

TWO-WAY REGIONALIZED CLASSIFICATION OF MULTIVARIATE DATA SETS
AND ITS APPLICATION TO THE ASSESSMENT OF HYDRODYNAMIC DISPERSION¹

by

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Suggested Running Head: Application of two-way RC in the assessment of hydrodynamic dispersion

ABSTRACT

Zones of mixing between shallow groundwaters of different composition were unravelled by “two-way regionalized classification”, a technique based on Correspondence Analysis, Cluster Analysis and Discriminant Analysis, aided by gridding, map-overlay and contouring tools. The shallow groundwaters are from a granitoid plutonite in the Fundão region (central Portugal). Correspondence Analysis detected three natural clusters in the working data set: 1 – weathering; 2 - domestic effluents; 3 - fertilizers. Cluster Analysis set an alternative distribution of the samples by the three clusters. Group memberships obtained by Correspondence Analysis and by Cluster Analysis were optimized by Discriminant Analysis, gridded over the entire Fundão region, and converted into “two-way regionalized classification” memberships as follows: codes 1, 2 or 3 were used when classification by Correspondence Analysis and Cluster Analysis produced the same results; code 0 when the grid node was first assigned to cluster 1 and then to cluster 2 or vice-versa (mixing between weathering and effluents); code 4 in the other cases (mixing between agriculture and the other influences). Code-3 areas were systematically surrounded by code-4 areas, an observation attributed to hydrodynamic dispersion. Accordingly, the extent of code-4 areas in two orthogonal directions was assumed proportional to the longitudinal and transverse dispersivities of local soils. The results (0.7-16.8 m and 0.4-4.3 m, respectively) are acceptable at the macroscopic scale. The ratios between longitudinal and transverse dispersivities (1.2-11.1) are also in agreement with results obtained by other studies.

KEY WORDS: Correspondence Analysis, Cluster Analysis, Discriminant Analysis, Surface Mapping Tools, Regionalized Classification, Hydrodynamic Dispersion

NOTATION

Below is the alphabetical list of mathematical symbols used throughout this paper.

Latin Symbols

- d - geometric mean diameter of a granular material (e.g. soil sample)
- D (D_L , D_T) - Coefficient of hydrodynamic dispersion (longitudinal and transverse)
- E_i - classification score of group i
- $f_i(\mathbf{x})$ - score of vector $\mathbf{x}$ in the frequency curve (f) of group i
- F - factor
- $grad(h)$ - hydraulic gradient
- h - number of rows along the height of a grid
- k - number of groups present in a multivariate site-related data set
- K - hydraulic conductivity
- l - number of columns along the width of a grid
- m_t - total porosity
- m_e - effective porosity
- n - number of samples (or sites) in the working database
- p - number of variables describing the samples (or sites) in the working database
- $prob_i$ - prior probability of group's i membership
- $Prob_i$ - posterior probability of group's i membership
- S - matrix of within-group variances and covariances
- t - time
- v - velocity of a solute dissolved in water along the mean direction of flow
- $\mathbf{x}_p$ - vector containing the values of the p original (or X) variables
- $\mathbf{x}'$ - transpose of $\mathbf{x}$
- $\bar{\mathbf{x}}$ - mean of $\mathbf{x}$
- $\bar{\mathbf{x}}'$ - transpose of $\bar{\mathbf{x}}$
- X - set of original variables in the working data set
- w_{ij} - loading of variable j in factor i
- $w\%-Pollution$ - hydrochemical parameter discriminating between waters with weathering-dominated chemistries and waters with chemistries controlled by anthropogenic inputs
- $w\%-Agriculture$ - hydrochemical parameter discriminating between waters with fertilizer-dominated chemistries and effluents-dominated chemistries

Greek Symbols

α (α_L , α_T) - mechanical dispersivity (longitudinal and transverse)

δ - log standard deviation of a grain size distribution

γ - identification code of a hybrid region

σ – standard deviation of a membership probability distribution

ψ – specific retention of a porous material

INTRODUCTION

Regionalized Classification (RC) is defined as the probabilistic assignment of sites to groups by using Discriminant Analysis (DA). Following Olea (1999) and his predecessors Harff and Davis (1990), we see nothing conceptually new in RC but agree that some novelty is introduced by this joint application of a number of well known mathematical, statistical and geostatistical techniques.

The start of RC requires a training set that usually is provided by Cluster Analysis (CIA). However, with conventional clustering algorithms the number of groups (k) is defined subjectively, either on the basis of external information or iteratively until a certain function is optimized. A second difficulty in applying RC is the assignment of sites to groups when probabilities are similar among clusters. Again, the problem is solved by assigning to group zero (i.e. by setting to hybrid) all sites for which the difference between the two highest probabilities are less than a pre-established (subjective) threshold.

The primary objective of this study is to clean RC from the reported drawbacks. To define k objectively we propose that it is selected by natural clustering. To identify the hybrid sites precisely, we propose that a RC based on the natural groupings (*first-way* RC) is combined with another RC based on the CIA groupings (*second-way* RC). By looking simultaneously at two different perspectives of a same reality, we expect that the typical sites maintain their group memberships no matter which clustering method is used, whereas the atypical ones alternate among groups when the clustering technique is changed. Consequently, the atypical sites are recast as hybrid sites and demarcated on a map as hybrid regions.

The spatial relation between true and hybrid regions of groundwater data sets may, in some cases, unravel the mixing between waters of different compositions. The distribution of membership probabilities within regions of fertilizer-dominated water chemistries resembles the distribution of solutes inside pulse-like contaminant plumes. Using the appropriate contaminant transport models, it is possible to quantify processes such as hydrodynamic

dispersion from solute distributions inside plumes. As a secondary objective we wished to assess hydrodynamic dispersion across the soils of our study area (Fundão region, central Portugal) using the membership distributions as analogs for solute distributions.

THE TWO-WAY RC APPROACH

The flowchart in Figure 1 summarizes the method of two-way RC. The sites of a multivariate database are initially assigned to k groups by natural clustering, and then the groups are interpreted in terms of controlling sources and/or processes. When working with groundwater databases, the selected method of natural clustering can be the RST algorithm used by Pacheco and Van der Weijden (1996), Pacheco (1998a) or Pacheco and others (1999), or can be the technique based on Correspondence Analysis (CA) that Pacheco (1998b) developed. The first-way RC can pass through an optimization process using Discriminant Analysis (DA) or terminates. To start the second-way RC we run a conventional clustering algorithm like Ward's method (1963) to obtain a sub-optimal non-natural distribution of the sites by the k groups that subsequently is optimized using DA. Node Analysis (NA) is a last step in two-way RC whereby the natural and non-natural group memberships are interpolated over grids of regularly spaced nodes. Nodes are then compared among grids, maintaining their original assignments or being reclassified as hybrid in a combined grid. Finally, constant membership contours are drawn across the study area that work as boundaries between different groups as well as between groups and hybrid regions.

The next sections outline the mathematical, statistical and geostatistical procedures involved in two-way RC. Detailed and more mechanically oriented descriptions of these methods are beyond the scope of this paper and can be found elsewhere (Kaufman and Rousseeuw, 1990; Jackson, 1991; Jobson, 1992; among many other neat textbooks). It also should be mentioned that we used Pacheco's (1998b) approach to CA to define the natural clusters and Ward's method to represent the technique of non-natural clustering.

Correspondence Analysis

In this study, CA is used as a natural clustering technique. As usual, the set of p original or X variables are first transformed onto a set of p factors or F variables in a manner that a major portion of the data variation is concentrated on just a few of the latter, the so-called k common factors. The relation between the F and X variables is set on the basis of a linear equation:

$$F_i = w_{i1}X_1 + w_{i2}X_2 + \dots + w_{ip}X_p. \quad (1)$$

If the signs of factor loadings (w_i coefficients) are equal, the corresponding X variables are correlated positively in F_i , otherwise they are correlated negatively. From the observation of these “sympathies” and “antipathies” among signs of factor loadings, Equation (1) may be rewritten in forms that encompass some physical or chemical meaning. That was the approach used by Pacheco (1998b). Working with a shallow groundwater database from a granitoid plutonite (Fundão, central Portugal), he separated waters with weathering-dominated chemistries from waters with compositions controlled by anthropogenic inputs, using the following hydrochemical parameter:

$$w\% - Pollution = \frac{Pollution}{Weathering + Pollution} \times 100, \quad (2)$$

where

$$\begin{aligned} Pollution &= w_{1,Cl} [Cl^-] + w_{1,SO_4} [SO_4^{2-}] + w_{1,NO_3} [NO_3^-] \\ Weathering &= w_{1,HCO_3} [HCO_3^-] + w_{1,SiO_2} [SiO_2] \end{aligned}$$

Square brackets denote molar concentrations of chloride, sulphate, nitrate, bicarbonate and silica in a spring. Springs with $w\%-Pollution$ less than 50% have weathering-dominated water chemistries and springs with $w\%-Pollution$ greater than 50% have pollution-dominated water chemistries. The extent to which each component contributes to $w\%-Pollution$ is determined by the w_i values. Contaminated spring waters were further linked to sources such as farmland fertilizers or domestic effluents by the following hydrochemical parameter:

$$w\% - Agriculture = \frac{Agriculture}{Dom. Effluents/Atm. Input + Agriculture} \times 100, \quad (3)$$

where

$$Agriculture = w_{2,SO_4} [SO_4^{2-}] + w_{2,NO_3} [NO_3^-]$$

$$Dom. Effluents/Atm. Input = w_{2,Cl} [Cl^-]$$

Springs with $w\%-Agriculture$ greater than 50% were assigned to agricultural activities and springs with $w\%-Agriculture$ less than 50% were attributed to urban pollution plus atmospheric inputs.

In total, the hydrochemical parameters defined above accounted for about 80% of the system variance. The bi-univocal association (extent and significance) between hydrochemical parameters and factors was checked by Multiple Linear Regression (MLR) with satisfactory results. Because the Fundão's spring water chemistries have been explained by three different sources (weathering, agriculture and domestic effluents), Pacheco (1998b) classified his data set as a system of triple influence. In this study, these sources or influences provide a value for k , the number of natural clusters feeding Ward's method of CIA.

Cluster Analysis (Ward's Method)

CIA in this study is used as an alternative clustering technique. The adopted Ward's method (1963) belongs to the category of agglomerative hierarchical methods. The aggregate is gradually built on a similarity coefficient between samples or sites. First the algorithm gathers all most-similar pairs and then aggregates the other samples/sites or already-formed groups according to their similarities until k groups are formed. Distinct from other hierarchical methods, Ward's method is a minimum variance agglomerative technique because the two clusters to be joined in each round of clustering are those generating the smallest increase in the within-cluster variation.

Discriminant Analysis

For the present case study, DA is used as a classification tool, namely for optimizing the location of sites pre-assigned by CA or CIA. A general approach to the problem of (re)classifying an observation $\mathbf{x}$ may be stated as follows:

$$E_i = \mathbf{x}' \times \mathbf{S}^{-1} \times \bar{\mathbf{x}}_i - \frac{1}{2} \bar{\mathbf{x}}_i' \times \mathbf{S}^{-1} \times \bar{\mathbf{x}}_i + \ln(prob_i), \quad i = 1, 2, \dots, k \quad (4)$$

where E_i is the classification score of group i ; $\mathbf{x}'$ is the transpose of $\mathbf{x}$; $\bar{\mathbf{x}}_i$ and $\bar{\mathbf{x}}_i'$ are the mean of group i observations and the transpose of that vector, respectively; $\mathbf{S}^{-1}$ is the inverse of the within-group variance-covariance matrix; $prob_i$ is the prior probability of group membership manifest in the observed n_i/n proportion, where n_i is the number of observations in group i and n the number of observations in the dataset. According to this criterion, an observation $\mathbf{x}$ will be (re)classified into the group for which the E value is highest. The new (posterior) probability of group membership ($Prob_i$) is given by:

$$Prob_i = \frac{prob_i \times f_i(\mathbf{x})}{\sum_{i=1}^k prob_i \times f_i(\mathbf{x})} \quad (5)$$

where $f_i(\mathbf{x})$ is the score of $\mathbf{x}$ in the frequency curve of group i . The relation between prior and post assignments is frequently reported in a confusion matrix that shows the number of correctly classified cases in the main diagonal and the number of misclassified cases in the off-diagonals. Confusion matrices are also useful to compare classification results obtained by different approaches [Eq. (2), Eq. (3), and Ward's method].

Node Analysis

The scope of NA, as employed in this study, is threefold. First we looked at this procedure as a gridding tool. Using methods such as kriging, gridding produces a regularly

spaced array of z values from randomly spaced (x,y,z) observation points. When the (x,y,z) observations are spaced randomly over the study area, there are usually many holes in their distribution. Gridding fills in the holes by extrapolating or interpolating z values in those locations where no data exists. We interpolated the CA/DA group memberships to be used in NA over a grid with $l \times h$ nodes, where l is the number of columns along the width and h the number of rows along the height of the study area, and did the same with the CIA/DA results. After gridding we compared nodes between the CA/CIA or one-way RC grids and constructed a combined or two-way RC grid. If the membership of a node was equal in the first grids, then the node stayed in its group in the combined grid. Otherwise the node was reclassified as group- γ node (hybrid), where γ is an arbitrary identification code. In the last stage of NA we drew constant membership contours across the grids that became boundaries between different groups and between groups and hybrid regions.

THE TWO-WAY RC MODEL FOR THE FUNDÃO AREA

In this study we used the set of 160 spring water samples that were collected in the Fundão area (central Portugal) by Van der Weijden and others (1983). The sampling was carried out in June-July. The samples' locations are plotted in Figure 2 and the chemical analyses are given in the Appendix.

Results of CA/DA

CA was applied by Pacheco (1998b) to the Fundão data set using the major anions and dissolved silica as variables (concentrations in $\mu\text{mol/l}$). The results are shown in Table 1.

From the observation of sympathies and antipathies between factor loadings, the first two factors were represented by:

- the *w%-Pollution* (factor one), with

$$Pollution=443.0[Cl^-]+370.8[SO_4^{2-}]+748.9[NO_3^-]$$

$$Weathering=313.4[HCO_3^-]+421.0[SiO_2]$$

- the *w%-Agriculture* (factor two), with

$$Agriculture=63.4[SO_4^{2-}]+591.6[NO_3^-]$$

$$Dom. Effluents/Atm. Input=377.0[Cl^-].$$

The water samples were assembled into three groups: 1 – weathering (*w%-Pollution* < 50%); 2 - domestic effluents (*w%-Pollution* > 50% and *w%-Agriculture* < 50%); 3 - farmland fertilizers (*w%-Pollution* > 50 % and *w%-Agriculture* > 50%). The results of this classification are listed in the Appendix under the heading CA/DA-Prior.

The relation between hydrochemical parameters and factors was set on the basis of MLR and the results are summarized in the last two rows of Table 1. The MLR model for *w%-Pollution* holds a $R^2 = 99.1\%$ indicating a tight regression between this parameter and F_1 , but no similar link exists between the *w%-Agriculture* parameter and F_2 (in the latter case $R^2 = 77.9\%$). In view of such uncertainty, we used DA to optimize the location of the samples with respect to the three pre-defined groups. The results are in column CA/DA-Post of the Appendix and reveal that 15 samples (9.4%) were reclassified into a different group. Using the optimized memberships of the samples and gridding as explained above, we drew Figure 3 that illustrates the areas of influence of each CA group.

Results of CIA/DA

The results from Ward's method are described in detail in the Appendix (column CIA/DA-Prior). These groupings were used as a training set for DA which provided the post assignments listed in column CIA/DA-Post.

The confusion matrix comparing the CA/DA and CIA/DA results is shown in Table 2. There is little doubt that group A is equivalent to group 1 (the weathering group), but the associations between groups 2/3 and B/C are less evident. The medians of *w%-Pollution* and

w%-Agriculture suggest that group B and group 3 are influenced by farmland fertilizers, whereas group C, although falling in the field of weathering, has a median *w%-Agriculture* compatible with group 2 (influence by domestic effluents). Based on these associations we drew Figure 4 to show the areas of influence of each CIA/DA group.

Results of Node Analysis

Employing NA we combined Figures 3 and 4 obtaining Figure 5. The grids used were rectangles with $l = 400$ columns and $h = 300$ rows. The recasting of grid nodes was performed as follows: (1) when nodes in the one-way RC grids (Fig. 3 and 4) had the same value (1, 2 or 3 depending on whether their group memberships were 1/A, 2/C or 3/B) they preserved this value in the two-way RC (Fig. 5); (2) when group memberships in the original grids differ but one had the a value of 3 (fertilizer's influence) they were recast as 4 (mixing between fertilizer and other influences) in the combined grid; (3) in all other cases the two-way RC nodes were recast as 0 (mixing between weathering and domestic effluents).

The areas with weathering-dominated water chemistries occupy most of the studied region, working out as areas of background hydrochemistry. The dominance of effluents is restricted to the region of Alcaria, where the Meimoa river intersects the Zêzere river and some streamlets intersect the Meimoa river (Fig. 2). However, a substantial surface area upstream from the Meimoa river is occupied by regions where effluents blur the background compositions generated by weathering (white areas). Apparently the direct discharge of domestic effluents into streams and streamlets produces regions of mixing that are converted by some concentration process into a region of effluent-dominated water chemistries south of Alcaria. In all cases the areas with fertilizer-dominated water chemistries are spots surrounded by a zone of fluid mixing.

TWO-WAY RC AND THE ASSESSMENT OF HYDRODYNAMIC DISPERSION

Hydrodynamic dispersion of a solute in groundwater occurs as a consequence of two different processes: mechanical dispersion and molecular diffusion. Mechanical dispersion is a process of fluid mixing that causes a zone of mixing to develop between a fluid of one composition that is adjacent to or is being displaced by a fluid of another composition. It occurs as a result of variations around some mean velocity of flow. These variations are caused by the porous medium heterogeneities at the microscopic, macroscopic and megascopic scales (e.g. variations in the hydraulic conductivity, grain's sorting, etc). Molecular diffusion originates because of mixing caused by random molecular motions due to the thermal kinetic energy of the solute, i.e. it is a chemical rather than a physical (advective) process.

The results of two-way RC regarding the areas with fertilizer-dominated water chemistries (cross-hatched areas in Figure 5) suggest that some dispersion of the fertilizers took place after their application on farmland, because these areas are completely surrounded by a region of mixing (dark grey areas). It seems like the fertilizers applied in Spring (starting in early March) to feed the Summer crops have moved downstream and formed pulse-like contaminant plumes, which in turn have grown large and get diluted in their outer rims due to hydrodynamic dispersion. The sampling made in June-July worked out as a snapshot of the plumes when they were four months old. The purpose now is to quantify the hydrodynamic dispersion, but first some mathematical background must be introduced.

Mathematical Background on Hydrodynamic Dispersion

When a solute is subject to effective leaching, as usually happens in soils and saprolites derived from granites, mechanical dispersion grows several orders of magnitude higher than molecular diffusion, swamping the effects of this latter phenomenon (Pfannkuch, 1962). In such cases hydrodynamic dispersion is represented mathematically by:

$$D = v \times \alpha \quad (6a)$$

with

$$v = \frac{K \times \text{grad}(h)}{m_e} \quad (6b)$$

where D is the coefficient of hydrodynamic dispersion, v is the solute's velocity in the mean direction of flow and α is a characteristic property of mechanical dispersivity; K , $\text{grad}(h)$ and m_e are the hydraulic conductivity, hydraulic gradient and effective porosity. Hydrodynamic dispersion may be expressed by longitudinal (in the direction of flow) and transverse (at right angles) spreadings where the D and α coefficients are represented with L or T subscripts (e.g. D_L or α_T).

Assessment of the dispersion coefficients is essential for models of contaminant transport to work. Among the models in use, we focus on those dealing with localized and non-continuous sources of contamination, like the periodic application of fertilizers to farmland. According to these pulse-type models, the movement of a contaminant (e.g. sulphate) across the porous medium generates a growing plume due to hydrodynamic dispersion. One important feature of the concentration distribution inside the plume is that after a short period of time it becomes normal. The mean of the distribution describes the position of the plume and the variance (σ_L^2 or σ_T^2) of the longitudinal and transverse dispersions. The corresponding coefficients of hydrodynamic dispersion are given by (Domenico and Schwartz, 1990):

$$\begin{aligned} D_L &= \frac{\sigma_L^2}{2t} \\ D_T &= \frac{\sigma_T^2}{2t} \end{aligned} \quad (7)$$

where t is the time passed since the contaminant entered the system.

The Analog Pulse-Type Model Based on Group Memberships

Application of pulse-type models [estimation of σ in Equation (7)] requires that concentration distributions within contaminant plumes are well defined. This occurs when plumes are composed of a solute introduced artificially in the system (a tracer). In these cases solute concentrations inside and outside the plumes usually contrast. Contrarily, when plumes result from dissolution of fertilizers in ground waters also affected by weathering and domestic effluents (present case), the overlapping of several and sometimes similar sources of solutes masks the boundaries between plumes and the natural environment, making it difficult to quantify the mass transport parameters. In these cases we would need first to define a sharp boundary around the plumes and then use a proxy to describe the concentration distributions inside them. We believe that this is performed adequately by the two-way RC approach: the boundary of a plume is defined by the outer limit of a dark grey area enclosing a cross-hatched area (Fig. 5). The concentrations are represented by the membership probabilities of groups linked to the agriculture influence ($1/2 \times (\text{group 3} + \text{group B})$), listed in the Appendix under the heading Prob-3/B.

In total there are four contaminant plumes in Figure 5, which were termed Telhado, South of Alcária, Fundão and North of Valverde in reference to the closest town. From data in column Prob-3/B of the Appendix, we drew contours of membership probability inside the plumes and shaded the space between those corresponding to the means and means minus standard deviations (Fig. 6a-d). The thicknesses of the shaded areas in the directions of elongation and at right angles are measures of σ_L and σ_T , respectively.

Hydrology of the Fundão Soils

Apart from the estimation of σ , quantification of dispersivities [Eq. 6a] requires that some hydrologic information is available on the studied porous media, namely mean

velocities of flow, which in turn are dependent on hydraulic gradients, hydraulic conductivities and effective porosities [Eq. 6b]. Hydraulic gradients may be approached by topographic gradients. The other necessary hydrologic information is compiled in the next paragraph.

Costa and others (1971) collected a set of 37 soil samples from the region of Fundão and analysed them for grain size (Table 3). Hydraulic conductivities were estimated from the grain size distributions using the formula of Krumbein and Monk (1943):

$$K = 760d^2e^{-1.31\delta} \quad (8)$$

where K is the hydraulic conductivity given in darcys (conversion to m/s implies a division by 104000), d is the geometric mean diameter (in millimeters) and δ the log standard deviation of the grain size distribution. The $\log(K)$ values are listed in the last column of Table 3 and their spatial distribution is shown in Figure 7. Effective porosities have been estimated by an analytical method cited in Custodio and Llamas (1983):

$$\begin{aligned} m_e &= m_t - \Psi \\ \Psi &= 0.03 \times sand + 0.35 \times loam + 1.65 \times clay \end{aligned} \quad (9)$$

where m_t and m_e are the total and effective porosities of the soil and ψ is its specific retention; *sand*, *loam* and *clay* are the proportions of the sand, loam and clay fractions in the sample (Table 3). For m_t we assumed a value of 50%, which is common for soils derived from granites. The m_e values obtained by Equation (9) were interpolated across the Fundão area and some contours were drawn (Fig. 8).

Dispersivities of the Fundão Soils

From Figures 6a-d we estimated the plumes' σ_L^2 and σ_T^2 and then calculated the plumes' hydrodynamic dispersions using Equation (7), assuming that $t = 4$ months (the age of the plumes). From Figures 7 and 8 we averaged the plumes' hydraulic conductivities and effective porosities. Using this information in combination with hydraulic gradients deduced

from Figures 6a-d, we determined flow velocities [Eq. 6b] that when combined with the previously calculated hydrodynamic dispersions gave estimates for the longitudinal and transverse dispersivities [Eq. 6a]. All results are shown in Table 4.

The values of α_L range from 0.7 to 16.8 m. They are acceptable because in this study we are dealing with the assessment of dispersivities at the macroscopic scale. As expected, the α_T values are always smaller than the α_L values. The ratios α_L/α_T are within the interval [1.2, 12.6] m, a range that has already been found by other authors. The use of a single t is obviously a source of uncertainty because application of fertilizers is not restricted to a single day. The value of 4 months is the largest gap between the actions of fertilizing and water sampling. A value for the smallest gap would be 2 months or so, for crops seeded in late April. Adoption of $t = 2$ months would raise the α_L and α_T dispersivities by a factor of 2, but their ranges would be kept under acceptable values.

CONCLUSIONS

Hydrodynamic dispersion at the macroscopic and larger scales is an interesting and still unsolved research topic. In the previous sections of this paper we showed how the shapes and concentration distributions of contaminant plumes can be assessed by the application of our two-way RC and, notwithstanding limitations in accounting for the age of the plumes, demonstrated that quantification of mechanical dispersivities by this method leads to reliable results not only at the level of absolute values of the longitudinal and transverse components but also at the level of the ratios between them.

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APPENDIX: Location of the sampling sites (Hayford-Gauss M and P coordinates). Concentrations of major anions and silica in the 160 spring water samples collected by Van der Weijden and others (1983); the values were scaled to $\mu\text{mol/l}$. For some reason, some of the values in this appendix were transferred incorrectly from the original data set to Pacheco and Van der Weijden (1996) and Pacheco (1998b). Some values regarding the cations (not shown in this appendix) are also incorrect in those papers, and the correct values are ($\mu\text{mol/l}$): K(215)=34, Mg(226)=65, Mg(269)=861, Ca(42)=107, Ca(85)=171, Ca(226)=131, Ca(267)=327, Ca(271)=128, and Ca(439)=157, where values within brackets represent sample numbers. The chart shows prior and post assignments of samples to the CA and ClA groups. Prob-3/B is the sample's average posterior probability of group 3 (CA) and group B (ClA) memberships (agriculture influence).

Identification			Raw data					CA/DA		ClA/DA		Prob-3/B
nr	M (m)	P (m)	[HCO ₃ ⁻]	[Cl ⁻]	[SO ₄ ²⁻]	[NO ₃ ⁻]	[SiO ₂]	Prior	Post	Prior	Post	
28	253614	353895	780	440	356	371	656	3	1	C	C	0.21
30	253789	353965	844	485	458	460	639	3	3	C	C	0.33
31	253263	353298	490	423	185	387	506	3	3	A	A	0.27
32	253228	353579	390	282	129	371	558	3	1	A	A	0.24
35	252491	352105	729	347	341	221	614	1	1	C	C	0.13
39	252631	354666	619	231	129	216	260	3	3	A	A	0.23
41	251789	355052	261	189	198	55	463	1	1	A	A	0.12
42	252526	355754	370	130	127	139	421	1	1	A	A	0.16
45	254526	358596	1280	668	464	121	571	1	2	C	C	0.03
51	253474	358982	780	499	458	189	100	2	2	C	C	0.06
59	252281	358526	2260	2115	635	150	674	2	2	B	C	0.02
60	253614	357403	560	248	158	63	524	1	1	A	A	0.05
61	254105	357684	580	231	83	18	560	1	1	A	A	0.02
63	253754	353298	229	790	735	998	399	3	3	B	B	1.00
66	251579	353719	480	296	325	366	474	3	3	A	A	0.37
67	251754	353509	1052	243	4	0	684	1	1	C	C	0.00
71	250526	353263	639	183	433	0	626	1	1	C	C	0.07
72	250421	352947	239	164	56	1	478	1	1	A	A	0.05
74	249930	353123	660	149	44	32	609	1	1	A	A	0.02
75	249719	352772	480	138	62	0	399	1	1	A	A	0.05
76	249754	352421	810	155	92	0	503	1	1	C	C	0.02
77	252035	352140	851	550	237	258	499	2	1	C	C	0.11
78	251474	351930	918	1664	473	874	438	2	2	B	B	0.61
79	250737	352035	410	181	125	121	634	1	1	A	A	0.05
84	251649	353158	451	307	323	211	426	3	3	A	A	0.27
85	251579	352982	590	169	94	82	606	1	1	A	A	0.03
86	255017	353403	870	279	35	60	663	1	1	C	C	0.01
87	256316	353158	451	243	177	1	613	1	1	A	A	0.03
90	257438	355474	760	248	125	47	506	1	1	C	A	0.03
92	258000	356737	580	186	117	0	552	1	1	A	A	0.03
96	258386	355228	480	336	58	32	652	1	1	A	A	0.01
99	259123	354982	600	567	366	37	353	2	2	C	C	0.06
202	250175	355017	239	1297	1307	839	573	3	3	B	B	0.91
203	250210	355579	610	372	417	185	440	2	3	C	C	0.23

Identification			Raw data					CA/DA		CIA/DA		Prob-3/B
nr	M (m)	P (m)	[HCO ₃ ⁻]	[Cl ⁻]	[SO ₄ ²⁻]	[NO ₃ ⁻]	[SiO ₂]	Prior	Post	Prior	Post	
204	251895	356807	352	254	172	158	657	1	1	A	A	0.07
205	252561	357052	716	536	404	379	485	3	3	C	C	0.30
206	251052	356281	472	677	289	37	441	2	1	C	A	0.05
207	250421	354737	244	621	580	500	489	3	3	B	C	0.50
208	250666	355298	328	181	171	92	474	1	1	A	A	0.12
209	250456	353895	367	231	323	240	532	3	3	A	A	0.28
210	250386	353368	388	183	76	82	626	1	1	A	A	0.03
211	251789	356035	1080	395	383	71	587	1	1	C	C	0.04
212	251930	355544	357	85	173	144	603	1	1	A	A	0.10
213	252702	356351	429	691	431	855	405	3	3	B	B	0.92
214	252351	354702	215	220	437	203	437	3	3	A	A	0.38
215	252702	354877	690	121	173	18	564	1	1	C	C	0.03
216	250245	352035	1113	189	227	53	660	1	1	C	C	0.02
217	251298	352456	787	243	90	3	654	1	1	C	C	0.01
218	252000	353754	2994	485	228	181	635	1	1	C	C	0.00
219	250140	354561	167	762	139	871	465	3	3	B	A	0.55
220	253403	359158	3655	2482	1047	1081	264	2	2	B	B	0.50
221	254456	357438	477	209	137	3	522	1	1	A	A	0.04
222	253544	357544	642	259	194	216	634	1	1	A	A	0.08
223	253158	356947	326	254	371	435	485	3	3	A	A	0.44
224	253509	356035	1155	130	138	77	411	1	1	C	C	0.04
225	253263	355474	372	133	227	58	472	1	1	A	A	0.13
226	253684	355579	436	113	158	85	545	1	1	A	A	0.08
227	253965	355895	367	124	154	226	581	1	1	A	A	0.15
228	252526	352245	836	268	342	177	750	1	1	C	C	0.05
229	255684	351684	557	536	162	205	666	1	1	A	A	0.04
230	257544	352456	664	203	318	21	546	1	1	C	C	0.07
231	255193	352351	626	178	448	124	508	1	1	C	C	0.22
232	254561	353333	334	175	81	435	745	3	1	A	A	0.17
233	254456	353965	690	790	514	2903	687	3	3	B	B	1.00
234	253579	354807	433	158	278	132	670	1	1	A	A	0.09
235	255403	356947	523	155	70	65	668	1	1	A	A	0.02
236	255649	357088	601	1354	1144	1387	586	3	3	B	B	0.99
237	254877	356175	400	118	96	248	207	3	3	A	A	0.35
238	255158	356386	438	141	135	68	535	1	1	A	A	0.06
239	254772	355193	600	324	274	500	558	3	3	A	A	0.38
241	260210	357193	231	79	24	61	514	1	1	A	A	0.06
242	259754	357509	136	65	10	71	445	1	1	A	A	0.09
243	254105	359333	1529	874	515	435	776	2	1	C	C	0.07
244	255859	355824	323	265	336	250	476	3	3	A	A	0.33
245	254912	354702	692	310	173	131	608	1	1	A	C	0.04
246	254631	356351	564	127	151	131	519	1	1	A	A	0.09

Identification			Raw data					CA/DA		CIA/DA		Prob-3/B
nr	M (m)	P (m)	[HCO ₃ ⁻]	[Cl ⁻]	[SO ₄ ²⁻]	[NO ₃ ⁻]	[SiO ₂]	Prior	Post	Prior	Post	
247	254947	357193	454	282	372	166	532	3	1	A	C	0.21
248	250596	355789	526	195	384	500	415	3	3	A	C	0.47
249	248877	352947	408	107	170	52	560	1	1	A	A	0.06
250	258561	357614	187	268	279	324	579	3	3	A	A	0.32
251	258842	357368	203	93	15	35	467	1	1	A	A	0.06
252	259088	356842	128	104	7	66	414	1	1	A	A	0.10
253	259438	356175	249	90	66	61	619	1	1	A	A	0.04
254	260000	355509	295	116	75	29	600	1	1	A	A	0.03
255	260105	355509	293	124	72	66	672	1	1	A	A	0.03
256	259614	356140	236	130	75	35	520	1	1	A	A	0.06
257	259438	355930	243	144	99	140	613	1	1	A	A	0.07
258	259193	356000	59	96	9	66	237	1	1	A	A	0.21
259	258456	353824	723	262	173	190	740	1	1	A	C	0.03
260	255403	353438	647	141	62	44	760	1	1	A	A	0.01
261	256140	353965	675	931	365	452	620	2	1	C	C	0.21
262	256035	354070	1047	3328	749	1516	617	2	2	B	B	0.51
263	256105	354281	1721	3159	1450	1242	740	2	2	B	B	0.50
264	255930	354737	451	333	204	250	550	3	1	A	A	0.16
265	256000	354526	567	152	43	9	697	1	1	A	A	0.01
266	256000	355052	533	1297	1784	532	486	2	2	B	B	0.54
267	256456	354877	1278	564	113	182	739	1	1	C	C	0.01
268	256526	355263	526	527	439	282	581	2	3	C	C	0.25
269	256316	354105	877	6770	1117	1048	567	2	2	B	B	0.50
270	257088	354702	1169	1326	675	726	452	2	2	B	B	0.58
271	257754	354386	449	214	50	139	842	1	1	A	A	0.01
272	257158	353789	367	259	12	187	573	1	1	A	A	0.06
273	252877	351684	652	164	24	4	723	1	1	A	A	0.01
274	255930	352631	470	305	105	150	530	1	1	A	A	0.07
275	256316	352316	516	282	25	105	662	1	1	A	A	0.02
276	256737	351895	531	480	71	176	615	1	1	A	A	0.03
277	256877	352596	606	361	119	113	736	1	1	A	A	0.02
278	257965	352210	375	203	37	113	760	1	1	A	A	0.02
279	258526	352631	688	592	134	118	692	1	1	C	A	0.01
280	259614	350912	434	152	23	13	583	1	1	A	A	0.02
402	256631	350421	150	115	14	22	211	1	1	A	A	0.16
404	256982	350526	308	188	19	32	399	1	1	A	A	0.06
406	254281	359684	853	623	151	60	692	1	1	C	C	0.01
407	254807	359474	2081	745	399	106	757	1	1	C	C	0.00
408	257088	359052	551	268	140	113	711	1	1	A	A	0.02
410	260666	354386	272	107	25	74	530	1	1	A	A	0.05
411	261333	353579	214	199	93	30	209	1	1	A	A	0.18
415	248631	355824	470	244	34	8	612	1	1	A	A	0.01

Identification			Raw data					CA/DA		CIA/DA		Prob-3/B
nr	M (m)	P (m)	[HCO ₃ ⁻]	[Cl ⁻]	[SO ₄ ²⁻]	[NO ₃ ⁻]	[SiO ₂]	Prior	Post	Prior	Post	
420	254702	350947	390	209	46	14	340	1	1	A	A	0.07
421	255859	350842	353	188	45	23	339	1	1	A	A	0.08
423	260421	354245	262	88	32	29	352	1	1	A	A	0.10
424	258596	351298	365	232	79	81	445	1	1	A	A	0.08
425	258596	351088	819	91	21	11	812	1	1	C	C	0.00
427	259649	351333	433	162	10	30	534	1	1	A	A	0.03
430	248702	357017	725	241	324	34	464	1	1	C	C	0.09
432	260596	352807	338	161	19	25	689	1	1	A	A	0.01
433	260386	352351	280	107	82	24	524	1	1	A	A	0.05
434	260772	352456	292	79	16	13	524	1	1	A	A	0.03
435	260456	351859	421	64	10	5	581	1	1	A	A	0.02
438	256035	359298	430	152	60	30	487	1	1	A	A	0.04
439	253719	351474	714	128	25	0	709	1	1	A	A	0.01
440	254140	351228	636	127	58	7	729	1	1	A	A	0.01
441	256702	351298	956	166	67	8	875	1	1	C	C	0.00
442	258561	352175	607	832	50	75	838	1	1	C	A	0.00
443	259649	354386	549	378	65	33	569	1	1	A	A	0.02
444	259649	353333	351	157	27	36	442	1	1	A	A	0.05
446	256526	354175	651	255	28	33	887	1	1	A	A	0.00
447	256105	353438	974	533	189	107	548	1	1	C	C	0.02
452	252631	352281	838	338	351	105	774	1	1	C	C	0.03
453	251579	354386	1123	276	92	17	752	1	1	C	C	0.00
457	250666	350631	566	93	3	1	568	1	1	A	A	0.02
458	255509	351438	526	195	18	22	670	1	1	A	A	0.01
463	248947	350386	231	241	67	31	366	1	1	A	A	0.09
514	254737	356035	558	161	133	27	497	1	1	A	A	0.05
522	253824	356281	1149	181	95	32	600	1	1	C	C	0.01
523	252702	353579	650	302	299	34	860	1	1	C	C	0.01
524	252842	354982	918	248	228	21	679	1	1	C	C	0.01
525	251754	355649	503	126	138	48	554	1	1	A	A	0.05
530	256140	353614	643	454	356	62	742	1	1	C	C	0.03
534	257509	353123	310	277	162	100	604	1	1	A	A	0.06
535	257754	352281	625	725	286	105	568	2	1	C	C	0.04
536	255824	351719	529	236	111	42	431	1	1	A	A	0.06
539	257509	354912	600	685	226	150	375	2	1	C	A	0.08
540	256491	354105	520	224	46	63	806	1	1	A	A	0.01
573	259298	355789	96	195	20	19	280	1	1	A	A	0.13
574	258561	356105	652	914	189	29	515	2	1	C	A	0.01
575	258842	355193	875	426	261	30	514	1	1	C	C	0.03
583	248947	357895	305	2350	269	284	415	2	2	B	A	0.19
589	256316	352316	501	205	39	24	679	1	1	A	A	0.01
591	250421	357403	572	412	418	20	228	2	2	C	C	0.08

TABLE LEGENDS

Table 1. Results of the CA procedure. Adapted from Pacheco (1998b). Symbols: $\%F_i$ - percentage of data variation explained by F_i ; Cum- $\%F$ - cumulative $\%F_i$; B_i - standardized regression coefficient of factor F_i ; R^2 - adjusted coefficient of multiple determination; $w\%-Pollution$ and $w\%-Agriculture$ – hydrochemical parameters calculated by Equations (2) and (3).

Table 2. Confusion matrix comparing the results obtained by CA/DA (1, 2 and 3) and CIA/DA (A, B and C) groupings. Associated medians of the $w\%-Pollution$ and $w\%-Agriculture$ parameters as determined by Equations (2) and (3).

Table 3. Grain size distributions, hydraulic conductivities and effective porosities of 37 soil samples from the Fundão region. Original data (grain sizes) compiled from Costa and others (1971). Hydraulic conductivities estimated by the method of Krumbein and Monk (1943), and effective porosities by a method cited in Custodio and Llamas (1983) assuming an average total porosity of 50%. Symbols: nr - number of the soil sample; M, P - Hayford-Gauss coordinates of the soil samples (locations in Figures 7 and 8); K - hydraulic conductivity; m_e - effective porosity.

Table 4. Results of the procedures used to estimate the longitudinal and transverse dispersivities of the Fundão soils. Symbols: m_e - effective porosity; K - hydraulic conductivity; $grad(h)$ - hydraulic gradient; v - mean velocity of flow; σ_L , σ'_L , σ_T , σ'_T - standard deviations of group-3/B membership probabilities (spatial representation); D_L , D_T - coefficients of hydrodynamic dispersion; α_L , α_T - mechanical dispersivities.

FIGURE CAPTIONS

Figure 1. Flowchart illustrating two-way regionalized classification of multivariate data sets.

Figure 2. Location of the Fundão area and water sampling sites. Adapted from Pacheco (1998b). Original drawings in Van der Weijden and others (1983).

Figure 3. Spatial distribution of group memberships determined by the results of CA optimized by DA.

Figure 4. Spatial distribution of group memberships determined by the results of CIA optimized by DA.

Figure 5. Results of node analysis.

Figure 6. Topography around the contaminant plumes: (a) Telhado, (b) South of Alcaria, (c) Fundão, and (d) North of Valverde. The plumes are represented by dashed thick polygons. The shaded areas describe the regions inside the plumes where group-3/B membership probabilities range from the mean to the mean minus standard deviation. The thickness of the shaded areas is a measure of σ [Eq. (7)]. The samples' group-3/B memberships are listed in the Appendix.

Figure 7. Spatial distribution of the Fundão soils' hydraulic conductivities. The numbers near the dots are sample numbers as listed in Table 3. The labelled polygons are the four contaminant plumes.

Figure 8. Spatial distribution of the Fundão soils' effective porosities. The numbers near the dots are sample numbers as listed in Table 3. The labelled polygons are the four contaminant plumes.

TABLE 1

Factor	F_1	F_2	F_3	F_4
	Distribution of variance			
Eigenvalue (x1000)	190.5	74.8	44.9	34.6
%F _i	55.3	21.7	13.0	10.0
Cum-%F	55.3	77.0	90.0	100.0
	Correspondence factor loadings (x1000)			
HCO ₃ ⁻	313.4	92.0	-202.6	164.6
Cl ⁻	-443.0	377.0	178.3	14.6
SO ₄ ²⁻	-370.8	-63.4	-346.5	-394.1
NO ₃ ⁻	-748.9	-591.6	35.7	235.5
SiO ₂	421.0	-160.3	210.3	-114.7
	MLR model relating hydrochemical parameters with factors			
	B_1	B_2	B_3	$R^2(\%)$
w%-Pollution	51.4	1.4	0.6	99.1
w%-Agriculture	22.1	68.5	12.0	77.9

TABLE 2

	A	B	C	Total	<i>w%-Pollution</i>	<i>w%-Agriculture</i>
1	88	0	36	124	29.0	35.6
2	1	7	5	13	74.2	36.1
3	12	5	6	23	63.3	64.4
Total	101	12	47	160		
<i>w%-Pollution</i>	30.5	78.4	40.8			
<i>w%-Agriculture</i>	37.5	56.7	38.7			

TABLE 3

Identification			Grain Size Distribution (ranges in mm, values in wt%)					Physical Parameters	
nr	M (m)	P (m)	Sand		Loam		Clay	LOG (K)	m_e
			>2	2-0.05	0.05-0.02	0.02-0.002	<0.002		
1	251980	355554	24.6	51.0	6.2	10.4	5.7	-2.08	0.32
2	253424	352614	5.9	36.9	14.5	24.1	18.4	-2.52	0.05
3	253144	352897	11.4	63.9	6.3	9.6	3.4	-2.17	0.36
4	253271	354764	25.1	52.9	4.7	12.1	5.0	-2.06	0.33
5	251206	351810	18.5	67.1	5.7	6.4	1.5	-2.06	0.41
6	254266	353084	28.4	51.4	6.2	10.0	2.2	-2.03	0.38
7	250099	354408	18.2	65.3	3.8	8.0	3.2	-2.07	0.38
8	249208	351786	10.0	71.7	5.3	7.8	4.3	-2.14	0.36
9	254393	354426	9.2	72.1	4.9	11.4	1.5	-2.15	0.39
10	254490	353072	29.1	49.5	5.0	10.3	4.2	-2.04	0.35
11	254691	353406	8.9	71.7	5.0	11.2	1.3	-2.15	0.40
12	251966	356192	18.1	65.7	4.3	7.6	3.4	-2.07	0.38
13	248191	352669	12.5	77.8	1.8	5.2	2.5	-2.07	0.41
14	253926	355384	2.2	80.6	6.0	8.3	1.7	-2.19	0.40
15	255549	353221	3.0	65.2	10.0	15.0	4.8	-2.30	0.31
16	253636	356950	18.8	69.6	3.8	4.2	2.8	-2.04	0.40
17	255132	356889	18.5	66.8	3.5	7.4	3.2	-2.06	0.38
18	257768	354582	1.6	80.3	5.0	10.5	2.2	-2.20	0.38
19	257059	355671	2.3	81.0	1.3	9.8	5.3	-2.19	0.35
20	250432	355914	7.2	67.8	11.5	4.8	4.6	-2.21	0.34
21	252911	351265	3.2	82.2	4.7	7.8	1.1	-2.16	0.41
22	251028	350888	5.2	50.9	10.4	20.3	11.7	-2.39	0.18
23	256420	355492	3.0	65.9	7.1	12.1	10.2	-2.29	0.24
24	257132	356479	1.3	76.8	5.9	10.9	4.5	-2.23	0.34
25	254075	358061	5.2	74.8	2.4	10.3	6.8	-2.19	0.32
26	259283	353968	2.1	68.7	4.3	12.7	11.5	-2.28	0.23
27	257763	353661	21.4	63.4	3.0	6.8	4.4	-2.05	0.37
28	255701	352352	1.6	66.3	7.0	16.4	8.0	-2.31	0.26
29	257728	352449	3.5	65.1	7.4	13.2	7.6	-2.29	0.27
30	254891	359752	17.0	53.1	9.8	14.3	4.8	-2.17	0.31
31	260713	354768	10.8	30.2	9.8	29.9	14.9	-2.48	0.08
32	248056	355286	13.2	61.0	5.8	12.0	7.0	-2.17	0.30
33	250026	352255	3.9	73.7	3.8	11.5	6.1	-2.21	0.32
34	250539	353009	7.8	69.7	5.4	10.9	5.6	-2.18	0.33
35	254066	358209	6.0	71.7	6.6	10.6	4.4	-2.20	0.34
36	257749	359193	24.6	51.0	6.2	10.4	5.7	-2.08	0.32
37	259381	356181	4.9	68.0	7.1	12.6	6.4	-2.24	0.30

TABLE 4

Direction	Parameter	Contaminant Plume			
		A	B	C	D
		Telhado	South of Alcaria	Fundão	North of Valverde
	Mean group-3/B probability	0.4	0.4	0.6	0.5
	Associated standard deviation	0.1	0.2	0.1	0.1
	m_e	0.35	0.38	0.35	0.33
	$LOG(K)$	-2.13	-2.08	-2.15	-2.18
	$grad(h)$	0.041	0.0068	0.0382	0.0094
	$v \times 10^{-4} (m/s)$	8.5	1.5	7.7	1.9
Longitudinal	$\sigma_L (m)$	328.75	445.47	117.85	276.54
	$\sigma'_L (m)$	200.18	13.21	92.8	202.47
	$D_L (cm^2/s)$	33.7	25.4	5.3	27.7
	$\alpha_L (m)$	3.9	16.8	0.7	14.8
Transverse	$\sigma_T (m)$	129.16	124.3	98.76	237.58
	$\sigma'_T (m)$	29.46	5	94.84	20.74
	$D_T (cm^2/s)$	3.0	2.0	4.5	8.0
	$\alpha_T (m)$	0.4	1.3	0.6	4.3
Cross	D_L/D_T	11.1	12.6	1.2	3.4

FIGURE 1

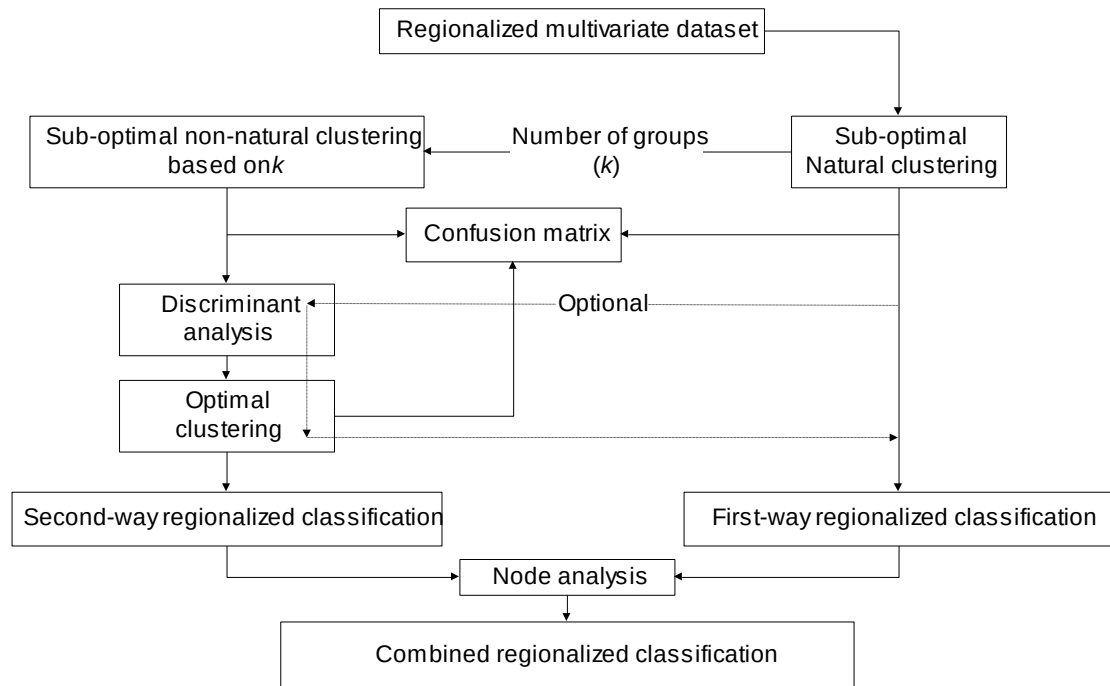


FIGURE 2

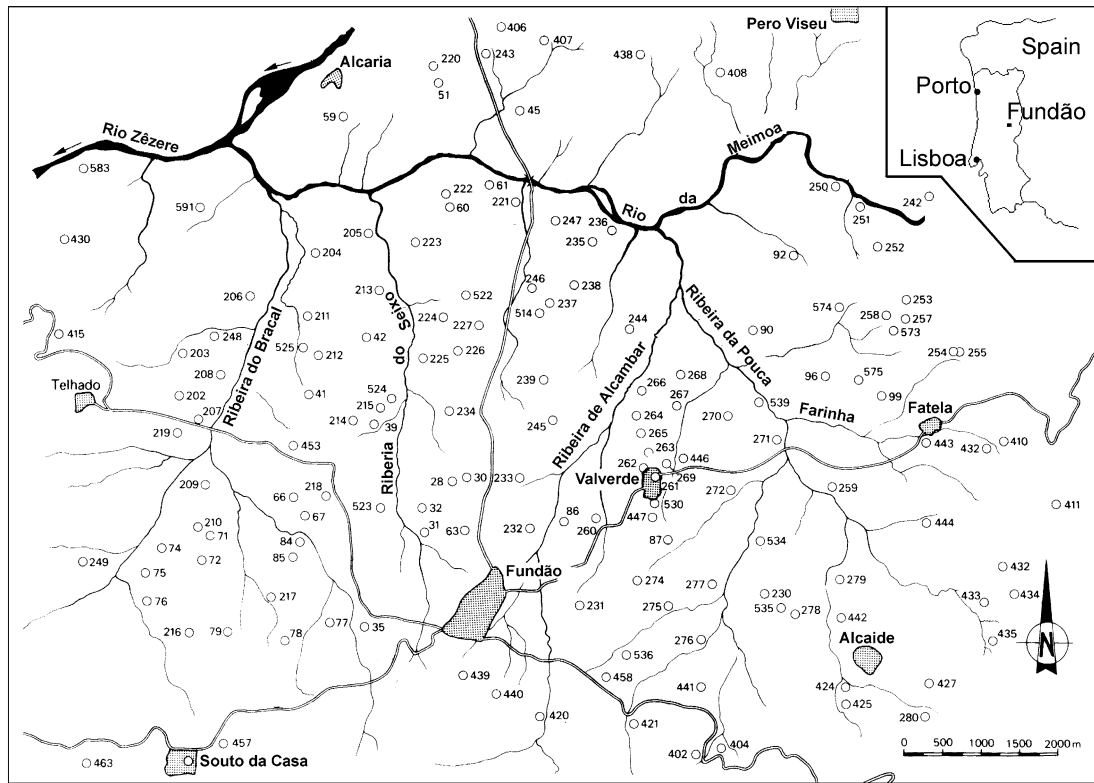


FIGURE 3

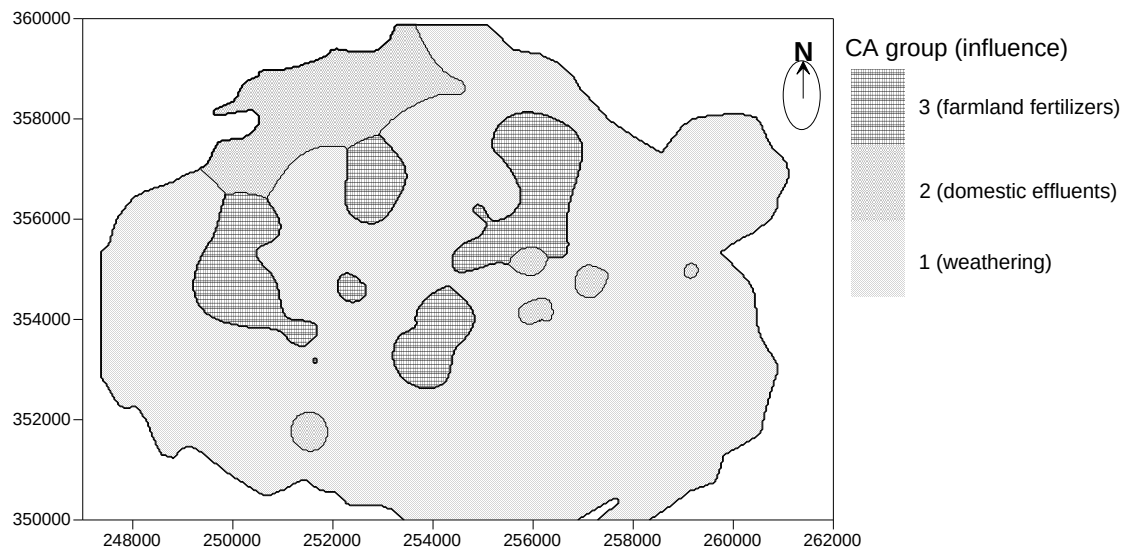


FIGURE 4

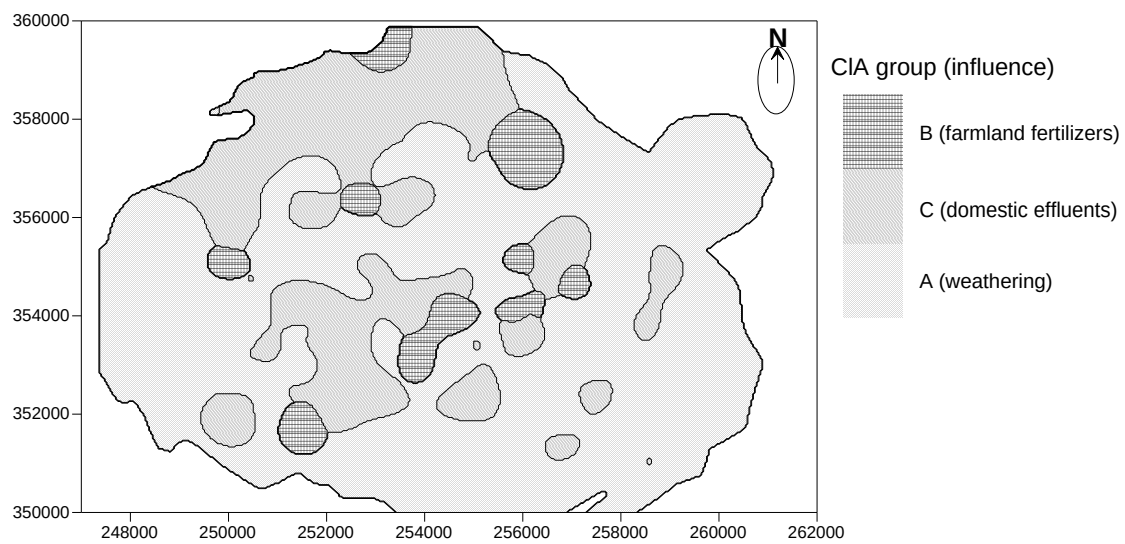


FIGURE 5

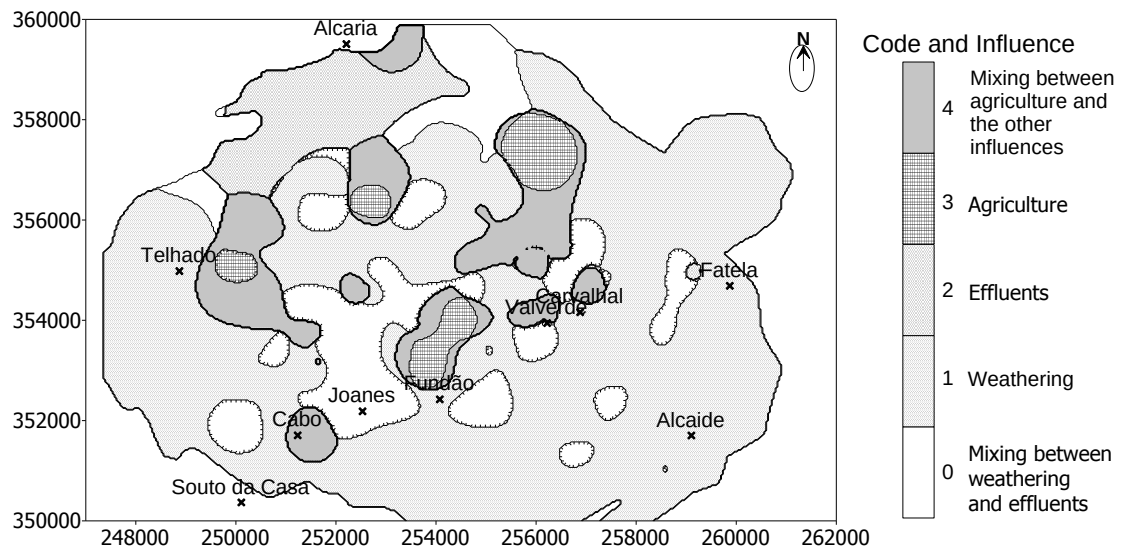


FIGURE 6A

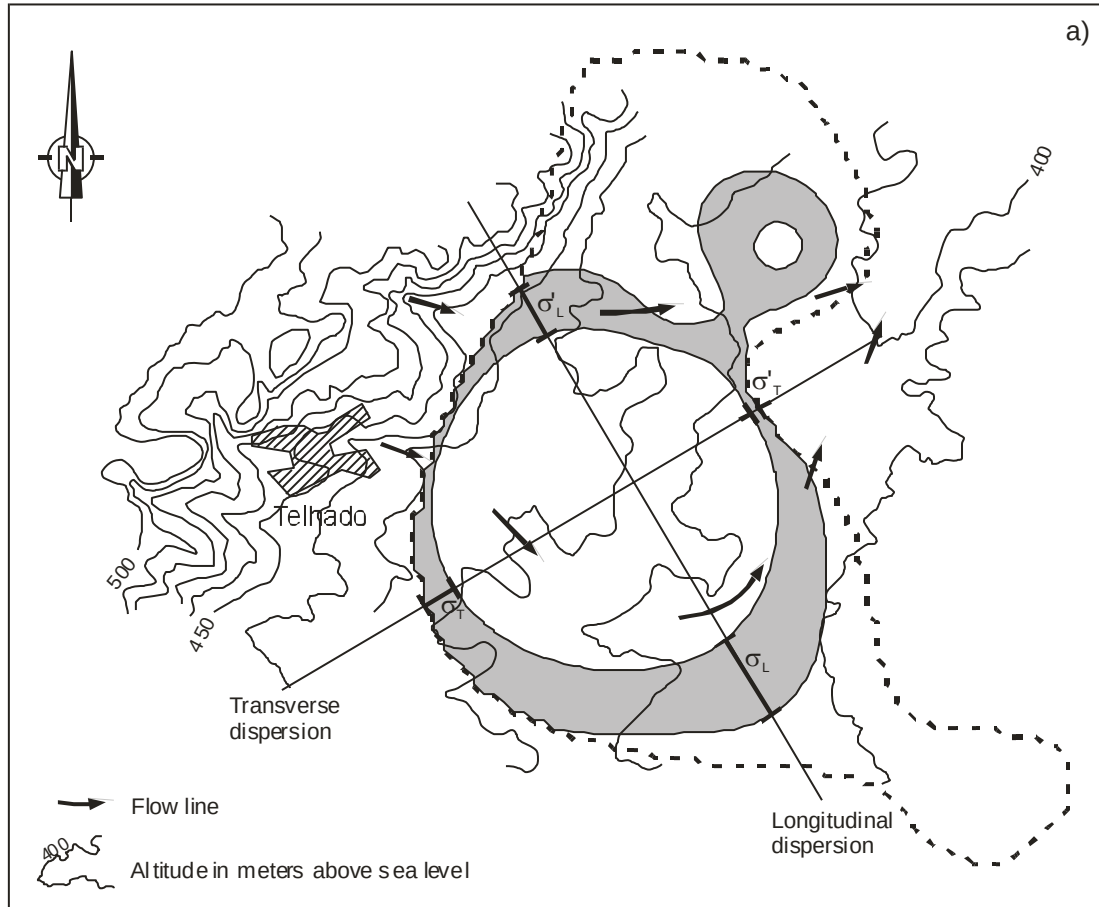


FIGURE 6B

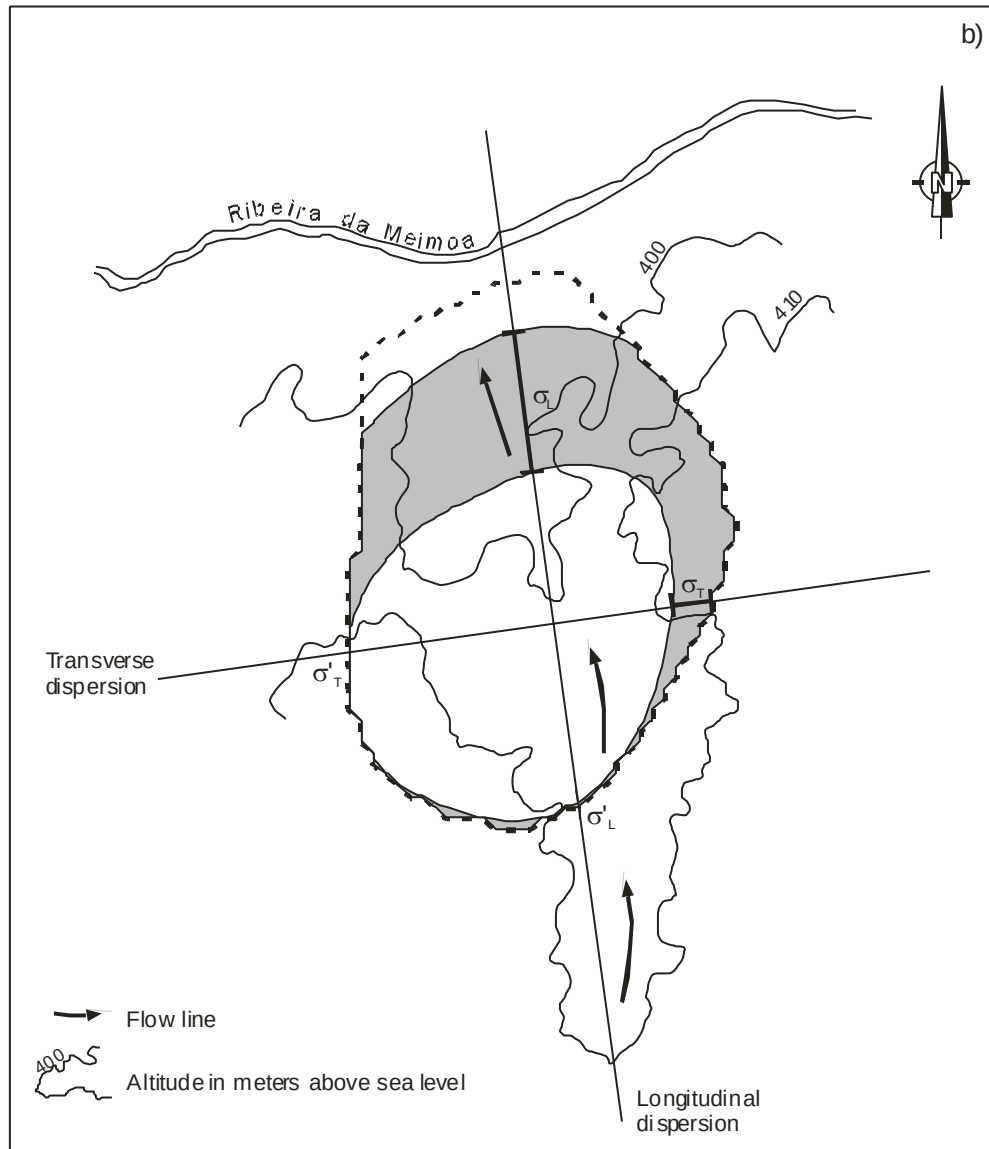


FIGURE 6C

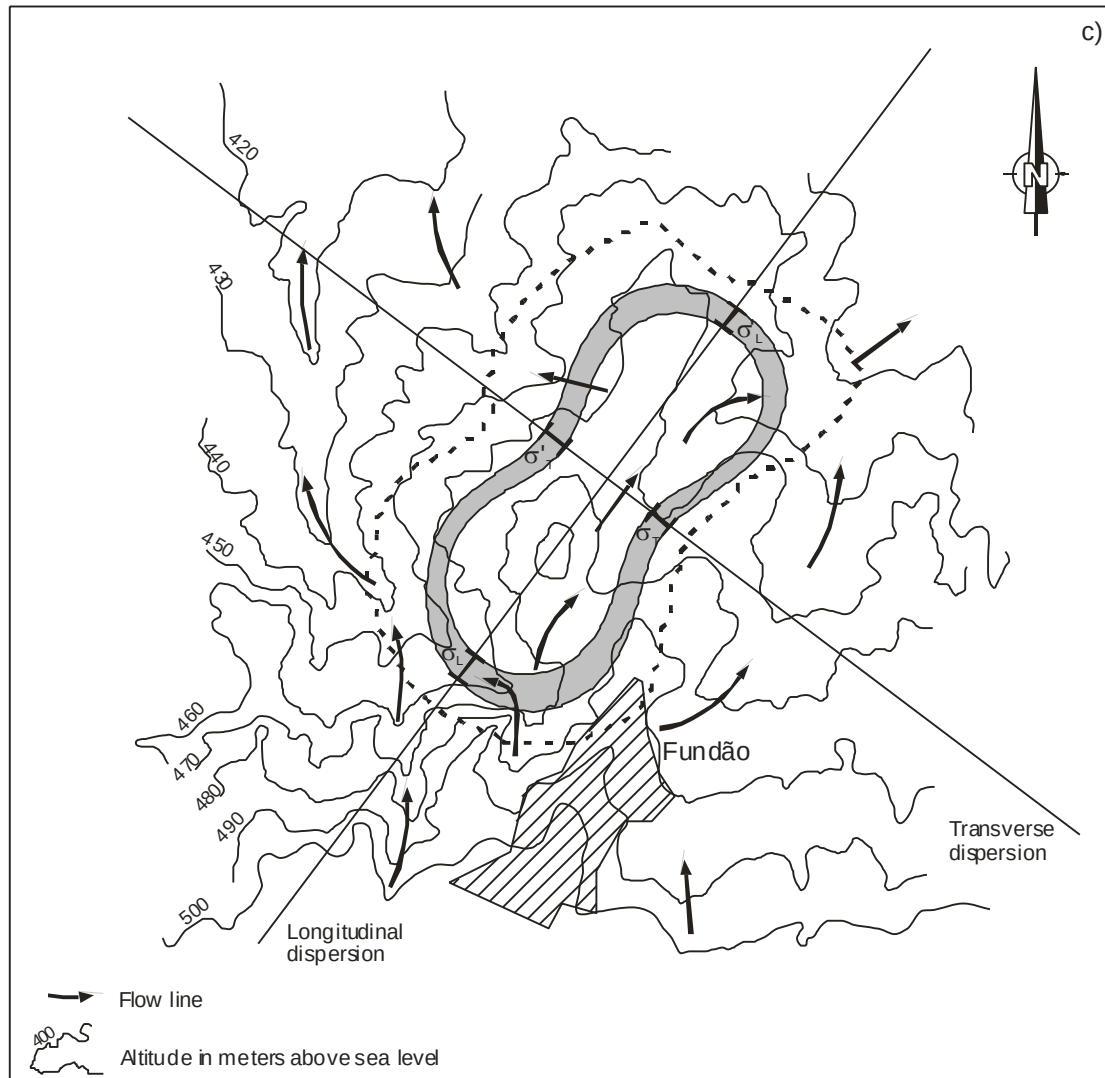


FIGURE 6D

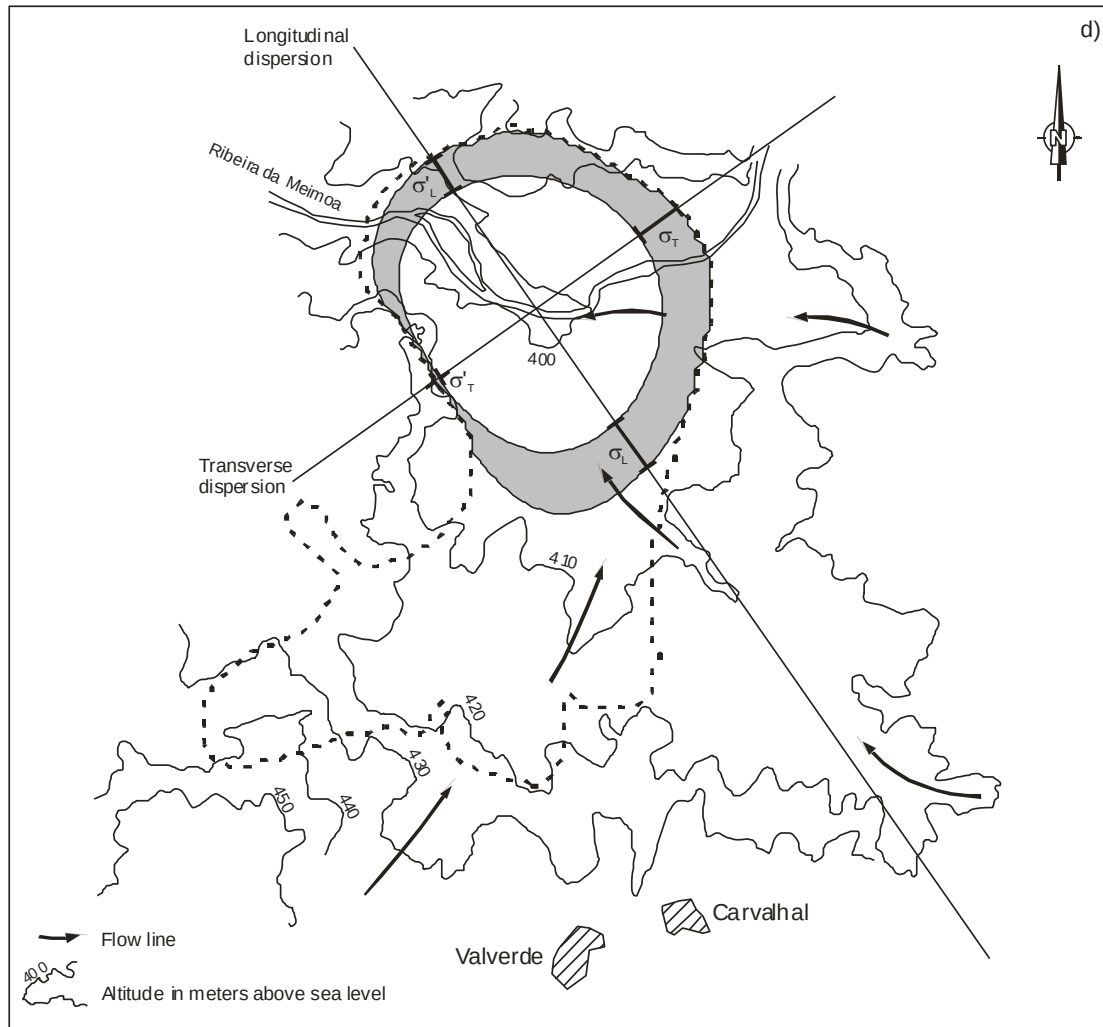


FIGURE 7

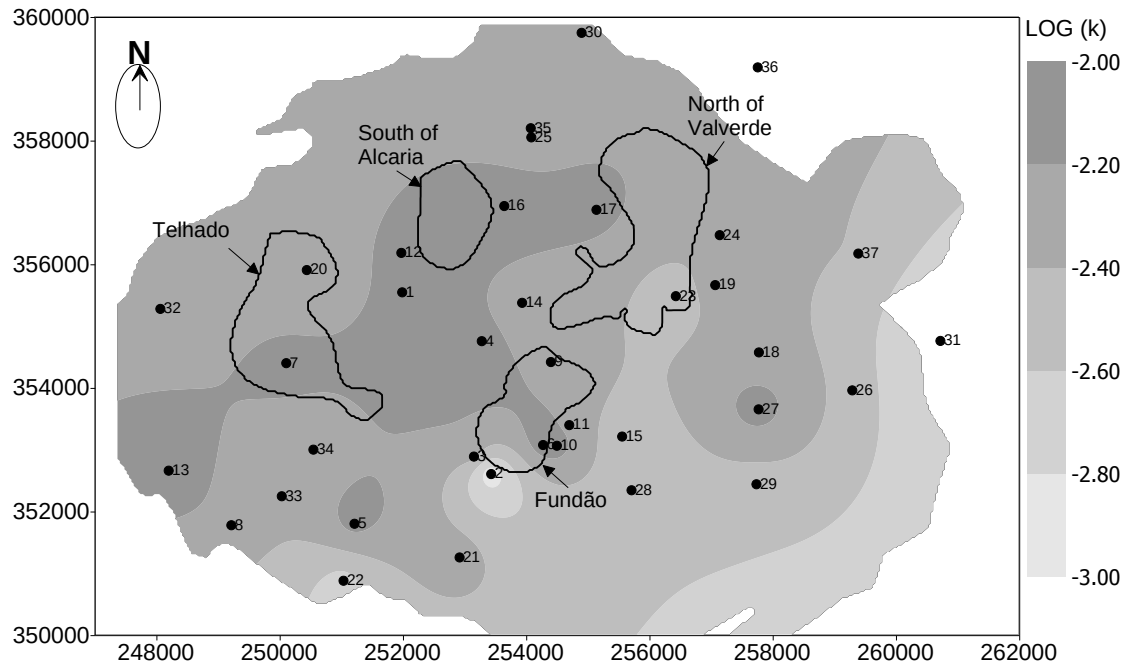


FIGURE 8

