

Standardized Schoeller Diagrams - A Matlab Plotting Tool

Rafael Schäffer¹ and Alexander Dietz²

¹Technical University of Darmstadt

²Technische Universität Darmstadt

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Abstract

Water analyses typically result in numerous characteristic values. The bunch of parameters hamper temporal or spatial comparisons of different samples. In order to facilitate the evaluation and interpretation of hydrochemical data, hydrogeologists use various special diagrams. One of them is the Schoeller diagram, in which concentrations of different species are plotted on logarithmic scales. Entries of an analysis are connected and form a characteristic signature. In the Schoeller diagram, parallel or subparallel signatures indicate relatedness of waters. Here we present the idea of standardized Schoeller diagrams: different logarithmic axes are shifted with respect to each other, in order for the signature of a selectable sample to form a straight line. This standardization greatly facilitates the comparison of water samples to the chosen standard and increases the informative value of a Schoeller diagram. As to our knowledge, there is no software that could generate standardized Schoeller diagrams, we have developed a Matlab tool for this purpose. The tool is available for free and allows fast generation of standardized Schoeller diagrams with many possibilities to implement user-specific wishes. We hope that this tool will contribute to a wider use of Schoeller diagrams.

Standardized Schoeller Diagrams – A Matlab Plotting Tool

R. Schäffer¹ and A. Dietz²

¹Institute of Applied Geosciences, Department of Materials and Earth Sciences, Technical University of Darmstadt, Schnittspahnstrasse 9, 64287 Darmstadt, Germany

²Geometry and Approximation, Department of Mathematics, Technical University of Darmstadt, Schlossgartenstrasse 7, 64289 Darmstadt, Germany

Corresponding author: Rafael Schäffer (rafael.schaeffer@tu-darmstadt.de)

Key Points

- A standardization creates more meaningful and powerful Schoeller diagrams.
- A freely accessible Matlab file allows to prepare, plot and print standardized Schoeller diagrams easily and quickly.
- Three application examples demonstrate the suitability of standardized Schoeller diagrams.

Abstract

Water analyses typically result in numerous characteristic values. The bunch of parameters hamper temporal or spatial comparisons of different samples. In order to facilitate the evaluation and interpretation of hydrochemical data, hydrogeologists use various special diagrams. One of them is the Schoeller diagram, in which concentrations of different species are plotted on logarithmic scales. Entries of an analysis are connected and form a characteristic signature. In the Schoeller diagram, parallel or subparallel signatures indicate relatedness of waters. Here we present the idea of standardized Schoeller diagrams: different logarithmic axes are shifted with respect to each other, in order for the signature of a selectable sample to form a straight line. This standardization greatly facilitates the comparison of water samples to the chosen standard and increases the informative value of a Schoeller diagram. As to our knowledge, there is no software that could generate standardized Schoeller diagrams, we have developed a Matlab tool for this purpose. The tool is available for free and allows fast generation of standardized Schoeller diagrams with many possibilities to implement user-specific wishes. We hope that this tool will contribute to a wider use of Schoeller diagrams.

1 Introduction

The analysis of a water sample results in a number of variables. When the quantity of analyses increases, it becomes more difficult to overview the data and to prepare it for addressees like water authorities, engineering consultants, researchers or enterprises. Therefore, graphical representations have been developed to facilitate evaluation, comparison, and interpretation of results in analyses. Such graphical presentations can range from simple graphics up to complex diagrams, especially tailored to describe hydrogeologic issues like groundwater composition. Examples are bar or column diagrams (Collins, 1923), ray diagrams (Dalmady, 1927), pie or circle diagrams (Udluft, 1953,) or Stiff diagrams (Stiff, 1951). Such diagrams are often combined with cross sections or maps (e.g. Carlé 1964, Habermahl, 2020, Schäffer et al., 2021) to illustrate groundwater quality.

Probably the most popular diagram among hydrogeologists is the Piper diagram (Piper, 1944), named after the US-American geochemist Arthur M. Piper (Upson, 1992), who slightly modified or further developed suggestions by Hill (1942) as well as Langelier and Ludwig (1942). Durov developed a similar diagram that was used primarily in the former Soviet Union (Durov, 1948, Chilingar, 1956). Decisive for the position of water samples within the Piper diagram are the ratio of the equivalent concentrations of calcium, magnesium, sodium, and potassium on the one hand, and bicarbonate, carbonate, sulfate, and chloride on the other hand. In principle, the total concentration does not influence the position, because the relative chemical composition is shown. Piper diagrams are therefore suitable to classify water types (e.g. Furtak and Langguth, 1967) or hydrochemical groups independently of the total concentration of samples. In addition, the Piper diagram is well suited to identify mixed waters, if end members are known.

An excellent complement to the Piper diagram is the Schoeller diagram (Schoeller, 1938), invented by the French engineering geologist Henri Schoeller. In this diagram, concentrations of any species are shown on a vertical, logarithmic scale, allowing to plot a wide concentration range. Schoeller drew the first version with calcium, magnesium, sodium, chloride,

sulfate, and carbonate displayed in equivalent concentrations (Schoeller, 1938). Nevertheless, Schoeller diagrams are versatile and can also display other species such as bicarbonate, potassium, nitrate, iron or sum parameters like total dissolved solids (TDS) or the total equivalent concentrations (TEC). Depending on the problem, any combination is possible, even including petrophysical parameters like electric conductivity, redox potential or oxygen saturation. Some authors use equal logarithmic axis and concentrations, given in equivalent concentrations (e.g., Güler et al., 2002, Nasrabadi et al., 2009), other authors prefer to use shifted logarithmic axis or to show mass concentrations (e.g., Schäffer and Sass, 2014, Babanezhad et al., 2018, Heldmann et al., 2020).

Independently of the chosen species and units, data points of the same sample are connected with straight lines. This results in a hydrochemical signature that is characteristic for each water sample. Hydrochemical similarities or differences become evident by comparing these signatures. Congruent signatures indicate water samples from the same aquifer or with a comparable genesis. Parallel or subparallel signatures suggest hydrochemical relationships, for example due to dilution. The informative value of Schoeller diagrams considerably increases, if a standardization is included, firstly presented by Schäffer et al. (2014). In a standardized Schoeller diagram, the axes of the different species are individually shifted in such a way that the signature of the standardizing sample forms a straight line. This simplifies comparisons of other water samples to the standard one. As far as we know, neither any free available software (e.g., Simler, 2020, Winston, 2020, R Core Team, 2021), nor commercial programs like Geochemist's Workbench (Aqueous Solutions LLC, 2020) can produce standardized Schoeller diagrams. However, manual drawing is time-consuming and laborious, even if graphical softwares are used. Authors will hesitate to create standardized Schoeller diagrams, unless an attractive solution is available. Thus, a Matlab tool is described here, which offers an easy data import and a variable generation of standardized Schoeller diagrams, due to the user's requirements and ideas.

2 Matlab Tool

The manual creation of a standardized Schoeller diagram involves considerable effort. On the one hand, it is not easy to transform the data in such a way that a data set shows a vertical line as well as coordinate systems in individual columns to be scaled correctly. On the other hand, it requires effort to adjust the plot in such a way that, in the end, it also meets the visual requirements for different purposes.

The plot tool for Matlab solves all these problems directly and has been designed to be as user-friendly as possible. Use and benefits of the tool contain three parts: importing the data, designing the plot in Matlab, and exporting the graphs. Here we presents a summarized description on how to handle these three parts and how easy it is to use this tool. A detailed tutorial with illustrated examples and sample code files has been created, so that you can adapt the plot to your own needs in just a few steps. Examples for the adaptability of the plots are the figures in this paper, which are all created with the given tool. All files (the Matlab code, the user manual, a sample .xlsx file, and the file that generates the tutorial graphics) can be downloaded from Dietz and Schäffer (2022).

Typically, measurement data are stored within data management systems in file formats such as .xlsx .csv .ods or .txt. The Matlab tool imports this data from these files. This means that raw data management can still be done in file formats mentioned above. There are only a few restrictions associated with the import into Matlab. More precisely, only the first two rows are reserved for identifying and labeling the columns of the plot and the first two columns are reserved for identifying and labeling the legend. The remaining cells can be designed freely. In addition, the tool allows any number of columns for elements and any number of rows for samples, from which either all or a desired selection can be plotted. A minimal example is given in table 1.

Table 1. Exemplarily minimal data set used in the manual. It already includes syntax for the import into Matlab.

		NH_4^+ $\backslash\text{bf NH}_{\{4\}}^{\{+\}}\backslash\text{rm}\backslash\text{newline}$ (mg/L)	K^+ $\backslash\text{bf K}^{\{+\}}\backslash\text{rm}\backslash\text{newline}$ (mg/L)	Mg^{2+} $\backslash\text{bf Mg}^{\{2+\}}\backslash\text{rm}\backslash\text{newline}$ (mg/L)	TEC $\backslash\text{bf TEC}\backslash\text{rm}\backslash\text{newline}$ (mmol(eq)/L)	TDS $\backslash\text{bf TDS}\backslash\text{rm}\backslash\text{newline}$ (mg/L)
S1	$\backslash\text{bf Sprudel-1 1898}$		862.5	432	1048.5	34980
S2	$\backslash\text{bf Sprudel-2 1901}$	3.51	548.7	377.8	938.2	30940.2
H1	$\backslash\text{bf Huttenquelle 1886}$		743.2	255.8	609.1	19959.8
O1	$\backslash\text{bf Ottoquelle 1886}$	6.18	160	161.5	643.5	21236.1
O2	$\backslash\text{bf Ottoquelle 1957}$		57.3	22.1		3406.9

Using the tool in Matlab is equally simple and requires no prior knowledge of Matlab. Only one command is required to create a plot. A minimal example of such a command line is:

```
plotSchoeller('ExampleDataSet.xlsx',1)
```

This command imports the raw data from the file 'ExampleDataSet.xlsx', plots the first data set as a vertical line and all other data sets relative to it. In doing so, the coordinate system is automatically adjusted so that all lines are within the plot, and a given distance to the top and bottom of the plot is maintained. To create a plot within Matlab, nothing more needs to be done than typing in the above mentioned line into the command line. With numerous additional options within the plot command, the plot can be customized according to personal preferences. Specifically, the following can be customized:

- Selection and order of different columns/elements and individual labeling. TEX code can be used for indices and superscripts (as in row 2 in table 1).
- Selection and order of the different rows/data sets. TEX code can also be used for their labeling in the legend (as in column 2 in table 1).
- Title of the graph
- Location and style of the legend, both related to the display and the font of the legend.
- Management for values below the detection limit and automatic indications that the value is below a given detection limit. The limit can be selected separately for each element.
- Automatic "zeroing" of values below the detection limit, if required.
- Distance of data curves to the upper and lower limit of the plot.

- Text size of all texts in the plot.
- Size and resolution of the plot.
- Any customization of the lines/data sets, such as color, line thickness, dash markers and much more, also separately for each line.
- Exporting the plot to all common file formats.

All these properties can be adjusted by a few entries in the plot command. Each of these commands is described in detail in the manual. In addition, graphical examples have been created for each command so that you can see the effects of the command directly. As an example, the command could be

```
plotSchoeller('ExampleDataSet.xlsx',1,'--','Markersize',15,'Color','r','LineWidth',4)
```

This example dots each line, equips it with markers at the data points, colors it red, and displays the lines with a thickness of 4 pixels. The manual also explains how to use various annotations, such as including text boxes and arrows. However, separate commands are required for this. Exporting the plot is also done with an addition in the plot command. For example:

```
plotSchoeller('ExampleDataSet.xlsx',1,'CreateFigure','Print','./mySubFolder/myNewPlot','-dpng')
```

This command creates the file 'myNewPlot.png' in the folder 'mySubFolder', which is an image of the plot. All common file formats such as .png .bmp .jpg .pdf .eps and many more are possible here. To elaborate publications, vector graphics are explicitly supported. For pixel graphics, like .png, the resolution is customizable.

In summary, you can see that you can still use the raw data in your preferred environment, that using Matlab is reduced to typing a command line, and that exporting the plot to a graph is supported for all common file formats. Beyond this brief description, the manual (Dietz and Schäffer, 2022) explains each command in detail and backs it up with examples. Thus, you will have easy access to the plot tool and a high degree of customization, whether you are a beginner or an expert in Matlab.

3 Application Examples

3.1. Comparison of spring waters from different tectonic units

At the northwestern edge of the Tauern Window, Tyrol, Austrian Alps, several overthrust faults occur within a few kilometers. The tectonic nappes are partly shingled and/or folded and consist of several rock types, making the geological situation quite complex (Schäffer et al., 2020, 2021a and citation therein). These metamorphic rocks are predominantly aquicludes. Only the Hochstegen formation, mainly consisting of calcite and dolomite marble, could act as a karst aquifer. Locally, numerous caves and other karst phenomena are known (Spötl & Mangini, 2010). However, it was unclear whether the entire Hochstegen formation is karstified and thus function as a connected karst aquifer. This is relevant because it could thus be assumed that the Tux valley would also be drained underground over a length of about 20 km and an elevation difference of more than 2000 m.

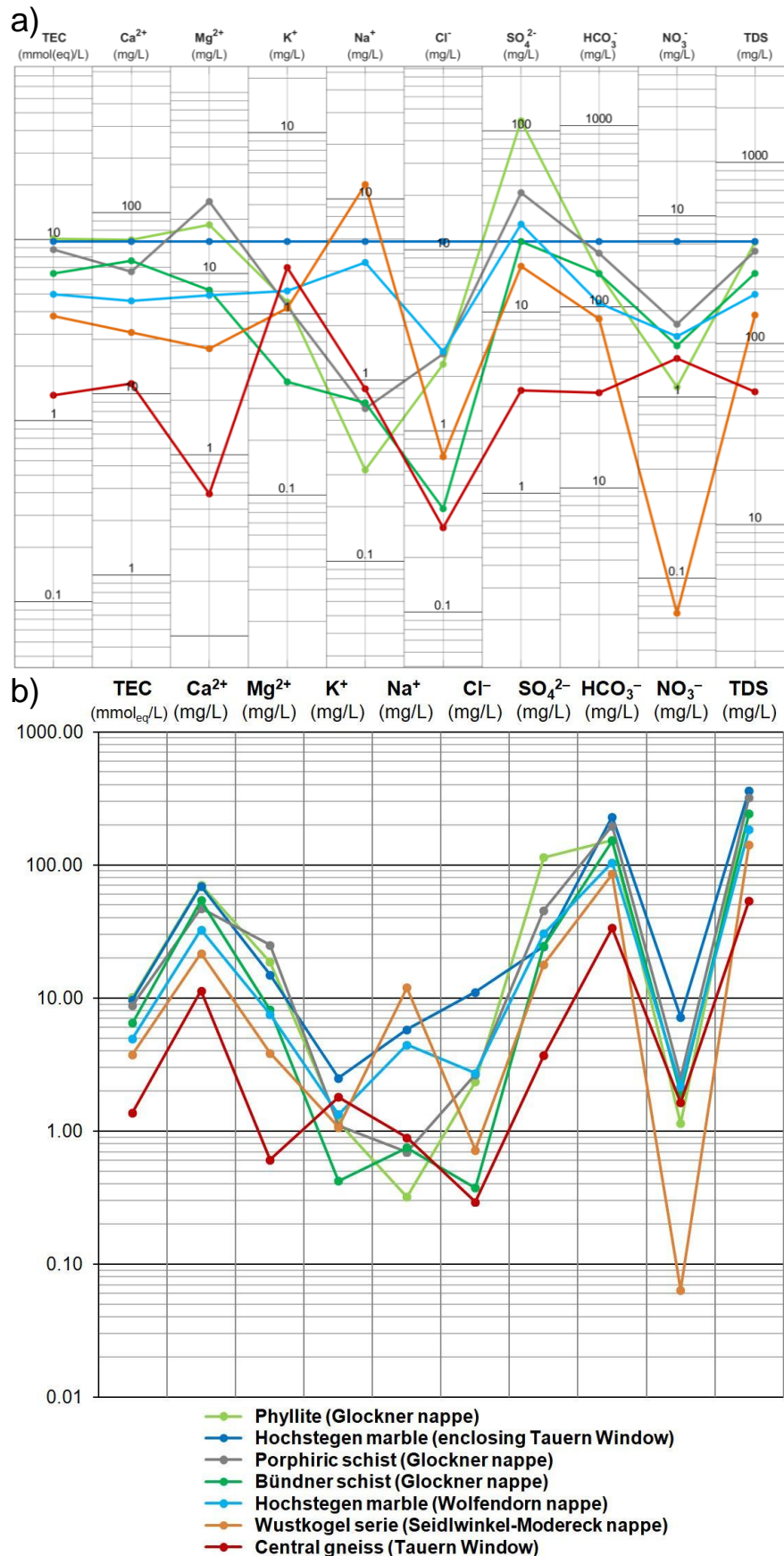


Figure 1. Comparison of a standardized (a) and a conventional (b) Schoeller diagram to compare the ascension and dilution of acidulous thermal brine through several aquifer levels. Water analyses are given in table 2.

To investigate this hypothesis, springs and streams have been sampled throughout the valley and assigned to rock units based on their catchment area (Sass et al., 2016, Schäffer et al., 2021a). Finally, mean values of hydrochemical parameters have been calculated for the respective rock units. For the Hochstegen marble, we distinguish an area in the upper valley belonging to the Wolfendorn nappe and an area in the lower valley directly enclosing the Tauern Window in a narrower sense (data in Table 2). The standardized Schoeller diagram (Figure 1a) shows the respective mean values. The Hochstegen marble enclosing the Tauern Window was chosen as the standard because the hydrochemical relationship to this unit is to be tested. In the standardized Schoeller diagram, the signature of the Hochstegen marble of the Wolfendorn appears subparallel with the exception of chloride and sulfate. Their concentrations are about half an order of magnitude lower compared to the standard. Thus, the standardized Schoeller diagram allows the interpretation that in the upper part of the valley surface, water infiltrates into the Hochstegen marble of the Wolfendorn nappe and then flows underground, following the hydraulic gradient. In this process, groundwater dissolves other minerals and accumulates dissolved solids as the flow distance increases. In addition, a mixture with water infiltrating along the flow path may also occur, resulting in a depletion of sulfate and an enrichment of chloride. Finally, the groundwater partially discharges at springs in the lower part of the valley (dark blue signature in Figure 1). Other relationships to other rock units are not visible in the standardized Schoeller Diagram.

In summary, the standardized Schoeller diagram visualized an evidence of a large-scale and connected karstification of the Hochstegen formation. This interpretation is much more difficult to make on the basis of a conventional Schoeller diagram (Figure 1b), because all waters are low mineralized Ca-HCO₃-waters, which yield a cloud of points or signatures that are difficult to differentiate without standardization.

3.2. Evaluation of rise and dilution of acidulous thermal brine

The thermal spa Bad Soden-Salmünster, Hesse, Germany, is located in the Mid-German Crystalline Zone (Zeh & Will, 2010). The crystalline basement is followed by the Permian Rotliegend formation of clastic sediments (Kowalczyk & Prüfert, 1974), the Permian Zechstein formation consisting mainly of carbonates and evaporites (Richter-Bernburg, 1953), the Triassic Buntsandstein formation of sandstones and mudstones (Lepper et al., 2014, Dersch-Hansmann et al., 2014), and Quaternary deposits. The spa has been using acidulous thermal brine from springs and boreholes for over 175 years (Hanna, 1986, Hansmann & Noll, 1987). The oldest available water analysis dates back to 1877 from the Barbarossaquelle (Himstedt et al., 1907), giving a nearly 150-year series of measurements (Schäffer et al., 2021b). Over this time, springs and shallow wells have been gradually replaced by deep wells (Schäffer et al. 2018). The deepest wells are the Pacificus-Sprudel (406 m, drilled in 1909), the Fritz-Hamm-Sprudel (503 m, drilled in 1972), and the König-Heinrich-Sprudel (539 m, drilled in 1931) (Mestwerdt, 1933). The Trinksprudel is a double borehole: well 1 was drilled to 122 m in 1970, and well 2 was drilled aside to 30 m in 1971. Except for the Pacificus-Sprudel, these wells are still in operation today.

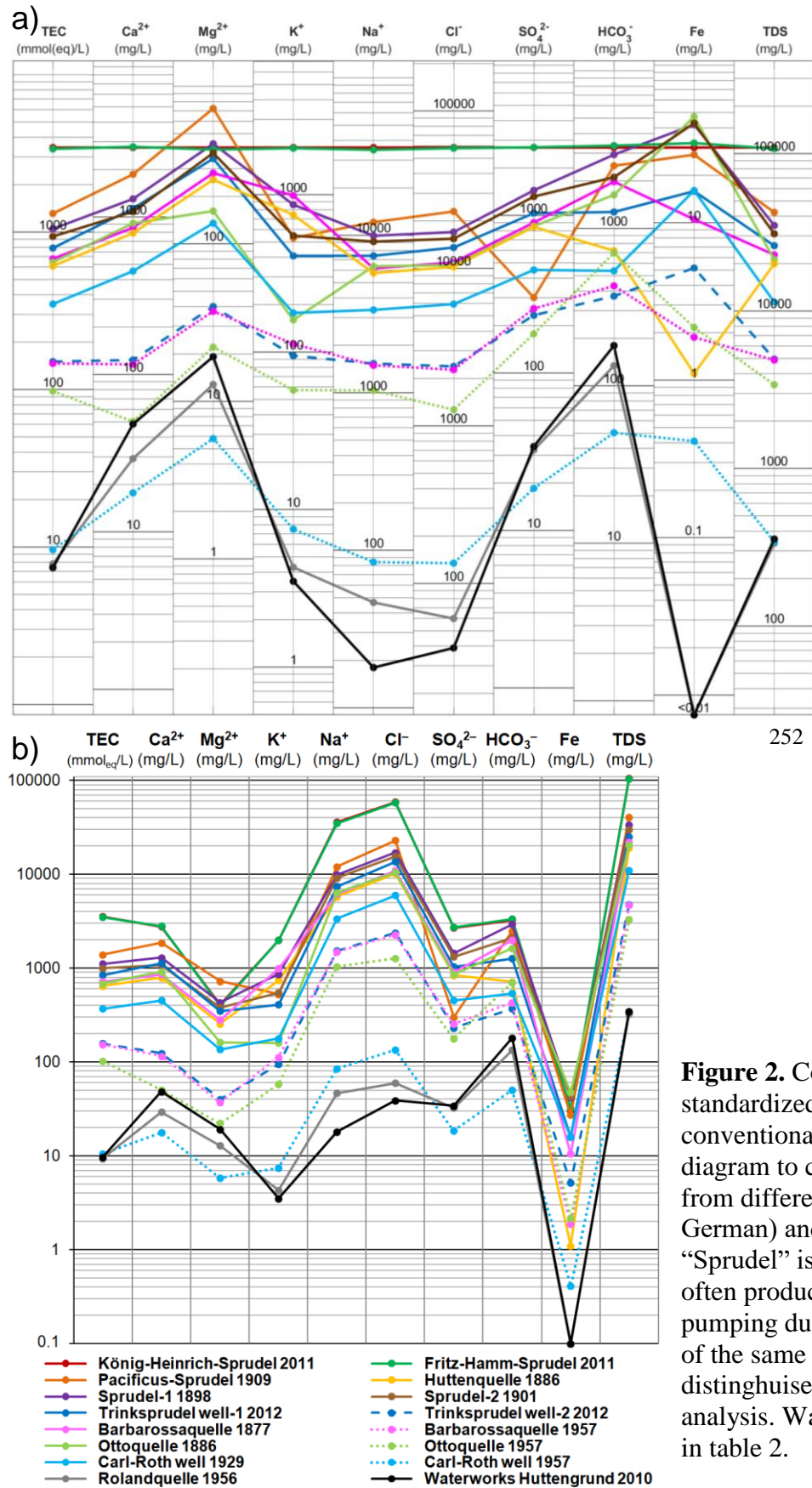


Figure 2. Comparison of a standardized (a) and a conventional (b) Schoeller diagram to compare spring waters from different springs (“Quelle” in German) and wells (“Brunnen”). “Sprudel” is a sparkling well, often producing brine without pumping due to gaslift. Analyses of the same spring or well are distinguished by the year of the analysis. Water analyses are given in table 2.

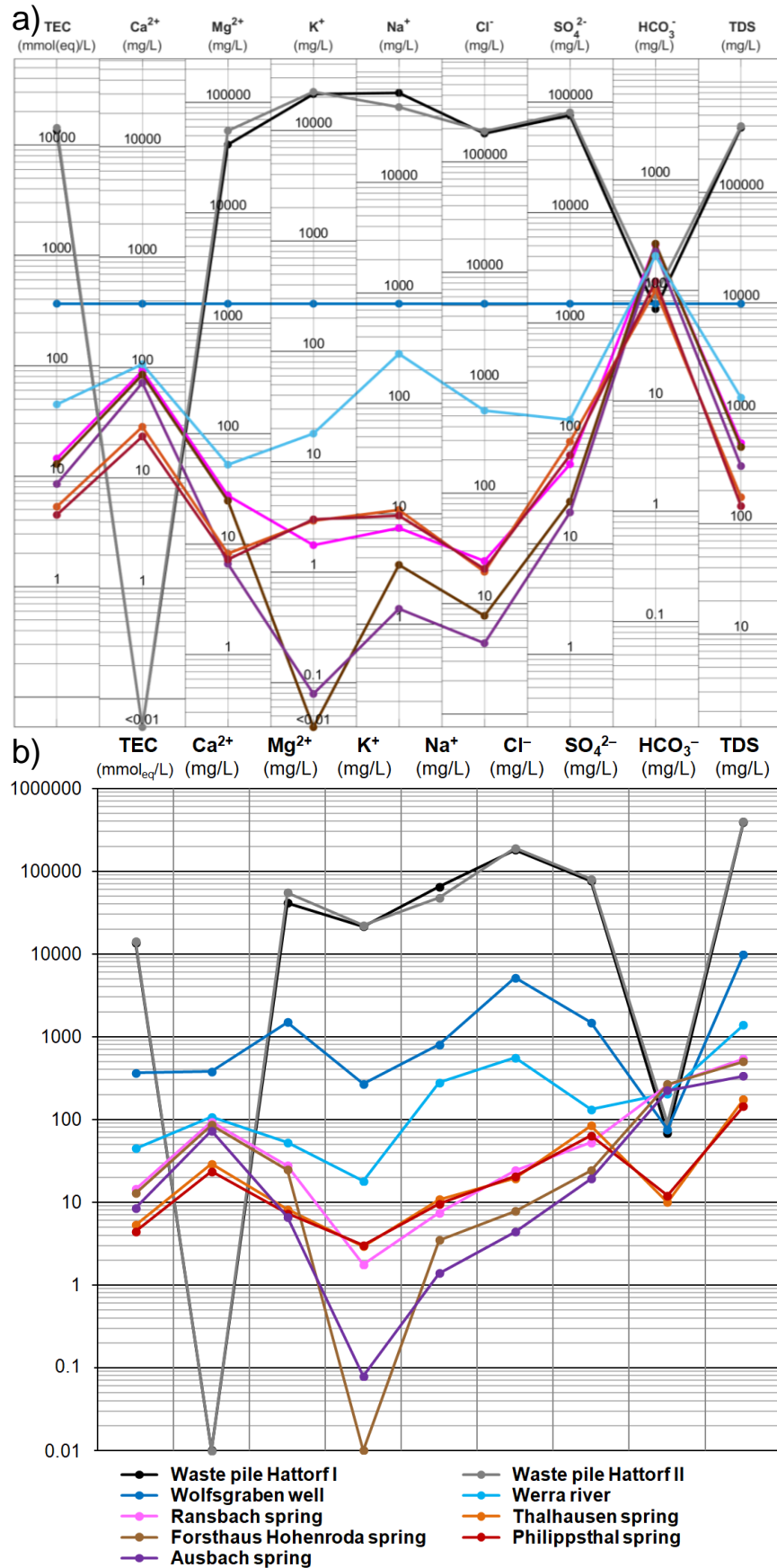
A standardized Schoeller diagram is used to clarify the genesis of the acidulous thermal brine. König-Heinrich-Sprudel serves as the standard because it shows the highest load of dissolved solids (Figure 2b). Rolandquelle and the waterworks Huttengrund are additionally plotted as representatives of the shallow groundwater. In comparison to the diagram in figure 1, iron is plotted instead of nitrate because nitrate is hardly present in the brine, while iron concentrations vary by several orders of magnitude between brine and shallow groundwater. Thus, iron is a good indicator of mixing processes here. Please note that iron concentrations in Rolandquelle and waterworks Huttengrund are below the detection limit of 0.01 mg/L.

The signatures of König-Heinrich-Sprudel and Fritz-Hamm-Sprudel are nearly congruent and represent the pure, undiluted brine from the Zechstein reservoir (Figure 2a). Signatures of the Rolandquelle and the waterworks Huttengrund are quite similar. Eight signatures of the analyses with a solid line between them are similar among themselves. Exceptions are magnesium in Ottoquelle 1886, potassium in Barbarossaquelle 1877, Huttenquelle, Pacificus-Sprudel, and Ottoquelle 1886, sulfate in Pacificus-Sprudel, bicarbonate in Huttenquelle as well as iron in Carl-Roth well 1929, Barbarossaquelle 1877 and Huttenquelle. Based on the parallel to subparallel course of the signatures, these eight analyses are classified as a hydrochemical group, originating from the mixture of brine and vadose groundwater. Here, the solution content increases with depth and due to different aquifer levels (Schäffer et al., 2018), illustrated, for example, by the analyses of Trinksprudel wells 1 and 2 (Figure 2a). In the standardized Schoeller diagram, a second effect is also evident from two analyses of Barbarossaquelle, Ottoquelle, and Carl-Roth well, respectively (same color but solid and dotted lines in Figure 2a). The signatures of the corresponding samples are similar, but the younger ones are shifted downward by one to two orders of magnitude. This indicates that there has been a uniform dilution of waters over decades. Thus, the increasing number of deep wells has reduced or completely stopped the natural rise of brine through the different aquifer levels to the springs at the surface, significantly reducing the proportion of brine in the mixed water.

This detailed interpretation of groundwater genesis is much more difficult to make with a normal Schoeller diagram (Figure 2b). Subtle similarities and differences are hardly apparent due to the missing standardization. The absolute concentration variabilities between potassium, sodium, chloride, sulfate as well as iron lead to signatures with steep slopes, and additionally mask similarities and differences.

3.3. Identification of groundwater contamination by mining residuals

In the Werra Potash Region in eastern Hesse and western Thuringia, Germany, evaporites of the Permian Zechstein formation have been mined for more than 100 years (Dietz, 1929). Since 1929, the potash wastewater has either been sunk into the Plattendolomit aquifer of the Zechstein or discharged into the Werra river (Finkenwirth, 1964). Although the injected brine remains predominantly in the Zechstein, it rises locally into the Triassic Buntsandstein formation or into Quaternary deposits, where it mixes with shallow groundwater or flows into the Werra river (Skowronek et al., 1999).



Solid residues from potash mining, mainly rock salt, are stored in waste piles. If the waste piles were constructed without base seal or if the seal does not work properly, precipitation can dissolve the salt, infiltrate into the subsurface and contaminate the shallow groundwater (Siefert et al., 2006). For the first time in 2016, controls in groundwater monitoring wells below the potash mining waste pile in Hattorf revealed remarkable high concentrations of aluminum, cadmium, iron, lead, manganese, nickel, and zinc. This prompted follow-up investigations to determine whether there is a hydraulic connection to the potash mining waste pile.

The standardized Schoeller diagram (Figure 3a) is standardized on the Wolfgraben well, one of the groundwater monitoring wells with remarkable high concentrations. Two samples from the drainage of the waste pile, as well as five samples from surrounding springs are also plotted. One sample from the Werra river is plotted for comparison. As expected, the signatures of the two samples from the waste pile are almost congruent. Except for potassium, the signatures of the spring waters are also quite similar among themselves. The concentrations of magnesium, potassium, sodium, chloride, sulfate, and total dissolved solids (TDS) are three to five orders of magnitude higher in the waste pile waters compared to the spring waters. The signatures of the Werra and Wolfgraben samples are in between and can be explained by the mixing of waste pile waters and uncontaminated groundwater (Figure 3a). However, this is not true for calcium and bicarbonate. While for calcium the Wolfgraben well shows the highest concentrations and calcium is not detectable at all in the waste pile waters, bicarbonate concentrations are highest in the Werra river and springs and lowest in the waste pile waters, with relatively small differences compared to the other species considered. Thus, the calcium concentration in the Wolfgraben well cannot be explained simply by mixing of these waters; obviously, other processes, such as ion exchange reactions in the aquifer, might play a role here. Overall, the standardized Schoeller diagram provides an evidence that the Wolfgraben well is a mixture of groundwater and waste pile water, and thus the contamination with heavy metals is also very likely due to the waste pile water.

Apart from being easier to interpret, the standardized Schoeller diagram (Figure 3a) has the advantage, compared to a normal Schoeller diagram (Figure 3b), that fewer orders of magnitude need to be represented, making it more compact.

4 Conclusions

On the one hand, standardized Schoeller diagrams are more meaningful and powerful than conventional Schoeller diagrams, but on the other hand, their preparation is laborious, because they had to be drawn manually. Here, we present a freely available Matlab tool which allows a fast and simple digital production of standardized Schoeller diagrams including many options to realize user-specific wishes or requirements. Three examples with different problems show that the standardization greatly facilitates the comparison of water samples to the chosen standard and increases the informative value of a Schoeller diagram. Interpretations and conclusions derived from the standardized Schoeller diagrams can hardly be gained with conventional Schoeller diagrams. Therefore, we hope that standardized Schoeller diagrams will be helpful and beneficial for many users and will be widely applied.

Acknowledgments, Samples, and Data

Lea Döpp, Claus-Dieter Heldmann and Philipp Zimmermann helped to collect water samples. Discussions with Ingo Sass lead to the idea of standardized Schoeller diagrams. Căcilia Tomoe Boller revised the manuscript. The authors declare that they have no conflict of interest. Data used in figures 1, 2 and 3 are summarized in table 2. The Matlab code, a detailed manual and additional information can be downloaded here: <https://doi.org/10.48328/tudatalib-877>

390 **Table 2.** Water analyses used in this technical report.

Example 1 (data from Schäffer et al., 2014, and Sass et al., 2016)	TEC	Ca ²⁺	Mg ²⁺	K ⁺	Na ⁺	Cl ⁻	SO ₄ ²⁻	HCO ₃ ⁻	NO ₃ ⁻	TDS
	[mmol _{eq} /L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]
Phyllite	10.09	70.84	18.59	1.16	0.32	2.34	113.7	153.2	1.14	362.3
Hochstegen marble (Tauern Window)	9.75	69.34	15.04	2.51	5.82	11.11	24.52	229.4	7.22	365.8
Porphyric schist	8.80	47.22	24.98	1.10	0.70	2.66	45.56	197.5	2.52	323.4
Bündner schist	6.49	54.25	8.10	0.42	0.75	0.37	24.49	152.4	1.92	243.7
Hochstegen marble (Wolfendorn nappe)	4.98	32.57	7.59	1.34	4.46	2.74	30.56	104.6	2.16	186.7
Wustkogel serie	3.78	21.81	3.85	1.07	12.00	0.72	17.89	85.76	0.06	143.5
Central gneiss	1.38	11.39	0.61	1.80	0.90	0.29	3.69	33.53	1.63	54.12
Example 2 (data from Schäffer et al., 2018)	TEC	Ca ²⁺	Mg ²⁺	K ⁺	Na ⁺	Cl ⁻	SO ₄ ²⁻	HCO ₃ ⁻	Fe	TDS
	[mmol _{eq} /L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]
König-Heinrich-Sprudel 2011	3557	2760	409	1990	36100	58600	2700	3258	30	105829
Fritz-Hamm-Sprudel 2011	3489	2790	397	1970	34900	58000	2710	3350	32	104129
Pacificus-Sprudel 1909	1391	1865	723.8	530.8	12118	23004	300.9	2495	27.35	41051
Huttenquelle 1886	648.2	789.8	255.8	743.2	5759	10236	845.8	720.4	1.1	19351
Sprudel-1 1898	1115	1302	432	862.5	9937	17020	1443	2935	41.9	33932
Sprudel-2 1901	995.2	1079	377.8	548.7	9126	15440	1318	2109	42.8	30002
Trinksprudel well-1 2012	845.5	1132	347.8	408.1	7414	13576	1034	1269	15.83	25210
Trinksprudel well-2 2012	157.6	123.5	40.01	94.76	1533	2387	232.4	371.0	5.15	4801
Barbarossaquelle 1877	718.7	855.2	281.6	986.6	6169	10910	901	1978	10.5	22081
Barbarossaquelle 1957	153.6	115.8	37.3	112.7	1494	2274	256.2	430.9	1.87	4738
Ottoquelle 1886	682.7	912	161.5	160	6364	10500	854.5	1629	47.1	20593
Ottoquelle 1957	101.8	50.21	22.14	57.34	1035	1267	177.2	697.7	2.16	3309
Carl-Roth-Brunnen 1929	370.7	453.1	135.3	177.3	3360	5937	450.9	536.5	15.80	11052
Carl-Roth-Brunnen 1957	10.46	17.72	5.83	7.47	84.14	134.4	18.53	50.32	0.41	332.6
Rolandquelle 1956	9.37	29.16	12.84	4.3	46.55	59.82	32.41	134	<0.01	327.7
Freshwater supply Huttengrund 2010	9.74	48.4	19.2	3.5	18	38.9	34.1	180	<0.01	349.4

Example 3	TEC	Ca ²⁺	Mg ²⁺	K ⁺	Na ⁺	Cl ⁻	SO ₄ ²⁻	HCO ₃ ⁻		TDS
	[mmoleq/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]		[mg/L]
Spoil tip I	13470	<0.01	41461	21349	64711	180578	75790	67.73		385427
Spoil tip II	14279	<0.01	55297	22382	48148	189429	80743	89.70		398335
Wolfsgraben well	364.5	377.8	1502	269.8	798	5190	1493	75.66		9816
Werra river	44.70	107.0	52.38	18.00	280.9	559.2	132.6	205.0		1383
Ransbach spring	14.47	93.12	27.48	1.76	7.43	24.29	52.60	258.7		537.2
Thalhausen spring	5.29	29.04	8.21	2.93	10.84	19.42	84.27	10.01		173.8
Forsthaus Hohenroda spring	12.89	86.03	24.67	<0.01	3.45	7.75	24.14	264.8		494.7
Philippsthal spring	4.46	23.75	7.27	3.01	9.62	20.64	63.45	12.08		144.3
Ausbach spring	8.50	72.63	6.63	0.08	1.38	4.38	19.26	224.5		332.7

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