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WHAT STORY DOES THE DUROV DIAGRAM TELL?

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Summary

The Durov diagram is a popular visualization technique applied in hydrogeology to display the major ions as percentages of milli-equivalents in two ternary (trilinear) graphs that form an additional two-dimensional projection (the Durov projection). The paper shows that the Durov diagram is not as useful as it is normally thought to be. We discuss that the Durov projection, which is the main idea behind the Durov diagram, offers a data picture that should not be interpreted as it normally is in the Durov diagram.

Key words and phrases: graphing, ions, ternary graph, trilinear graph, visualization

Classification AMS 2010: 86A05, 68U05

1. Introduction

The Durov diagram (Durov, 1948) displays the major ions as percentages of milli-equivalents in two ternary (trilinear) graphs, one for cations and one for anions. The sum of ions in each of these two groups is forced to be 100% for each sample element; so, when interpreting such data, we look at the compositions of the cations and anions.

The Durov diagram has been used in various hydrogeological applications (e.g., Fraser et al. 1996; Crandall et al. 1999; Parnachev et al. 1999; Banks et al. 2001; Rabemanana et al. 2005; Khayat et al. 2006; Demlie et al. 2007; Brodie et al. 2008). The main idea behind this display is to make a projection of two ternary displays for anions and cations: the ternary displays are drawn perpendicularly to each other, onto a square plot (which we will hereafter call the 'Durov projection'). Figure 1 shows an example of the Durov diagram for artificial data presented in Table 1 We used R (R Core Team 2017) to construct the graph. It is commonly accepted that this type of display helps to indicate clusters of samples: samples that are close in the Durov projection are assumed to have similar compositions of anions and cations.

In this note, we show that the Durov diagram is not as useful as it is normally considered, and that conclusions drawn based on this display can be misleading.

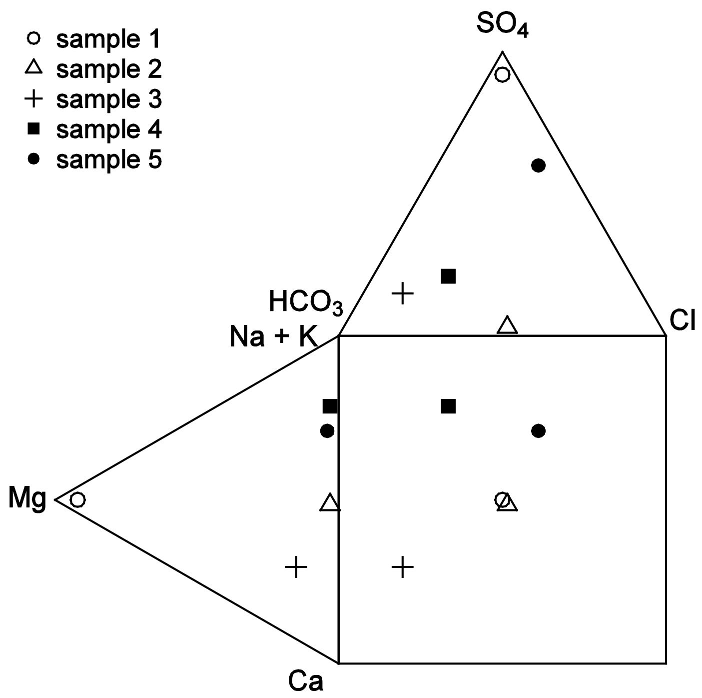

Fig. 1. The Durov diagram of the data presented in Table 1.

Table 1. An artificial data set consisting of five samples, used in Figures 1 and 2.

Sample		Cations [%]			Anions [%]		
		NaK	Mg	Ca	Cl	SO_4	HCO_3
1	○	4	92	4	4	92	4
2	Δ	47	3	50	50	3	47
3	+	22	15	63	12	15	73
4	■	77	3	20	23	21	56
5	●	69	4	27	31	60	9

2. Durov diagram

The Durov diagram bases on two ternary (trilinear) graphs. A ternary graph aims to display compositional data consisting of three variables x, y and z for which the following condition holds:

$$x + y + z = 1 = 100\%. \tag{2.1}$$

For the Durov diagram, two such compositions are used, one for cations:

$$(Na + K) + Mg + Ca = 1 = 100\%$$

(Na and K are summed up and considered together as one variable), and another one for anions:

$$Cl + SO_4 + HCO_3 = 1 = 100\%.$$

In practice, a ternary plot is displayed in Cartesian coordinates by the following projection (Wilkinson, 2005):

$$u = \frac{\left(2\tan\left(\frac{\pi}{3}\right)x + \tan\left(\frac{\pi}{3}\right)y\right)}{x + y + z}, \tag{2.2a}$$

$$v = \frac{y}{x + y + z}, \tag{2.2b}$$

u and v forming the horizontal and vertical coordinates, respectively. Of course, since $x + y + z = 1 = 100\%$, the denominators in (2.2a) and (2.2b) are not needed, but these formulas are more general because they work also for variables in original units.

After replacing the tangent with its value of $\sqrt{3}$, the ternary plots in the Durov diagram are displayed based on the following projections:

$$u_{cations} = \frac{2\sqrt{3}(\mathrm{Na}+\mathrm{K})+\sqrt{3}\,\mathrm{Mg}}{(\mathrm{Na}+\mathrm{K})+\mathrm{Mg}+\mathrm{Ca}},\; v_{cations} = \frac{\mathrm{Mg}}{(\mathrm{Na}+\mathrm{K})+\mathrm{Mg}+\mathrm{Ca}} \quad (2.3a)$$

and

$$u_{anions} = \frac{2\sqrt{3}\mathrm{Cl}+\sqrt{3}\mathrm{SO}_4}{\mathrm{Cl}+\mathrm{SO}_4+\mathrm{HCO}_3},\; v_{anions} = \frac{\mathrm{SO}_4}{\mathrm{Cl}+\mathrm{SO}_4+\mathrm{HCO}_3}. \quad (2.3b)$$

For simplicity, let us assume that the anions and cations are already presented in percentages, thus the denominators in (2.3a) and (2.3b) can be removed, yielding the following scaled coordinates:

$$u^s_{cations} = 2\sqrt{3}(\mathrm{Na}+\mathrm{K})+\sqrt{3}\mathrm{Mg},\; v^s_{cations} = \mathrm{Mg} \quad (2.4a)$$

and

$$u^s_{anions} = 2\sqrt{3}\mathrm{Cl}+\sqrt{3}\,\mathrm{SO}_4,\; v^s_{anions} = \mathrm{SO}_4. \quad (2.4b)$$

These scaled coordinates are presented in the original percentage values (for anions and cations), having the minimum of 0% and the maximum of 346.4% for the scaled coordinate u^s and the minimum of 0% and the maximum of 100% for the scaled coordinate v^s.

Note the coordinates of the Durov projection are

$$x_{Durov} = u^s_{anions}, y_{Durov} = u^s_{cations}.$$

The Durov projection is plotted in the full range of the variables: 0-3.46 (which follows from equations (2.3a) and (2.3b)) for the coordinates for u_{anions} and $u_{cations}$ and 0-346.4% for the scaled coordinates u^s_{anions} and $u^s_{cations}$. Note that changing scales in (2.3a) and (2.3b), which is done in (2.4a) and (2.4b), will affect only the tick mark labels in the projection, but not the appearance of the graph. Thus, the Durov projection can be redrawn in the coordinates u^s_{anions} (2.4a) and $u^s_{cations}$ (2.4b); see Fig. 2.

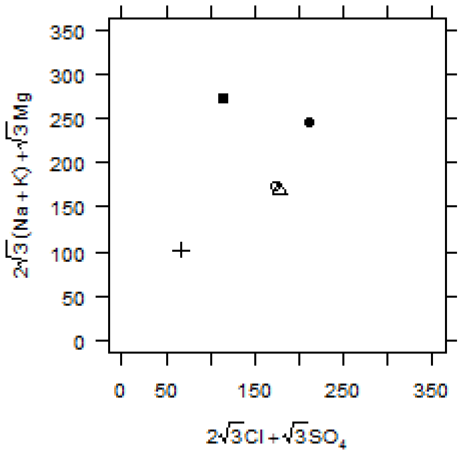

Fig. 2. The Durov projection constituting the part of the Durov diagram presented in Fig. 1.

3. Discussion and conclusion

Let us recall what story the Durov diagram is to tell: clusters of similar samples are to be detected, in that way offering interpretation about samples' similarities in the compositions of anions and cations. This interpretation is done by the visual grouping of samples in the Durov projection, and those from the same cluster are assumed to have similar compositions of anions and cations.

Does the Durov diagram tell such a story indeed? To answer this question, let us recall what the Durov projection (Fig. 2) displays:

$$2\sqrt{3}(\mathrm{Na}+\mathrm{K})+\sqrt{3}\mathrm{Mg} \ \ \textit{versus} \ \ 2\sqrt{3}\mathrm{Cl}+\sqrt{3}\,\mathrm{SO}_4 . \tag{3.1}$$

So, grouping samples based on the Durov projection does not offer clusters of samples with similar anion and cation compositions, but with similar values given in (3.1), so, similar $u^s_{cations}$ and u^s_{anions}. We have thus two groupings: one based on anion-cation composition and another one based on the Durov projection. Are they similar? It will depend on the data, but the sad truth is that *they do not have to be similar*. In fact, the Durov projection substitutes HCO_3

with the value for Cl (so, instead of HCO_3 + Cl, the Durov projection uses 2Cl) and Ca with the value for Na + K. So, instead of Ca + Na + K, the Durov projection uses 2(Na + K).

Below, we will use the term “axis” to mean the line used in the displays to provide information about the coordinates of the points in the graph, and the term “scale” to mean this information. Such differentiation is normally made in information graphics (see, e.g., Harris 1999, although different authors may use different terms), but as we will show, for the Durov diagram this differentiation is crucial and thus needs to be emphasized.

The problem is that the appearance of the Durov diagram (Fig. 1) suggests that the scales of the Durov projection have to do with the corresponding scales of the ternary plots. Thus, two axes are presented as one axis, but they represent two different scales: one from the ternary graph and one from the Durov projection. These two axes are related only in terms of how the Durov projection is constructed, but they do not represent the same scales. The bottom axis in a ternary plot is projected into Cartesian coordinates by the formula in (2.2a). However, the ternary diagram is not read in these coordinates, but in barycentric coordinates (and actually the scales presented in the sides of the triangle refer to the scale having representation in the corresponding heights in the triangle), and the axis has its own scale that is *not* formed by the values of u in (2.2a). The Durov projection’s axes are formed by u values and its scales should be understood as representing u values, and so treating the corresponding scales from the Durov projection and from the ternary plot as the same scales is incorrect. Thus, the main reason why Durov diagram may give a falsified picture is that triangles (for cations and anions) are projected only on one axis (the u coordinate)—v is ignored. So, when Mg and SO_4 are quite variable in the dataset, this may lead to incorrect clustering.

Let us return to Figure 1. Samples 1 and 2 are almost indistinguishable in the Durov projection, while in fact they do differ a lot in both anion and cation compositions (Table 1). Would anyone want to conclude based on these data that sample 1 and sample have the same compositions of anions and cations?

The question is, then, why should one use the Durov projection and risk a rather likely situation that the projection does not reflect the true anion and cation compositions? Of course, one can check that, as we did above with Figure 1. But if there are many samples, such checking would be troublesome, and in fact would seldom work—as the formulas for the projection (2.3a-2.4b) themselves show, the Durov projection is not what one wants to interpret.

To the best of our knowledge, this simple but problematic feature of the Durov diagram has not yet been posed in the literature. This paper does not aim to show that the Durov diagram is incorrect: it is just a type of projection of six variables onto Cartesian coordinates, offering one of many possible simplifications. But the bottom line is that the Durov projection, and hence the Durov diagram, tells a different story than that which its users want it to. Ergo, the Durov diagram should *not* be recommended for the interpretation of compositions of major cations and anions.

We would be happy to suggest a better visualization method—but for the moment we cannot. Analyzing the two ternary plots can provide proper interpretation, although indeed a simplistic one—because such an approach does not link anions and cations. Anyone deciding to use the Durov diagram should be very careful and remember that, depending on the data, it is possible that the interpretation made based on it will be incorrect. For this very reason, we would suggest that hydrogeologists and other researchers give up using the Durov diagram for analyzing composition of anions and cations in samples. Instead, they may use exploratory data analysis, also with the help of two separate ternary plots (for anions and cations). Additional research might reveal a better graphical method to visualize these two compositions in one graph.

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