GROUND WATER

Computer Notes

DurovPlot: A Computer Program for Processing and Plotting Hydrochemical Data

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Abstract

The expanded Durov diagram has been widely used to represent the dissolved constituents of natural water and to show plausible hydrochemical processes occurring within the hydrological systems. Because of the time required to calculate Durov diagram coordinates and to plot the points, especially when dealing with large numbers of chemical analyses, the treatment of such data is often quite a tedious process. To alleviate this problem, DurovPlot program is designed to help users in calculating and plotting the diagram in a very short time. The program is written in BASIC as a special menu-driven hydrochemical data analyses code. It was compiled using Microsoft QuickBASIC version 4.5 compiler. The utilization of this program requires the acquisition of an IBM-PC or compatible with at least 512K bytes of memory, one disk drive (at least 360K bytes), a graphic card (EGA or VGA), and at least DOS version 5.0. DurovPlot possesses several advantages such as the ease with which the data can be entered, edited, and retrieved. The results of computation and plotting are obtained in seconds, depending on the amount of data analyzed and the speed of the computer processor.

Introduction

The Durov diagram is one of the most widely used forms of trilinear graphical representation for hydrochemical data. It was primarily designed by Durov (1948) and then expanded by Burdon and Mazloom (1958) and Lloyd (1965). The early form of these diagrams consisted of two triangles whose bases occupy the two neighboring sides of the main rectangular field of projection (Figure 1). The diagram plotting is based on the milliequivalent percentage of the total major cations and the total major anions in the water samples. The cations and the anions are plotted on their respective triangles (normally cations occupy the upper triangle, and anions occupy the left-side triangle). In their expanded form, Burdon and Mazloom (1958) and Lloyd (1965) split both triangles along the 50 percent lines so that the main rectangular field of projection could be subdivided into nine subfields of representation (Figure 2). This allows not only representation of the hydrochemical data, but also definition of the plausible hydrochemical processes dominating the groundwater chemistry. Classification of water into "types" according to the dominating cations and anions can then be undertaken. Several parameters such as the total dissolved solids (TDS) and the pH or any other desired parameter, may be added to occupy the remaining sides of the main rectangular field of projection as shown in Figure 1. The major problem with the use of Durov diagrams is the time and effort needed in their formulation.

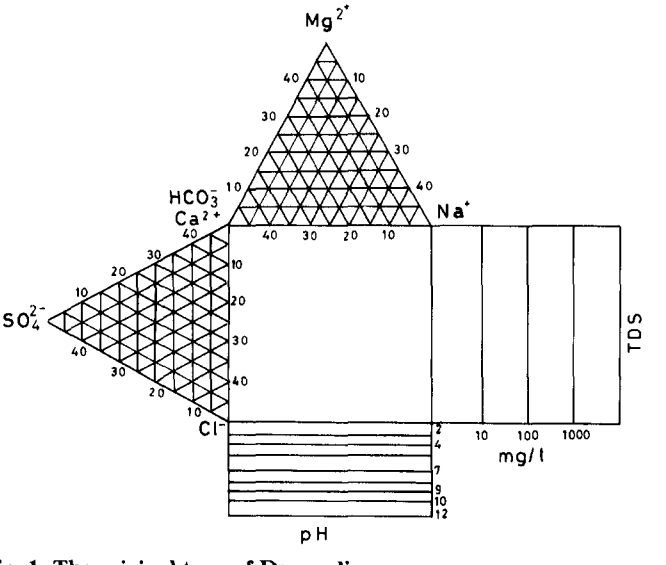

Fig. 1. The original type of Durov diagram.

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Received March 1995, revised February 1996, accepted July 1996.

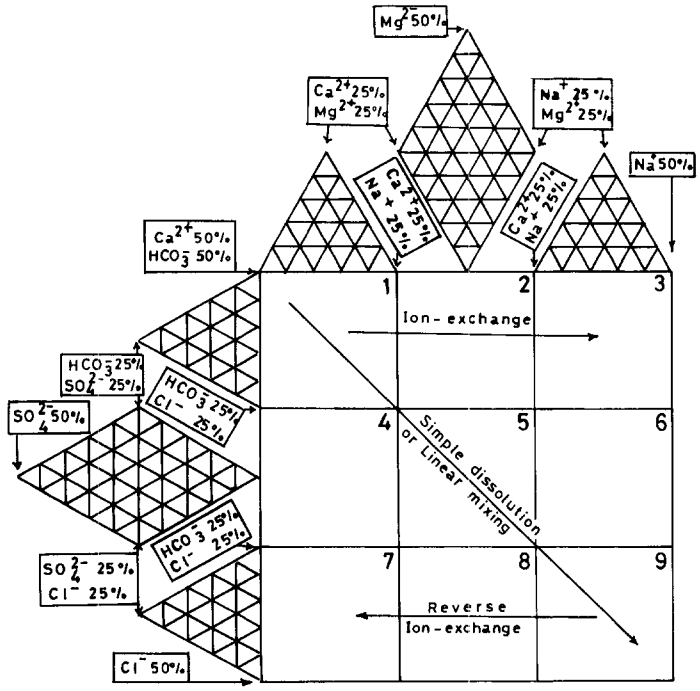

Fig. 2. Expanded Durov diagram with subdivision and processes demonstrated (after Lloyd and Heathcote, 1985).

Significance of Durov Diagrams

The Durov diagram is considered a useful graphical tool for representing hydrochemical data. This diagram represents the data in a very simple and easy way to understand. Durov diagrams also permit the achievement of a more complete characterization of ground water (Zaporozec, 1972). For example, its application removes some of the shortcomings of other trilinear plots such as Hill diagrams (Hill, 1940) and Piper diagrams (Piper, 1944). The Durov diagram is of simple construction and widely used to classify water into types representing each type by a single point, to determine the concentration of chemical constituents and total dissolved solids, and to study the origin of chemical composition of water. It is also used for correlating chemical analyses, grouping water points that are closely related to each other, and specifying water quality. Desai et al. (1979) used Durov diagrams to compare the major ionic constituents in the ground water from wells in the Mangrol-Chorwad coast, Saurashtra Gujarat, to determine the water types, to group water, and to discern evidence of sea-water intrusion. Lawrence et al. (1976) also used Durov diagrams to depict water types and groups, and to illustrate hydrochemical zonation across part of the Lincolnshire Limestone Aquifer of England. Lloyd and Heathcote (1985) have reviewed the usefulness of Durov diagrams in discerning processes that control ground-water chemical properties and discussed the significance of the nine subfields of projection on the expanded Durov diagram (Figure 2). They successfully applied the diagram to represent minor ion chemistry for ground-water designation purposes. They also used the expanded Durov diagram to illustrate the chemistry of the Suffolk and Essex, England, ground waters.

General Features of DurovPlot

Many computer programs have been developed to plot geochemical and hydrogeological data on trilinear diagrams (e.g., Morris et al., 1983; Garcia and Frias, 1990; Ong, 1990). Generally, such programs have been written to satisfy specific needs of the authors and most required specialized data input format. In our reviewing of published and commercial software such as ROCKWARE and PLOTCHEM, we have not observed any program specifically designed for representing hydrochemical data in the form of a Durov diagram. DurovPlot was designed as a special purpose, menu-driven, hydrochemical data analysis program. The program accepts input data, then processes and plots these data in the form of a Durov diagram. DurovPlot was written and compiled using Microsoft QuickBASIC version 4.5 compiler. To run the program, the following hardware is required: an IBM-PC or compatible with at least 512K bytes of memory, one disk drive (at least 360K bytes), a graphics card (EGA or VGA), and at least DOS version 5.0.

Computational and Plotting Procedures

The drawing of the diagram outline and the plotting of points are done in Cartesian coordinates on the graphic screen of the computer, so that all trilinear coordinates are converted to Cartesian coordinates. This procedure is well explained by Morris et al. (1983).

The primary trilinear diagram is an equilateral triangle with each side representing a range of 0 to 100 concentration percentage. The base length of each triangle is 160 units, and its height is 138.56 units of screen coordinates (pixels). In the expanded form of the Durov diagram each of the cation and anion triangles is split into two subtriangles and a diamond. The base of each subtriangle takes 80 units to represent a range of 0 to 50% of specified constituents. Figure 3 shows the screen physical coordinate system. Plotting of points within the cation triangle is based on the percentage of Ca^{2+} and Mg^{2+} compared to the total cations. The following equations were derived for converting trilinear coordinates into X-Y coordinates of the screen.

$$X_{coord} = X_Q - (Ca\% \cdot 1.6) - [(Mg\% \cdot 1.3856)/\tan 60] \quad (1)$$

$$Y_{coord} = Y_Q - (Mg\% \cdot 1.3856) \quad (2)$$

where X_{coord} and Y_{coord} are the Cartesian coordinates of a single

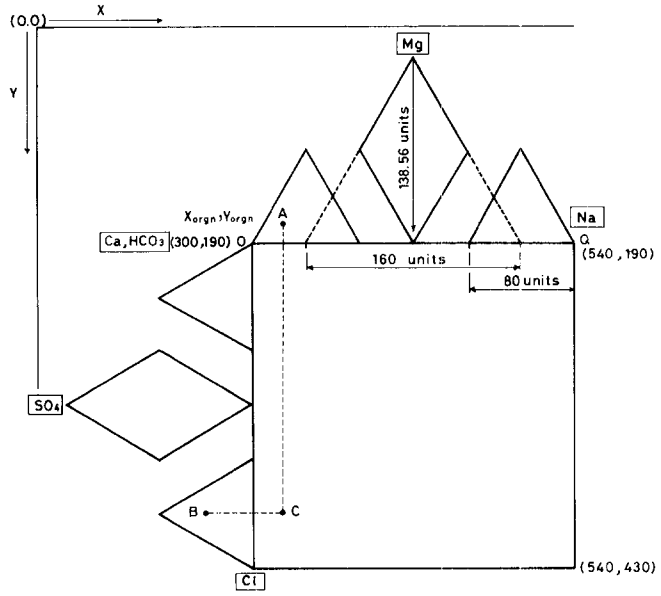

Fig. 3. Coordinate system in the triangular and rectangular fields of Durov diagram.

Table 1. Calculated Durov Coordinates Using DurovPlot

Well	*Ca*	*Mg*	*Na*	*K*	*HCO_3*	*Cl*	*SO_4*	*NO_3*
Major ions concentrations in mg/l:								
2033	100.00	37.20	184.00	8.20	110.00	330.00	307.00	18.00
2036	60.00	37.20	185.00	12.50	120.00	266.00	283.00	27.90
2039	68.00	39.60	196.00	8.60	112.00	309.00	288.00	22.90
2040	96.20	24.90	70.80	7.40	65.00	227.00	173.00	22.30
2041	123.00	35.70	177.00	15.20	100.00	288.00	384.00	57.70
2045	86.40	71.20	312.00	14.80	134.00	508.00	336.00	34.10
2048	272.00	94.40	607.00	17.80	89.10	1164.00	787.00	19.20
2049	130.00	35.50	104.00	3.50	65.90	291.00	197.00	9.90
2066	68.20	27.50	112.00	5.50	105.00	217.00	154.00	13.00
2071	101.00	61.70	370.00	18.30	203.00	643.00	432.00	13.60
2073	122.00	74.00	434.00	15.20	179.00	643.00	557.00	17.40
2075	162.00	56.30	322.00	11.70	143.00	589.00	528.00	13.00
2078	127.00	62.20	421.00	24.60	176.00	799.00	595.00	16.10
2082	89.80	54.10	177.00	10.50	121.00	401.00	298.00	14.90
2084	73.80	28.60	116.00	5.10	101.00	195.00	206.00	63.20
2088	43.00	25.00	162.00	8.60	89.10	217.00	211.00	21.10
2091	226.00	95.40	284.00	0.00	106.00	767.00	451.00	18.00
2026	28.00	10.40	70.20	3.90	63.40	90.20	106.00	21.10
2027	40.00	16.40	59.30	5.50	73.20	114.00	106.00	16.10
2030	64.00	11.30	80.00	4.30	57.30	153.00	144.00	18.60
5210	134.00	20.20	92.90	3.90	117.00	229.00	194.00	35.30
5220	57.00	8.90	71.50	2.00	132.00	110.00	71.50	19.80
5230	66.00	10.70	64.40	3.10	112.00	105.00	106.00	25.40
5240	167.00	78.00	311.00	12.10	254.00	685.00	300.00	14.30
5247	71.20	26.70	110.00	5.90	234.00	179.00	92.20	32.20

Well	*Ca meq%*	*Mg meq%*	*Na + K meq%*	*HCO_3 meq%*	*SO_4 meq%*	*Cl + NO_3 meq%*
Durov's coordinates:						
2033	30.69	18.81	50.50	10.13	35.94	53.93
2036	20.76	21.22	58.02	12.44	37.28	50.28
2039	22.04	21.15	56.80	10.85	35.46	53.69
2040	47.45	20.24	32.31	9.32	31.53	59.15
2041	35.77	17.11	47.13	8.77	42.80	48.43
2045	17.88	24.28	57.84	9.12	29.08	61.80
2048	28.16	16.11	55.73	2.86	32.15	64.98
2049	46.27	20.82	32.90	7.97	30.29	61.74
2066	31.87	21.18	46.94	15.29	28.49	56.22
2071	18.89	19.02	62.08	10.85	29.33	59.82
2073	19.36	19.36	61.28	8.90	35.21	55.88
2075	29.92	17.14	52.94	7.77	36.47	55.76
2078	20.85	16.83	62.32	7.58	32.56	59.87
2082	26.52	26.33	47.15	10.05	31.45	58.50
2084	32.85	20.98	46.17	13.28	34.43	52.29
2088	18.71	17.93	63.36	11.86	35.69	52.45
2091	35.83	24.93	39.25	5.26	28.42	66.32
2026	25.85	15.82	58.33	16.95	36.01	47.04
2027	32.91	22.24	44.85	17.43	32.08	50.48
2030	41.41	12.05	46.54	10.98	35.07	53.95
5210	53.54	13.30	33.15	14.77	31.12	54.11
5220	42.22	10.86	46.92	30.58	21.05	48.36
5230	46.69	12.47	40.83	24.76	29.78	45.46
5240	29.15	22.44	48.41	13.90	20.86	65.24
5247	33.25	20.55	46.19	33.87	16.96	49.16

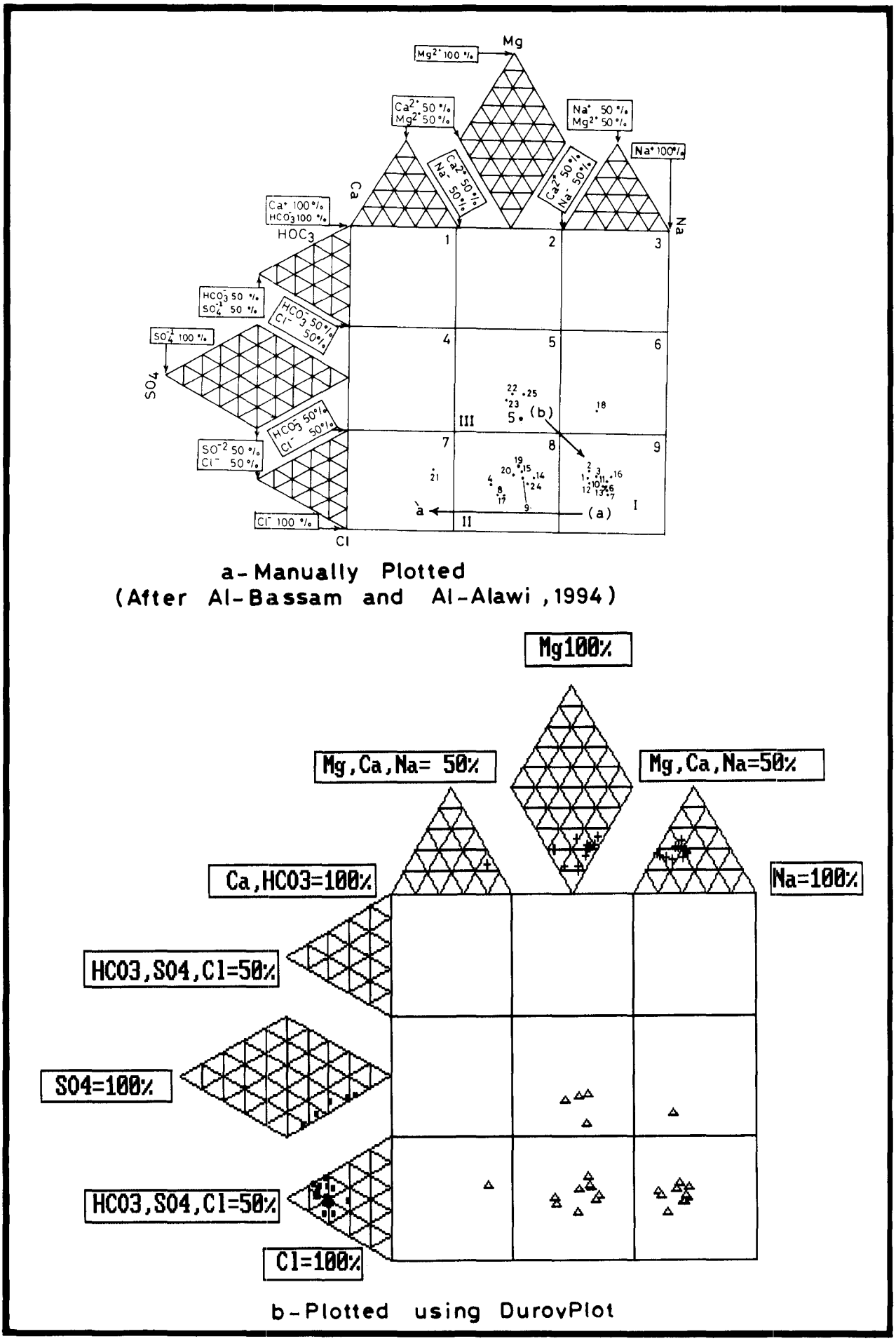

Fig. 4. Durov representation for data from Saudi Arabia.

point on the cation triangle; X_Q and Y_Q are the coordinates of the rightmost point of the cation triangle. The calculated X_{coord} and Y_{coord} are adjusted to the local coordinates (X_{orgn}, Y_{orgn}), and then shifted to fit within the location of the cation triangle split segments of the expanded Durov diagram. These shifted local coordinates are used to plot the cation position. In a similar fashion the calculation and plotting of points within the anion triangle are done based on the HCO_3^- and SO_4^{2-} percentages. The use of Ca^{2+} and Mg^{2+} to plot the cations and SO_4^{2-} and HCO_3^- to plot the anions is an arbitrary choice, where a combination of any two of the constituents can be used with slight modifications to the previous equations.

The location of a point in the rectangular field of projection on Durov diagram (point C on Figure 3), lies at the intersection of two lines projected from two points in the cation and anion triangles (points A and B on Figure 3). Therefore, the X_{coord} of point C is the same as the X_{coord} of point A on the cation triangle, and consequently the Y_{coord} of point C is the same as the Y_{coord} of point B on the anion triangle. The X_{coord} and Y_{coord} of points A and B are used to plot these points.

To test the usefulness of DurovPlot a real data set (Table 1, Figure 4) was processed by the program. The computational results and graphic output printed on a Hewlett Packard Laser Jet II printer using PIZZAZPlus (screen dumping package), are shown in Figure 4b. We could not recognize any difference in the position of data points between the manually plotted (Figure 4a) and the computer generated ones (Figure 4b).

Operation of DurovPlot

The program has been designed in a menu-driven format that can be easily understood by anyone who has any computer experience. DurovPlot consists of three parts: data entry, calculation, and plotting routines. All these routines are accessed through the main menu (Figure 5). The program receives unprocessed data from the keyboard or a disk file. Input of directory and file names are checked for error through various error trapping procedures.

The DurovPlot main menu offers four selections:

1 - Input. The program asks for concentrations of various chemical constituents (Ca^{2+}, Mg^{2+}, Na^+, K^+, HCO_3^-, NO_3^-, SO_4^{2-}, Cl^-) in units of parts per million (ppm, mg/l). Data entry is performed on a template displayed on the screen. After completion of data entry, the program moves to an editing mode that offers a wide range of editing commands. The edited data are then passed to the calculation routine that converts the entered and edited data into meq/l and further to percentage of the total dissolved ions.

2 - Read, 3 - Add. These options are used to process or append data to an existing file. The program asks for the name of the file containing data, then the program displays the file. If the user chooses (Add) option, the program turns to data entry mode and then to the calculation routine.

4 - Plot. After calculations, the processed data are passed to the plotting routine. The plotting routine constructs the diagram, plots each data point on the two triangles of Durov diagram, then projects these points into the rectangular field of the diagram.

Graphic Output

Due to the diversity of computer screens and printer types, it is not easy for individual programmers to write an independent screen dumping subroutine that incorporates a wide range of these screens and printers. Therefore, it was necessary to employ the available public domain or commercial softwares for dumping screen graphics. Three options were introduced to DurovPlot for producing hard copies of screen graphics. The first option employs EGADUMPL.COM that transfers the screen output to an EPSON or compatible dot-matrix printer. The second option utilizes the DOS utility GRAPHICS.COM that gives the user a wide range of 16 printer types. The third option transfers the user to the DOS command line to activate any screen dumping program that fits his computer facility. After the activation of the screen dumping program in option 3, the user can exit the DOS command line and transfers the control to DurovPlot. In all three options, the user can request the number of graphic hard copies he desires.

Conclusions

DurovPlot is an easy to use interactive MS-DOS based program for processing and graphically presenting hydrochemical data. The menu-driven format of the program also makes it easy to use.

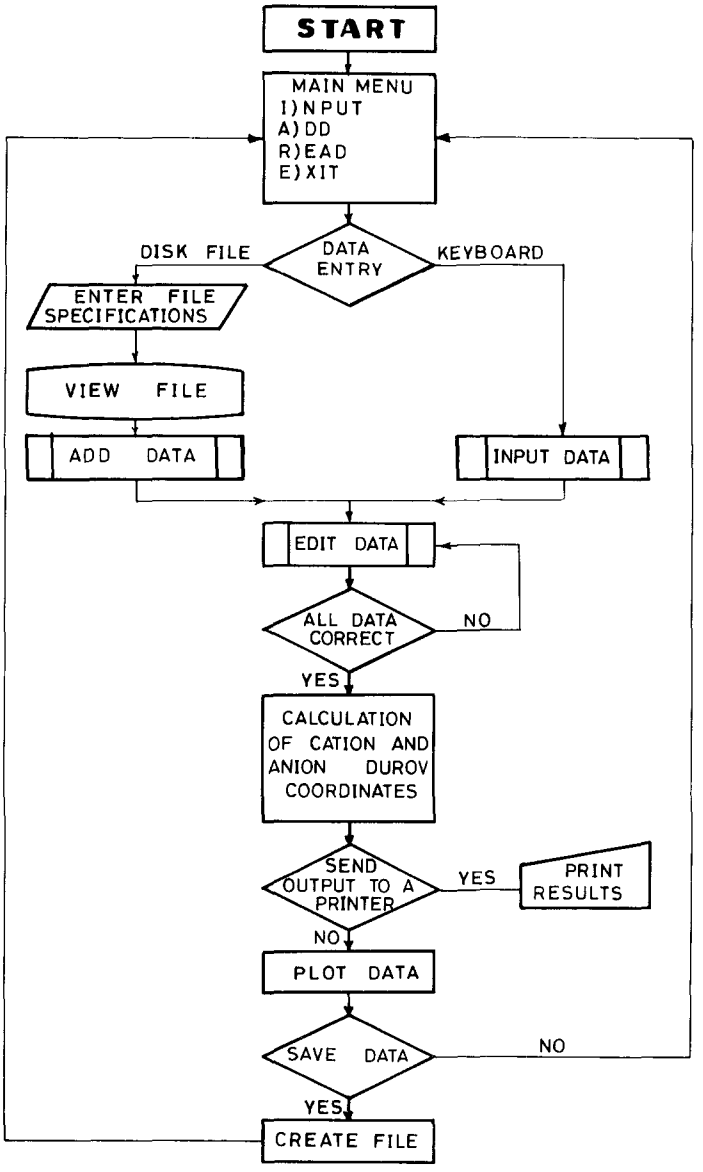

Fig. 5. Flow chart for DurovPlot.

The program has several advantages: data can be entered, edited, and retrieved easily. The results of computations and plotting are obtained in a very short time depending upon the amount of data processed and the speed of the computer processor.

Availability

A copy of the executable code of DurovPlot and a sample data file may be acquired upon request from A. Al-Bassam or H. S. Awad at the Department of Geology, at King Saud University.

Acknowledgments

The authors acknowledge with gratitude Dr. M. Al-Dabbagh, Dr. A. Al-Aswad, and Dr. M. Al-Bassam for their editing and helpful suggestions. We are also indebted to Aftab Aziz for drafting the figures. Our deep appreciation goes to all those who provided us with consultation and helpful discussions, including three anonymous reviewers who greatly improved the original manuscript.

References

Al-Bassam, A. M. and J. A. Al-Alawi. 1994. Hydrogeological and hydrochemical study of Al-Ula area, Kingdom of Saudi Arabia. Middle East Research Center, Ain Shams Univ., Earth Sci. Ser. v. 8, pp. 88-100.

Burdon, D. J. and S. Mazloom. 1958. Some chemical types of groundwater from Syria. UNESCO Symp., Tehran. UNESCO, Paris. pp. 73-90.

Desai, B. I., S. K. Gupta, M. V. Shah, and S. C. Sharma. 1979. Hydrochemical evidence of sea water intrusion along the Mangrol-Chorwad coast for Saurashtra, Gujarat. Hydrological Science Bulletin, Blackwell Scientific Publication. v. 24, no. 1, pp. 71-82.

Durov, S. A. 1948. Natural waters and graphic representation of their composition. Dokl. Akad. Nauk SSSR. v. 59, pp. 87-90.

Garcia, R. B. and J. M. Frias. 1990. BITERCLA:GW-BASIC program to plot classification diagrams. Computers & Geosciences. v. 16, no. 2, pp. 265-271.

Hill, R. A. 1940. Geochemical patterns in Coachella Valley, California. Amer. Geophys. Union Trans. v. 21, pp. 46-53.

Lawrence, A. R., J. W. Lloyd, and J. M. Marsh. 1976. Hydrochemistry and ground-water mixing in part of Lincolnshire Limestone Aquifer, England. Ground Water. v. 14, no. 5, pp. 12-20.

Lloyd, J. W. 1965. The hydrochemistry of the aquifers of north-eastern Jordan. Journal of Hydrology. v. 3, pp. 319-330.

Lloyd, J. W. and J. A. Heathcote. 1985. Natural Hydrochemistry in Relation to Groundwater. Clarendon Press, Oxford. 296 pp.

Morris, M. D., J. A. Berk, J. W. Krulik, and Y. Eckstein. 1983. A computer program for a trilinear diagram plot and analysis of water mixing system. Ground Water. v. 21, no. 1, pp. 67-78.

Ong, C. 1990. CatTrack: A Pascal program to display ternary diagram on a Macintosh computer. In: Microcomputer Application in Geology II. Edited by J. T. Hanley and D. F. Merriam. Series 1990, Pergamon Press. pp. 175-179.

Piper, A. M. 1944. A graphic procedure in the geochemical interpretation of water analyses. Trans. Am. Geophys. Union. v. 25, pp. 914-924.

Zaporozec, A. 1972. Graphical interpretation of water-quality data. Ground Water. v. 10, no. 2, pp. 32-43.