining high temperatures in  
591 the crust.

592 Our modeling results are consistent with the conventional view that there is a downward  
593 decrease in the concentration of HPEs in the lower crust, based on seismological evidence and  
594 bulk rock composition analyses (Rudnick and Gao, 2014 and references therein). In these works,  
595 some lower crust of many Archean cratons (e.g. Kaapvaal craton, North China craton) are  
596 characterized by slow *P*-wave velocities and low heat flow, which were interpreted as highly  
597 evolved pelitic rocks depleted in HPEs (Durrheim and Green, 1992; Liu *et al.*, 2001; Nguuri *et*  
598 *al.*, 2001; Niu & James, 2002). In recent works, however, some chemical analyses and theoretical  
599 modeling work suggest a conservation of deep crustal heat production (e.g. Alessio *et al.*, 2018;  
600 Yakymchuk & Brown, 2019). Yakymchuk and Brown (2019) interpreted the contradictory  
601 between equilibrium modeling and natural rocks reported by Alessio *et al.* (2018) as a result of  
602 new monazite growth near the metamorphic peak driven by upward percolation of  
603 LREE-saturated melt. Alternatively, phase equilibrium modeling cannot consider the shielding of

604 accessory mineral grains within porphyroblasts, which removes them from the matrix. As a  
605 result, this imbalance at UHT conditions may be resolved , In addition, theoretical modeling also  
606 indicates that an initial high LREE concentrations in the protolith would preserve monazite from  
607 being totally resorbed at UHT conditions (Kelsey et al., 2008). All of these factors might  
608 plausibly explain the slight increase of Th in the residue during heating, but U does decrease  
609 up-temperature, as shown from both natural rocks and theoretical modeling (Alessio et al., 2018;  
610 Yakymchuk and Brown, 2019). Nonetheless, the heat production rate of Th ( $0.072 \mu\text{W m}^{-3}$ ) is  
611 much lower than that of U ( $0.265 \mu\text{W m}^{-3}$ ) (Bea, 2012), therefore bulk-rock heat production  
612 would decrease due to U loss, even if Th becomes more concentrated in the residue. Such an  
613 occurrence is shown for the metapelitic residue in this work at  $< 850 \text{ }^\circ\text{C}$  at 0.8 GPa.

614 In general, granulite and UHT terranes do not only comprise pelitic and mafic granulites.  
615 Granitic rocks, which usually have high heat production, are also often emplaced into these high  
616 grade terranes due to earlier metamorphic episodes (Huang et al., 2019). In such cases, all  
617 lithologies should be considered when evaluating the contributions of heat production on  
618 bulk-terrane heat flow. Based on the review work of granite heat production by Artemieva et al.  
619 (2017), granite formed before the Early Proterozoic usually has a low heat production ( $< 2 \mu\text{W}$   
620  $\text{m}^{-3}$  on average), which increases forwards in time to peak during the Mesoproterozoic (*c.*  $4.5$   
621  $\mu\text{W m}^{-3}$  on average). Granite formed after this period of time generally shows a steady decrease  
622 in heat production to the present day ( $2.7 \mu\text{W m}^{-3}$  in average). Given the pervasiveness of UHT  
623 metamorphism in the Precambrian (Brown & Johnson, 2018), we suggest that heat production  
624 would not be the only mechanism driving UHT metamorphism on the early Earth, but it must  
625 have been be a contributor in many cases.

626

#### 627 **7.4 Implications for heat budget of melting reaction under open-system**

628           Among various lithologies in a granulite-UHT terrane, and assuming the presence of  
629 fluid, metapelite is the most fertile rock, metabasites are the second-most fertile, and most other  
630 lithologies such as meta-granitoids and meta-sandstone are usually highly refractory. It is well  
631 known that a number of subsolidus and suprasolidus metamorphic reactions and melting  
632 reactions are endothermic, buffering temperature increase during the heating process (e.g. Bea,  
633 2012; Lyubetskaya & Ague, 2009; Stüwe, 1995; Thompson & Connolly, 1995; Vielzeuf,  
634 Clemens, Pin, & Moinet, 1990). As a result, a disparity of peak metamorphic temperature would  
635 be revealed among various lithologies, among which metapelite usually registered the lowest  
636 temperature, whereas other refractory rocks record a 60–70 °C higher peak metamorphic  
637 temperature (e.g. Namaqua-Natal Metamorphic Complex, South Africa, Schorn & Diener, 2019).

638           A comparison of enthalpy changes for an average metapelite during prograde  
639 metamorphism between closed- and open-system was modeled by Schorn et al. (2018). For  
640 open-system conditions, they modeled episodic melt extraction (extracting 5 mol.% melt as soon  
641 as threshold of 7 mol.% is reached) and continuous melt extraction (extracting all melt in excess  
642 of 2 mol.% threshold as soon as it is produced). Both show consistent enthalpy change with that  
643 in a closed-system for major melting reactions (e.g. sillimanite + biotite + quartz  $\rightarrow$  garnet +  
644 cordierite + K-feldspar + melt). After biotite is totally consumed, the residue in an open system  
645 is able to transform heat to temperature more efficiently.

646           In this study, the temperature at which biotite is totally consumed in an open-system (c.  
647 850 °C at 0.8 GPa) is identical to that in a closed-system, which is consistent with the results by  
648 Schorn et al. (2018). From the view of heat transformation to temperature, whether or not melts  
649 can drain away from the system will not have a significant influence. However, melt extraction

650 would strengthen the crust, leading to an increase of mechanical heat production (Clark et al.,  
651 2011; Nabelek, Whittington, & Hofmeister, 2010). Given that the production and redistribution  
652 of heat in the lithosphere would be a combination of heat conduction, heat advection, and heat  
653 production (Stüwe, 2007), we proposed that most UHT metamorphism would be driven by a  
654 hybrid mechanism, including advective heat from mantle, radioactive heat production as well as  
655 mechanical heat production.

656

## 657 **8 CONCLUSIONS**

658 Phase equilibria modeling of open-system melting of metapelite and metabasalt suggest  
659 that progressive melt loss events caused by crossing the melt connectivity threshold make a key  
660 contribution to intracrustal differentiation, leading to an increase of Al and Mg in metapelitic  
661 paleosomes, which provide a possible mechanism for forming sapphirine + quartz in residual  
662 Mg–Al rich domains in an originally Mg-rich metasedimentary rocks. Metabasalt assemblages  
663 are less sensitive to bulk compositional changes at UHT conditions. More than three and two  
664 melt loss events are modeled to occur as the rocks evolve to UHT conditions in pelitic and  
665 basaltic bulk compositions, respectively. Partial melting in an open system environment would  
666 produce 22–27 vol. % S-type granite and 12–17 vol. % I-type granite, respectively. Further, the  
667 heat production values of the residuum would attenuate in an open-system environment. Most  
668 UHT metamorphism is likely therefore driven by a combination of advective heat supplied from  
669 the mantle, internal radioactive heat production, as well as mechanical heat production.

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#### 944 **SUPPORTING INFORMATION**

945 Additional Supporting Information may be found online in the supporting information tab for  
946 this article.

947 **Table S1** Bulk composition used for phase equilibria modeling

948 **Table S2** Modeled results of major composition of extracted melt

949 **Table S3** Modeled amount of accessory minerals in the rocks

950 **Table S4** Modeled U and Th concentrations in the rocks and calculated results of heat  
951 production value

## 952 **FIGURE CAPTIONS**

953 **Figure 1**  $P$ – $T$  pseudosection calculated for an average amphibolite-facies pelite at closed system,  
954 contoured with isopleth of mol. % melt. The black bold solid arrow representing  
955 isobaric heating at 0.8 GPa is proposed  $P$ – $T$  path 1. The mineral proportion against  
956 temperature for isobaric heating at 0.8 GPa is shown below.

957 **Figure 2**  $P$ – $T$  pseudosection calculated for an average MORB at closed system, contoured with  
958 isopleth of mol. % melt. The bold solid line representing isobaric heating at 0.8 GPa is  
959 proposed  $P$ – $T$  path 1. The mineral proportion against temperature for isobaric heating at  
960 0.8 GPa is shown below.

961 **Figure 3**  $P$ – $T$  mosaic pseudosection panels of metapelite at open system along proposed  $P$ – $T$   
962 path 1, contoured with isopleth of mol. % melt. The mineral proportion against  
963 temperature is shown below.

964 **Figure 4**  $P$ – $T$  mosaic pseudosection panels of metabasalt at open system along proposed  $P$ – $T$   
965 path 1, contoured with isopleth of mol. % melt. The mineral proportion against  
966 temperature is shown below.

967 **Figure 5** The evolution of the compositions of the metapelite along various  $P$ – $T$  paths against  
968 temperature.

969 **Figure 6** The evolution of composition of extracted melts from metapelite along various  $P-T$   
970 paths against temperature.

971 **Figure 7** The evolution of the compositions of the metabasalt along various  $P-T$  paths against  
972 temperature.

973 **Figure 8** The evolution of composition of extracted melts from metabasalt along various  $P-T$   
974 paths against temperature.

975 **Figure 9** Modeled U, Th, K concentrations in the pelitic residual and calculated results of heat  
976 production values.

977 **Figure 10** Modeled U, Th, K concentrations in the basaltic residual and calculated results of heat  
978 production values.

979 **Figure 11**  $P-T$  mosaic pseudosection panels of metapelite at open system along proposed  $P-T$   
980 path 2, contoured with isopleth of mol. % melt. The mineral proportion against  
981 temperature is shown below.

982 **Figure 12**  $P-T$  mosaic pseudosection panels of metabasalt at open system along proposed  $P-T$   
983 path 2, contoured with isopleth of mol. % melt. The mineral proportion against  
984 temperature is shown below.

985 **Figure 13**  $P-T$  mosaic pseudosection panels of metapelite at open system along proposed  $P-T$   
986 path 3, contoured with isopleth of mol. % melt. The mineral proportion against  
987 temperature is shown below.

988 **Figure 14**  $P-T$  mosaic pseudosection panels of metabasalt at open system along proposed  $P-T$   
989 path 3, contoured with isopleth of mol. % melt. The mineral proportion against  
990 temperature is shown below.

991 **Figure 15** Geochemical classification diagrams for extracted melts. (a) Total alkali against silica  
992 diagram (TAS, after Middlemost, 1994) for metapelite-derived melts; (b) A/NK against  
993 A/CNK classification diagram (Maniar & Piccoli, 1989) for metapelite-derived melts;  
994 (c) TAS diagram for metabasite-extracted melts; (d) A/NK against A/CNK  
995 classification diagram for metabasite-extracted melts. Compositions of melts generated  
996 along  $P$ - $T$  path 1 to  $P$ - $T$  path 3 for open system are labeled with orange cubes, grey  
997 triangles and yellow circles, respectively.