soil systems

MDPI

Supplementary information

Supplementary Information to: Soil Development under Continuous Agriculture at the Morrow Plots Experimental Fields from X-Ray Diffraction Profile Modelling

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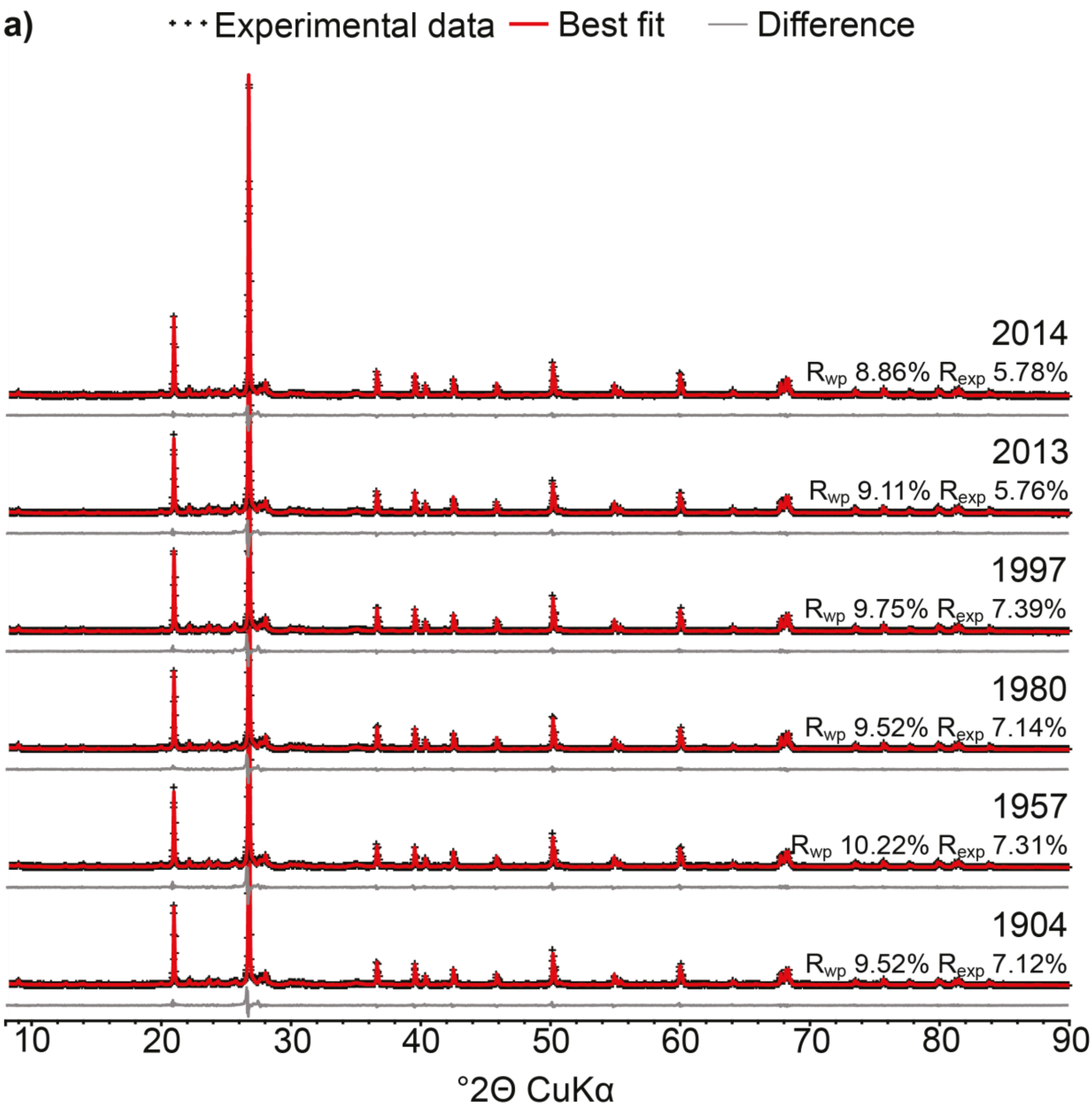

Figure S1a. Quantitative phase analysis of the 50–2 μm fraction for 1904–2014 soil samples. Best fit to the XRD patterns obtained from the 50–2 μm fraction of all samples. Experimental data is shown as black crosses, best fit as solid red lines, and the difference plots as solid grey lines.

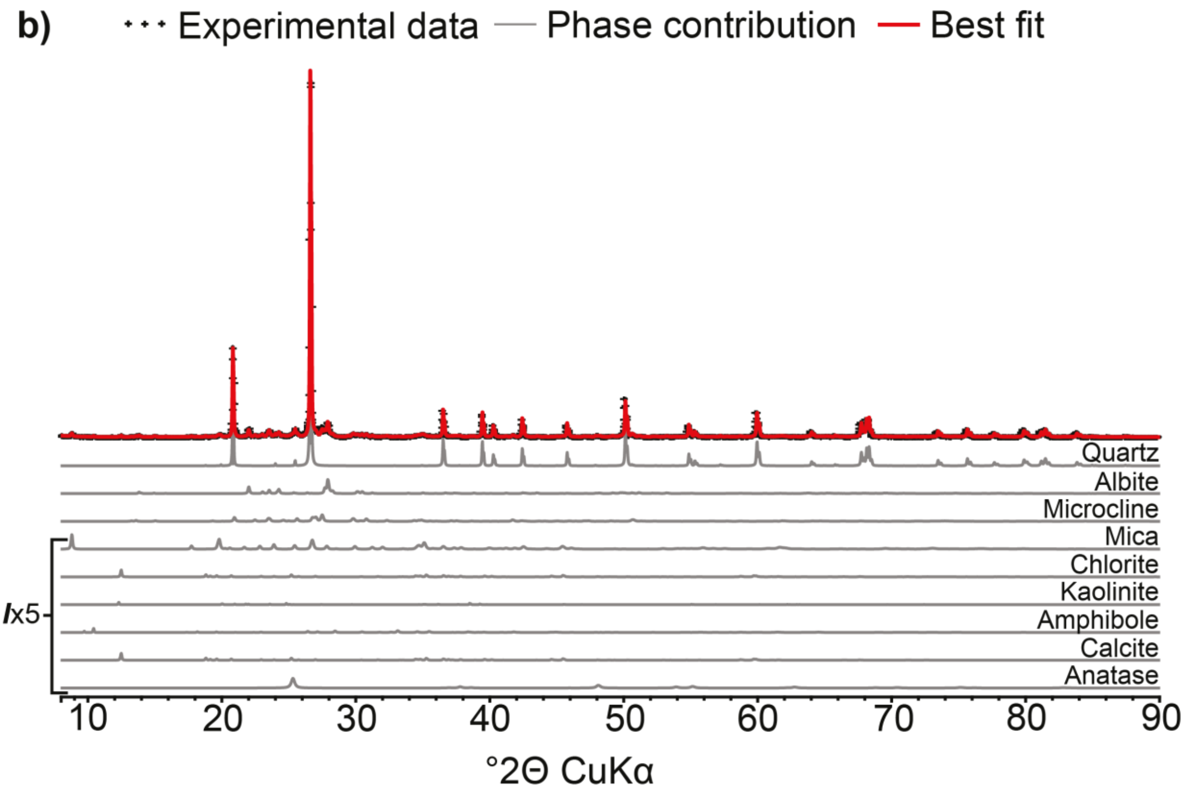

Figure S1b. Quantitative phase analysis of the 50–2 μm fraction for 1904–2014 soil samples. Best fit to sample 2014 RU. Experimental data is shown as black crosses, best fit as solid red lines and individual contributions to the intensity as solid grey lines.

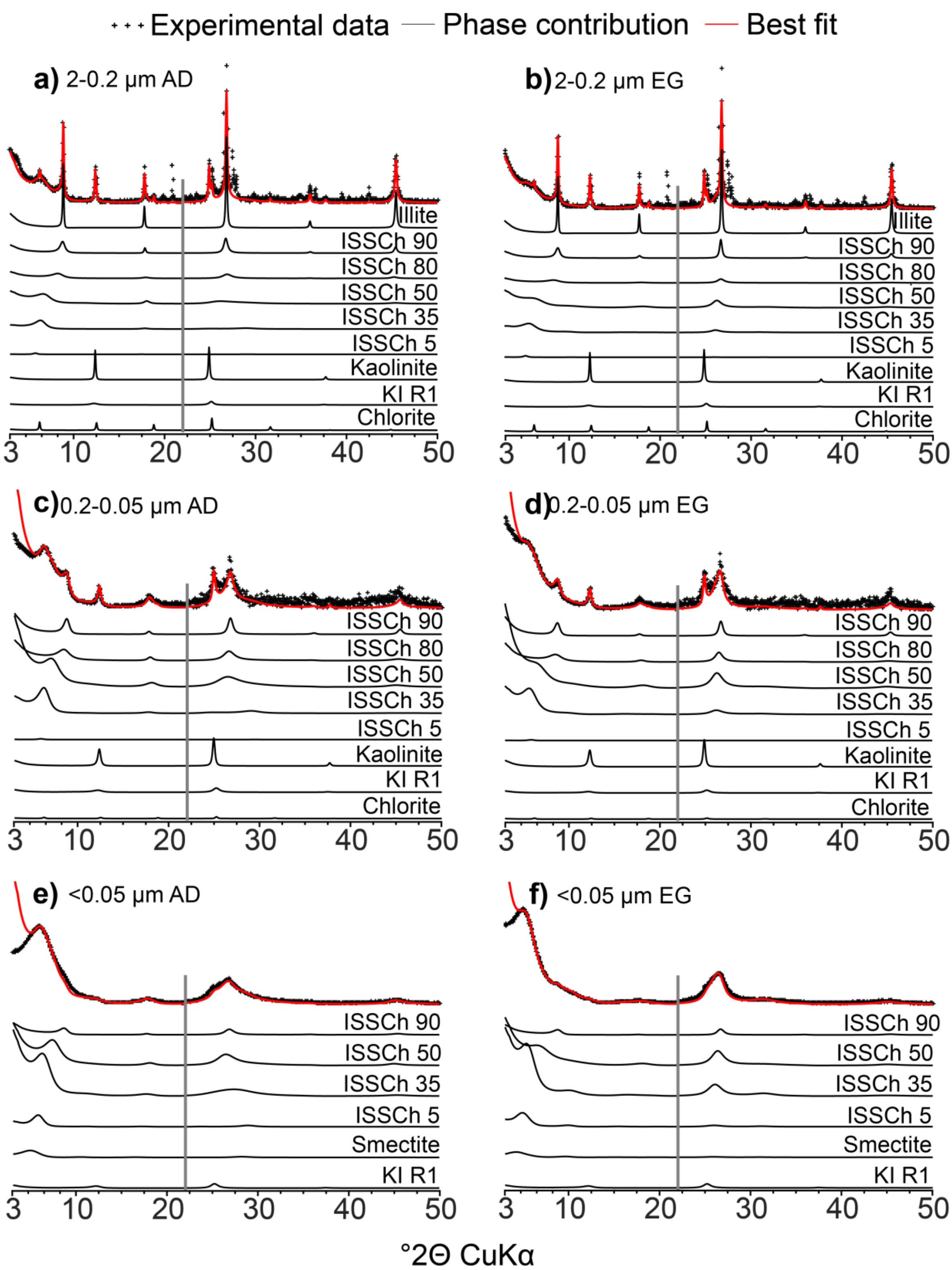

Figure S2. Elementary contributions to the intensity diffracted by the different clay subfractions of soil sample 2014: (**a**) Ca-AD pattern of the 2–0.2 μm subfraction; (**b**) Ca-EG pattern of the 2–0.2 μm subfraction; (**c**) Ca-AD pattern of the 0.2–0.05 μm subfraction; (**d**) Ca-EG pattern of the 0.2–0.05 μm subfraction; (**e**) Ca-AD pattern of the <0.05 μm subfraction; (**f**) Ca-EG pattern of the <0.05 μm subfraction. The structural parameters for the optimal models are given in Table S2. Experimental data is shown as black crosses, best fit as solid red lines and individual contributions to the intensity as solid black lines.

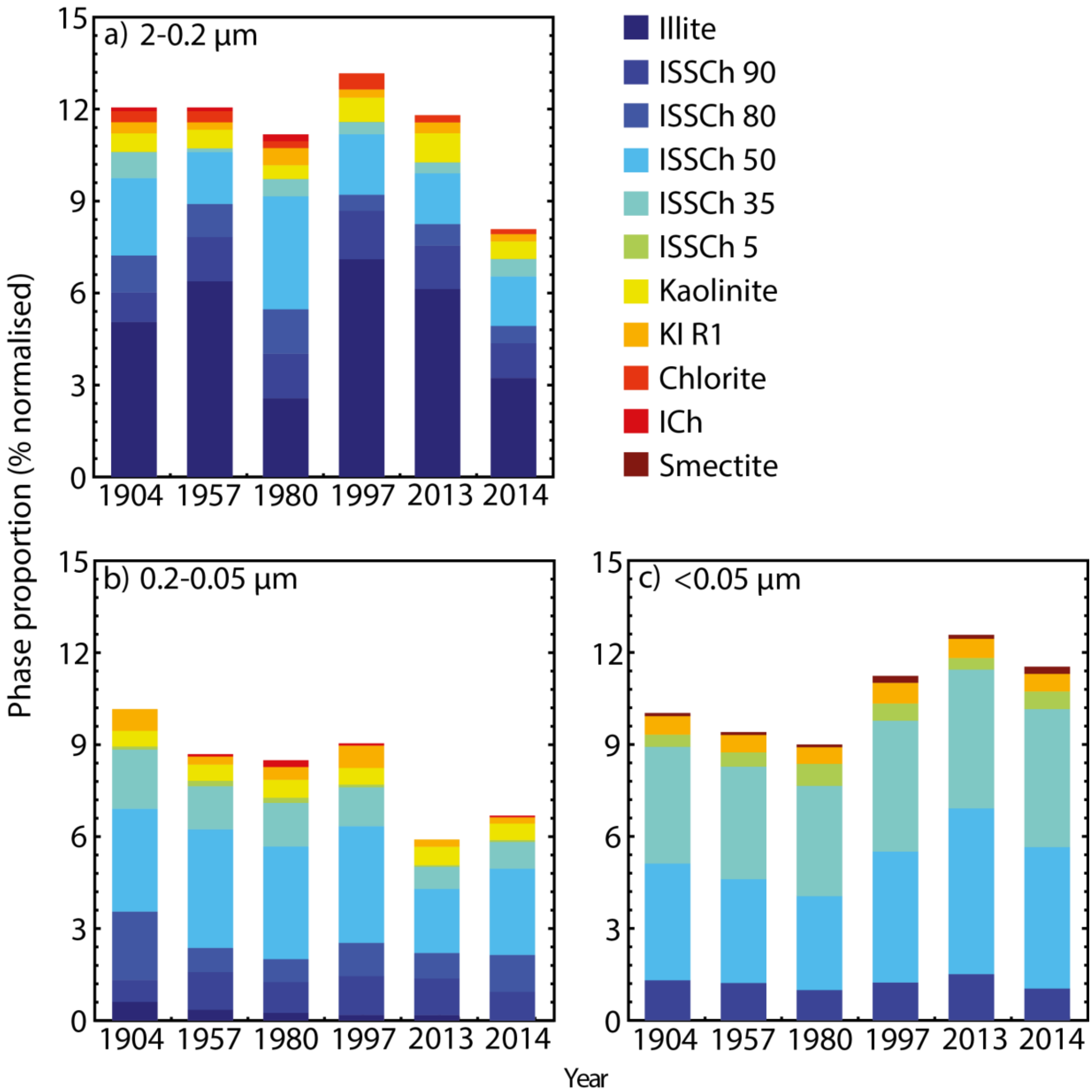

Figure S3. Relative proportions of the different mineral phases used to fit experimental XRD patterns of soil sample 2014. (**a**) 2–0.2 µm, (**b**) 0.2–0.05 µm, and (**c**) <0.05 µm subfractions. Proportions are normalized to the relative proportion of the size subfraction.

Table S1. Relative proportions (wt%) of the different mineral phases used to fit experimental XRD patterns of the 50–2 μm fraction for 1904–2014 samples.

Mineral / Mineral Group	1904	1957	1980	1997	2013	2014
Albite	11.1	11.6	10.4	10.4	10.0	11.1
Anatase	0.3	0.6	0.5	0.8	0.8	1.0
Calcite	0.4	0.2	0.3	0.3	0.2	0.3
Chlorite[1]	1.7	1.9	2.0	1.8	1.7	1.7
Amphibole[1]	0.6	0.9	0.8	0.7	0.5	0.5
Kaolinite[1]	1.1	1.2	1.2	1.1	0.8	0.7
Microcline	12.0	12.2	11.8	11.6	11.3	11.4
Mica[1]	4.8	4.9	6.0	5.4	5.4	5.5
Quartz	68.3	67.1	67.5	68.8	69.9	68.8

[1]amphibole was refined as a magnesio-ferri-hornblende; chlorite, kaolinite and mica were refined using PDF files 01-079-1270, 00-014-0164 and 01-076-0637, respectively.

Table S2. Relative proportions (wt%) of the different mineral phases used to fit experimental XRD patterns of <2 μm subfractions for 1904–2014 samples.

Contribution	1904	1957	1980	1997	2013	2014
			2–0.2 μm			
Illite	42	53	26	51	56	51
ISSCh 90	8	12	13	12	13	8
ISSCh 80	10	9	6	4	5	11
ISSCh 50	21	14	27	16	10	15
ISSCh 35	7	1	10	1	1	2
ISSCh 5						
Kaolinite	5	5	8	7	10	8
KI R1	3	2	6	5	3	3
Chlorite	3	3	4	4	2	2
ICh	1	1				
Smectite						
			0.2–0.05 μm			
Illite	6	4	3	2	3	1
ISSCh 90	7	14	12	14	20	19
ISSCh 80	22	9	9	12	14	12
ISSCh 50	33	44	44	42	35	41
ISSCh 35	19	16	17	14	12	14
ISSCh 5	1	2	2	1	1	1
Kaolinite	5	6	7	6	10	8
KI R1	7	3	5	8	4	3
Chlorite						
ICh		2	1	1	1	1
Smectite						
			<0.05 μm			
Illite						
ISSCh 90	13	13	11	11	12	9
ISSCh 80						
ISSCh 50	38	36	34	38	43	40
ISSCh 35	38	39	40	38	36	39
ISSCh 5	4	5	8	5	3	5
Kaolinite						
KI R1	6	6	6	6	5	5
Chlorite						
ICh						
Smectite	1	1	1	2	1	2