

Supplementary Material

Evaluation of the Rietveld method for determining content and chemical composition of inorganic X-ray amorphous materials in soils

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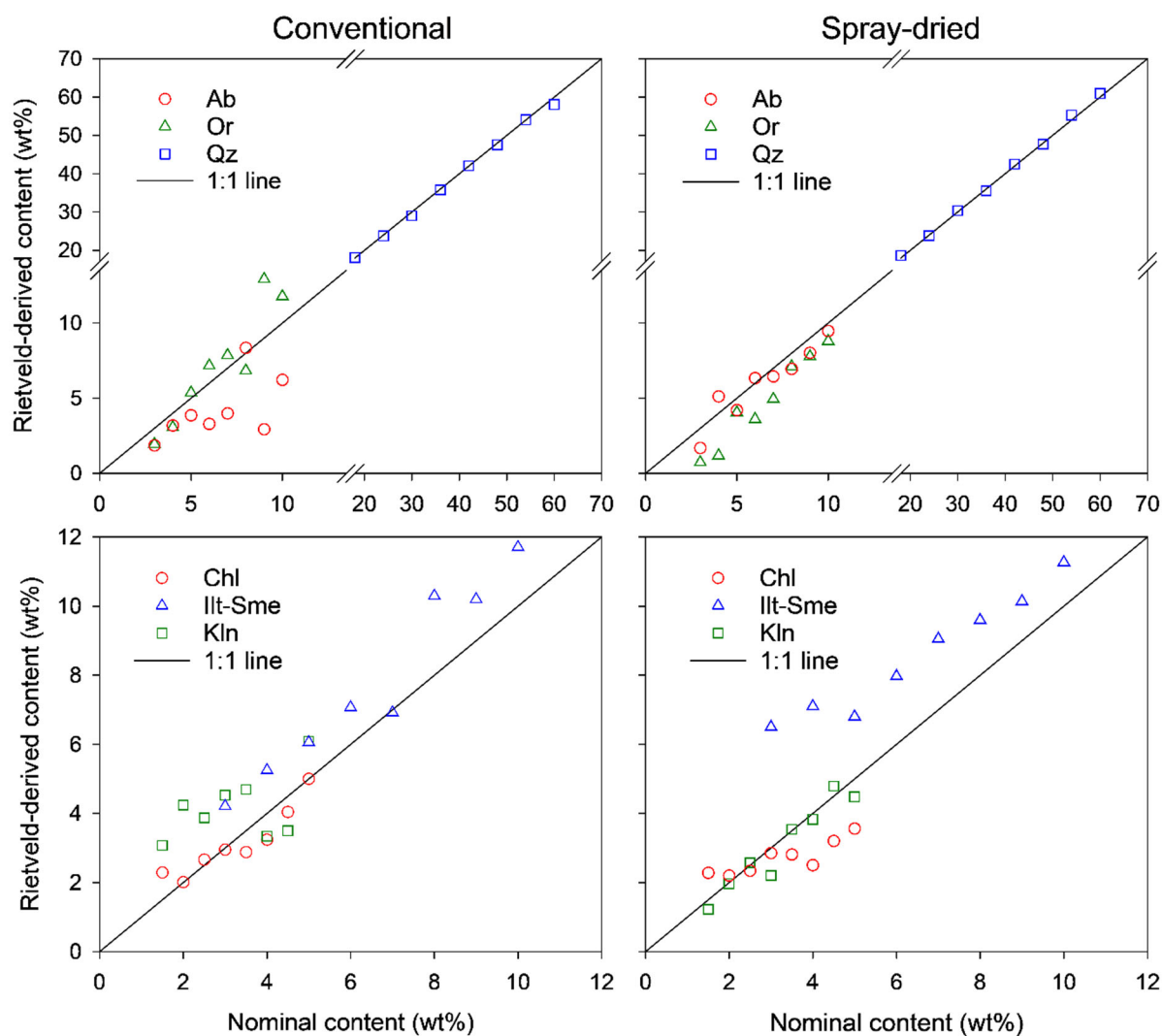


Figure S1. Plots of nominal versus Rietveld-derived contents of crystalline non-clay and clay minerals in mineral mixture A amended with 0–70 wt% iXAMs and analyzed after conventional sample preparation and spray drying. Mineral abbreviations: Ab = albite; Chl = chlorite; Ill-Sme = illite-smectite; Kln = kaolinite; Or = orthoclase; Qz = quartz.

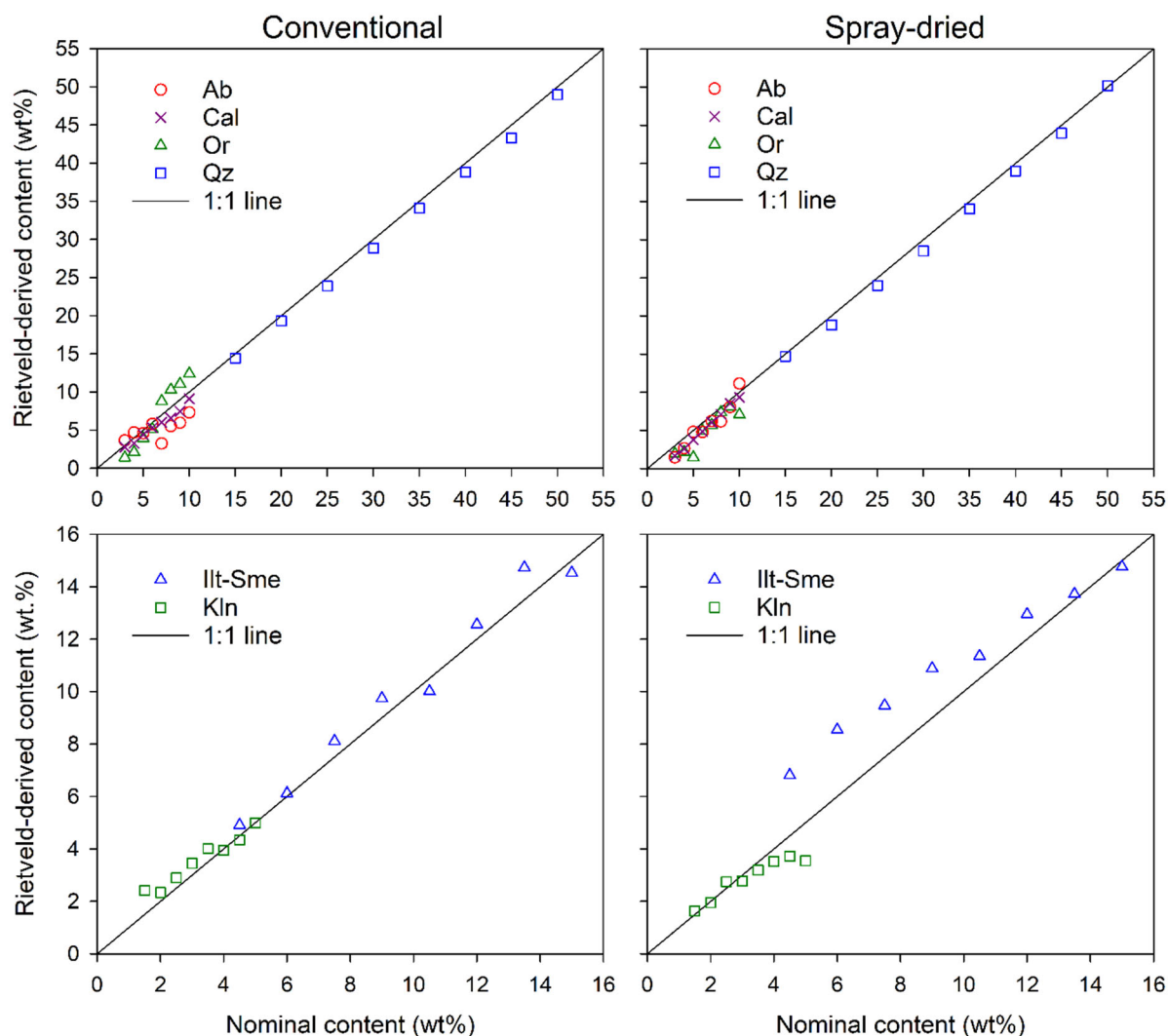


Figure S2. Plots of nominal versus Rietveld-derived contents of crystalline non-clay and clay minerals in mineral mixture B amended with 0–70 wt% iXAMs and analyzed after conventional sample preparation and spray drying. Mineral abbreviations: Ab = albite; Cal = calcite; Ill-Sme = illite-smectite; Kln = kaolinite; Or = orthoclase; Qz = quartz.

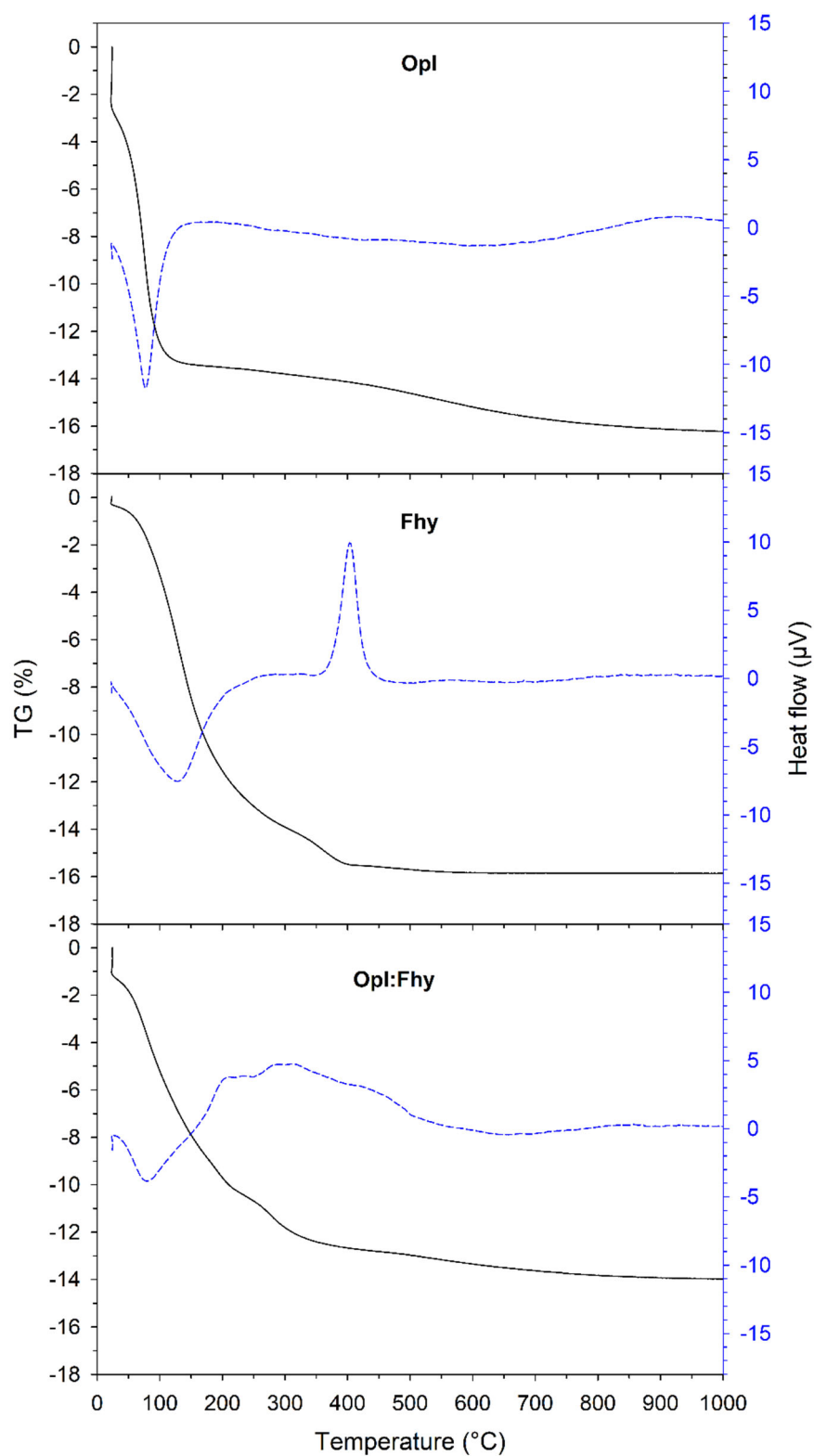


Figure S3. TGA-DSC data of opal-A (Opl), ferrihydrite (Fhy), and a 1:1 (w/w) Opl:Fhy mixture. Solid black lines: TGA curves, dashed blue lines: DSC curves.

Table S1. Rietveld refinement results for mineral mixtures A–D amended with 0–70 wt% iXAMs and analyzed after conventional sample preparation and spray drying. GOF is R_{wp} (%) divided by R_{exp} (%). Nominal and Rietveld derived values are given in wt%. Mineral abbreviations: Ab = albite; Cal = calcite; Chl = chlorite; Ilt-Sme = illite-smectite; Kln = kaolinite; Lb = labradorite; Or = orthoclase; Qz = quartz; Sme = smectite.

Mixture		A – Conventional								A – Spray-dried							
iXAMs (nominal)		0	10	20	30	40	50	60	70	0	10	20	30	40	50	60	70
	R _{wp}	7.69	8.12	9.13	7.57	7.83	7.95	8.62	9.48	9.93	9.34	8.52	8.55	8.51	9.70	10.29	9.98
	R _{exp}	5.35	5.45	5.53	5.63	5.68	5.76	5.73	5.81	5.24	5.28	5.52	5.53	5.69	5.72	5.72	5.84
	GOF	1.44	1.49	1.65	1.34	1.38	1.38	1.50	1.63	1.90	1.77	1.54	1.55	1.50	1.70	1.80	1.71
	Qz	58.02	54.08	47.58	42.07	35.77	29.04	23.74	18.10	60.93	55.31	47.71	42.52	35.54	30.35	23.81	18.63
	Or	11.78	12.92	6.84	7.86	7.17	5.37	3.07	1.95	8.80	7.78	7.11	4.94	3.61	4.05	1.19	0.74
	Ab	6.22	2.94	8.35	3.99	3.29	3.87	3.19	1.86	9.47	8.02	6.95	6.45	6.34	4.21	5.12	1.69
	Ilt-Sme	11.71	10.20	10.30	6.92	7.07	6.06	5.25	4.21	11.27	10.14	9.60	9.05	7.97	6.80	7.10	6.50
	Chl	5.00	4.04	3.24	2.88	2.95	2.66	2.01	2.29	3.56	3.20	2.50	2.81	2.85	2.34	2.20	2.28
	Kln	6.09	3.50	3.34	4.69	4.53	3.87	4.24	3.07	4.48	4.79	3.83	3.54	2.20	2.57	1.97	1.22
iXAMs (Rietveld)		1.18	12.39	20.34	31.58	39.21	49.16	58.50	68.52	1.49	10.77	22.30	30.69	41.48	49.68	58.61	68.95
Mixture		B – Conventional								B – Spray-dried							
iXAMs (nominal)		0	10	20	30	40	50	60	70	0	10	20	30	40	50	60	70
	R _{wp}	7.19	7.23	7.26	6.95	7.49	7.58	7.90	8.34	9.05	8.45	8.04	8.39	8.46	8.82	9.39	9.81
	R _{exp}	5.44	5.59	5.61	5.63	5.80	5.67	5.85	5.87	5.29	5.29	5.59	5.64	5.65	5.71	5.77	5.83
	GOF	1.32	1.29	1.29	1.23	1.29	1.34	1.35	1.42	1.71	1.60	1.44	1.49	1.50	1.54	1.63	1.68
	Qz	48.99	43.28	38.83	34.09	28.86	23.91	19.31	14.43	50.20	43.97	39.00	34.04	28.52	24.01	18.82	14.71
	Or	12.41	11.05	10.30	8.80	5.13	3.95	2.11	1.41	7.08	8.11	7.38	5.68	4.94	1.47	2.17	1.94
	Ab	7.32	5.96	5.52	3.26	5.81	4.60	4.70	3.66	11.14	8.05	6.17	6.21	4.78	4.80	2.64	1.46
	Cal	9.12	7.46	6.56	6.02	5.31	4.43	3.28	2.77	9.35	8.53	7.11	6.05	4.87	3.79	2.60	1.67
	Ilt-Sme	14.53	14.73	12.56	10.01	9.74	8.11	6.12	4.91	14.76	13.72	12.95	11.35	10.88	9.47	8.54	6.81
	Kln	4.99	4.34	3.95	4.01	3.45	2.90	2.34	2.41	3.55	3.72	3.52	3.19	2.77	2.75	1.95	1.63
iXAMs (Rietveld)		2.64	13.19	22.28	33.82	41.71	52.11	62.15	70.42	3.92	13.90	23.86	33.48	43.25	53.69	63.28	71.78

Table S1. *Continued*

Mixture		C – Conventional							C – Spray-dried								
iXAMs (nominal)		0	10	20	30	40	50	60	70	0	10	20	30	40	50	60	70
R _{wp}		8.25	8.17	7.95	7.49	8.19	8.36	8.23	8.65	9.14	8.63	8.47	8.50	9.22	9.28	10.02	10.74
R _{exp}		5.38	5.44	5.51	5.60	5.66	5.62	5.77	5.81	5.48	5.42	5.65	5.49	5.70	5.78	5.78	5.81
GOF		1.53	1.50	1.44	1.34	1.45	1.49	1.43	1.49	1.67	1.59	1.50	1.55	1.62	1.61	1.73	1.85
Qz		39.86	35.45	31.58	27.86	24.01	19.63	16.00	12.04	39.61	36.08	31.67	27.99	23.85	19.63	15.89	11.53
Or		13.49	12.40	10.26	9.30	7.47	6.27	3.79	2.73	14.07	13.14	10.67	8.94	6.81	5.47	3.93	4.16
Cal		18.00	16.65	14.36	12.61	10.32	8.60	6.85	5.19	19.24	17.17	14.77	13.07	11.09	8.20	6.26	4.27
Ilt-Sme		21.15	18.95	16.37	13.30	11.65	10.37	7.80	6.82	19.35	16.93	15.67	14.68	12.66	10.36	9.25	8.32
Chl		5.28	4.62	3.82	4.73	3.33	2.77	2.89	3.04	5.41	4.34	4.39	4.20	3.05	3.37	1.93	1.68
iXAMs (Rietveld)		2.23	11.92	23.61	32.19	43.23	52.37	62.66	70.18	2.33	12.33	22.82	31.12	42.54	52.96	62.73	70.02
Mixture		D – Conventional							D – Spray-dried								
iXAMs (nominal)		0	10	20	30	40	50	60	70	0	10	20	30	40	50	60	70
R _{wp}		8.62	7.27	7.05	7.18	7.38	8.08	7.99	8.72	8.60	8.41	7.61	8.20	8.30	8.72	9.46	9.42
R _{exp}		4.68	4.88	5.09	5.23	5.33	5.50	5.63	5.67	4.79	4.94	5.11	5.27	5.40	5.43	5.63	5.67
GOF		1.84	1.49	1.39	1.37	1.38	1.47	1.42	1.54	1.80	1.70	1.49	1.56	1.54	1.61	1.68	1.66
Qz		20.43	18.12	15.91	14.00	11.8	9.81	7.48	5.90	20.55	18.83	15.96	15.04	11.85	10.30	8.08	5.79
Or		20.60	17.49	16.1	13.62	14.05	11.12	5.57	3.35	20.26	18.49	15.05	11.44	11.23	7.98	5.82	3.70
Lb		9.82	8.20	5.92	6.50	2.66	3.20	3.01	1.73	9.44	7.80	5.50	5.46	3.86	3.43	2.70	1.18
Ilt-Sme		23.51	21.99	20.26	17.36	14.67	11.80	11.11	8.77	22.90	19.77	18.48	17.42	16.08	13.92	11.63	8.77
Chl		2.72	2.69	2.55	2.36	2.23	2.26	1.72	1.82	3.13	3.14	3.53	1.88	2.11	1.24	2.48	1.39
Kln		13.72	12.15	11.18	10.13	9.16	6.47	6.06	4.79	14.54	13.69	12.76	10.45	8.82	7.71	5.88	6.40
Sme		7.05	7.38	7.55	5.68	5.64	4.72	2.95	3.37	6.20	5.73	6.24	5.07	5.16	5.41	3.77	2.38
iXAMs (Rietveld)		2.15	11.98	20.52	30.34	39.78	50.61	62.10	70.26	2.98	12.53	22.47	33.24	40.89	50.14	59.65	70.38

Table S2. Analysis of variance (ANOVA) and Student's t-tests for Rietveld GOF values of mineral mixtures A–D amended with 0–70 wt% iXAM and analyzed after conventional sample preparation and spray drying. Significant p-values are marked in bold. SD: standard deviation; SEM: standard error of the mean; df: degrees of freedom; SS: sum of squares; MS: mean squared errors.

Conventional								
Kruskal-Wallis ANOVA on Ranks					Post-hoc tests (Tukey)			
	N	Median	25%	75%	Comparison	Diff. of Ranks	q	p
A	8	1.46	1.38	1.60	A vs. B	116.0	4.37	0.01
B	8	1.31	1.29	1.35	A vs. C	0.00	0.00	1.00
C	8	1.47	1.43	1.50	A vs. D	4.00	0.15	1.00
D	8	1.44	1.49	1.53	B vs. C	116.0	4.37	0.01
		df	p		B vs. D	112.0	4.22	0.01
		3	0.003		C vs. D	4.00	0.15	1.00
Spray-dried								
	N	Mean	SD	SEM				
A	8	1.68	0.14	0.05				
B	8	1.57	0.10	0.03				
C	8	1.64	0.11	0.04				
D	8	1.63	0.10	0.04				
		df	SS	MS	F	p		
	Between groups	3	0.05	0.02	1.23	0.317		
	Within groups	28	0.36	0.01				
	Total	31	0.41					
Conventional vs. Spray-dried								
		N	Mean	SD	SEM	df	p	
A ^a	Conventional	8	1.48	0.12	0.04	14	0.007	
	Spray-dried	8	1.68	0.14	0.05			
B ^a	Conventional	8	1.32	0.05	0.02	14	< 0.001	
	Spray-dried	8	1.57	0.10	0.03			
C ^a	Conventional	8	1.46	0.06	0.02	14	0.001	
	Spray-dried	8	1.64	0.11	0.04			
		N	Median	25%	75%	p		
D ^b	Conventional	8	1.44	1.39	1.53	0.028		
	Spray-dried	8	1.63	1.54	1.70			
Sum ^{b,c}	Conventional	32	1.42	1.35	1.45	< 0.001		
	Spray-dried	32	1.61	1.54	1.71			

^a Student's t-test.

^b Mann-Whitney rank sum test.

^c Combined GOF values of mineral mixtures A–D for each sample preparation method.

Table S3. Deviations of Rietveld-derived crystalline phase contents in mineral mixtures A–D amended with 0–70 wt% iXAMs and analyzed after conventional sample preparation and spray drying. Total bias is the sum of absolute deviations in each mineral mixture. All values are given in wt%. Mineral abbreviations: Ab = albite; Cal = calcite; Chl = chlorite; Ill-Sme = illite-smectite; Kln = kaolinite; Lb = labradorite; Or = orthoclase; Qz = quartz; Sme = smectite.

Mixture		A – Conventional								A – Spray-dried							
iXAMs (nominal)		0	10	20	30	40	50	60	70	0	10	20	30	40	50	60	70
Qz		-1.98	0.08	-0.42	0.07	-0.23	0.96	-0.26	0.10	0.93	1.31	-0.29	0.52	-0.46	0.35	-0.19	0.63
Or		1.78	3.92	-1.16	0.86	1.17	-0.37	-0.93	-1.05	-1.20	-1.22	-0.89	-2.06	-2.39	-0.95	-2.81	-2.26
Ab		-3.78	-6.06	0.35	-3.01	-2.71	1.13	-0.81	-1.14	-0.53	-0.98	-1.05	-0.55	0.34	-0.79	1.12	-1.31
Ill-Sme		1.71	1.20	2.30	-0.08	1.07	-1.06	1.25	1.21	1.27	1.14	1.60	2.05	1.97	1.80	3.10	3.50
Chl		0.00	-0.46	-0.76	-0.62	-0.05	-0.16	0.01	0.79	-1.44	-1.30	-1.50	-0.69	-0.15	-0.16	0.20	0.78
Kln		1.09	-1.00	-0.66	1.19	1.53	-1.37	2.24	1.57	-0.52	0.29	-0.17	0.04	-0.80	0.07	-0.03	-0.28
Total bias		10.34	12.72	5.65	5.83	6.76	5.05	5.50	5.86	5.89	6.24	5.50	5.91	6.11	4.12	7.45	8.76
Mixture		B – Conventional								B – Spray-dried							
iXAMs (nominal)		0	10	20	30	40	50	60	70	0	10	20	30	40	50	60	70
Qz		-1.01	-1.72	-1.17	-0.91	-1.14	-1.09	-0.69	-0.57	0.20	-1.03	-1.00	-0.96	-1.48	-0.99	-1.18	-0.29
Or		2.41	2.05	2.30	1.80	-0.87	-1.05	-1.89	-1.59	-2.92	-0.89	-0.62	-1.32	-1.06	-3.53	-1.83	-1.06
Ab		-2.68	-3.04	-2.48	-3.74	-0.19	-0.40	0.70	0.66	1.14	-0.95	-1.83	-0.79	-1.22	-0.20	-1.36	-1.54
Cal		-0.88	-1.54	-1.44	-0.98	-0.69	-0.57	-0.72	-0.23	-0.65	-0.47	-0.89	-0.95	-1.13	-1.21	-1.40	-1.33
Ill-Sme		-0.47	1.23	0.56	-0.49	0.74	0.61	0.12	0.41	-0.24	0.22	0.95	0.85	1.88	1.97	2.54	2.31
Kln		0.01	-0.16	-0.05	0.51	0.45	0.40	0.34	0.91	-1.45	-0.78	-0.48	-0.31	-0.23	0.25	-0.05	0.13
Total bias		7.46	9.74	8.00	8.43	4.08	4.12	4.46	4.37	6.60	4.34	5.77	5.18	7.00	8.15	8.36	6.66

Table S3. Continued

Mixture		C – Conventional								C – Spray-dried							
iXAMs (nominal)	0	10	20	30	40	50	60	70	0	10	20	30	40	50	60	70	
Qz	-0.14	-0.55	-0.42	-0.14	0.01	-0.37	0.00	0.04	-0.39	0.08	-0.33	-0.01	-0.15	-0.37	-0.11	-0.47	
Or	-1.51	-1.10	-1.74	-1.20	-1.53	-1.23	-2.21	-1.77	-0.93	-0.36	-1.33	-1.56	-2.19	-2.03	-2.07	-0.34	
Cal	-2.00	-1.35	-1.64	-1.39	-1.68	-1.40	-1.15	-0.81	-0.76	-0.83	-1.23	-0.93	-0.91	-1.80	-1.74	-1.73	
Ilt-Sme	1.15	0.95	0.37	-0.70	-0.35	0.37	-0.20	0.82	-0.65	-1.07	-0.33	0.68	0.66	0.36	1.25	2.32	
Chl	0.28	0.12	-0.18	1.23	0.33	0.27	0.89	1.54	0.41	-0.16	0.39	0.70	0.05	0.87	-0.07	0.18	
Total bias	5.08	4.07	4.35	4.66	3.90	3.64	4.45	4.98	3.14	2.50	3.61	3.88	3.96	5.43	5.24	5.04	
Mixture		D – Conventional								D – Spray-dried							
iXAMs (nominal)	0	10	20	30	40	50	60	70	0	10	20	30	40	50	60	70	
Qz	0.43	0.12	-0.09	0.00	-0.20	-0.19	-0.52	-0.10	0.55	0.83	-0.04	1.04	-0.15	0.30	0.08	-0.21	
Or	0.60	-0.51	0.10	-0.38	2.05	1.12	-2.43	-2.65	0.26	0.49	-0.95	-2.56	-0.77	-2.02	-2.18	-2.30	
Lb	-0.18	-0.80	-2.08	-0.50	-3.34	-1.80	-0.99	-1.27	-0.56	-1.20	-2.50	-1.54	-2.14	-1.57	-1.30	-1.82	
Ilt-Sme	3.51	3.99	4.26	3.36	2.67	1.80	3.11	2.77	2.90	1.77	2.48	3.42	4.08	3.92	3.63	2.77	
Chl	-2.28	-1.81	-1.45	-1.14	-0.77	-0.24	-0.28	0.32	-1.87	-1.36	-0.47	-1.62	-0.89	-1.26	0.48	-0.11	
Kln	-1.28	-1.35	-0.82	-0.37	0.16	-1.03	0.06	0.29	-0.46	0.19	0.76	-0.05	-0.18	0.21	-0.12	1.90	
Sme	-2.95	-1.62	-0.45	-1.32	-0.36	-0.28	-1.05	0.37	-3.80	-3.27	-1.76	-1.93	-0.84	0.41	-0.23	-0.62	
Total bias	11.23	10.19	9.25	7.07	9.55	6.46	8.44	7.77	10.40	9.11	8.96	12.16	9.05	9.69	8.02	9.73	

Table S4. Analysis of variance (ANOVA) and Student's t-tests for feldspar quantification errors (wt%) in mineral mixtures A–D amended with 0–70 wt% iXAMs and analyzed after conventional sample preparation and spray drying. Significant p-values are marked in bold. SD: standard deviation; SEM: standard error of the mean; df: degrees of freedom; SS: sum of squares; MS: mean squared errors.

Conventional									
Feldspars ^a	Kruskal-Wallis ANOVA on Ranks								
	N	Median	25%	75%					
	A	16	-0.87	-2.32	1.06				
	B	16	-0.64	-2.33	1.53				
	C	8	-1.52	-1.76	-1.21				
D	16	-0.66	-2.01	0.03					
		df	p						
		3	0.388						
Orthoclase	Kruskal-Wallis ANOVA on Ranks					Post-hoc tests (Tukey)			
	N	Median	25%	75%	Comparison	Diff. of ranks	q	p	
	A	8	0.25	-1.02	1.63	A vs. B	9.50	0.36	0.99
	B	8	0.47	-1.46	2.24	A vs. C	104.0	3.90	0.03
	C	8	-1.52	-1.76	-1.21	A vs. D	33.00	1.24	0.82
D	8	-0.14	-1.95	0.99	B vs. C	94.00	3.54	0.06	
		df	p						
		3	0.025						
B vs. D					B vs. D	23.50	0.89	0.92	
C vs. D					C vs. D	70.50	2.66	0.24	
Albite	Student's t-test								
	N	Mean	SD	SEM	df	p			
A	8	-2.00	2.35	0.83	14	0.569			
B	8	-1.40	1.78	0.63					
Spray-dried									
Feldspars ^a									
	N	Mean	SD	SEM					
	A	16	-1.72	0.72	0.18				
	B	16	-1.25	1.05	0.26				
	C	8	-1.35	0.75	0.26				
D	16	-1.42	0.92	0.23					
		df	SS	MS	F	p			
	Between groups	3	1.93	0.64	0.82	0.49			
	Within groups	52	40.89	0.79					
	Total	55	42.82						
Orthoclase									
	N	Mean	SD	SEM					
	A	8	-1.72	0.74	0.26				
	B	8	-1.65	1.04	0.37				
	C	8	-1.35	0.75	0.26				
D	8	-1.25	1.19	0.42					
		df	SS	MS	F	p			
	Between groups	3	1.26	0.42	0.46	0.712			
	Within groups	28	25.28	0.90					
	Total	31	26.53						
Albite	Student's t-test								
	N	Mean	SD	SEM	df	p			
A	8	-1.72	0.74	0.26	14	0.058			
B	8	-0.84	0.94	0.33					

^aFor all feldspars (albite, labradorite, and orthoclase) in mineral mixtures.

Table S5. Analysis of variance (ANOVA) and Student's t-tests for clay mineral (chlorite, illite-smectite, kaolinite, smectite) quantification errors (wt%) in mineral mixtures A–D amended with 0–70 wt% iXAMs and analyzed after conventional sample preparation and spray drying. Significant p-values are marked in bold. SD: standard deviation; SEM: standard error of the mean; df: degrees of freedom.

Conventional							
Kruskal-Wallis ANOVA on Ranks							
	N	Median	25%	75%			
A	24	0.40	-0.58	1.24			
B	16	0.41	-0.04	0.60			
C	16	0.35	-0.11	0.94			
D	32	-0.32	-1.25	1.44			
	df	p					
	3	0.188					
Spray-dried							
Kruskal-Wallis ANOVA on Ranks							
	N	Median	25%	75%			
A	24	0.06	-0.46	1.52			
B	16	0.18	-0.29	1.65			
C	16	0.38	-0.14	0.70			
D	32	-0.12	-1.17	1.87			
	df	p					
	3	0.792					
Conventional vs. Spray-dried							
		N	Mean	SD	SEM	df	p
A	Conventional	24	0.46	1.09	0.22	46	0.984
	Spray-dried	24	0.45	1.35	0.28		
B	Conventional	16	0.32	0.47	0.12	30	0.632
	Spray-dried	16	0.47	1.17	0.29		
C	Conventional	16	0.43	0.62	0.16	30	0.749
	Spray-dried	16	0.35	0.79	0.20		
		N	Median	25%	75%	p	
D ^a	Conventional	32	-0.32	-1.25	1.44	0.697	
	Spray-dried	32	-0.12	-1.17	1.87		
Total ^b	Conventional	88	0.22	-0.47	1.09	0.991	
	Spray-dried	88	0.10	-0.48	1.22		

^a Mann-Whitney rank sum test.

^b For all mixtures of each sample preparation method.

Table S6. Analysis of variance (ANOVA) of individual clay mineral quantification errors (wt%) in mineral mixtures A–D amended with 0–70 wt% iXAMs and analyzed after conventional sample preparation and spray drying. Significant p-values are marked in bold. SD: standard deviation; SEM: standard error of the mean; df: degrees of freedom; SS: sum of squares; MS: mean squared errors.

Conventional									
Chlorite					Post-hoc tests (Holm-Sidak method)				
	N	Mean	SD	SEM	Comparison	Diff. of means	t	p	
A	8	-0.16	0.48	0.17	A vs. C	0.72	2.13	0.053	
C	8	0.56	0.60	0.21	A vs. D	0.80	2.38	0.053	
D	8	-0.96	0.88	0.31	C vs. D	1.52	4.51	<0.001	
		df	SS	MS	F	p			
Between groups		2	9.21	4.60	10.17	<0.001			
Within groups		21	9.50	0.45					
Total		23	18.70						
Illite-smectite					Post-hoc tests (Holm-Sidak method)				
	N	Mean	SD	SEM	Comparison	Diff. of means	t	p	
A	8	0.95	1.05	0.37	A vs. B	0.61	1.54	0.302	
B	8	0.34	0.59	0.21	A vs. C	0.65	1.64	0.302	
C	8	0.30	0.67	0.24	A vs. D	2.23	5.63	<0.001	
D	8	3.18	0.78	0.28	B vs. C	0.04	0.09	0.925	
		df	SS	MS	F	p			
Between groups		3	44.37	14.79	23.52	<0.001			
Within groups		28	17.61	0.63					
Total		31	61.98						
Kaolinite					Kruskal-Wallis ANOVA on Ranks				
	N	Median	25%	75%					
A	8	1.14	-0.92	1.56					
B	8	0.37	-0.04	0.50					
D	8	-0.60	-1.22	0.14					
		df	p						
		3	0.064						
Spray-dried									
Chlorite					Post-hoc tests (Holm-Sidak method)				
	N	Mean	SD	SEM	Comparison	Diff. of means	t	p	
A	8	-0.53	0.83	0.30	A vs. C	0.83	2.36	0.055	
C	8	0.30	0.36	0.13	A vs. D	0.36	1.01	0.324	
D	8	-0.89	0.80	0.28	C vs. D	1.18	3.37	0.009	
		df	SS	MS	F	p			
Between groups		2	5.90	2.95	5.98	0.009			
Within groups		21	10.36	0.49					
Total		23	16.27						
Illite-smectite					Post-hoc tests (Holm-Sidak method)				
	N	Mean	SD	SEM	Comparison	Diff. of means	t	p	
A	8	2.05	0.84	0.29	A vs. B	0.74	1.58	0.125	
B	8	1.31	1.02	0.36	A vs. C	1.65	3.51	0.006	
C	8	0.40	1.09	0.39	A vs. D	1.07	2.27	0.091	
D	8	3.12	0.79	0.28	B vs. C	0.91	1.93	0.124	
		df	SS	MS	F	p			
Between groups		3	31.83	10.61	11.99	<0.001			
Within groups		28	24.78	0.89					
Total		31	56.62						
Kaolinite									
	N	Mean	SD	SEM					
A	8	-0.18	0.35	0.12					
B	8	-0.37	0.55	0.19					
D	8	0.28	0.75	0.26					
		df	SS	MS	F	p			
Between groups		2	1.78	0.88	2.69	0.091			
Within groups		21	6.87	0.33					
Total		33	8.63						

Table S7. Student's t-tests of the effect of sample preparation on quantification errors (wt%) of individual clay minerals in mineral mixtures A–D amended with 0–70 wt% iXAMs. Significant p-values are marked in bold. SD: standard deviation; SEM: standard error of the mean; df: degrees of freedom.

Chlorite		N	Mean	SD	SEM	df	p
A	Conventional	8	-0.16	0.48	0.17	14	0.290
	Spray-dried	8	-0.53	0.84	0.30		
C	Conventional	8	0.56	0.60	0.21	14	0.303
	Spray-dried	8	0.30	0.37	0.13		
D	Conventional	8	-0.96	0.88	0.31	14	0.872
	Spray-dried	8	-0.89	0.80	0.28		
Total ^a	Conventional	24	-0.18	0.90	0.18	46	0.453
	Spray-dried	24	-0.38	0.84	0.17		
Illite-Smectite		N	Mean	SD	SEM	df	p
A	Conventional	8	0.95	1.05	0.37	14	0.036
	Spray-dried	8	2.05	0.84	0.30		
B	Conventional	8	0.34	0.59	0.21	14	0.035
	Spray-dried	8	1.31	1.02	0.36		
C	Conventional	8	0.30	0.67	0.24	14	0.826
	Spray-dried	8	0.40	1.09	0.39		
D	Conventional	8	3.18	0.78	0.28	14	0.876
	Spray-dried	8	3.12	0.79	0.28		
Total	Conventional	32	1.19	1.41	0.25	62	0.132
	Spray-dried	32	1.72	1.35	0.24		
Kaolinite		N	Mean	SD	SEM	df	p
A	Conventional	8	0.57	1.37	0.48	14	0.156
	Spray-dried	8	-0.18	0.35	0.12		
B	Conventional	8	0.30	0.35	0.13	14	0.012
	Spray-dried	8	-0.37	0.55	0.19		
D	Conventional	8	-0.54	0.66	0.24	14	0.035
	Spray-dried	8	0.28	0.75	0.26		
Total	Conventional	24	0.11	0.99	0.20	46	0.453
	Spray-dried	24	-0.09	0.61	0.13		
Smectite		N	Mean	SD	SEM	df	p
D	Conventional	8	-0.96	1.03	0.36	14	0.403
	Spray-dried	8	-1.51	1.47	0.52		

^aFor all mixtures of each sample preparation method.

Table S8. Chemical compositions (wt%) of initial mineral mixtures A–D (no iXAMs added) as determined by XRF spectrometry and Rietveld-based QPA of XRD data, including their difference.

Mixture		SiO ₂	TiO ₂	Al ₂ O ₃	Fe ₂ O ₃	MgO	CaO	Na ₂ O	K ₂ O	LOI ^a	Total ^b
Conventional											
A	XRF	82.02	0.11	9.64	0.30	1.96	0.18	1.63	1.48	2.53	99.80
	XRD	81.03	0.00	10.69	0.99	2.50	0.27	1.52	1.82	0.00	98.82
	Diff.	0.99	0.11	-1.05	-0.69	-0.54	-0.09	0.11	-0.34	2.53	
B	XRF	73.07	0.11	10.35	0.14	0.32	5.70	1.62	1.86	6.60	99.80
	XRD	72.98	0.00	9.69	0.47	0.94	5.36	1.59	2.32	4.01	97.36
	Diff.	0.09	0.11	0.66	-0.33	-0.62	0.34	0.03	-0.46	2.59	
C	XRF	61.58	0.04	9.82	0.29	2.19	11.13	0.95	2.52	11.31	99.80
	XRD	61.99	0.00	9.05	1.57	3.06	10.36	0.80	3.03	7.91	97.77
	Diff.	-0.41	0.04	0.77	-1.28	-0.87	0.77	0.15	-0.52	3.40	
D	XRF	62.18	0.38	20.98	0.86	2.54	1.30	1.82	2.97	6.69	99.80
	XRD	64.58	0.00	21.51	1.86	2.04	2.60	1.68	3.58	0.00	97.85
	Diff.	-2.40	0.38	-0.53	-1.00	0.50	-1.31	0.14	-0.61	6.69	
Spray-dried											
A	XRF	82.02	0.11	9.64	0.30	1.96	0.18	1.63	1.48	2.53	99.80
	XRD	83.12	0.00	9.20	1.21	1.39	0.16	1.60	1.82	0.00	98.50
	Diff.	-1.10	0.11	0.44	-0.91	0.57	0.02	0.03	-0.34	2.53	
B	XRF	73.07	0.11	10.35	0.14	0.32	5.70	1.62	1.86	6.60	99.80
	XRD	72.64	0.00	8.66	0.60	0.95	5.35	1.64	2.13	4.11	96.08
	Diff.	0.43	0.11	1.69	-0.46	-0.63	0.35	-0.02	-0.27	2.49	
C	XRF	61.58	0.04	9.82	0.29	2.19	11.13	0.95	2.52	11.31	99.80
	XRD	61.09	0.00	8.71	1.49	3.13	11.07	0.83	2.88	8.46	97.66
	Diff.	0.49	0.04	1.11	-1.20	-0.94	0.06	0.12	-0.37	2.85	
D	XRF	62.18	0.38	20.98	0.86	2.54	1.30	1.82	2.97	6.69	99.80
	XRD	64.16	0.00	21.86	0.98	2.30	2.34	1.37	4.00	0.00	97.01
	Diff.	-1.98	0.38	-0.88	-0.12	0.24	-1.05	0.45	-1.03	6.69	

^a Includes the amount of CO₂ from Rietveld-based QPA of XRD data.

^b The difference of ‘total XRD’ to 100 equals the intrinsic amorphous content of initial mixtures.

Table S9. Chemical compositions (wt%) of mineral mixtures B–D amended with 10–70 wt% iXAMs as determined by XRF spectrometry and nominal chemical compositions of iXAMs in mineral mixtures calculated from XRF data of the 1:1 (w/w) mixture of ferrihydrite and opal-A.

Nominal iXAMs	SiO ₂	TiO ₂	Al ₂ O ₃	Fe ₂ O ₃	MgO	CaO	Na ₂ O	K ₂ O	LOI	Total
Mixture B										
10	69.98	0.10	9.29	4.47	0.28	5.18	1.48	1.68	7.35	99.88
20	66.84	0.10	8.29	8.74	0.26	4.59	1.31	1.49	8.17	99.90
30	63.60	0.08	7.28	13.03	0.22	4.05	1.18	1.30	9.05	99.89
40	60.61	0.08	6.24	17.35	0.20	3.51	1.01	1.11	9.66	99.89
50	57.27	0.07	5.21	21.59	0.17	2.94	0.82	0.94	10.80	99.88
60	54.16	0.05	4.19	25.76	0.14	2.36	0.69	0.75	11.70	99.92
70	51.25	0.05	3.19	30.23	0.11	1.80	0.53	0.57	12.09	99.91
Mixture C										
10	59.54	0.04	8.81	4.66	1.97	10.07	0.87	2.27	11.57	99.89
20	57.64	0.04	7.87	8.99	1.74	8.95	0.80	2.02	11.78	99.89
30	55.42	0.03	6.85	13.30	1.52	7.82	0.69	1.77	12.27	99.74
40	53.53	0.03	5.91	17.59	1.31	6.76	0.63	1.51	12.51	99.90
50	51.76	0.03	4.95	22.02	1.10	5.65	0.52	1.28	12.49	99.91
60	49.80	0.03	3.95	26.34	0.87	4.54	0.42	1.01	12.86	99.92
70	47.70	0.03	2.99	30.42	0.66	3.41	0.32	0.76	13.53	99.90
Mixture D										
10	60.19	0.34	18.97	5.19	2.29	1.19	1.67	2.66	7.22	99.84
20	58.20	0.31	16.85	9.46	2.04	1.07	1.49	2.40	7.95	99.85
30	56.08	0.27	14.73	13.69	1.78	0.94	1.29	2.07	8.90	99.87
40	53.97	0.24	12.57	17.92	1.52	0.82	1.11	1.77	9.85	99.86
50	52.15	0.20	10.58	22.14	1.27	0.69	0.94	1.49	10.33	99.87
60	49.92	0.17	8.46	26.39	1.02	0.57	0.78	1.19	11.28	99.91
70	48.07	0.13	6.36	30.72	0.77	0.45	0.58	0.90	11.84	99.90
iXAMs^a										
10	4.13	0.00	0.01	4.30	0.00	0.01	0.00	0.00	1.53	10.00
20	8.25	0.00	0.02	8.61	0.00	0.01	0.01	0.00	3.07	19.99
30	12.38	0.01	0.02	12.91	0.01	0.02	0.01	0.00	4.60	29.99
40	16.51	0.01	0.03	17.22	0.01	0.02	0.02	0.00	6.13	39.98
50	20.64	0.01	0.04	21.52	0.01	0.03	0.02	0.01	7.67	49.98
60	24.76	0.01	0.05	25.82	0.01	0.04	0.02	0.01	9.20	59.98
70	28.89	0.01	0.06	30.13	0.01	0.04	0.03	0.01	10.73	69.97
100	41.27	0.02	0.08	43.04	0.02	0.06	0.04	0.01	15.33	99.96

^a Values for nominal iXAM contents of 10–70 wt% were calculated from the 1:1 (w/w) mixture of ferrihydrite and opal-A.

Table S10. Chemical compositions (wt%) of conventionally prepared and spray-dried mineral mixtures B–D amended with 10–70 wt% iXAMs as determined by XRF-spectrometry and their respective iXAM chemical compositions obtained from oxide mass balances.

Nominal iXAMs	SiO ₂	Al ₂ O ₃	Fe ₂ O ₃	MgO	CaO	Na ₂ O	K ₂ O	LOI ^a	SiO ₂	Al ₂ O ₃	Fe ₂ O ₃	MgO	CaO	Na ₂ O	K ₂ O	LOI ^a
B – Conventional									B – Spray-dried							
10	65.12	8.75	0.63	0.95	4.40	1.35	2.24	3.28	64.50	8.09	0.56	0.88	4.94	1.41	1.96	3.75
iXAMs ^b	4.86	0.54	3.84	-0.67	0.78	0.13	-0.56	4.07	5.48	1.20	3.91	-0.60	0.24	0.07	-0.28	3.60
20	58.55	7.91	0.45	0.81	3.88	1.24	2.01	2.89	57.21	7.14	0.72	0.83	4.12	1.14	1.84	3.13
iXAMs	8.29	0.38	8.29	-0.55	0.71	0.07	-0.52	5.28	9.63	1.15	8.02	-0.57	0.47	0.17	-0.35	5.04
30	49.80	6.32	0.76	0.64	3.58	0.99	1.44	2.65	49.98	5.92	1.14	0.72	3.48	1.00	1.62	2.66
iXAMs	13.80	0.96	12.27	-0.42	0.47	0.19	-0.14	6.40	13.62	1.36	11.89	-0.50	0.57	0.18	-0.32	6.39
40	43.59	6.16	0.17	0.63	3.06	0.94	1.43	2.33	42.71	5.83	0.24	0.71	2.82	0.84	1.47	2.14
iXAMs	17.02	0.08	17.18	-0.43	0.45	0.07	0.07	7.33	17.90	0.41	17.11	-0.51	0.69	0.17	0.17	7.52
50	35.73	4.74	0.53	0.52	2.54	0.72	1.17	1.95	35.13	4.70	0.32	0.61	2.15	0.63	1.09	1.67
iXAMs	21.54	0.47	21.06	-0.35	0.40	0.10	-0.23	8.85	22.14	0.51	21.27	-0.44	0.79	0.19	-0.15	9.13
60	28.50	3.44	0.76	0.38	1.85	0.60	0.87	1.44	27.93	3.68	0.47	0.55	1.50	0.44	1.01	1.14
iXAMs	25.66	0.75	25.00	-0.24	0.51	0.09	-0.12	10.26	26.23	0.51	25.29	-0.41	0.86	0.25	-0.26	10.56
70	21.84	2.92	0.61	0.31	1.55	0.43	0.72	1.22	22.31	3.49	0.01	0.51	0.99	0.28	0.86	0.76
iXAMs	29.41	0.27	29.62	-0.20	0.25	0.10	-0.15	10.87	28.94	-0.30	30.22	-0.40	0.81	0.25	-0.29	11.33
C – Conventional									C – Spray-dried							
10	55.36	7.67	1.89	2.80	9.58	0.72	2.75	7.32	55.49	8.56	0.43	2.77	9.90	0.80	2.57	7.55
iXAMs	4.18	1.14	2.77	-0.83	0.49	0.15	-0.48	4.25	4.05	0.25	4.23	-0.80	0.17	0.07	-0.30	4.02
20	48.41	6.37	1.80	2.31	8.25	0.58	2.35	6.31	48.80	7.41	0.21	2.80	8.48	0.58	2.40	6.49
iXAMs	9.23	1.50	7.19	-0.57	0.70	0.22	-0.34	5.47	8.84	0.46	8.78	-1.06	0.47	0.22	-0.39	5.29
30	42.55	5.86	1.68	2.41	7.24	0.52	2.00	5.55	43.99	6.25	0.06	2.70	7.50	0.51	2.13	5.75
iXAMs	12.87	0.99	11.62	-0.89	0.58	0.17	-0.23	6.72	11.43	0.60	13.24	-1.18	0.32	0.18	-0.36	6.52
40	36.18	4.58	1.64	1.80	5.92	0.41	1.70	4.54	36.67	4.98	0.94	1.47	6.34	0.37	1.80	4.88
iXAMs	17.35	1.33	15.95	-0.49	0.84	0.22	0.22	7.97	16.86	0.93	16.65	-0.16	0.42	0.26	0.26	7.63
50	30.18	3.94	1.41	1.56	4.93	0.34	1.49	3.78	30.03	4.69	0.32	1.93	4.71	0.32	1.43	3.61
iXAMs	21.58	1.01	20.61	-0.46	0.72	0.18	-0.22	8.71	21.73	0.26	21.70	-0.83	0.94	0.20	-0.16	8.88
60	23.98	2.93	0.83	1.40	3.91	0.20	1.09	3.01	24.50	3.43	0.52	1.04	3.59	0.23	1.21	2.75
iXAMs	25.82	1.02	25.51	-0.53	0.63	0.22	-0.08	9.85	25.30	0.52	25.82	-0.17	0.95	0.19	-0.20	10.11
70	18.79	2.52	1.04	1.19	2.95	0.11	0.95	2.28	19.65	3.14	0.60	0.81	2.43	0.12	1.34	1.88
iXAMs	28.91	0.47	29.38	-0.53	0.46	0.21	-0.19	11.25	28.05	-0.15	29.82	-0.15	0.98	0.20	-0.58	11.65

Table S10. Continued

Nominal iXAMs	SiO ₂	Al ₂ O ₃	Fe ₂ O ₃	MgO	CaO	Na ₂ O	K ₂ O	LOI ^a	SiO ₂	Al ₂ O ₃	Fe ₂ O ₃	MgO	CaO	Na ₂ O	K ₂ O	LOI ^a
	D – Conventional									D – Spray-dried						
10	57.92	19.33	1.29	2.48	2.35	1.43	3.23	0.00	58.32	19.46	0.63	2.27	2.05	1.26	3.47	0.00
iXAMs ^b	2.27	-0.36	3.90	-0.19	-1.16	0.24	-0.57	7.22	1.87	-0.49	4.56	0.02	-0.86	0.41	-0.81	7.22
20	52.59	17.55	0.78	2.28	2.03	1.25	3.00	0.00	50.72	17.91	0.91	2.18	1.74	0.99	3.06	0.00
iXAMs	5.61	-0.70	8.68	-0.24	-0.97	0.24	-0.60	7.95	7.48	-1.06	8.55	-0.14	-0.68	0.50	-0.66	7.95
30	45.72	16.01	0.39	2.02	1.84	1.11	2.57	0.00	44.73	14.81	0.62	1.64	1.57	0.92	2.47	0.00
iXAMs	10.36	-1.28	13.30	-0.24	-0.90	0.18	-0.50	8.90	11.35	-0.08	13.07	0.14	-0.63	0.37	-0.40	8.90
40	39.53	13.54	0.98	1.51	1.32	0.98	2.35	0.00	39.05	13.26	0.57	1.66	1.35	0.79	2.42	0.00
iXAMs	14.44	-0.97	16.94	0.01	-0.50	0.13	0.13	9.85	14.92	-0.69	17.35	-0.14	-0.53	0.32	0.32	9.85
50	32.50	10.67	1.15	1.16	1.23	0.84	1.82	0.00	32.81	11.17	1.01	1.12	1.27	0.65	1.83	0.00
iXAMs	19.65	-0.09	20.99	0.11	-0.54	0.10	-0.33	10.33	19.34	-0.59	21.13	0.15	-0.58	0.29	-0.34	10.33
60	24.70	8.64	0.74	1.02	0.87	0.45	1.49	0.00	25.74	9.43	0.88	1.11	0.82	0.46	1.48	0.00
iXAMs	25.22	-0.18	25.65	0.00	-0.30	0.33	-0.30	11.28	24.18	-0.97	25.51	-0.09	-0.25	0.32	-0.29	11.28
70	18.97	6.80	1.18	0.74	0.71	0.31	1.02	0.00	20.97	3.95	1.69	0.84	0.73	0.31	1.14	0.00
iXAMs	29.10	-0.44	29.54	0.03	-0.26	0.27	-0.12	11.84	27.10	2.41	29.03	-0.07	-0.28	0.27	-0.24	11.84

^a Includes the amount of CO₂ from Rietveld-based QPA of XRD data.

^b Chemical composition of iXAMs in mineral mixtures calculated from XRF spectrometry (Table S9) and Rietveld results.

Table S11. Minor oxide compositions (wt%) for iXAMs in mineral mixtures B–D amended with 10–70 wt% iXAMs determined by oxide mass balancing using XRF spectrometry and Rietveld results obtained after conventional sample preparation and spray drying.

Mixture		B – Conventional							B – Spray-dried						
iXAMs (nominal)		10	20	30	40	50	60	70	10	20	30	40	50	60	70
Al ₂ O ₃		0.54	0.38	0.96	0.08	0.47	0.75	0.27	1.20	1.15	1.36	0.41	0.51	0.51	-0.30
CaO		0.78	0.71	0.47	0.45	0.40	0.51	0.25	0.24	0.47	0.57	0.69	0.79	0.86	0.81
K ₂ O		-0.56	-0.52	-0.14	-0.32	-0.23	-0.12	-0.15	-0.28	-0.35	-0.32	-0.36	-0.15	-0.26	-0.29
MgO		-0.67	-0.55	-0.42	-0.43	-0.35	-0.24	-0.20	-0.60	-0.57	-0.50	-0.51	-0.44	-0.41	-0.40
Na ₂ O		0.13	0.07	0.19	0.07	0.10	0.09	0.10	0.07	0.17	0.18	0.17	0.19	0.25	0.25
Sum		0.21	0.09	1.07	-0.15	0.39	0.98	0.27	0.62	0.87	1.30	0.40	0.90	0.94	0.07
Mixture		C – Conventional							C – Spray-dried						
iXAMs (nominal)		10	20	30	40	50	60	70	10	20	30	40	50	60	70
Al ₂ O ₃		1.14	1.50	0.99	1.33	1.01	1.02	0.47	0.25	0.46	0.60	0.93	0.26	0.52	-0.15
CaO		0.49	0.70	0.58	0.84	0.72	0.63	0.46	0.17	0.47	0.32	0.42	0.94	0.95	0.98
K ₂ O		-0.48	-0.34	-0.23	-0.19	-0.22	-0.08	-0.19	-0.30	-0.39	-0.36	-0.29	-0.16	-0.20	-0.58
MgO		-0.83	-0.57	-0.89	-0.49	-0.46	-0.53	-0.53	-0.80	-1.06	-1.18	-0.16	-0.83	-0.17	-0.15
Na ₂ O		0.15	0.22	0.17	0.22	0.18	0.22	0.21	0.07	0.22	0.18	0.26	0.20	0.19	0.20
Sum		0.47	1.52	0.61	1.71	1.24	1.26	0.42	-0.61	-0.29	-0.45	1.16	0.42	1.29	0.29
Mixture		D – Conventional							D – Spray-dried						
iXAMs (nominal)		10	20	30	40	50	60	70	10	20	30	40	50	60	70
Al ₂ O ₃		-0.36	-0.69	-1.30	-0.97	-0.09	-0.18	-0.44	-0.49	-1.06	-0.08	-0.69	-0.59	-0.97	2.41
CaO		-1.16	-0.97	-0.90	-0.50	-0.54	-0.30	-0.26	-0.86	-0.68	-0.63	-0.53	-0.58	-0.25	-0.28
K ₂ O		-0.57	-0.60	-0.50	-0.58	-0.33	-0.30	-0.12	-0.81	-0.66	-0.40	-0.65	-0.34	-0.29	-0.24
MgO		-0.19	-0.24	-0.24	0.01	0.11	0.00	0.03	0.02	-0.14	0.14	-0.14	0.15	-0.09	-0.07
Na ₂ O		0.24	0.24	0.18	0.13	0.10	0.33	0.27	0.41	0.50	0.37	0.32	0.29	0.32	0.27
Sum		-2.05	-2.26	-2.73	-1.91	-0.75	-0.45	-0.53	-1.74	-2.03	-0.59	-1.69	-1.07	-1.28	2.08

Table S12. Summed SiO₂, Fe₂O₃, and LOI contents of iXAMs and their individual quantification errors for mineral mixtures B–D amended with 10–70 wt% iXAMs determined by oxide mass balancing using XRF spectrometry and Rietveld results obtained after conventional sample preparation and spray drying. All values are given in wt%.

Mixture		B – Conventional							B – Conventional						
iXAMs (nominal)		10	20	30	40	50	60	70	10	20	30	40	50	60	70
Sum ^a		12.77	21.86	32.47	41.53	51.45	60.92	69.90	12.99	22.69	31.90	42.53	52.54	62.08	70.49
SiO ₂		0.73	0.04	1.42	0.51	0.90	0.90	0.52	1.35	1.38	1.24	1.39	1.51	1.47	0.05
Fe ₂ O ₃		-0.46	-0.32	-0.64	-0.04	-0.46	-0.82	-0.51	-0.39	-0.59	-1.02	-0.11	-0.25	-0.53	0.09
LOI ^b		2.54	2.21	1.80	1.20	1.19	1.06	0.14	2.07	1.97	1.79	1.39	1.47	1.36	0.60
Mixture		C – Conventional							C – Conventional						
iXAMs (nominal)		10	20	30	40	50	60	70	10	20	30	40	50	60	70
Sum		11.20	21.89	31.21	41.27	50.90	61.18	69.54	12.30	22.91	31.19	41.14	52.31	61.23	69.52
SiO ₂		0.05	0.98	0.49	0.84	0.94	1.06	0.02	-0.08	0.59	-0.95	0.35	1.10	0.54	-0.84
Fe ₂ O ₃		-1.53	-1.42	-1.29	-1.27	-0.91	-0.31	-0.75	-0.07	0.17	0.33	-0.57	0.18	0.00	-0.31
LOI ^b		2.72	2.40	2.12	1.84	1.05	0.65	0.52	2.49	2.22	1.92	1.50	1.22	0.91	0.92
Mixture		D – Conventional							D – Conventional						
iXAMs (nominal)		10	20	30	40	50	60	70	10	20	30	40	50	60	70
Sum		13.39	22.24	32.56	41.23	50.97	62.15	70.48	13.65	23.98	33.32	42.12	50.80	60.67	67.97
SiO ₂		-1.86	-2.64	-2.02	-2.07	-0.99	0.46	0.21	-2.26	-0.77	-1.03	-1.59	-1.30	-0.58	-1.79
Fe ₂ O ₃		-0.40	0.07	0.39	-0.28	-0.53	-0.17	-0.59	0.26	-0.06	0.16	0.13	-0.39	-0.31	-1.10
LOI ^b		5.69	4.88	4.30	3.72	2.67	2.08	1.11	5.69	4.88	4.30	3.72	2.67	2.08	1.11

^a Sum of SiO₂, Fe₂O₃ and LOI/CO₂ derived by the balance sheet method (Table S10).

^b Includes the amount of CO₂ from Rietveld-based QPA of XRD data.