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Supporting Information

Decomposing Bulk Electrical Conductivity of Streamflow to Recover Individual Solute Concentrations at High Frequency

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Contents

S1 Introduction to the Supporting Information material

The Supporting Information material includes theoretical and operational details to compute the electrical conducticity (EC) of an aqueous solution starting from the mass concentration of the dissolved species. Files and instructions for the implementation of the main equations using the software PHREEQC, as well as details on the Upper Hafren (UHF) data preparation, are here provided.

S2 Implementing main equations relating EC to ion concentration

The set of equations used to represent EC as the sum of different ion species can be easily implemented in any programming software. The use of a specific geochemical program, however, can be convenient as useful chemical properties (e.g., the electrochemical activity coefficient) and elementary operations (like the charge balance) are typically built-in. For this reason, we implemented all model equations using the free software PHREEQC (version 3.3.8), which is a general purpose geochemical model made available for free by the U.S. Geological Survey (USGS). PHREEQC has a built-in function to calculate the electrical conductivity (or Specific Conductance) of a solution at a given temperature from the specified concentrations, the calculated activity coefficients, and the given diffusion coefficients of all the charged species. The methodology is described in the PHREEQC version 3 manual[1], in more detail at http://www.hydrochemistry.eu/exmpls/sc.html, and it is briefly summarized here.

EC is computed by PHREEQC as (main text, equation (1)):

$$EC = \sum_i \left(\Lambda_m^0 \, m \, \gamma_{EC}\right) \tag{S1}$$

where for each solute species: Λ_m^0 is the molar conductivity [S/m/(mol/m^3)], m is the molar concentration [mol/m^3], and γ_{EC} $[-]$ is the electrochemical activity coefficient.

The molar conductivity of a solute species and its diffusion coefficient are related by

$$\Lambda_m^0 = \frac{z^2\, F^2}{R\, T}\, D_w \tag{S2}$$

where z is the charge number [-], F is Faraday's constant (96485.33289 Coulomb/mol), R is the gas constant (8.3144621 J/°K/mol), T is the absolute temperature [°K], and D_w the diffusion coefficient [m^2/s] of the solute species. The diffusion coefficient is corrected for the given temperature with:

$$(D_w)_T = (D_w)_{298} \cdot (T/298) \cdot (\eta_{298}/\eta_T) \tag{S3}$$

where η is the viscosity of water. To remove the temperature effect on Λ^0 and γ_{EC}, EC measurements are typically reported at the standard temperature of 25°C (EC$_2$5).

The electrochemical activity coefficient of a solute species, γ_{EC}, is related to the Debye-Hückel activity coefficient,γ_{DH}, and is calculated by PHREEQC for an ionic strength $I < 0.36|z|$ as:

$$\log(\gamma_{EC}) = \log(\gamma_{DH})\frac{0.6}{|z|^{0.5}} \tag{S4}$$

Equations (S1-S4) were manually implemented for each individual solute in the PHREEQC input file *compute_EC* reported in section S6. The file only needs to be filled with solute concentrations and it is set to create two output tables: *output_a.dat*, which includes the chemical coefficients $a_i = \Lambda^0\, \gamma_{EC}\, /M$ [(μS/cm) / (mg/L)], where M is the solute molar mass; and *output_EC.dat*, which includes EC_i for each individual solute and can be used to evaluate the individual solute contribution f_i. Further details about input and output data are provided directly within the file. The application to the UHF dataset is described below.

S3 Upper Hafren water quality dataset: data source, selection and preparation

The Upper Hafren (UHF) dataset is part of the Plynlimon high-frequency water quality dataset[2,3], which includes 7-hour frequency grab samples of precipitation and streamflow for the Hafren catchment (mid-Wales). Data were collected in the period 2007-2009 and comprise more than 40 elements. It is to be noted that water quality parameters as pH, EC (at 25°C) and Gran Alkalinity were measured in the lab (and not in the field) for the same 7-hour frequency samples as all other elements (although measurements were done on unfiltered samples for these parameters). The complete dataset can be downloaded through the data portal of the UK Centre for Ecology and Hydrology, together with metadata about field and analytical methods. For the analyses, we selected UHF data over the period 04/12/2007 12:00 - 27/01/2009 05:00, to avoid major gaps in EC measurements. The major solute species selected for the analysis were: sodium (Na^+), calcium (Ca^{2+}), magnesium (Mg^{2+}), potassium (K^+), chloride (Cl^-), sulphate (SO_4^{2-}) and nitrate (NO_3^-). Further, H^+ concentration was derived from pH [-] and HCO_3^- was computed from speciation calculation with Gran Alkalinity [μEq/l], pH, and main ions as input. Dissolved organic carbon (DOC) could contribute to Gran Alkalinity[4], but we expect its part to be small in this catchment as negative Gran Alkalinities in half of the samples could largely be explained by pH and did not point to a DOC contribution. Some large gaps in the Gran Alkalinity dataset were filled through a linear regression with pH, where available (Figure S1). Such an approximation, although rough, is better than assuming a fixed value for the missing Gran Alkalinity and it allows extending EC computations to a much larger number of samples. Samples with missing values of EC, pH, SO_4^{2-}, Cl^-, Na^+, or Mg^{2+} (total amount 188) were disregarded for the analyses. A final number of 1252 samples was hence used in the computations. The mean values of major ions, pH, Gran Alkalinity and EC are reported in Table S1.

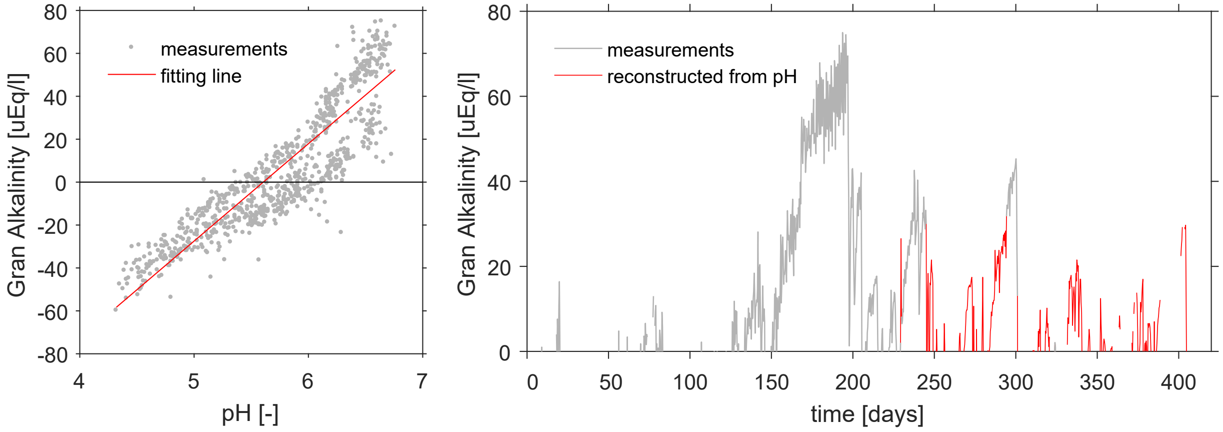

Figure S1: Reconstruction of missing Gran Alkalinity values (right panel) through a regression with pH (left panel). Only positive Gran Alkalinity values are reported in the plot, as bicarbonates become negligible for negative alkalinity values. Regression line is $Alk = 43 \cdot pH - 235$, coefficient of determination R^2=0.78. Total number of reconstructed (positive) Alkalinity values is 185. Alkalinity could not be computed on the 188 samples where a pH value was missing.

Table S1: Mean values of the measured variables used in the analyses

variable	mean value
Na^+ (mg/l)	3.28
Ca^{2+} (mg/l)	0.48
Mg^{2+} (mg/l)	0.56
K^+ (mg/l)	0.12
Cl^- (mg/l)	5.54
SO_4^{2-} (mg/l)	1.97
NO_3^- (mg/l)	0.15
pH (-)	5.66
Gran Alkalinity (μEq/l)	3.57
EC (μS/cm)	29.06

S4 Details of the application to the Upper Hafren dataset

The prepared UHF dataset was inserted into the PHREEQC input file to compute EC for each individual solute in the solution. All the computations are done for the standard temperature of 25°C.

S4.1 Measured and computed EC

EC obtained from the implementation of equation (S1) is compared to the measured values in Figure S2. The result is generally accurate, with 95% of the errors within ±10% and 66% of the error within ±5%. The mean error is slightly negative (-3%), reflecting that some minor elements that can contribute EC may have not been accounted for, but their contribution is rather limited as the 9 major elements are able to cover, on average, 97% of EC. It is worth noting that the UHF stream presents rather challenging conditions for EC estimation as it is a dilute, low-conductivity system with acidic conditions during high flows. The overall correct representation of the measured EC signal indicates that solute contributions to EC computed through equation (S1) are generally appropriate. Local inaccuracies like the errors around day 50 are likely related to the low pH conditions (<5) which make the relationship between H^+ and EC more complicated. In these conditions, it was shown[5] that equation (S1) may overestimate the actual contribution of H^+ to EC, but the contributions of the other ions, which are the main focus of our approach, are not affected.

S4.2 Coefficients a_i

The coefficients a_i were directly taken from the generated PHREEQC output files. Such coefficients can vary with time because Λ_m^0 and γ_{EC} can change in time. The former does not change in our case because all computations are referred to a fixed temperature of 25°C. The latter, instead, changes with the Ionic strength I of the solution (γ_{EC} decreases for increasing I), but as the total ion concentration has little changes in the observed timeseries

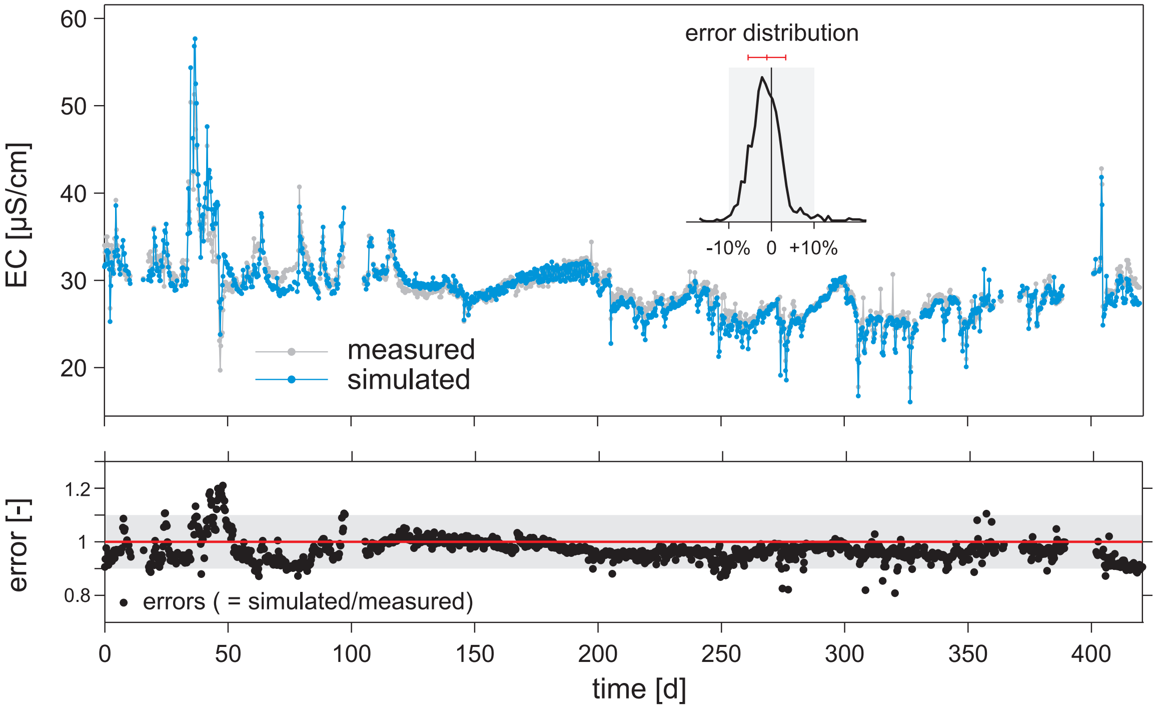

Figure S2: Top: comparison between EC computed through equation (S1) and measured EC on the 7-hour Upper Hafren dataset. The inset shows the error distribution, with the red bar indicating the mean and the standard deviation of the distribution. Bottom: timeseries of simulation errors expressed as EC_{simul}/EC_{meas}.

(as typically in natural fresh water systems), I and hence γ_{EC} have very little variations. Therefore, the coefficients a_i only have minor variations in time, as illustrated in Figure S3.

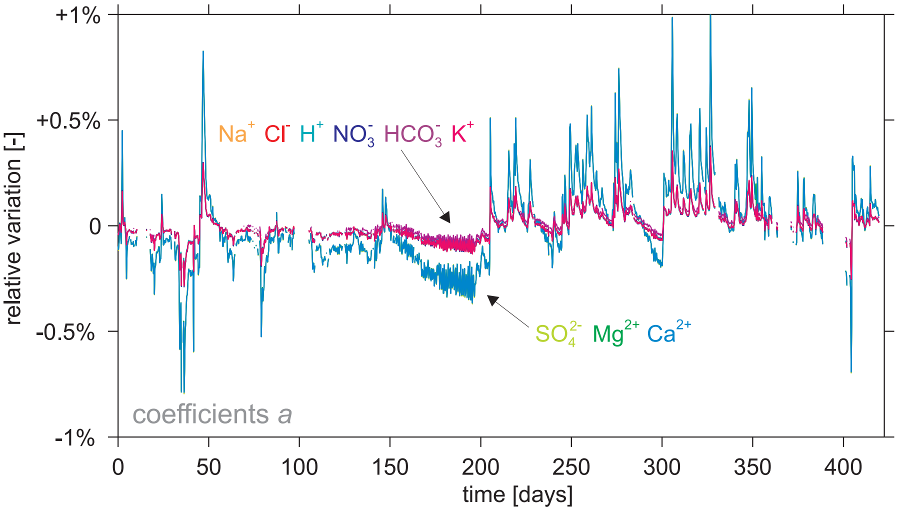

Figure S3: Relative variations of the coefficients a with respect to their mean. Maximum variations are roughly ±1%. Ions with absolute charge 2 have slightly larger variations with respect to ions with unitary absolute charge. Although all coefficients are plotted, some are not visible because of almost perfect overlappings.

S4.3 Weights f_i and interpolation error

For the 9 major ions, the weights f_i are computed as the ratio between EC_i (computed from equation (S1) and the measured EC signal. For this reason, the sum of the weights f_i can be different from 1 according to the error on EC estimation (Figure S2, lower panel). As the different contributions EC_i are evaluated independently from one another, the weights can be computed for the available measured ions even if other ion's concentrations are missing. The only consequence in this case is that one cannot verify the overall accuracy of equation (S1) in simulating the measured EC.

The weights analysis for the complete UHF dataset is described in the main text (Section Proof of Concept). Here, we investigate the error of the weights f_i arising from a linear interpolation of low-frequency subsamples of f_i. Figure S4 shows, for each ion, the "true" value of the weight (as obtained from high-frequency measurements) and the estimate from the linear interpolation of biweekly samples. As the UHF dataset includes 7-hour samples, biweekly subsamples are obtained by selecting 1 every 48 samples, hence they always occur at the same time of the day (which depends on the choice of the first extracted sample). Occasionally, 3-week subsamples were considered if the biweekly samples corresponded to a missing value (as this is what happens in real field conditions). The relative error of the interpolation was evaluated by taking the relative difference between the true and the interpolated value (Figure S5). For Cl, Na, Mg, SO_4 and Ca, the error timeseries is rather similar in shape but differs in magnitude. Solutes with higher contributions to EC like Cl and Na tend to have lower relative errors. For example, the mean absolute error for Cl or Na is about 3 times lower than for Ca.

The computed weights can be used to obtain solute concentraion estimates at high frequency (main text equation (4)). By further developing equation (4), one can explicitly account for the error in the estimation of the term $f_i(t)/a_i(t)$:

$$C_i(t) = EC(t)\,\left[\frac{f_i(t)}{a_i(t)}\right]_{est.} = EC(t)\,\left[\frac{f_i(t)}{a_i(t)}\right]_{true} + EC(t)\,\left[\frac{f_i(t)}{a_i(t)}\right]_{err} \tag{S5}$$

and by indicating with r_e the relative error on $f_i(t)/a_i(t)$ one gets:

$$C_i(t) = (1 + r_e)\,EC(t)\,\left[\frac{f_i(t)}{a_i(t)}\right]_{true} = (1 + r_e)\,C_{i,true} \tag{S6}$$

As shown in Section S4.2, the coefficients a_i only have minor fluctuations, so the error on f_i directly transfers to the error on concentration estimate C_i. Therefore, solutes that are likely to be better estimated using EC are those with the more predictable weights f_i. This sets a first criterion to identify the solutes that can be better quantified with the EC-aided methodology. Weights are more predictable if their contribution is stable in time, e.g., when they have low *relative* variability. Weight variability arises when a solute behaves differently from EC, i.e., when it behaves differently from the ensemble of the other solutes.

At UHF, solutes tend to have a contrasting behavior during acidic conditions at high flows, where positive concentration peaks occur in H^+, but mostly negative peaks occur in other solutes' concentration. During these occurrences, most solutes get diluted more than EC (indeed, because of the H^+ increase), hence the ratio $f_i = EC_i/EC$ is characterized by sudden depressions (Figure 1, especially around days 150-200). This example suggests a potential in using pH estimates, either using relationships with flow or by deploying high-frequency sensors, to achieve better estimates of the weight variability (and, in turn, of solute concentration).

S4.4 Solute concentration estimates for all ions

The weights interpolated starting from biweekly measurements are here combined with high-frequency EC measurements (main text, equation 4) to provide solute concentration at high frequency. Results are reported for all ions in Figure S6. For solutes with lower weight-interpolation errors (like Cl and Na) the proposed approach is able to accurately reproduce most of the measured high-frequency solute dynamics. The period between day 0-100 is particularly illustrative because it shows that even when starting from a linear estimation of the weights f_i, the prediction can correctly reproduce the high-frequency fluctuations of the concentration signal as they are embedded in the EC signal. During such periods, the contribution of chloride and sodium to EC is rather stable (Figure S4), hence the weights could be well approximated by a linear interpolation. The estimate is instead less accurate where the contribution to EC has large fluctuations, as around days 200-250. For solutes with low contributions to EC (Ca, NO_3, K, HCO_3) the approach provides, as expected, a poor performance because the interpolation error on f_i is high. For solutes that are in an intermediate position (like Mg and SO_4, with average weights $\langle f_{Mg} \rangle \approx 8\%$ and $\langle f_{SO_4} \rangle \approx 11\%$) the model can reproduce some high-frequency peaks, but it also misses the solute behavior in some other events, hence the overall model error is not significantly better than the simple interpolation of measured concentrations.

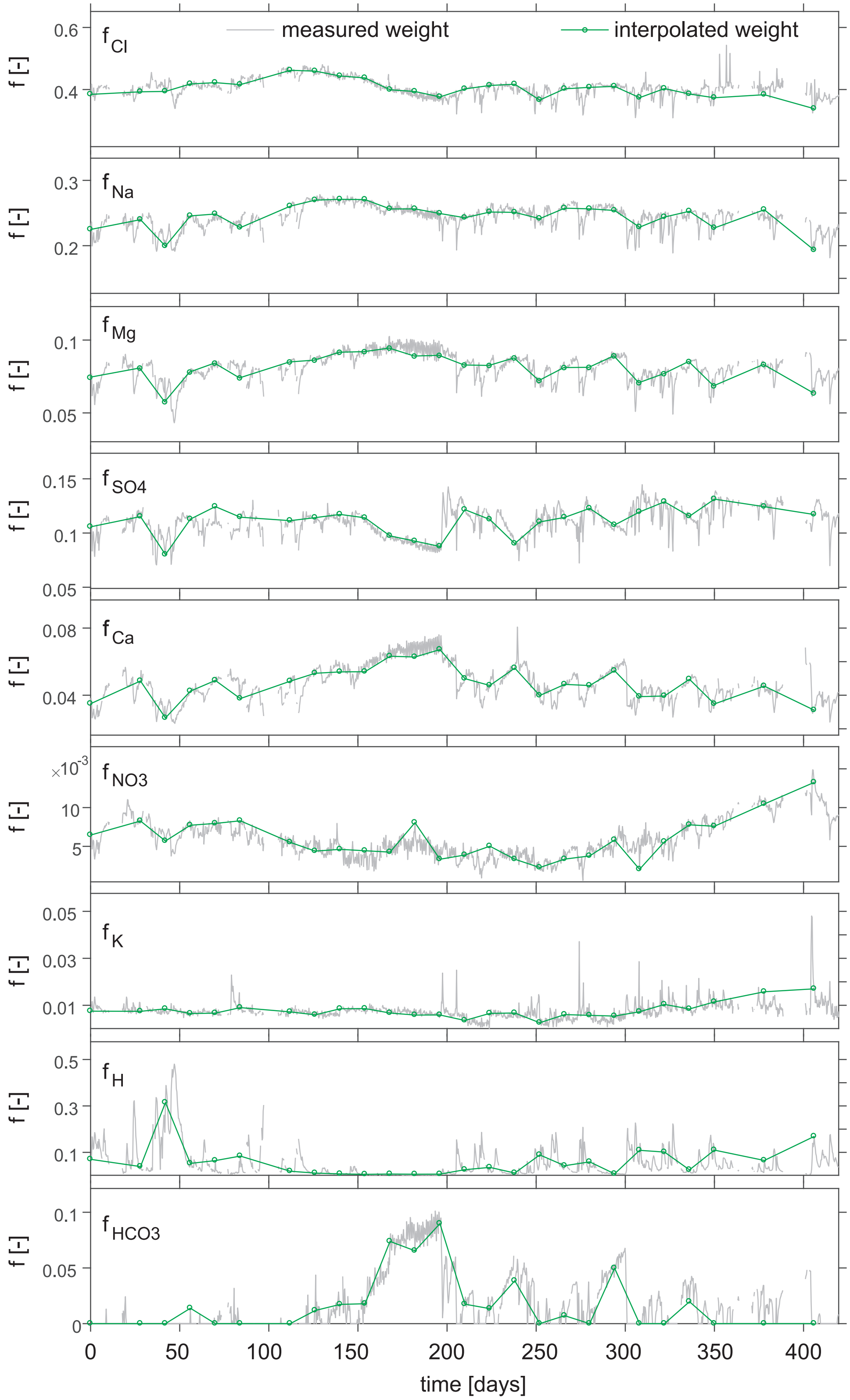

Figure S4: Weights f_i computed from high-frequency measurements (grey) and from interpolation of biweekly measurements (green).

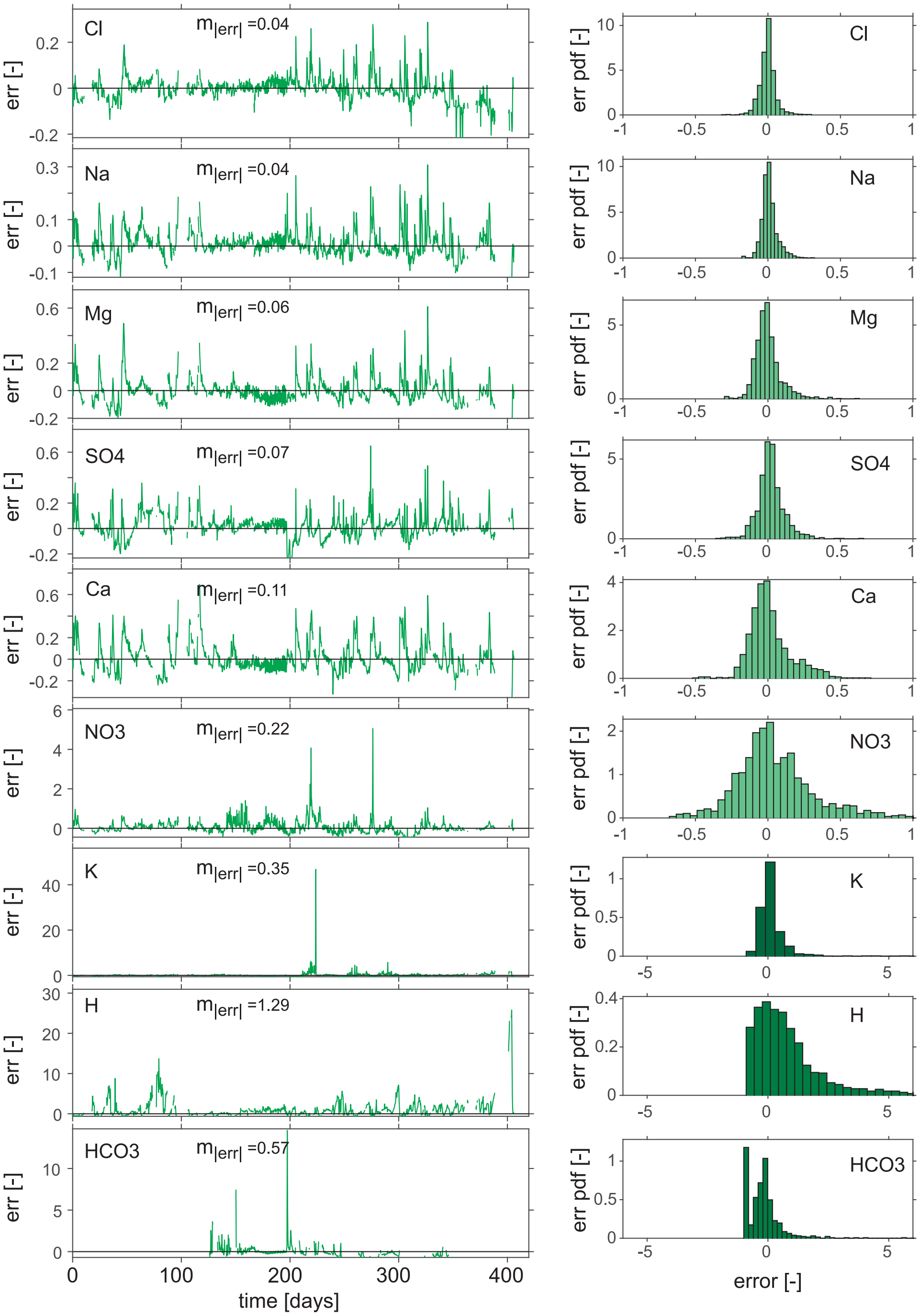

Figure S5: Weight interpolation errors, computed as the relative difference between the true and the interpolated values. Error timeseries (left) and error distribution (right). The color used for the error distribution of K, H and HCO_3 is darker to highlight that the x-axis is different.

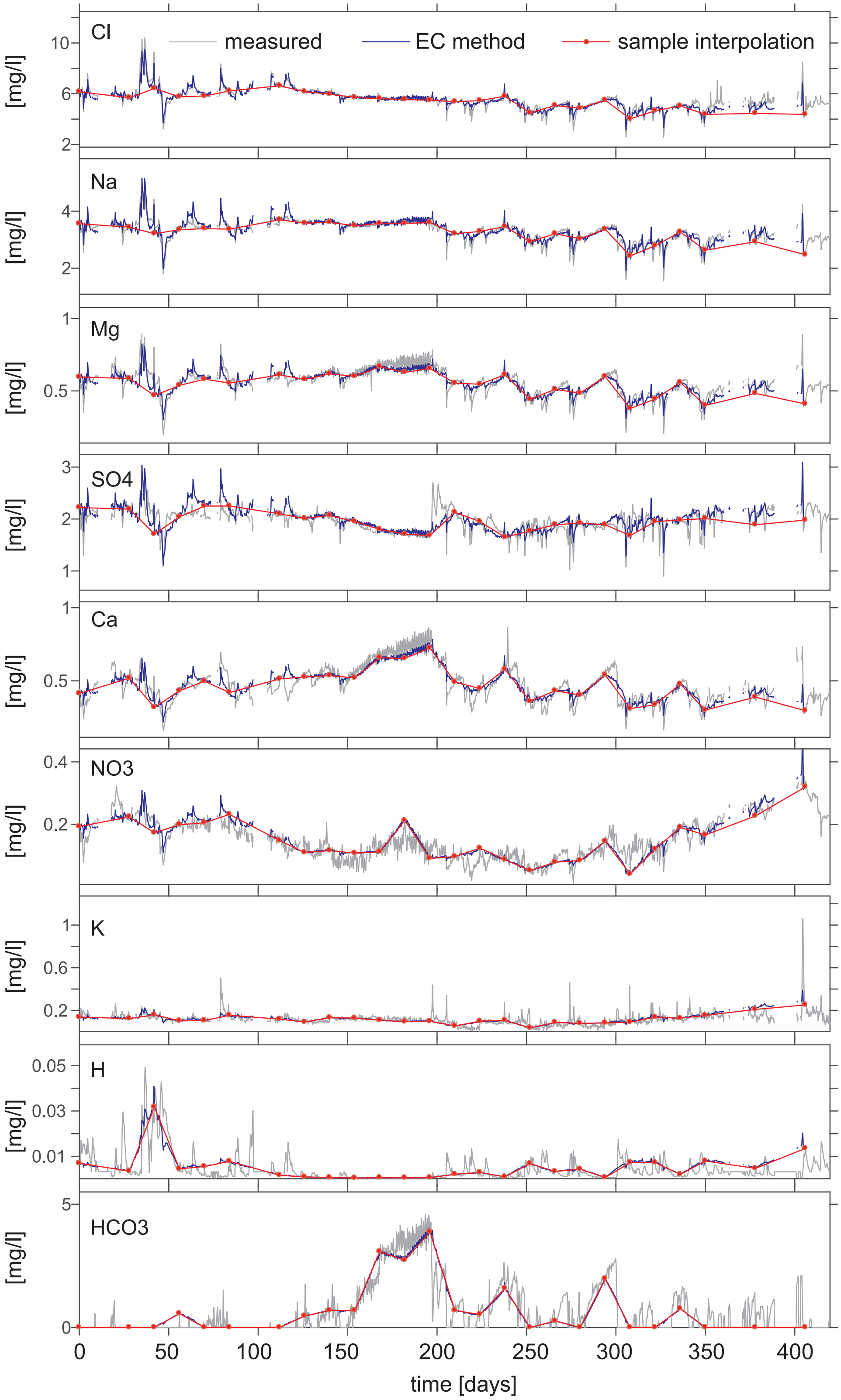

Figure S6: Solute concentration predicted through the EC-aided approach (blue) compared to high-frequency measured values (grey) and linear interpolation of biweekly measured values (red).

S5 Linear regressions between EC and solute concentration

S5.1 Ordinary regressions with EC for Cl and Na

Estimates of solute concentration obtained from a linear regression with EC are useful to understand and assess the performance of the EC-aided methodology. For chloride and sodium measured at UHF, we computed least-square linear regressions of the kind:

$$C(t) = p_1\, EC(t) + p_0 \tag{S7}$$

where concentrations are expressed in $[mg/l]$ and EC in $[\mu S/cm]$. The regression lines are plotted in Figure S7 and the regression coefficients are reported in Table S2.

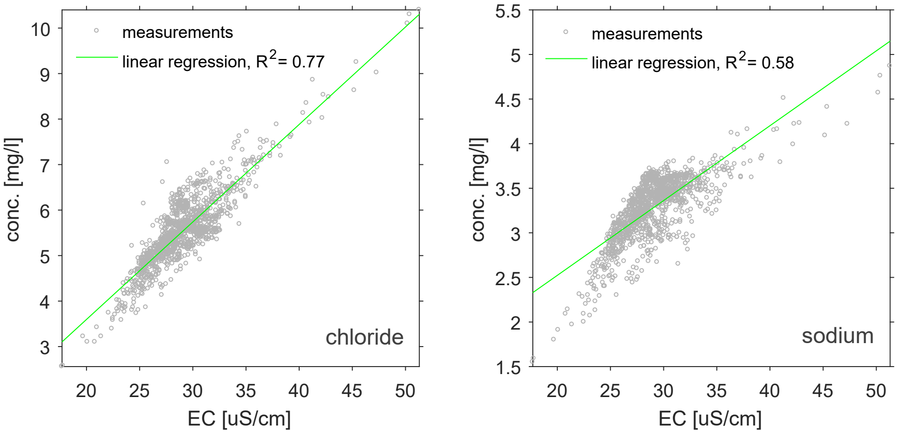

Figure S7: Regression plots for chloride (left) and sodium (right)

Table S2: Regression coefficients for chloride and sodium

	p_1	p_0
chloride	0.214	-0.69
sodium	0.084	0.84

S5.2 Comparisons between the proposed methodology and linear regressions

Linear regressions can be further investigated to understand the relationship between the weights f_i resulting from EC decomposition and the slope of the regression line. When the intercept (p_0) of the regression is close to zero, the slope (p_1) tends to approximate the 'zero-intercept' regression line, i.e., the regression line which is forced to pass by the axis origin:

$$C(t) = m\, EC(t) \tag{S8}$$

where the slope m can be expressed analytically as:

$$m = \frac{\sum_k C_k\, EC_k}{\sum_k EC_k^2} \tag{S9}$$

with the summation spanning all the available k samples for which both EC and C are known. Equation (S8) recalls main text equation 4, which reads:

$$C_i(t) = \frac{f_i(t)}{a_i(t)}\, EC(t) \tag{S10}$$

and by expressing $g(t) = f(t)/a(t)$, equation (S10) can be reformulated as:

$$C(t) = g(t)\, EC(t) = \bar{g}\, EC(t) + g'(t)\, EC(t) \tag{S11}$$

where $\bar{g}_i$ is the mean of $g(t)$ and $g'(t) = g(t) - \bar{g}$ are the deviations from the mean. The question is then how m is related to $\bar{g}$. If we substitute eq. (S11) into eq. (S9) we obtain:

$$m = \frac{\sum_k \bar{g}\, EC_k^2}{\sum_k EC_k^2} + \frac{\sum_k g'_k\, EC_k^2}{\sum_k EC_k^2} \tag{S12}$$

which simplifies into:

$$m = \bar{g} + \frac{\sum_k g'_k \, EC_k^2}{\sum_k EC_k^2} \tag{S13}$$

Equation (S13) shows that when the fluctuations in g are poorly correlated to EC^2, then $\bar{g}$ tends to coincide with the slope of the zero-intercept regression line.

At UHF, the correlation between g' and EC^2 is poor for both Cl and Na, causing $\bar{g}$ and m to only differ by a factor of 10^{-4}. Hence, the use of a constant, mean weight f_i in equation (S10) is equivalent to approximating solute concentration through a zero-intercept linear regression with EC. Further, as for both Cl and Na the intercept of the linear regression is rather close to zero, the use of mean f_i is very similar to a 'classic' linear regression. Results from both regressions are plotted against measurements in Figure S8. Mean absolute errors for classic and zero-intercept regressions are 5.23% and 5.33% respectively for chloride and 5.59% and 5.77% for sodium. This line of reasoning shows that in some circumstances linear

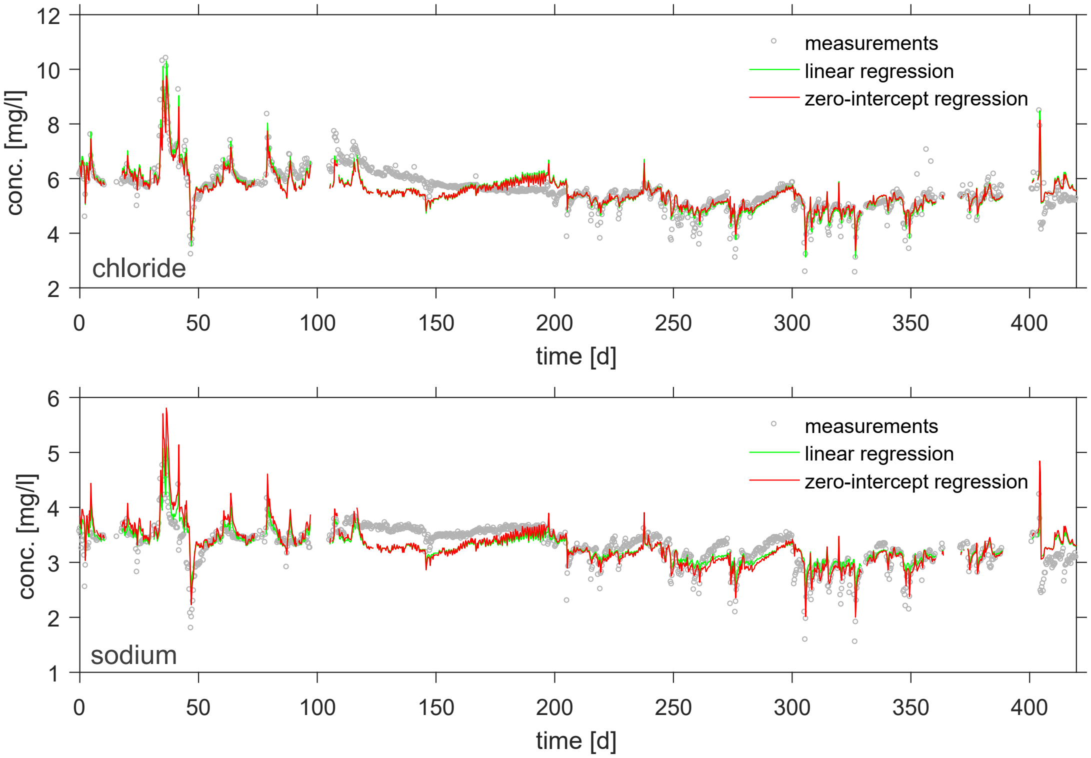

Figure S8: Measured and estimated solute concentrations for chloride (top) and sodium (bottom) obtained from a classic linear regression and from a zero-intercept linear regression.

regressions can be seen as a special case of the proposed EC approach (equation (S10)) where, instead of time-variable weights $f_i(t)$, the long-term mean value is used.

S6 PHREEQC input file

The following PHREEQC input file was used in the computations of EC, EC_i and a:

```
DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 3.3.9-11951\database\phreeqc.dat
# DATABASE (insert here the path to phreeqc.dat file, e.g. C:\Program Files\...\database\
    phreeqc.dat)

######
# PHREEQC file to compute the Electrical Conductivity (EC) of the individual ion species
    of a solution
# Input chemical analytes are to be inserted in the SOLUTION_SPREAD block
# Outputs are printed to file according to SELECTED_OUTPUT and USER_PUNCH blocks
# by Boris van Breukelen and Paolo Benettin, April 2017
######

# the SOLUTION_SPREAD block allows inserting a table with chemical analytes for the
    computations
# note: default units are here set to mg/l, but variations for individual elements can be
     specified (see Alkalinity below)
# note: default temperature is 25 degrees C
# note: a "description" column with IDs (e.g. A1, A2,.. An) is required.
# note: headings needs to respect PHREEQC standard: NO3- is N(5), SO4-2 is S(6)
# note: gram formula weight has to be specified for nitrate if mass units are grams of
    NO3
# note: empty entries are allowed and considered as zero concentration or missing values

SOLUTION_SPREAD
    -units mg/l
```

```
#----------------------------------------------------------------
 Description pH Alkalinity N(5) S(6) Cl Na Mg K Ca
                          ueq/l gfw 62
         A1 5.10 -17.10 0.123 1.22 7.15 3.96 0.682 0.09 0.521
# A2 etc
# ...
# An etc
#----------------------------------------------------------------

SELECTED_OUTPUT 1 # this block allows writing an output file. Here we print the result of
     EC computation
-reset false # avoid printing default output
-file output_EC.dat # output file name

USER_PUNCH 1  # print user-defined quantities to the selected_output file
    -headings Sample_ID EC_tot EC_majel EC_error[%] EC_H EC_Ca EC_Cl EC_K EC_NO3 EC_Na
        EC_Mg EC_SO4 EC_HCO3 charge_error [%]
    -start

# define some useful constant for the computations
10 F = 96485.33289 # C per mol
20 R = 8.3144621 # J per K per mol
30 ff1 = 0.6 / 1^0.5 # group together some constants
40 ff2 = 0.6 / 2^0.5 # group together some constants
50 temp25_corr = 1 # no temperature correction needed to get the default EC at 25 C
# 50 temp25_corr = TK/298 * (viscosity298) / (viscosityTK) # to get EC at TK temperature

# calculate conductivity for the individual species
# note: lg("species") is the log10 of the Debye-Huckel activity coefficient of a solution
     species
# note: DIFF_C("species") is the diffusion coefficient at 25 C of a solution species
# note: the molar conductivity is in S/m / (mol/m3 = mmol/L), so multiply mol("species")
    by 1000 to obtain mmol/L
```

```
# note: to report EC is in uS/cm, multiplication by 10’000 is needed
110 EC_H = ((1^2 * F^2)/(R*TK)) * (DIFF_C("H+") * temp25_corr) * mol("H+") * 1000 * 10^(
    lg("H+") * ff1) * 10000
120 EC_Ca = ((2^2 * F^2)/(R*TK)) * (DIFF_C("Ca+2") * temp25_corr) * mol("Ca+2") * 1000 *
    10^(lg("Ca+2") * ff2) * 10000
130 EC_Cl = ((1^2 * F^2)/(R*TK)) * (DIFF_C("Cl-") * temp25_corr) * mol("Cl-") * 1000 *
    10^(lg("Cl-") * ff1) * 10000
140 EC_K = ((1^2 * F^2)/(R*TK)) * (DIFF_C("K+") * temp25_corr) * mol("K+") * 1000 * 10^(
    lg("K+") * ff1) * 10000
150 EC_NO3 = ((1^2 * F^2)/(R*TK)) * (DIFF_C("NO3-") * temp25_corr) * mol("NO3-") * 1000 *
     10^(lg("NO3-") * ff1) * 10000
160 EC_Na = ((1^2 * F^2)/(R*TK)) * (DIFF_C("Na+") * temp25_corr) * mol("Na+") * 1000 *
    10^(lg("Na+") * ff1) * 10000
170 EC_Mg = ((2^2 * F^2)/(R*TK)) * (DIFF_C("Mg+2") * temp25_corr) * mol("Mg+2") * 1000 *
    10^(lg("Mg+2") * ff2) * 10000
180 EC_SO4 = ((2^2 * F^2)/(R*TK)) * (DIFF_C("SO4-2") * temp25_corr) * mol("SO4-2") * 1000
     * 10^(lg("SO4-2") * ff2) * 10000
190 EC_HCO3 = ((1^2 * F^2)/(R*TK)) * (DIFF_C("HCO3-") * temp25_corr) * mol("HCO3-") *
    1000 * 10^(lg("HCO3-") * ff1) * 10000
195 EC_majel = EC_H + EC_Ca + EC_Cl + EC_K + EC_NO3 + EC_Na + EC_Mg + EC_SO4 + EC_HCO3

# print results to output
198 PUNCH DESCRIPTION
200 PUNCH sc #total EC as computed by PHREEQC
205 PUNCH EC_majel #total EC by considering major species only
207 PUNCH 100*((sc-EC_majel)/sc) #relative error on EC by considering major species only
210 PUNCH EC_H
220 PUNCH EC_Ca
230 PUNCH EC_Cl
240 PUNCH EC_K
250 PUNCH EC_NO3
260 PUNCH EC_Na
270 PUNCH EC_Mg
```

```
280 PUNCH EC_SO4
290 PUNCH EC_HCO3
300 PUNCH PERCENT_ERROR # Percent charge-balance error: 100*(cations-|anions|)/(cations+|
    anions|)
    -end

SELECTED_OUTPUT 2 # this block allows writing an output file. Here the coefficients 'a'
    are printed
-file output_a.dat # output file name

USER_PUNCH 2  # print user-defined quantities to the selected_output file
    -headings Sample_ID a_H a_Ca a_Cl a_K a_NO3 a_Na a_Mg a_SO4 a_HCO3
    -start

# define some useful constant for the computations
10 F = 96485.33289 # C per mol
20 R = 8.3144621 # J per K per mol
30 ff1 = 0.6 / 1^0.5 # group together some constants
40 ff2 = 0.6 / 2^0.5 # group together some constants
50 temp25_corr = 1 # no temperature correction if EC is needed at 25 degrees C
# 50 temp25_corr = 298/TK * (viscosityTK) / (viscosity298) # to get standard EC at 25
    degree C

# calculate the variable a = molar_conductivity*electrochemical_activity_coefficient/
    molar_mass [uS/cm / (mg/L)] for the individual species
# note: lg("species") is the log10 of the Debye-Huckel activity coefficient of a solution
     species
# note: GFW("species") is the molar mass of the species [grams]
# note: DIFF_C("species") is the log10 of the Debye-Huckel activity coefficient of a
    solution species
# note: to report EC is in uS/cm, multiplication by 10'000 is needed
110 a_H = ((1^2 * F^2)/(R*TK)) * (DIFF_C("H+") * temp25_corr) * 10^(lg("H+") * ff1) / GFW
    ("H+") * 10000
```

```
120 a_Ca = ((2^2 * F^2)/(R*TK)) * (DIFF_C("Ca+2") * temp25_corr) * 10^(lg("Ca+2") * ff2)
    / GFW("Ca+2") * 10000
130 a_Cl = ((1^2 * F^2)/(R*TK)) * (DIFF_C("Cl-") * temp25_corr) * 10^(lg("Cl-") * ff1) /
    GFW("Cl-") * 10000
140 a_K = ((1^2 * F^2)/(R*TK)) * (DIFF_C("K+") * temp25_corr) * 10^(lg("K+") * ff1) / GFW
    ("K+") * 10000
150 a_NO3 = ((1^2 * F^2)/(R*TK)) * (DIFF_C("NO3-") * temp25_corr) * 10^(lg("NO3-") * ff1)
     / GFW("NO3-") * 10000
160 a_Na = ((1^2 * F^2)/(R*TK)) * (DIFF_C("Na+") * temp25_corr) * 10^(lg("Na+") * ff1) /
    GFW("Na+") * 10000
170 a_Mg = ((2^2 * F^2)/(R*TK)) * (DIFF_C("Mg+2") * temp25_corr) * 10^(lg("Mg+2") * ff2)
    / GFW("Mg+2") * 10000
180 a_SO4 = ((2^2 * F^2)/(R*TK)) * (DIFF_C("SO4-2") * temp25_corr) * 10^(lg("SO4-2") *
    ff2) / GFW("SO4-2") * 10000
190 a_HCO3 = ((1^2 * F^2)/(R*TK)) * (DIFF_C("HCO3-") * temp25_corr) * 10^(lg("HCO3-") *
    ff1) / GFW("HCO3-") * 10000

# print results to output
198 PUNCH DESCRIPTION
210 PUNCH a_H
220 PUNCH a_Ca
230 PUNCH a_Cl
240 PUNCH a_K
250 PUNCH a_NO3
260 PUNCH a_Na
270 PUNCH a_Mg
280 PUNCH a_SO4
290 PUNCH a_HCO3
    -end
END
```

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