Matlab-Based Implementation of Durov Trilinear Diagrams: Postprint

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Abstract

Hydrochemical classification is one of the important prerequisites for achieving sustainable development and utilization of water resources. The Durov diagram, as a primary hydrochemical classification chart, has limited practical application due to its plotting complexity, and some common hydrochemical software also lacks the functionality to plot Durov diagrams. The Durov diagram includes the original Durov diagram and the extended Durov diagram evolved based on it. This paper elaborates on the differences, compositional characteristics, and projection principles of the two types of Durov diagrams, proposes a method for establishing coordinate systems in Durov diagrams, and derives formulas for projecting hydrochemical data onto Durov diagrams. On this basis, this paper describes the methods and procedures for implementing the original and extended Durov diagrams through Matlab programming, and plots both types of Durov diagrams using published data. Based on comparisons using the same data, it is found that the original Durov diagrams plotted by relevant hydrochemical software and the extended Durov diagrams from some published research results are consistent with those plotted using Matlab in this study, demonstrating that the program is accurate and feasible. This program can not only plot the original Durov diagram but also plot the extended Durov diagram, which cannot be accomplished by common hydrochemical software. The implementation of this program will facilitate the efficient application of Durov diagrams, particularly the extended Durov diagram, which can serve not only as a basis for hydrochemical classification but also indicate certain hydrochemical processes.

Full Text

Plotting Durov Diagrams Based on Matlab

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1. Introduction

Hydrochemical classification of water resources is one of the vital preconditions for sustainable water resource utilization. Although numerous methods exist for hydrochemical classification, the diagram method remains the most effective and simplest approach. As one of the most important diagram methods for hydrochemical classification, Durov diagrams (including both the original Durov diagram and the expanded Durov diagram) are widely used not only because they can reveal the hydrochemical characteristics of water, but also because they can illustrate the hydrochemical processes occurring within different hydrogeological systems. However, compared with other diagrams (such as the Piper diagram), these diagrams are very complex and difficult to plot. Few commercial software packages are designed to plot Durov diagrams, which limits researchers' ability to use them.

This paper introduces both the original Durov diagram and the expanded Durov diagram, comparing their similarities and differences. To better understand the diagrams, we interpret the composition of the original Durov diagram, particularly its cation triangle, anion triangle, and square field components. We also interpret the composition of the expanded Durov diagram, in which each of the cation and anion triangles is split into two sub-triangles and a diamond, while the square field is divided into nine fields. We emphasize how to establish coordinate systems for plotting both diagram types and derive formulas to transform hydrochemical data for projection into both the original and expanded Durov diagrams. Using these principles, we developed Matlab programs for outputting both diagram types.

2. Coordinate Transformation Formulas

The coordinate transformation formulas for plotting Durov diagrams are derived based on the percentage composition of major ions. The following equations establish the relationship between ion concentrations and their graphical coordinates:

For the cation triangle when $25\% < \mathrm{Ca}^2 \quad 50\%$:

$$x_1 = 0.5 \times (50\% - a_1 + b_1)$$

$$y_1 = 0.5\% \times \tan 60^\circ \times (50\% - a_1 - b_1)$$

For the anion triangle when 25% < Cl 50%:

$$x_2 = -0.5 \times \tan 60^\circ \times (50\% - a_2 - b_2)$$

$$y_2 = -0.5 \times (50\% - a_2 + b_2)$$

For the diamond field:

$$x_3 = x_1$$

$$y_3 = y_2$$

Where a_1, b_1, a_2, and b_2 represent the percentage values of specific cations and anions, respectively. Additional conditional formulas are applied based on different ion concentration ranges, with appropriate offsets (12.5 or 25 units) added to position the points correctly within the expanded diagram structure.

3. Implementation and Validation

3.1 Data Input Requirements The program accepts hydrochemical data in either mg · L ^{1} or meq · L ^{1} units. Users must input the concentrations of six major ions: Ca^{2} , Mg^{2} , Na , K , HCO , SO^{2} , and Cl . The data should be organized in a matrix format where each row represents a water sample and each column represents an ion. The program automatically converts mg · L ^{1} to meq · L ^{1} and calculates the percentage composition of each ion relative to the total cations or anions. The input data must be numeric, and the program validates that the sum of percentages for cations and anions each equals 100%.

3.2 Validation Testing To test the validity of our Matlab programs, we plotted the original Durov diagram using published data from Lloyd and Heathcote [8] and compared the results with those generated by commercial software. Table 1 shows the anion and cation data from Lloyd and Heathcote [8] used for validation.

The Matlab-generated diagram (Figure 5) was compared with the original Durov diagram plotted using AquaChem (Version 2014.2) (Figure 6). The results demonstrate that our program produces identical results to the commercial software, confirming its correctness and reliability.

[Figure 5: see original paper]
[Figure 6: see original paper]

3.3 Program Features The Matlab implementation offers several advantages: cross-platform compatibility (Windows, Linux, Mac), customizable plotting parameters, batch processing capabilities, and the ability to handle large datasets efficiently. The program flow is illustrated in Figure 4, showing the sequential steps from data input through coordinate transformation to final diagram output.

[Figure 4: see original paper]

4. Discussion

The expanded Durov diagram provides a more detailed representation of hydrochemical processes by subdividing the traditional triangular fields. This enhanced resolution allows researchers to better identify subtle hydrochemical evolution patterns and mixing processes. While commercial software packages like AquaChem can plot the original Durov diagram, none currently support the expanded version. Our Matlab program fills this gap, offering researchers a free, flexible, and powerful tool for advanced hydrochemical data visualization.

The program' s modular design facilitates integration with existing hydrochemical analysis workflows. Users can easily modify the code to accommodate specific research needs, such as adding custom classification fields or implementing automated sample classification algorithms. The ability to process data in batch mode significantly improves efficiency when analyzing large hydrogeological datasets.

5. Conclusion

Both the original and expanded Durov diagrams plotted using Matlab provide reliable tools for hydrochemical data interpretation. The programs produce results consistent with established commercial software while offering greater flexibility and control over the plotting process. The expanded Durov diagram, in particular, provides enhanced capability for indicating hydrochemical processes through its refined field subdivisions. These Matlab programs will enable researchers to conveniently apply graphical methods for hydrochemical data interpretation, particularly for studies requiring detailed process identification.

Abstract: Hydrochemical classification of water resource is one of the vital preconditions for water resource sustainable utilization. There are numerous methods with regard to hydrochemical classification for water resource, but the most effective and simplest method is the diagram method. As one of the most important diagram methods for hydrochemical classification, the Durov diagrams (including both the original type of Durov Diagram and the expanded Durov Diagram) are used widely not only because it can reveal the hydrogeochemical characteristics of water, but also because it can show the hydrochemical processes occurring within different hydrogeological systems. However, comparing with other diagrams (such as the Piper Diagram), these diagrams are very complex and difficult to plot. Few commercial software packages are designed to plot Durov diagrams, which limits researchers to use the diagrams. In this paper, we introduced both the original type of Durov Diagram and the expanded Durov Diagram, and we also compared the similarities and differences in them. To better understand the diagram, we interpreted the composition of the original type of Durov Diagram, especially the part of cation triangle, anion triangle and the square field. We also interpreted the composition of the expanded Durov Diagram, in which each of the cation and anion triangles

is split into two sub-triangles and a diamond, while the square field is split into nine fields. We stressed how to establish a coordinate to plot the original type of Durov Diagram and the expanded Durov Diagram respectively. And we deduced formulas to transform the hydrochemical data so that they can be projected in both the original type of Durov Diagram and the expanded Durov Diagram. Using these principles, we wrote programs for the output of both the original type of Durov Diagram and the expanded Durov Diagram based on Matlab. To test the validity of the programs, we plotted the original type of Durov Diagram with published data based on our Matlab programs. And we also plot the original type of Durov Diagram with the same data based on commercial software. The results showed that our program was as correct as the commercial software, which indicated our program is feasible. However, because none of commercial software packages we found has the function of plotting the expanded Durov Diagram, we compared the diagram plotted by our Matlab program with diagram appearing in some classical literature that used the same data. The results also confirmed that our Matlab program is reliable. Both the original type of Durov Diagram and the expanded Durov Diagram plotted by Matlab will help researchers to interpret hydrochemical data in graphical methods conveniently. Especially, the expanded Durov Diagram provides a method to indicate hydrochemical processes.

Keywords: hydrochemistry; the Durov diagrams; Matlab; plotting

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Note: Figure translations are in progress. See original paper for figures.