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# PROCESSING OF WATER-QUALITY DATA BY DIGITAL COMPUTER

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## INTRODUCTION

During an investigation of groundwater quality in Western Holland (G e i r n a e r t, 1969) it became apparent that large quantities of data had to be digested. We have developed a program to process water-quality data. This program was written in Fortran IV and tested on the IBM 360/50 of Leiden University (see also R o p e s, M o r g a n and M c N e l l i s, 1969; M c N e l l i s and M o r g a n, 1969). The running time of the program is about one minute, compared with at least one man-day work. The program can be obtained from the Geological Institute of Leiden University.

## DESCRIPTION OF THE COMPUTER PROGRAM

1. Program 1 reads, tabulates and transfers the data from punched cards to a tape. This data consists of the results of analyses (in ppm) from the archives of the Government Institute of Drinking Water Supply.
2. Program 2 reads this tape and calculates the concentrations of the main cations and anions: $Cl^-$, $HCO_3^-$, $SO_4^{2-}$, $Na^+$, $Mg^{2+}$, $Ca^{2+}$, in meq/1. When a value is missing, it tries to derive it from the following relationships (H e m, 1959).
   (a) $\frac{\text{Hardness in } ^\circ D}{2.8}$ (German degrees) = $Ca^{2+}$ + $Mg^{2+}$ (meq/1), where 2.8 is the conversion factor from German degrees to meq/1.
   (b) main anions = main cations (meq/1). The relative quantity of the remaining ions in solution is negligible. The calculated values are printed, and together with the original data they are written on to a second tape.
3. Program 3 is designed to process information selected from this second tape. There is a procedure to reject any analysis for which the variables do not satisfy any logical condition.

The memory of the IBM 360/50 computer is not large enough to contain all the variables of all the analyses simultaneously. The program transfers a maximum of 9 variables from the tape to core storage, and executes the following operations.

a. Listing of the basic data (subroutine LIST)
b. Printing a frequency distribution of each variable (subroutine DIST)
c. Plotting a scatter diagram for two variables (subroutine CORL)
d. Printing the values of a variable on a map (subroutine AREA)

A flow chart of the entire set of programs is shown in figure 1.

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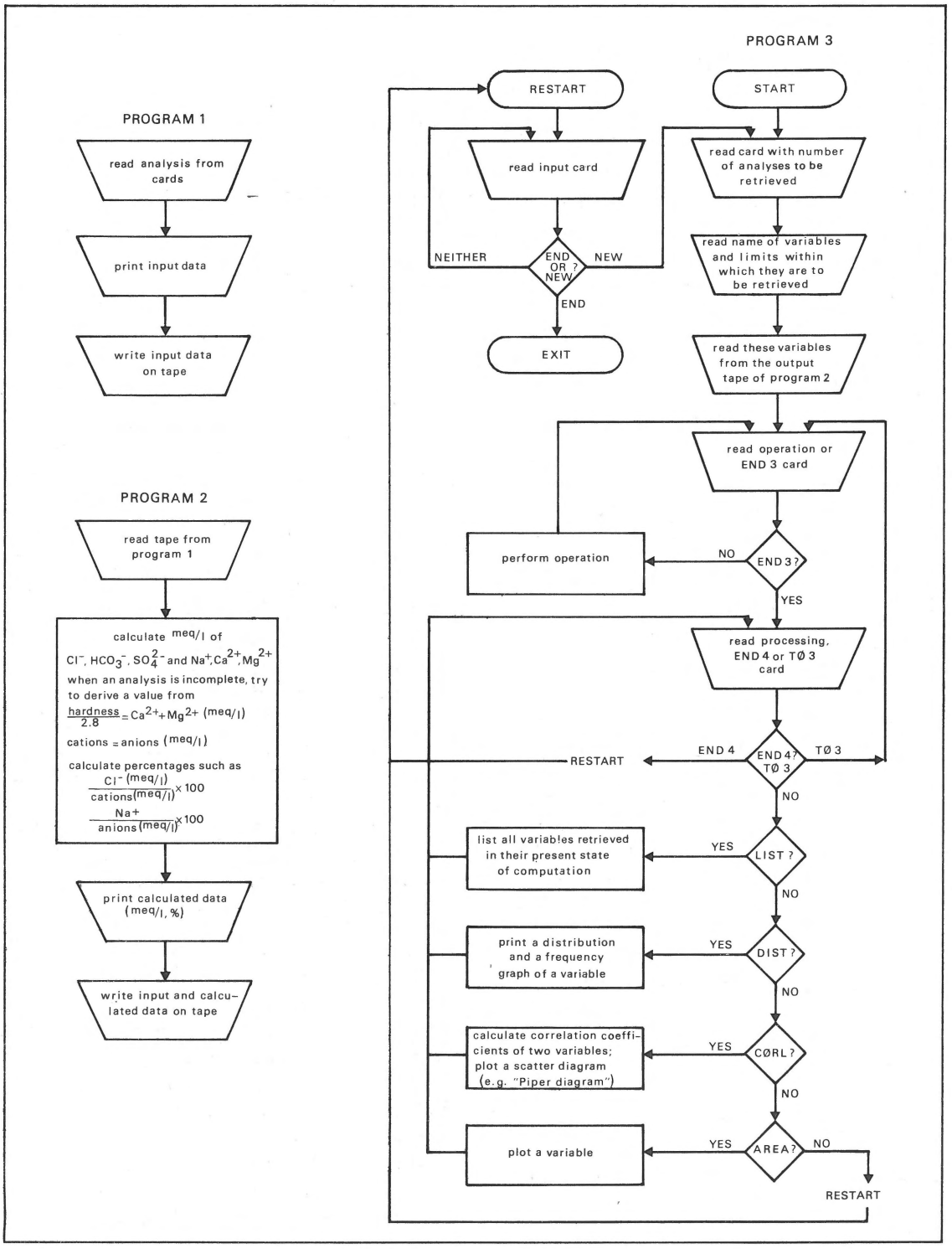


Fig. 1
Flow chart of the programmes.

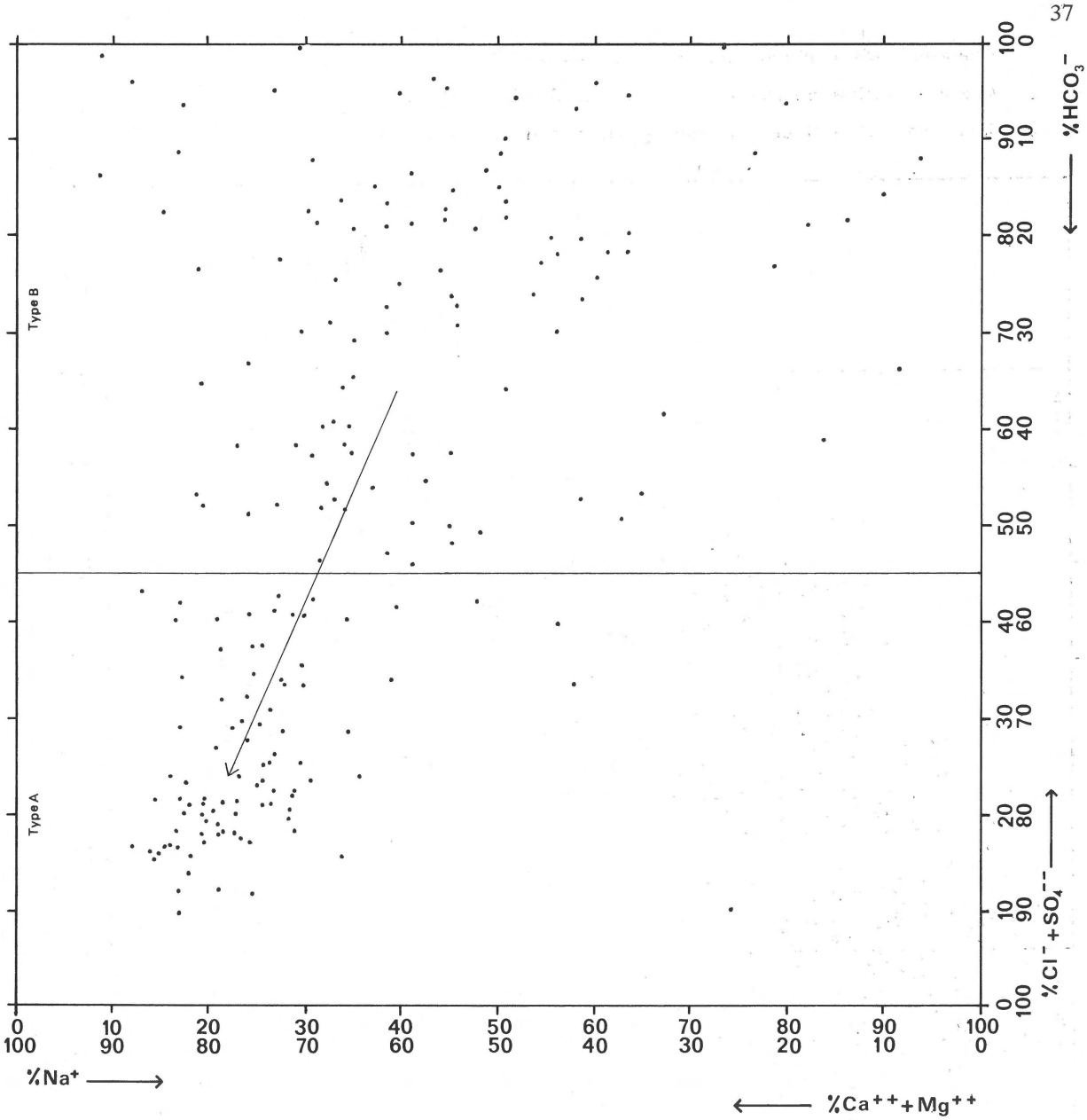


Fig. 2
Modified Piper diagram of the analyses with a hardness less than 7°D.

## EXAMPLE OF AN APPLICATION OF THE PROGRAM

An example of the use of this program is the plotting of different types of water on modified Piper diagrams by using the CORL subroutine. The x-coordinate corresponds to the $Na^+$ content as a percentage of the main cations $Ca^{2+}$, $Mg^{2+}$, $Na^+$ and the y-coordinate corresponds to the $Cl^- + SO_4^{2-}$ content as a percentage of the main anions $HCO_3^-$, $SO_4^{2-}$, $Cl^-$ (fig. 2 and 3). One important restriction in the use of this kind of diagram is that the ion content is expressed as a percentage of total cations or anions. This leads to a larger spread in values when the total

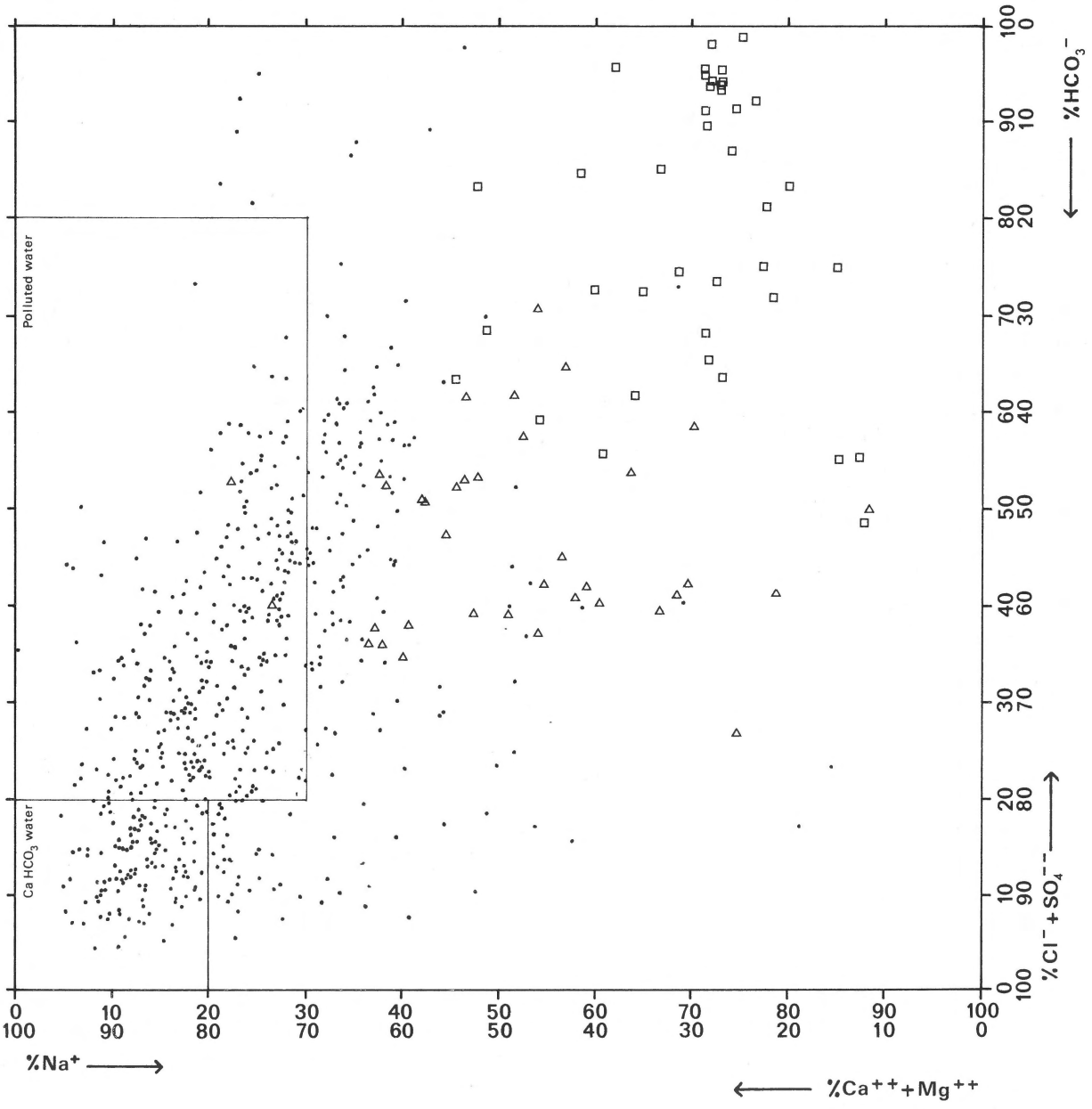


Fig. 3
Modified Piper diagram of the analyses with a hardness greater than 7°D.

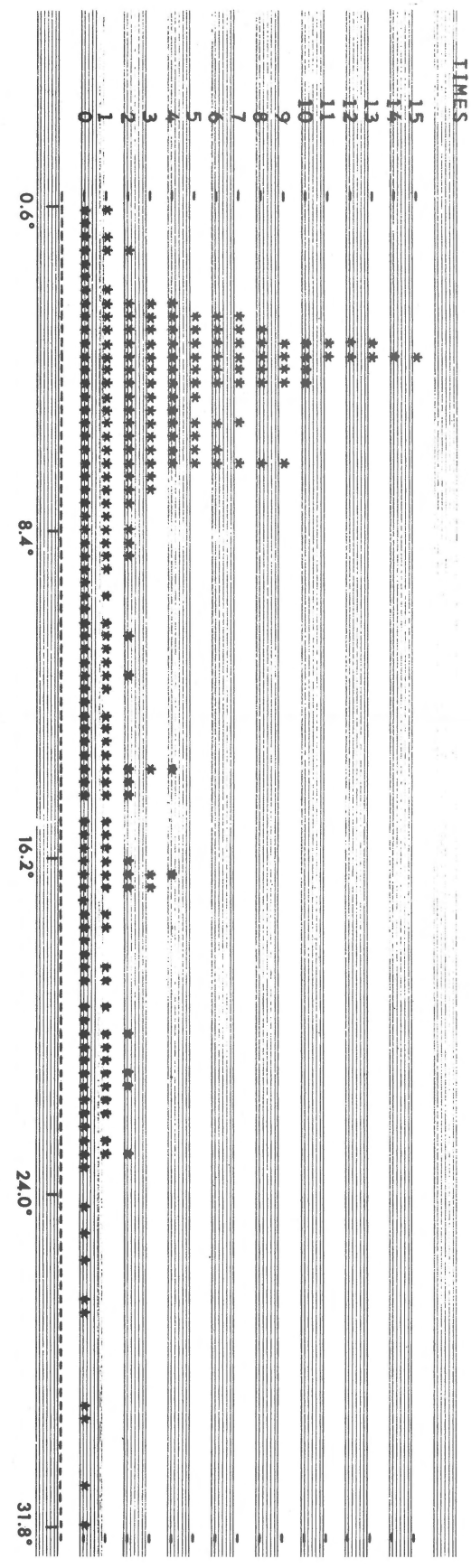


Fig. 4
Distribution of the hardness (°D) in the eastern part of the area.

dissolved solids is small. We found that the hardness was a good criterion for the total dissolved solids. On the basis of the distribution of hardness, shown in fig. 4 we examined the Piper diagrams for values of hardness above and below 7°D separately.

The modified Piper diagram for a hardness less than 7 is shown in fig. 2. In spite of the wide scatter of the points we can see the general trend shown by the arrow in which $HCO_3^-$ and $Ca^{2+} + Mg^{2+}$ contents increase, due to sulphate reduction and the solution of carbonates by the water.

This water has been arbitrarily divided into types A and B. Eventually, as the dissolved $Ca^{2+} + Mg^{2+}$ increases, the hardness becomes greater than 7 and we have to look at fig. 3 to follow the trend. The "$CaHCO_3$" water is reached when the $HCO_3^-$ and the $Ca^{2+} + Mg^{2+}$ contents are more than 80% of the cations and anions respectively.

Pollution of this water increases the $SO_4^{2-}$ and the $Cl^-$ content. However, the $Cl^-$ content of most polluted water is generally below 200 ppm (fig. 3). We used the AREA subroutine to plot the different types of water on the map (fig. 5). Polluted areas stand out clearly near rivers and around urban areas. The groundwater in the western part (near Leiden and Rotterdam) has a high salt content of marine origin (greater than 200 ppm). We have not taken the depth at which the water sample was taken into account and to some extent this masks the increasing carbonate content with distance from the infiltration areas (NE and SE part of fig. 5).

## REFERENCES

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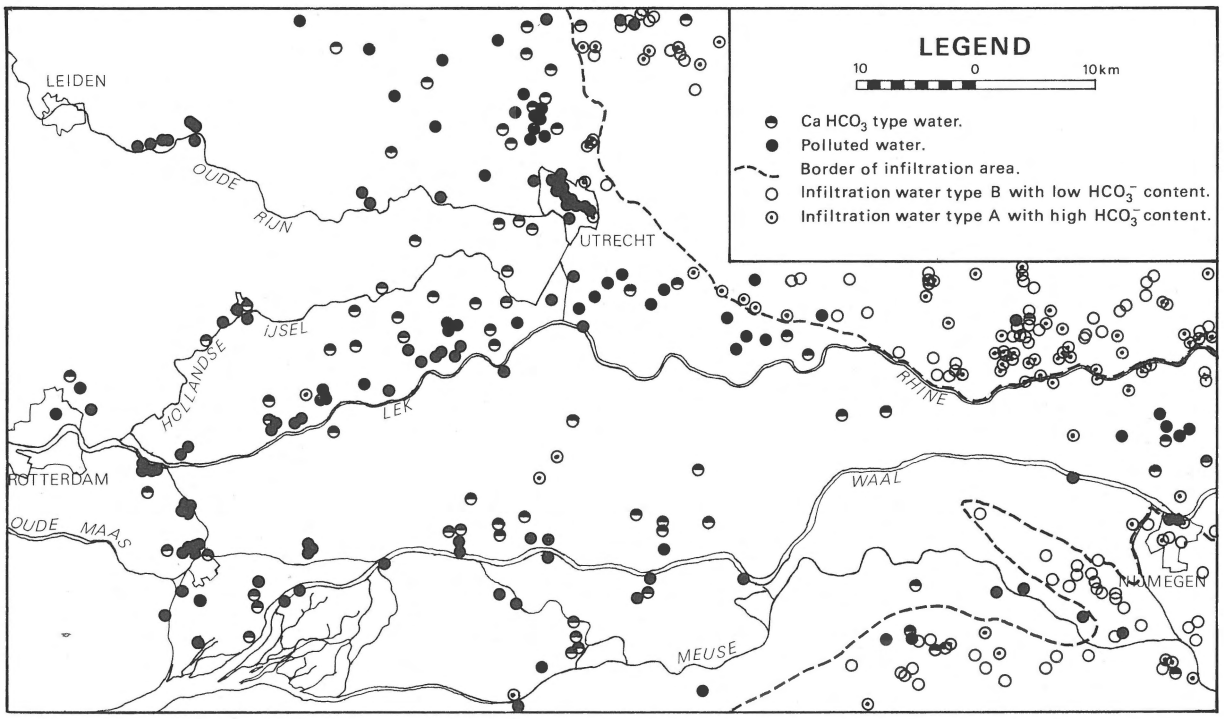


Fig. 5
Map of the area with the locations of the different types of water.