Supporting Information

for

Predicting current and future background ion concentrations in German surface water under climate change

Le Trong Dieu Hien[a,b], Mira Kattwinkel[a], Klaus Schützenmeister[a], John R.Olson[c], Charles P. Hawkins[d], Ralf B. Schäfer[a]

[a] Institute for Environmental Sciences, University Koblenz-Landau, Fortstraße 7, 76829 Landau, Germany.

[b] Faculty of Resources & Environment, University of Thu Dau Mot, 06 Tran Van On street, Thu Dau Mot city, Binh Duong, Vietnam.

[c] School of Natural Sciences, California State University Monterey Bay, Seaside, USA.

[d] Watershed Science, Utah State University, Logan, USA.

Tables

Table S1. Attributes assigned for each unit of lithology.

Lith	%CaO	%MgO	%S	Uniaxial Compressive Strength (Mpa)	Geometric Mean Hydraulic Conductivity (µm/sec)
Amphibolite	9.9000	6.7000	0.0244	181.9100	0.0016
Andesite	6.5000	3.5000	0.0140	128.5600	0.2380
Anhydrite	39.3000	0.3000	58.7014	89.8300	0.0018
Aplite	0.8000	0.2000	0.0200	136.0800	0.0045
Arkose	1.3500	0.5400	0.0142	130.9300	0.0054
Basalt	9.3000	6.5000	0.0300	193.8200	0.6070
Basaltic-andesite	8.2000	4.1000	0.0050	55.4000	0.0551
Biotite-gneiss	2.0000	0.6000	0.0050	152.2000	0.0253
Biotite-schist	2.3000	1.7000	0.6900	68.8000	0.2500
Black-shale	0.5000	0.4000	1.7900	19.0500	0.0001
Boulders	0.4500	0.4900	0.0200	5.0000	106.0000
Calcarenite	54.3600	0.6700	0.0471	17.6500	0.4510
calcareous-Conglomerate	27.3600	1.1200	NA	NA	NA
calcareous-Sandstone	21.1400	8.4600	NA	NA	NA
calcareous-Siltstone	13.9000	4.5000	NA	NA	NA
Calc-silicate	15.5000	3.5000	0.0200	97.4000	0.3800
Carbonate	47.7800	0.5900	0.0459	76.5600	0.1400

Lith	%CaO	%MgO	%S	Uniaxial Compressive Strength (Mpa)	Geometric Mean Hydraulic Conductivity (µm/sec)
Chalk	53.4000	0.3000	0.0190	18.9800	0.0013
Clay	0.5000	1.8000	0.0385	0.3300	0.0011
Claystone	0.9700	2.2000	0.2700	16.1500	0.0000
Conglomerate	0.6100	0.6400	0.0400	103.1000	0.0159
Conglomerate-sandstone	1.0600	0.8200	0.0350	95.6000	0.0846
Dacite	0.0000	0.0000	0.0200	90.7800	0.1270
Diorite	6.3000	3.2000	0.0600	226.1400	0.0013
dolomitic-Claystone	2.8900	2.9000	NA	NA	NA
dolomitic-Limestone	28.2000	13.4000	NA	NA	NA
dolomitic-Marlstone	23.5000	3.1000	NA	NA	NA
Dolostone	0.0000	0.0000	0.0320	138.2000	0.0870
Eclogite	11.5000	6.9000	0.0120	400.0000	0.0042
Foidite	10.8000	4.1000	0.1123	43.4000	1.3900
Gabbro	9.7000	6.5000	0.0600	224.0100	0.7040
Gneiss	2.3000	1.1000	0.0100	152.2100	0.0253
Granite	0.0000	0.0000	0.0300	188.6800	0.0001
Granodiorite	3.4000	1.4000	0.0070	135.6500	0.0012
Granulite	9.9000	6.6000	0.0280	214.6700	0.2910
Gravel	0.4100	0.4800	0.0208	2.2900	8.3000
Graywacke	0.8400	1.8100	0.0058	81.8800	0.0137
Greenschist	8.5000	6.7000	0.1586	49.8100	0.0086
Gypsum	31.3000	2.0000	41.5189	21.5800	0.0434
Hornblende-gneiss	2.1000	0.6000	0.0090	152.2000	0.0253
Hornfels	1.2000	2.8000	0.2900	256.9500	0.0001
Ice	NA	NA	NA	NA	NA
Igneous	6.7900	5.3100	0.0501	128.8000	0.0083
Lamprophyre	0.0000	0.0000	0.0494	137.0800	0.0001
Latite	3.1000	1.3000	0.0500	136.5000	0.0338
Limestone	0.0000	0.0000	0.0500	102.9500	0.0244
Marble	33.2000	2.7000	0.1000	108.6200	0.1480
Marl	25.2500	6.1400	0.6500	30.9000	0.0028
Marlstone	27.6000	1.6000	0.6800	85.9200	0.0343
Metaandesite	7.7000	4.0000	0.0030	101.3000	1.4000
Metabasalt	8.7000	5.7000	0.0154	101.3000	1.4000
Metadacite	2.2000	0.5000	0.0025	101.3000	1.4000
Metadiabase	8.9000	5.8000	0.0270	131.7000	0.8000
Metagabbro	9.5000	6.8000	0.0060	131.7000	0.8000
Metagranite	1.6000	0.7000	0.0070	131.7000	0.8000
Metagraywacke	1.9000	1.4000	0.0005	117.3000	0.0122
Metamorphic	4.4700	3.4800	0.0468	151.9600	2.5900
Metarhyolite	1.0000	0.2000	0.0040	101.3000	1.4000
Mica-schist	1.7000	2.3000	0.0900	68.8000	0.2500
Migmatite	2.2000	1.1000	0.0045	172.1700	0.0473
Monzogranite	1.7000	0.5000	0.0192	155.7900	0.0004
Monzogranite	1.7000	0.5000	0.0192	155.7900	0.0004
Monzonite	2.3000	0.9000	0.1850	174.6000	0.0000

Lith	%CaO	%MgO	%S	Uniaxial Compressive Strength (Mpa)	Geometric Mean Hydraulic Conductivity (µm/sec)
Muscovite-gneiss	1.1000	0.4000	0.0030	152.2000	0.0253
Muscovite-schist	0.3000	3.5000	0.0300	68.8000	0.2500
Mylonite	NA	NA	NA	146.0000	50.0000
Orthogneiss	2.1000	1.5000	0.0100	152.2100	0.0300
Paragneiss	2.5000	2.7000	0.2880	152.2100	0.0300
Peat	7.0600	1.5400	3.1333	0.0300	0.0444
Pegmatite	0.8000	0.2000	0.0500	140.8800	0.0000
Peridotite	3.5000	32.5000	0.0900	125.7300	0.0398
Phonolite	2.7000	0.8000	0.0144	98.0000	0.0110
Phyllite	0.7000	2.6000	0.0450	75.0300	0.0233
Picrite	7.8000	13.3000	0.0300	76.0000	0.1350
Pyroxenite	14.6000	17.0000	0.0900	130.7100	2.0500
Quartz-diorite	6.8000	3.6000	0.0365	181.8700	0.0000
Quartz-feldspar-schist	1.3000	2.9000	0.0600	68.8000	0.2500
Quartzite	0.6000	1.1000	0.0100	242.4300	0.0343
Rhyolite	1.1000	0.4000	0.0200	203.7300	2.2400
Salt	7.7000	3.3000	22.4600	22.3100	0.0001
Sand	1.4700	1.1100	0.0200	0.9600	16.0000
Sandstone	1.5000	1.0000	0.0300	88.0600	0.4510
Sedimentary	NA	NA	0.5643	68.6000	0.0063
Sedimentary-breccia	9.7000	0.7300	0.1880	65.6600	0.0001
Serpentinite	0.3000	35.1000	0.1700	86.5900	0.0297
Silt	3.0900	1.4300	0.0700	0.3800	0.0066
Siltstone	0.9900	1.7000	0.1300	62.4500	0.0016
Skarn	27.6000	2.3000	0.0200	202.8300	0.3160
Slate	0.4000	1.6000	0.1400	144.2800	0.0000
Syenite	2.1000	0.7000	0.1700	218.4200	0.0000
Syenogranite	0.6000	0.2000	0.0110	188.6800	0.0001
Tectonite	NA	NA	NA	118.2500	0.0842
Tonalite	4.9000	2.1000	0.0100	124.3700	0.0000
Trachyte	0.0000	0.0000	0.0200	232.5500	0.0775
tuff	NA	NA	NA	30.3700	0.0048
tuff-Andesite	NA	NA	NA	30.3700	0.0048
tuff-Basalt	NA	NA	NA	30.3700	0.0048
tuff-Rhyolite	NA	NA	NA	30.3700	0.0048
tuff-Trachyte	NA	NA	NA	30.3700	0.0048
Volcanic	7.5900	5.9800	0.0265	95.0000	0.1110
Water	NA	NA	NA	NA	NA

Source: Olson & Hawkins, 2012 [1]

Table S2. Sources of environmental data

Properties	Sources	Type	Extent	Resolution	Year
Geology	Institute for Geosciences and Natural Resources (BGR) [2]	Vector	Germany	1:200,000	2007
Climate	DWD Climate Data Center [3]	Raster	Germany	1km x 1km	1981-2015
Available water capacity	Institute for Geosciences and Natural Resources (BGR) [4]	Raster	Germany	250m x 250m	2015
Bulk density	European Soil Data Centre (ESDAC) [5]	Raster	Europe	1km x 1km	2013
Organic matter content	European Soil Data Centre (ESDAC) [6]	Raster	Europe	1km x 1km	2015
Soil erodibility	European Soil Data Centre (ESDAC) [7]	Raster	Europe	500m x 500m	2014
Soil permeability	Institute for Geosciences and Natural Resources (BGR) [8]	Vector	Europe	1:200,000	2016
Soil depth	Institute for Geosciences and Natural Resources (BGR) [9]	Raster	Germany	250m x 250m	2015
Water table depth	Fan, Y., H. Li, G. Miguez Macho (2013) [10]	Raster	World	1km x 1km	2013
Enhanced vegetation index (EVI)	MODIS Vegetation Indices [11]	Raster	Germany	1km x 1km	2005-2016
Groundwater recharge veolcity	Institute for Geosciences and Natural Resources (BGR) [4]	Raster	Germany	1km x 1km	2008

Table S3. Highly correlated variables

Var 1	Var 2	Correlation coeffficient (EC model)	Correlation coeffficient (Ca^{2+}/Mg^{2+}) model)	Correlation coefficient (SO_4^{2-})
Mean catchment elevation	Mean compressive strength	0.76	0.70	0.75
Mean catchment elevation	Mean annual precipitation	0.75	0.71	0.73
Mean catchment elevation	Mean freeze days	0.89	0.87	0.86
Mean catchment elevation	Mean water table depth	0.79	0.77	0.78
Mean catchment elevation	Mean recharge speed	0.72	0.70	0.72
Mean annual precipitation	Mean recharge speed	0.89	0.91	0.91
Mean catchment elevation	Mean annual temperature	-0.95	-0.94	-0.94
Mean compressive strength	Mean annual temperature	-0.72		-0.71
Mean freeze days	Mean annual temperature	-0.94	-0.94	-0.94
Mean water table depth	Mean annual temperature	-0.74	-0.74	-0.72

Table S4: Values of α and λ values of optimal models in elastic net regression

Models	Alpha (α)	Lamda (λ)
EC	1	0.0001
Ca^{2+}	0	0.0405
Mg^{2+}	1	0.0102
SO_4^{2-}	0.78	0.0001

Table S5: The size of tree (mtry) and out of bag (OOB) errors for RF models

Models	mtry	OOB error
EC	3	0.028
Ca^{2+}	3	0.053
Mg^{2+}	4	0.042
SO_4^{2-}	6	0.036

Table S6: Coefficient and order of important variables in LR and RF models

Random forest model				Linear Regression model with elastic net			
Predictor	**Direction**	**%IncMSE**	**Rank**	**Predictor**	**Direction**	**Coefficient**	**Rank**
Electrical Conductivity (log EC)							
				Intercept	+	3.69E+00	
Mean annual precipitation	-	61	1	Percent CaO	+	3.05E-01	1
Percent CaO	+	39	2	Mean annual temperature	+	9.15E-02	2
Percent S	+	39	3	Percent S	+	6.88E-02	3
Mean annual temperature	+	38	4	Mean annual precipitation	-	-1.57E-02	4
Mean soil depth	+	36	5	Percent MgO	+	1.70E-02	5
Mean EVI	+	35	6	Log catchment area	+	1.34E-02	6
Soil mean organic matter content	+	34	7	Mean EVI	+	5.87E-03	7
Mean hydraulic conductivity	+	30	8	Mean hydraulic conductivity	+	2.67E-03	8
				Mean soil depth	+	4.86E-04	9
				Mean water table depth	-	-1.19E-03	10
				Mean catchment elevation	-	-1.09E-03	11
				Mean compressive strength	-	-6.39E-04	12
				Mean soil permeability	-	-2.69E-04	13
				Mean available water capacity	-	-1.59E-04	14
				Mean recharge speed	-	-1.46E-04	15
Calcium (log Ca^{2+})							
				Intercept	+	1.68E+00	
Mean annual precipitation	-	55	1	Percent CaO	+	1.64E+00	1
Percent CaO	+	44	2	Mean annual temperature	+	6.66E-01	2
Mean EVI	+	42	3	Percent S	+	1.50E-01	3
Percent S	+	41	4	Mean annual precipitation	-	-6.55E-02	4
Mean hydraulic conductivity	+	36	5	Log soil mean organic matter content	+	5.18E-02	5
Mean compressive strength	+	36	6	Mean hydraulic conductivity	+	3.78E-02	6
Mean annual temperature	+	30	7	Mean soil erodibility	+	1.87E-02	7
				Percent MgO	+	1.08E-02	8

Random forest model				Linear Regression model with elastic net			
Predictor	**Direction**	**%IncMSE**	**Rank**	**Predictor**	**Direction**	**Coefficient**	**Rank**
				Mean soil permeability	-	-1.17E-02	9
				Log catchment area	+	1.03E-02	10
				Mean soil depth	+	9.54E-03	11
				Mean water table depth	-	-2.39E-03	12
				Mean EVI	+	5.33E-03	13
				Mean freeze days	-	-2.16E-03	14
				Mean available water capacity	-	-9.04E-04	15
				Mean recharge speed	-	-6.92E-04	16
				Mean compressive strength	-	-5.24E-04	17
				Mean bulk density	+	3.53E-04	18
				Mean catchment elevation	-	-3.67E-04	19
Magnesium (log Mg^{2+})							
				Intercept	+	1.24E+00	1
Mean annual precipitation	+	59	1	Percent S	-	1.69E-01	2
Percent MgO	+	47	2	Percent MgO	+	1.36E-01	3
Percent S	+	36	3	Mean EVI	+	8.23E-02	4
Mean annual temperature	+	35	4	Annual precipitation	-	-2.32E-02	5
Mean EVI	+	32	5	Annual freezed days	-	-5.35E-03	6
Mean compressive strength	-	38	6	Mean soil permeability	-	-4.25E-03	7
Mean soil erodibility	+	27	7	Log catchment area	-	-2.52E-03	8
Mean soil permeability	-	20	8	Mean recharge speed	-	-8.19E-04	9
				Mean bulk density	+	5.45E-04	10
				Mean compressive strength	-	-3.39E-04	11
				Mean available water capacity	-	-9.85E-05	12
				Mean catchment elevation	-	-5.11E-05	13
Sulphate (log SO_4^{2-})							
				Intercept	+	2.00E+00	
Mean annual precipitation	-	98	1	Percent CaO	+	1.28E+00	1
Mean soil permeability	-	37	2	Mean annual temperature	+	5.86E-01	2

Random forest model				Linear Regression model with elastic net			
Predictor	**Direction**	**%IncMSE**	**Rank**	**Predictor**	**Direction**	**Coefficient**	**Rank**
Mean hydraulic conductivity	+	30	3	Percent S	+	1.17E-01	3
Mean soil depth	+	28	4	Log soil mean organic matter content	+	6.04E-02	4
Mean available water capacity	+	27	5	Mean bulk density	+	5.57E-02	5
Mean annual temperature	+	25	6	Percent MgO	+	3.13E-02	6
Percent S	+	24	7	Mean EVI	+	2.35E-02	7
Mean bulk density	+	24	8	Mean hydraulic conductivity	+	1.40E-02	8
Mean EVI	+	20	9	Mean soil permeability	-	-1.23E-02	9
Percent MgO	+	12	10	Annual freezed days	-	-1.04E-02	10
				Log catchment area	-	-5.19E-03	11
				Mean water table depth	+	1.33E-03	12
				Mean catchment elevation	-	-1.15E-03	13
				Mean soil erodibility	+	8.07E-04	14
				Mean annual precipitation	-	-6.16E-04	15
				Mean soil depth	+	2.82E-04	16
				Mean compressive strength	-	-2.22E-04	17
				Mean available water capacity	+	2.11E-04	18
				Mean recharge speed	-	-1.05E-04	19

Table S7. Change in temperature and precipitation for Germany in period from 2070-2100

Period	**Temperature (^{0}C)**			**Precipitation (mm/year)**		
	Min	**Mean**	**Max**	**Min**	**Mean**	**Max**
Current (1981-2015)	-3.62	8.93	11.38	399.00	807.02	3258.47
RCP2.6 (2070-2100)	-0.52	10.92	13.83	421.00	698.77	1785.00
RCP8.5 (2070-2100)	2.62	13.64	16.49	418.00	691.43	1740.00

Figures

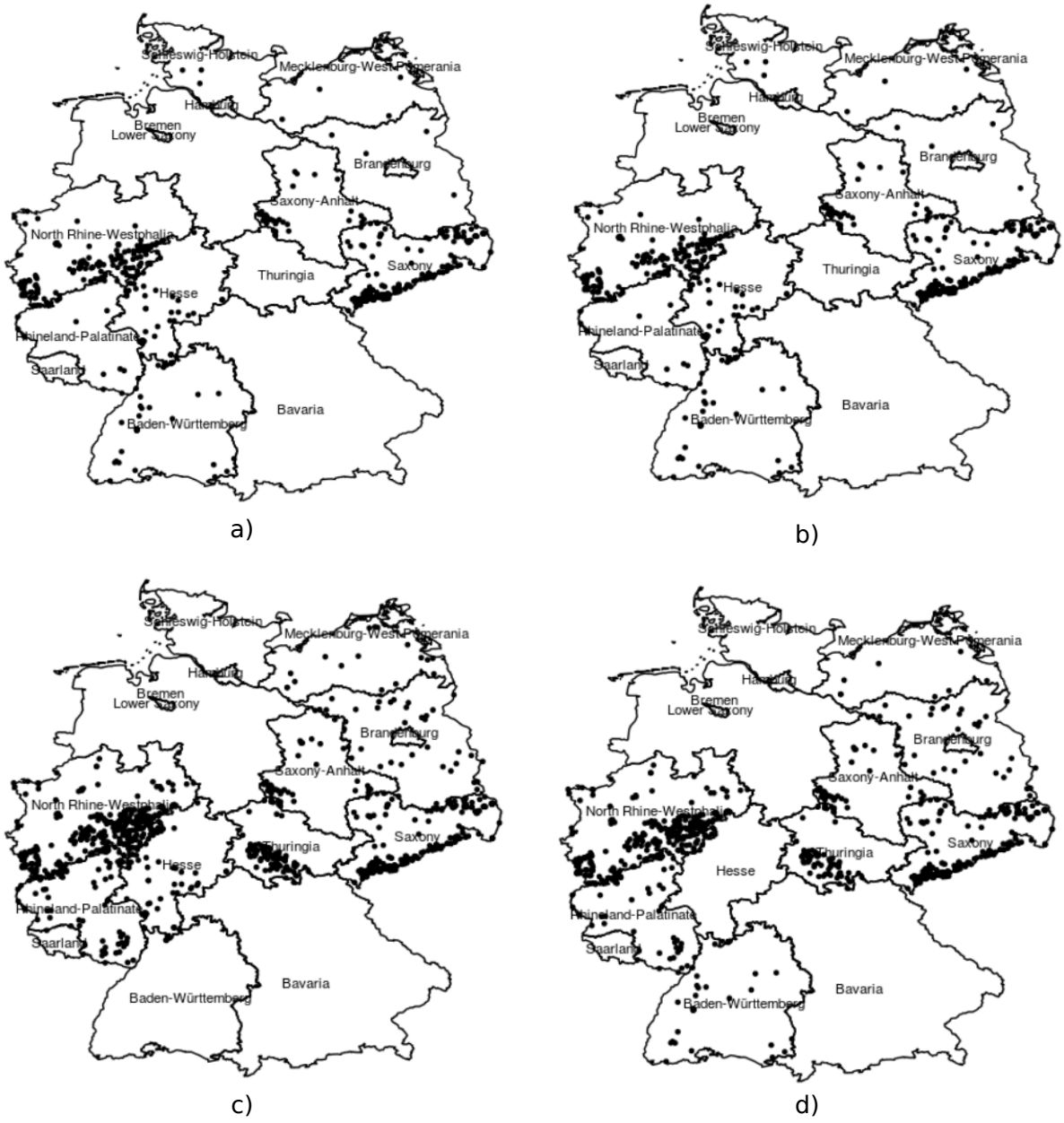
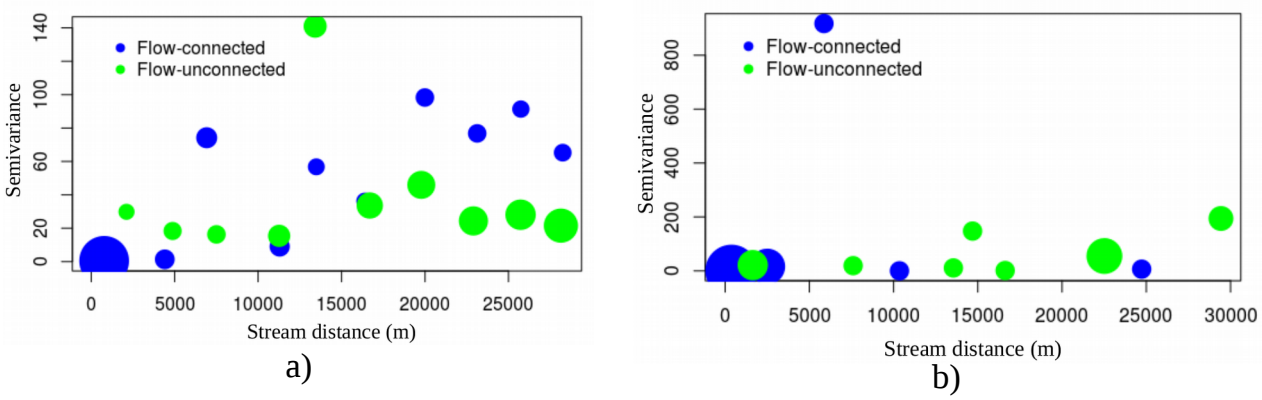
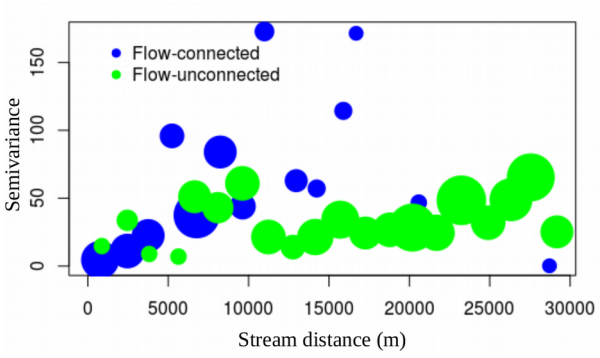


Fig S1. Location of monitoring sites a) Ca sites (266 sites) b) Mg sites (266 sites) c) EC sites (410 sites) d) SO_4^{2-} sites (357 sites)





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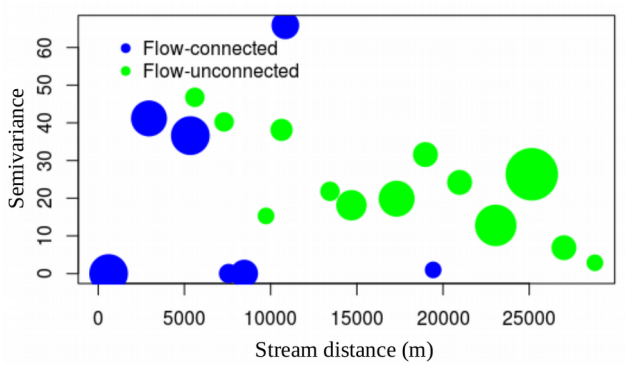
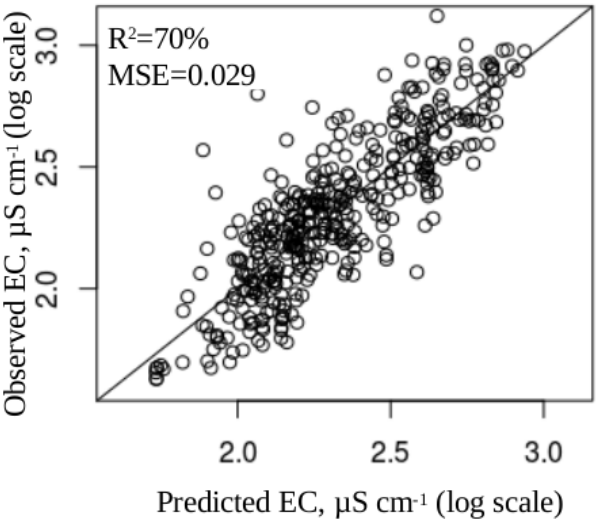


d)

Fig S2: Semivariogram of EC measurements in the German states a) Saxony b) Hesse c)North Rhine-Westphalia d)Thuringia



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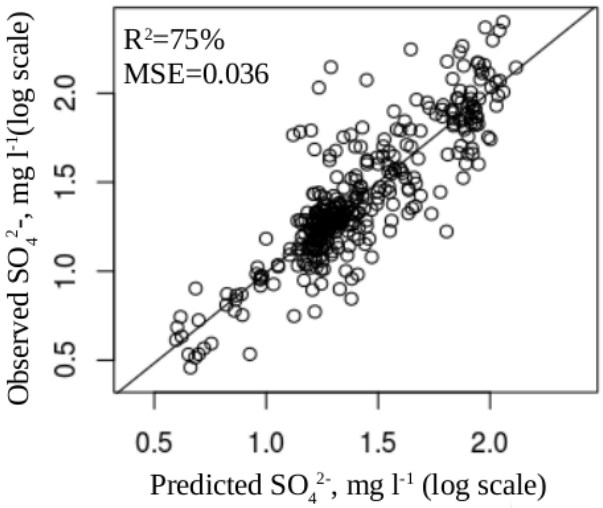

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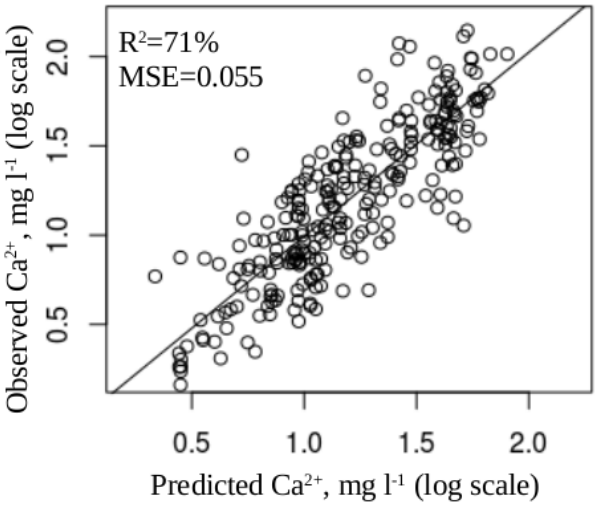

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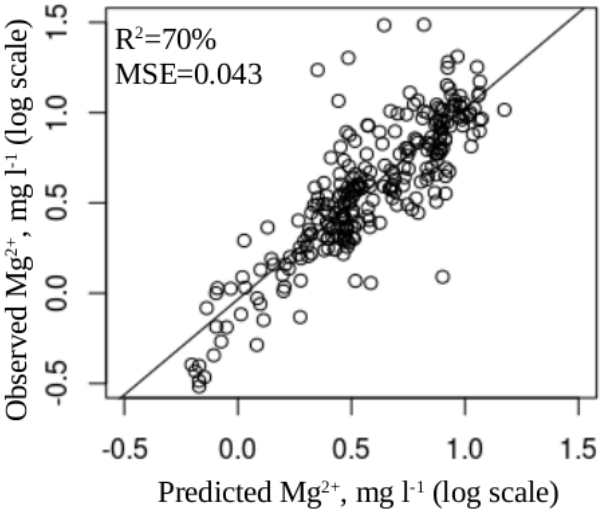

d)

Fig S3 Plots of predicted versus observed values in LR a) Electrical conductivity b) Sulfate c) Calcium d) Magnesium

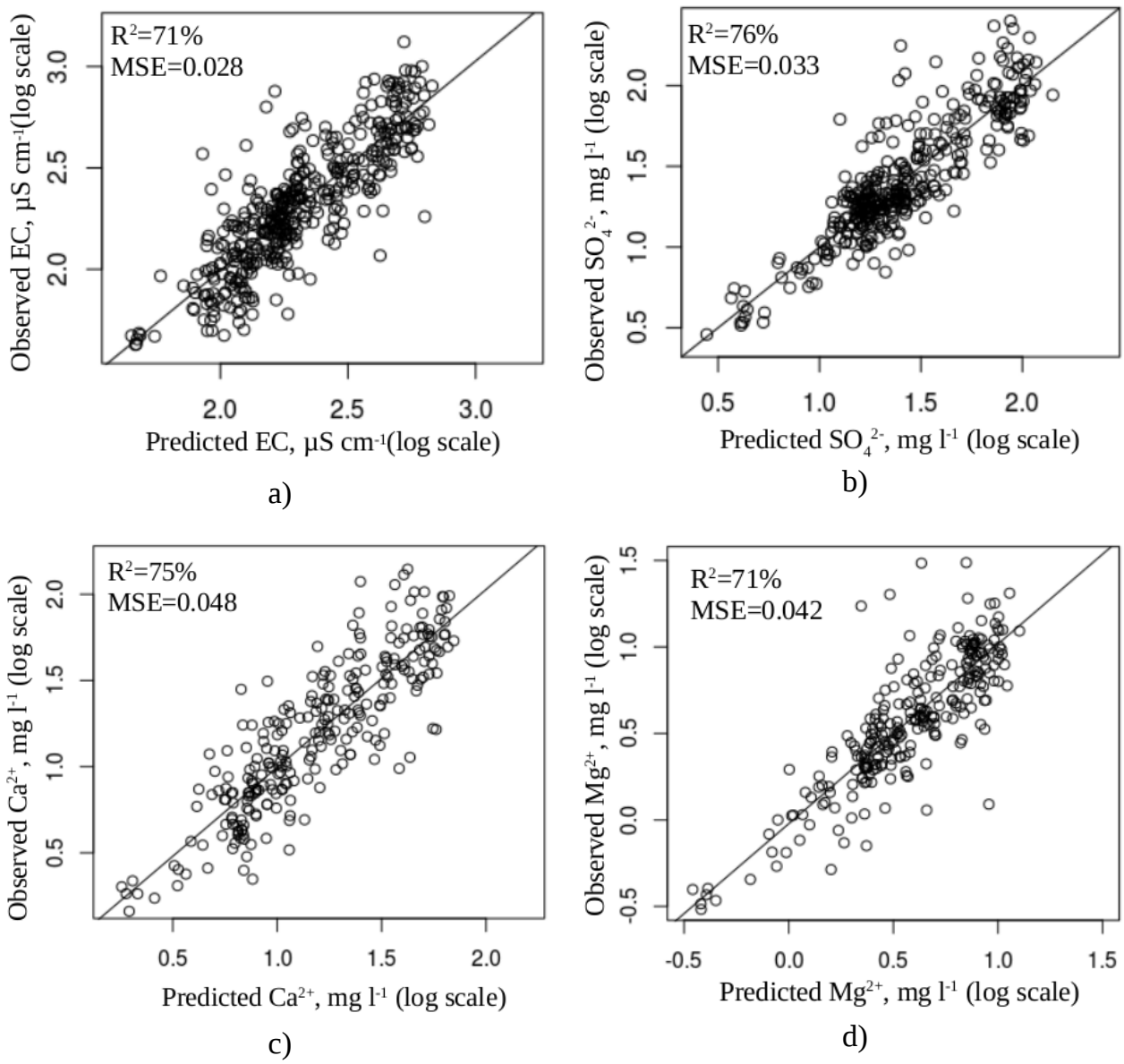

Fig S4 Plots of predicted versus observed values in RF a) Electrical conductivity b) Sulfate c) Calcium d) Magnesium

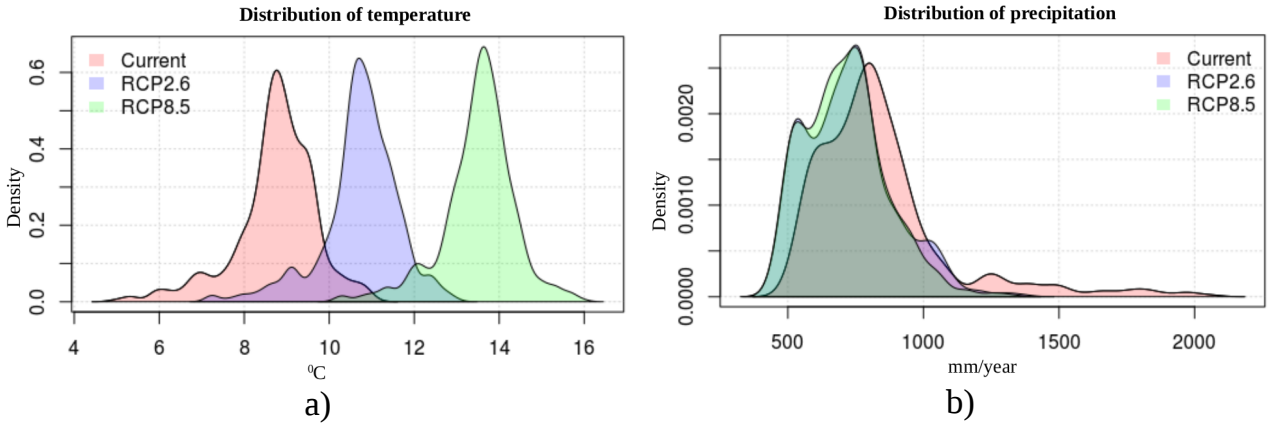

Fig S5. Distribution of temperature and precipitation in 610 sample sites in Germany in period from 2070-2100 a) Temperature b) Precipitation

Reference

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