Revision 3

Supplementary Information for

Quantifying the potential for mineral carbonation of processed kimberlite with the Rietveld-PONKCS method

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Table S1. Detailed parameters for each of three XRDs.

XRD	Goniometer radius (mm)	Divergence slit size (mm or °)	Zero error (°)	Primary Soller angle (°)	Secondary Soller angle (°)
XRD A1	200.5	10 mm	-0.02849353	5.0	5.0
XRD B1	250	0.6 mm	-0.01717877	2.5	2.5
XRD B2	250	0.6 mm	-0.01979303	2.5	2.5

Table S2. Refined mineral abundances (wt.%) using PONKCS models calibrated to each of three XRDs.

Sample	wcskim1			wcskim2			wcskim3			wcskim4			wcskim5		
Phase/XRD	A1	B1	B2	A1	B1	B2	A1	B1	B2	A1	B1	B2	A1	B1	B2
Lizardite	61.9	60.3	60.7	53.5	49.4	48.1	38.2	35.1	35.5	20.0	22.9	22.0	21.4	12.9	12.2
bias	2.5	1.0	1.3	4.0	0.0	-1.3	3.6	0.5	0.9	0.2	3.1	2.3	11.5	3.0	2.3
esd	1.7	0.5	0.6	0.8	0.5	0.4	0.7	0.6	0.3	0.8	0.6	0.4	1.9	0.5	0.4
Ca-montmorillonite	9.5	7.7	9.9	14.0	19.2	22.9	33.4	35.8	34.1	48.7	49.7	41.1	58.9	59.3	50.2
bias	0.1	-1.7	0.5	-4.8	0.4	4.2	0.6	3.0	1.3	1.8	2.8	-5.8	2.6	3.0	-6.1
esd	2.2	0.3	0.5	0.5	0.3	0.3	0.5	0.6	0.3	0.7	0.7	0.4	1.5	0.6	0.5
Calcite	4.6	4.5	5.1	5.7	4.3	4.8	4.8	3.8	5.1	5.9	2.9	6.1	3.9	3.3	5.6
bias	-1.0	-1.1	-0.6	0.1	-1.2	-0.8	-0.6	-1.5	-0.3	0.7	-2.3	0.9	-1.2	-1.9	0.5
esd	0.2	0.2	0.1	0.2	0.2	0.1	0.2	0.2	0.1	0.2	0.2	0.2	0.2	0.2	0.2
Quartz	5.4	3.2	5.1	5.6	3.7	4.9	5.4	3.4	5.9	6.0	4.0	7.8	4.9	4.7	9.1
bias	-0.2	-2.4	-0.5	-0.6	-2.6	-1.4	-1.8	-3.8	-1.3	-2.1	-4.1	-0.3	-3.8	-4.0	0.4
esd	0.3	0.1	0.1	0.2	0.1	0.1	0.1	0.1	0.1	0.2	0.1	0.1	0.2	0.1	0.2
Clinochlore	2.8	8.7	3.2	3.9	7.5	5.6	3.8	6.4	5.2	3.0	5.8	6.2	1.8	6.4	6.6
bias	-2.5	3.5	-2.0	-1.4	2.2	0.4	-1.5	1.1	-0.1	-2.3	0.5	0.9	-3.5	1.2	1.4
esd	0.4	0.4	0.3	0.4	0.4	0.3	0.4	0.4	0.2	0.4	0.4	0.3	0.3	0.4	0.4
Phlogopite	5.6	5.6	5.6	5.9	6.3	5.0	4.7	5.9	5.0	4.7	5.9	6.4	1.8	5.5	6.5
bias	0.6	0.6	0.6	0.9	1.3	0.0	-0.3	0.9	0.0	-0.3	0.9	1.4	-3.2	0.5	1.5
esd	0.4	0.3	0.2	0.4	0.3	0.2	0.3	0.3	0.2	0.3	0.3	0.2	0.3	0.3	0.3
Brucite	3.9	5.0	4.1	4.1	4.9	4.1	4.3	4.3	4.2	4.1	3.6	4.2	2.3	3.5	3.9
bias	-0.8	0.2	-0.6	-0.6	0.1	-0.7	-0.5	-0.4	-0.6	-0.7	-1.2	-0.5	-2.5	-1.3	-0.8
esd	0.2	0.3	0.2	0.2	0.3	0.1	0.2	0.3	0.1	0.2	0.2	0.2	0.2	0.2	0.2
Talc	6.2	4.9	6.3	7.2	4.7	4.5	5.4	5.3	5.0	7.6	5.2	6.1	5.1	4.5	5.8
bias	1.5	0.2	1.6	2.5	0.0	-0.2	0.7	0.6	0.3	2.9	0.5	1.4	0.4	-0.3	1.1
esd	0.4	0.3	0.3	0.3	0.3	0.2	0.3	0.4	0.2	0.3	0.4	0.3	0.3	0.3	0.3
Total	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
R_{wp} (%)	5.6	13.8	11.0	5.7	12.6	8.8	4.3	10.9	7.9	4.8	10.2	8.8	4.9	9.8	9.7
Total absolute bias (wt.%)	9.3	10.7	7.8	14.9	7.9	8.8	9.4	11.8	4.8	11.0	15.4	13.4	28.6	15.1	14.1

R_{wp}: weighted profile R-factor, a function of the least-squares residual (%). esd: estimated standard deviation.

Table S3. Refined mineral abundances (wt.%) using PONKCS models calibrated to XRD B1.

Sample	wcskim1		wcskim2		wcskim3		wcskim4		wcskim5	
Phase	A1	B2	A1	B2	A1	B2	A1	B2	A1	B2
Lizardite	51.6	54.2	45.4	48.2	38.2	35.4	23.7	22.4	34.5	17.8
bias	-7.7	-5.1	-4.1	-1.3	3.6	0.8	3.9	2.6	24.6	7.9
esd	0.7	0.8	0.6	0.5	0.8	0.5	0.9	0.6	1.2	0.7
Ca-montmorillonite	1.5	5.9	5.2	16.8	10.9	28.1	18.8	36.7	23.7	41.2
bias	-7.9	-3.5	-13.6	-1.9	-21.9	-4.7	-28.1	-10.2	-32.6	-15.1
esd	0.3	1.0	0.3	0.6	0.4	0.7	0.4	1.0	0.6	1.1
Calcite	5.4	4.7	6.6	4.6	5.8	4.4	6.8	6.0	5.4	5.0
bias	-0.3	-1.0	1.0	-0.9	0.4	-1.0	1.6	0.8	0.3	-0.1
esd	0.2	0.2	0.2	0.2	0.3	0.2	0.3	0.2	0.3	0.2
Quartz	7.8	5.4	8.3	5.8	9.8	6.8	12.4	8.6	11.5	10.8
bias	2.2	-0.2	2.1	-0.4	2.6	-0.3	4.3	0.5	2.7	2.1
esd	0.2	0.2	0.2	0.1	0.2	0.2	0.3	0.2	0.3	0.3
Clinochlore	12.0	11.4	9.3	8.6	13.2	8.9	11.4	7.9	8.4	6.5
bias	6.8	6.1	4.0	3.3	7.9	3.7	6.1	2.6	3.2	1.2
esd	0.6	0.5	0.5	0.4	0.8	0.4	0.8	0.5	0.8	0.5
Phlogopite	5.9	5.3	8.5	5.3	5.6	5.8	6.7	6.9	2.7	6.6
bias	0.9	0.3	3.5	0.3	0.6	0.8	1.7	1.9	-2.3	1.6
esd	0.5	0.3	0.4	0.2	0.6	0.2	0.7	0.2	0.4	0.4
Brucite	5.5	4.6	5.5	4.5	5.2	4.1	4.8	4.0	4.1	3.7
bias	0.8	-0.1	0.8	-0.2	0.4	-0.6	0.0	-0.7	-0.7	-1.1
esd	0.3	0.2	0.2	0.2	0.3	0.2	0.3	0.2	0.3	0.2
Talc	10.3	8.6	11.3	6.2	11.5	6.4	15.6	7.6	9.9	8.4
bias	5.5	3.9	6.6	1.5	6.7	1.7	10.8	2.9	5.2	3.6
esd	0.4	0.3	0.4	0.3	0.5	0.4	0.6	0.4	0.5	0.4
Total	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
R_{wp} (%)	6.2	12.1	6.0	11.2	6.2	10.4	6.7	10.2	6.2	11.4
Total absolute bias (wt.%)	32.1	20.1	35.6	9.8	44.1	13.6	56.5	22.1	71.6	32.7

Table S4. Carbonation potentials (g CO_2/kg kimberlite) calculated from the known composition of wcskim samples and refinement results using correctly calibrated PONKCS models with XRD B2 data, and incorrectly calibrated PONKCS models (calibrated to XRD B1) with XRD B2 data and XRD A1 data.

Sample	wcskim1				wcskim2				wcskim3				wcskim4				wcskim5			
Units (g/kg)	Actual	Calibrated B2	Uncal B2	Uncal A1	Actual	Calibrated B2	Uncal B2	Uncal A1	Actual	Calibrated B2	Uncal B2	Uncal A1	Actual	Calibrated B2	Uncal B2	Uncal A1	Actual	Calibrated B2	Uncal B2	Uncal A1
Lizardite	593	607	542	516	495	481	482	454	346	355	354	382	198	220	224	237	99	122	178	345
Mg in lizardite	156	160	143	136	130	127	127	119	91	93	93	100	52	58	59	62	26	32	47	91
Hydromagnesite eq (lizardite)	601	614	549	522	501	487	488	459	350	359	359	387	200	223	227	240	100	124	180	349
Carbonation potential of lizardite	*226*	*231*	*207*	*197*	*188*	*183*	*184*	*173*	*132*	*135*	*135*	*145*	*75*	*84*	*85*	*90*	*38*	*47*	*68*	*131*
Brucite	47	41	46	55	47	41	45	55	47	42	41	52	47	42	40	48	47	39	37	41
Mg in Brucite	20	17	19	23	20	17	19	23	20	17	17	22	20	18	17	20	20	16	15	17
Hydromagnesite eq (brucite)	76	66	74	88	76	66	73	89	76	67	66	83	76	68	64	76	76	63	59	65
Carbonation potential of brucite	*29*	*25*	*28*	*33*	*29*	*25*	*27*	*33*	*29*	*25*	*25*	*31*	*29*	*26*	*24*	*29*	*29*	*24*	*22*	*24*
Ca-montmorillonite	94	99	59	15	188	229	168	52	328	341	281	109	469	411	367	188	563	502	412	237
Mg in Ca-montmorillonite	2	2	1	0	3	4	3	1	6	6	5	2	8	7	7	3	10	9	7	4
Hydromagnesite eq (Ca-montmorillonite)	6	7	4	1	13	16	11	4	22	23	19	7	32	28	25	13	38	34	28	16
Carbonation potential of Mg in Ca-montmorillonite	*2*	*3*	*2*	*0*	*5*	*6*	*4*	*1*	*8*	*9*	*7*	*3*	*12*	*11*	*9*	*5*	*14*	*13*	*11*	*6*
Ca in Ca-montmorillonite	1	1	0	0	2	2	1	0	3	3	2	1	4	3	3	2	5	4	3	2
Calcite eq (Ca-montmorillonite)	2	2	1	0	4	5	4	1	7	7	6	2	10	9	8	4	12	11	9	5
Carbonation potential of Ca in Ca-montmorillonite	*1*	*1*	*1*	*0*	*2*	*2*	*2*	*0*	*3*	*3*	*3*	*1*	*4*	*4*	*3*	*2*	*5*	*5*	*4*	*2*
Total carbonation potential	**258**	**259**	**237**	**230**	**224**	**216**	**217**	**208**	**172**	**172**	**170**	**181**	**120**	**124**	**122**	**126**	**86**	**88**	**105**	**164**

Carbonation potentials calculations

The emissions offset potential results are reported in Table S4 and Fig. 6. Carbonation potential was calculated using (1) the known composition of the wcskim samples (Table 1), (2) Rietveld refinement results (wt.%) utilizing PONKCS models calibrated to XRD B2 (Table S2), which gave the most accurate results, and Rietveld refinement results (wt.%) using PONKCS models calibrated to XRD B1 with data collected on (3) XRD B2 and (4) XRD A1 (Table S3). Ideal stoichiometries were assumed for lizardite [$Mg_3Si_2O_5(OH)_4$] and brucite [$Mg(OH)_2$]. Average values for Mg (1.773 wt.%) and Ca (0.841 wt.%) content in SWy-2 (Mermut and Cano, 2001) were used for montmorillonite. Considering a sample mass of 1 kg, *E eq*, the equivalent proportion (in g/kg) of Mg in lizardite, brucite or montmorillonite or Ca in montmorillonite were then calculated using (1).

$$E\ eq = C \times M \qquad (1)$$

Where *C* is the weight proportion of lizardite or brucite in g/kg *and M* is the mass fraction (%) of the element in the mineral (*e.g.*, Mg comprises 26.31 % and 41.58 % of the mass of lizardite and brucite, respectively).

Assuming hydromagnesite [$Mg_5(CO_3)_4(OH)_2{\cdot}4H_2O$] forms from Mg released during complete dissolution of lizardite, brucite and montmorillonite and that calcite ($CaCO_3$) forms from Ca during complete cation-exchange reactions and dissolution of montmorillonite in the presence of aqueous carbonate. *Mineral eq*, the equivalent proportion (in g/kg) of either hydromagnesite or calcite that would contain these amounts of Mg and Ca were then calculated using (2).

$$Mineral\ eq = \frac{E\ eq}{M} \qquad (2)$$

Where M is the mass fraction (%) of the element in hydromagnesite or calcite (*e.g.,* Mg comprises 25.99 % of hydromagnesite and Ca comprises 40.04 % of calcite).

The carbonation potential, $CO_2\ eq$, in units of g CO_2 / kg of kimberlite, was calculated with (3) using the mass fraction of CO_2, which we name the storage factor (*SF*), in a given carbonate mineral (0.3764 for hydromagnesite and 0.4397 for calcite).

$$CO_2\ eq = Mineral\ eq \times SF \qquad (3)$$