STOCHASTIC MODELLING AND PROBABILITY RISK MAPS OF NITRATE POLLUTION IN THE VICINITIES OF BEJA (Alentejo, south Portugal)

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ABSTRACT

The groundwater resources study of the Alentejo region (CCR Alentejo, 1996-1999) was carried out in several places namely Beja`s Gabbros Aquifer to assess water quality for public supply and agriculture.

A geostatistical study of nitrate diffuse pollution in the vicinities of Beja based on probabilistical technics was developed in the context of a MSc Thesis in co-operation with CVRM - Geosystems Center. Several basic statistics between July 1997 and July 2000 were computed.

Indicator variograms for nitrate ion with 50 mg/l cut-off are presented and Indicator Kriging is performed based on parameters fitted to spherical models.

Risk and probability maps used in environmental management are also included.

Key-words: Hidrogeology; Geostatistics; nitrate; variogram; Kriging.

INTRODUCTION

The Alentejo region (south Portugal) is one of the poorest areas in the European Community. Beja is a major town of the Alentejo region (20 000 inhabitants), located at 150 km SE of Lisbon.

The Alentejo region, like many other Mediterranean areas, suffers from periods of acute water shortages. This situation greatly limits human activity and economical development and in extreme cases of cyclical droughts, actually threatens the public water supply as occurried between 1991 and 1995.

The Alentejo region is extremely dependent on groundwater resources for public supply and agriculture. In fact 66% of Alentejo counties depend on wells and boreholes for public supply. Groundwater represents 77% of total water resources used in public supply, 48% in agriculture and 40% of total water used in industry.

The Mining and Geological Institute has been developing hidrogeological studies and geophysical surveys in the vicinities of Beja since 1985 [Vieira da Silva, 1985; Costa, 1987; Paralta, 1997] in co-operation with Beja Municipality.

Beja public supply depends partially on groundwater resources of the gabbro-dioritic aquifer surrounding the city and surface reservoir of the Rôxo dam.

Together, both origins have productive qualities able to sustain public water supplies (6000 m^3/day) and agricultural projects of major importance.

The aim of this studies is to assess nitrate pollution in order to optimise urban and agriculture water management as well as ecological aspects related to large scale diffuse pollution by agricultural practices on the basis of several European and national directives (80/778/EEC, 91/676/EEC, 91/2078/EEC, European Water Directive, Environmental Farming Proposals, D.L. 236/98, D.L. 159/99, D.L. 382/99).

A hydrochemical monitoring was carried out between July 1997 and July 2000 to assess spatial and temporal variability of nitrate contents in the aquifer due to seasonal fertilization and rainfall episodes.

Outputs such as diagrams, hydrogeochemical indexes and risk/probability maps could be of major importance in groundwater management and also in the implementation of quality monitoring network systems [Ribeiro, 1998].

The hydrogeologic characterisation of the study area was performed through a multidisciplinary approach using geology, geophysics, geostatistics and GIS. The study of groundwater quality and aquifer vulnerability using PHREEQC modelling [Parkhurst, 1995] and DRASTIC pollution methodology [Aller et al., 1987] were also made and already described [Paralta & Francés 2000; Paralta et al. 2000].

GEOLOGY AND HIDROGEOLOGY

The study area is located in a wider region, between Ferreira do Alentejo (NW) and Serpa (SE) (see figure 1), covering an area of about 350 km^2 in the Ossa-Morena geotectonic unit.

It is composed mainly of two units: the Maphic and Ultramaphic Beja-Acebuches Complex and the Beja Gabbros Complex. Its northern limit is the Beja fault, and the southern limit is the Ferreira-Ficalho Overthrust, which is also the transition to the South-Portuguese Zone. In the Beja area predominant formations are gabbro-dioritic rocks.

The altered zone varies locally, and it may reach 30 meters thickness [Paralta, 1997]. It creates an unconfined aquifer, hydraulically homogeneous. Recharge in the study area is estimated in 20% of average annual rainfall.

The gabbro-dioritic aquifer is one of the most productive formations of the Alentejo region when comparing it with other fissured compact rocks, except karst systems. It has transmissivity values that may reach, in some areas, about 350 m^2/day. It produces water flows that range from 1 to 15 l/s (exceptionally), with most frequent average values between 3 and 6 l/s. Under the impermeable unaltered gabbro-dioritic rocks, water circulation occurs mostly through secondary porosity.

Hydrochemical characterisation indicates that these waters are mineralised (with TDS reported to range from about 400 mg/l to 900 mg/l), mainly as calcium-magnesium bicarbonate or magnesium-calcium bicarbonate.

Chemical weathering of the gabbro-dioritic rocks results in the production of clay minerals, such as illite, chlorite and montmorilonite [Vieira e Silva, 1991]. Up to the surface, as a direct result of the arid and dry climate, may occur “caliços”, as a result of mobilisation and re-precipitation of Ca^{2+} in the solution.

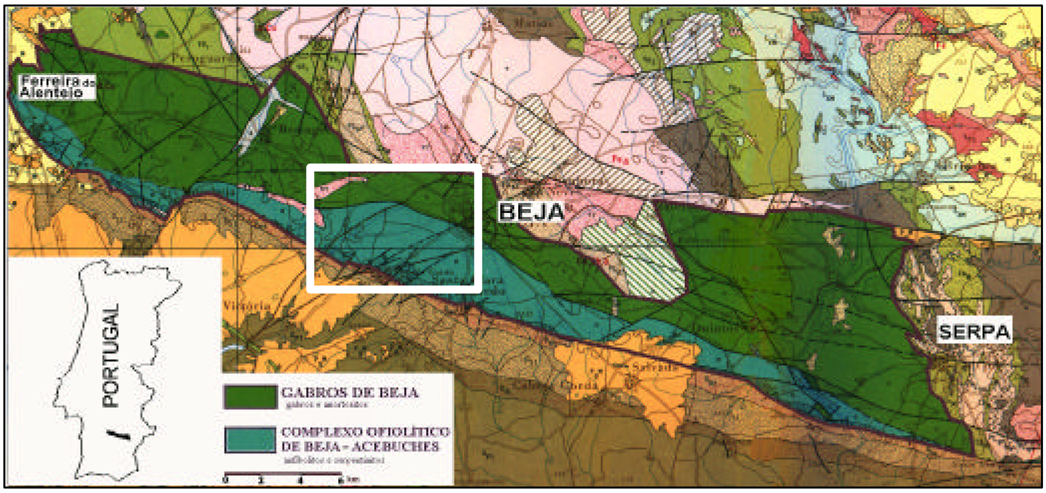


Figure 1 – Geographical location of Beja´s Gabbro Aquifer (350 km^2) and study area (50 km^2). Extracted from Portuguese Geological Map, sheet 8 [Oliveira *et al.*, 1992].

CLIMATOLOGY, AGRICULTURE AND NITRATES

Beja region is influenced by the Mediterranean climate with large temperature intervals between summer and winter and cyclical droughts. The annual average temperature is 16ºC and average rainfall is about 584 mm/year (Beja meteorological station 1958-88). There are 2 distinct periods. The warm and dry period between June and September and the wet period between October and March with 75% of total annual rainfall.

In the vicinities of Beja land use is mainly cereal (wheat) and sunflower or corn as alternative crops. Under intensive cereal cultivation it is common fertilizer application in the range of 100-120 KgN/ha/a. The sunflower and corn cultivation usually don't need fertilizer but groundwater pumping for irrigation is important in the range of 4000-5500 m^3/ha/a. For an average nitrate content of 50 mgNO_3/l irrigation flux represents 45 KgN/ha/a to 62 KgN/ha/a.

The irrigation return flow under semi-arid climate conditions induces impact on groundwater composition as already described [Paralta et al., 2000].

Seasonal rainfall and variation of nitrate leaching at the shallow water-table in 5 observation wells is shown in figure 2.

Results show a slightly trend to the increase of nitrate contents in the beginning of spring and a large range variation reaching 100 mg/l.

The relationship between nitrogen leaching, cultivation practices, type of culture and seasonal rainfall it is not evident due to climate irregularity and alternative crops but annual variations are significant.

The nitrate ion content on groundwater is due mainly to processes of natural nitrification, decomposition of organic material and human pollution, namely agriculture related to the use of nitrogenous fertilizers in farming.

Increasing concentrations of nitrate in groundwater supplies in Beja was recognized early in the 1940s. The actual situation is the long-term consequence of major changes in agricultural cultivation in Alentejo during 1930-1940 directed to increase national grain production. The following decades will lead to substantial increase in application of inorganic fertilizers to sustain more continuous cereal cultivation.

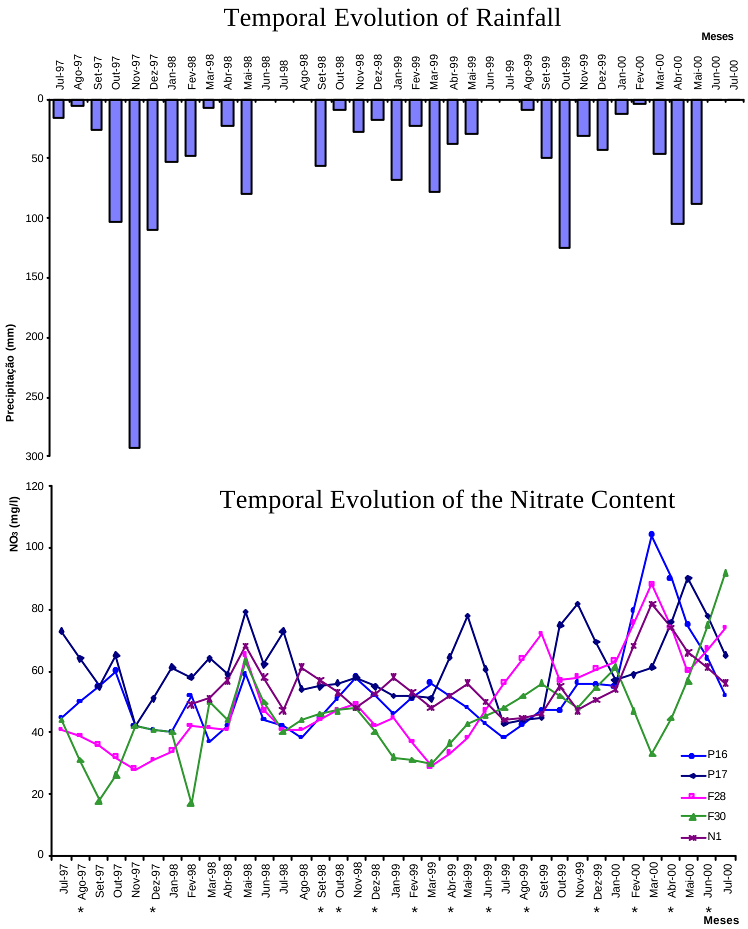


Figure 2 – Rainfall and related nitrate concentration in five observation wells between July 1997 and July 2000.

Diffuse agricultural pollution of groundwater is perhaps the major European groundwater quality concern of the last 25 years.

In northern European countries large-scale environmental pollution due to agriculture practices has been monitored since the mid-eighties with positive results in some issues (GSI -150th Environmental Geology Symposium, 1995).

Concerning environmental management and groundwater protection and monitoring, European countries are making serious efforts in determining vulnerability areas and source protection zones according to the EU Framework Directive on groundwater protection (4th Technical Workshop of Lawa and Environment Agency, 1998).

In Portugal nitrate pollution was first recognized in the Algarve in the mid-eighties (Almeida & Silva, 1987) and after in several places namely the Alentejo region (Chambel, 1992; Duque, 1997; Paralta & Ribeiro, 1998, 2000).

STATISTICAL ANALYSIS

The hydrochemical characterization of the aquifer water, with regard to the nitrate content was based on 24 monthly samplings in the period of July 1997 to July 2000 with a total of 1096 sampling points measured (wells, boreholes and springs).

The experimental area began with 35 km^2 and 28 monitoring points and ended with 50 km^2 and 69 points that represent 15% of the Beja Gabbro`s Aquifer System.

Measurements were made with portable instrument RQFlex 2 (Merck) with detection range from 5 to 225 mgNO_3/l and accuracy of $\pm$ 5%. Basic statistics are given in figure 3.

Boxplot

Temporal Evolution of the Nitrate Content

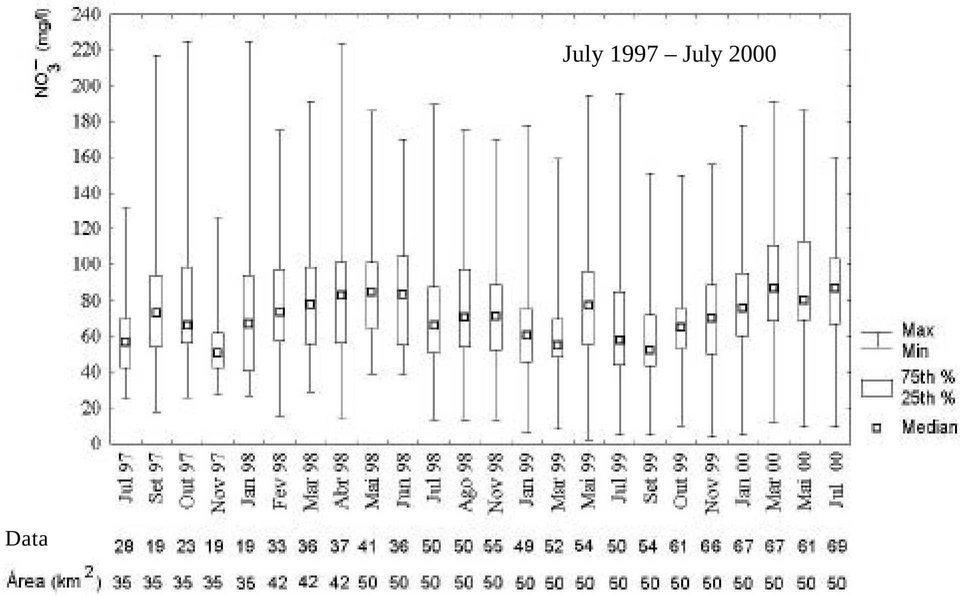


Figure 3 – Boxplot of nitrate monitoring with indication of available data.

There is a large range of values but more frequently classes are 50-60 and 70-80 mgNO_3/l.

The median fluctuates between 53 and 86 mgNO_3/l and maximum nitrate content during monthly sampling ranged from 126 to 225 mg/l.

Frequency distribution is highly skewed (Lognormal) and the coefficient of variation ranges from 37% to 63% with median around 47%.

The extreme variability of time-space nitrate diffuse pollution makes it difficult to establish accurate predictive models for environmental management.

STOCHASTIC MODELLING AND PROBABILITY RISK MAPS

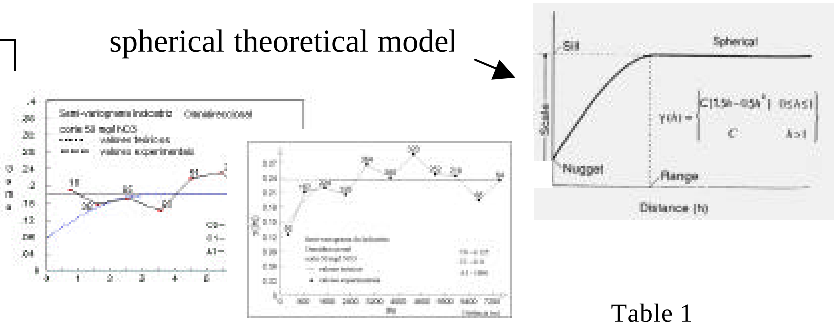
A non-parametrical geostatistical methodology was implemented in order to produce contamination risk maps that represent the iso-probability that nitrate content exceeds the specified threshold value of 50 mg/l (maximum admissible content for human consumption).

The structural indicator analysis was performed to all 24 monthly samplings based in a binary code, 0 ($Z \leq 50$ mg/l) or 1 ($Z > 50$ mg/l). The general methodology for Indicator Kriging (IK) purposes is shown in figure 4.

Binary code

$Z \leq 50$ mg/l ⇒ 0
$Z > 50$ mg/l ⇒ 1

spherical theoretical model



spherical models fitted

Table 1
Parameters for indicator variogram models

Indicator	C_0	C	A (m)
October 97	0.104	0.170	1206
November 98	0.100	0.160	1320
July 99	0.171	0.236	2465
March 00	0.050	0.069	540

Legend : C_0 – nugget effect; C - sill; A - range

Figure 4 - Structural analysis and Indicator Kriging parameters fitted to spherical models.

The main objective of IK is not to provide an indicator value estimate but to build probalilistic models of uncertainty at unsampled locations. That model of uncertainty takes the form of a conditional cumulative distribution function of a continuous Random Variable Z(u), [Deutsch & Journel, 1998]:

$$F(u; z\} = \text{Prob}\,\{Z(u) \leq z\} \qquad [1]$$

The study of 2D spatial structure of nitrate diffuse pollution during 36 months was based in the assumption that nitrate content in groundwater could be considered the realization of a Random Variable [Delhomme, 1976].

Space-time analysis assumed the field to be isotropic in order to compute the omnidirectional variogram fitted to spherical theoretical models with a nugget effect.

Variogram modelling uses software Variowin 2.2 [Pannatier, 1995] and Indicator Kriging estimation was performed with a 100x100m grid file using software Surfer® corresponding to 1410 nodes.

Almost all variograms have a large uncertainty with a nugget effect of 50% to 90% of the total variance. The range of indicator variograms is 400 to 3000 meters.

Figure 5 give the omnidirectional indicator variogram for 4 of the 24 sampling months studied.

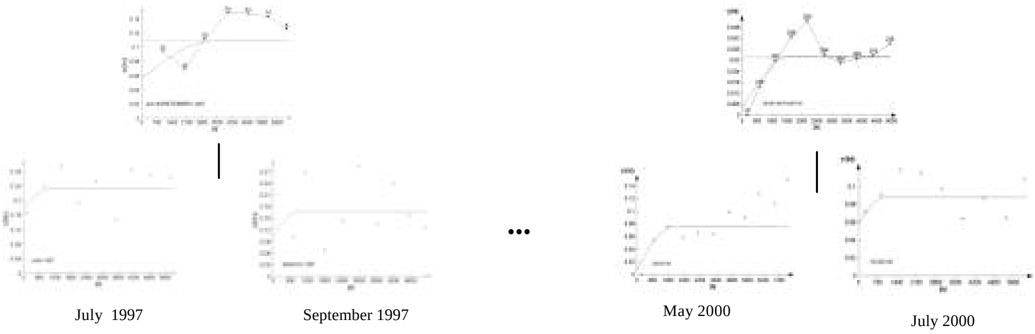


Figure 5 - Indicator variograms and cross-variograms computed between July 1997 and July 2000.

This situation reflects field data with a large range of distribution in a small area that represents not only an average diffuse pollution but also some point contamination with high contents.

Kriging has been widely applied in hydrosciences since Delhomme [1976, 1978] and it is appropriate as an estimation method to assess diffuse nitrate pollution because Kriging algorithm smooth variability giving a more continuous pattern better adjusts to diffuse pollution reality.

As a result of stochastic simulations some probability maps are given in figure 6. These maps represent equally probable images of unknown nitrate content exceeds the specific threshold value of 50 mg/l.

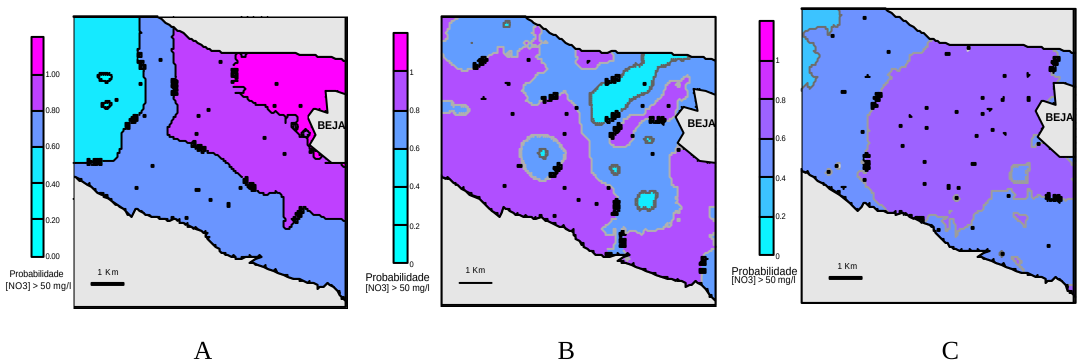
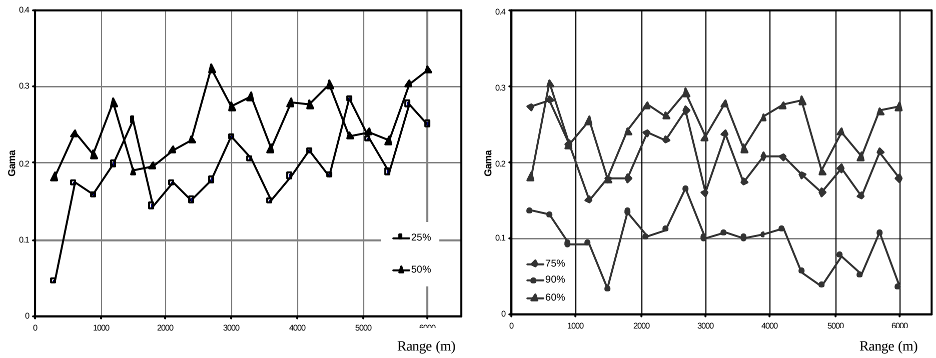


Figure 6 - Probability maps. Probability of exceeding 50 $mgNO_3/l$ in October 1997 (A), November 1998 (B) and July 1999 (C).

Another methodological approach uses probability function and structural analysis is performed by indicator variograms.

We intend to determine the nitrate diffuse pollution index on the basis of spatial correlation patterns meaning pollutant continuity/non continuity in relation with de-structuration for increasing percentiles.

For probabilistic calculations 5 indicator variables were build on 45, 58, 71, 84 and 112 $mgNO_3/l$ which correspond respectively to 25%, median, 60%, 75% and 90% percentile. Indicator variograms are given in figure 7 and table 2 indicates parameters fitted to spherical models.



A B

Figure 7– Omnidirectional indicator variograms for 25% and 50% percentile (A) and 60%, 75% and 90% percentile (B).

Table 2
Parameters for the indicator variogram models of July 1999

Indicator	C_0	C	A (m)	C_0/C(%)
25%	0.086	0.192	1220	45
50%	0.183	0.250	1525	73
60%	0.210	0.240	1400	88
75%	no	structure		....
90%	no	structure		....

Legend: C_0 – nugget effect; C - sill; A – range; C_0/C – uncertainty (%)

Note that, until 50% percentile, at cut-off 58 mgNO_3/l, variogram model is relatively well structured with a range of 1525 meters. For upper percentiles occurs a clearly de-structuration that could be interpreted as point contamination with no meaning in terms of diffuse pollution in the study area.

We might conclude that diffuse agriculture pollution in July 1999 had a maximum around 60 mg/l. For upper cut-offs it is not possible to establish the spatial continuity pattern using indicator variogram.

Figure 8 provides the isopleth maps of the probability of exceeding 45 mgNO_3/l and 71 mgNO_3/l corresponding to 25% and 60% percentile.

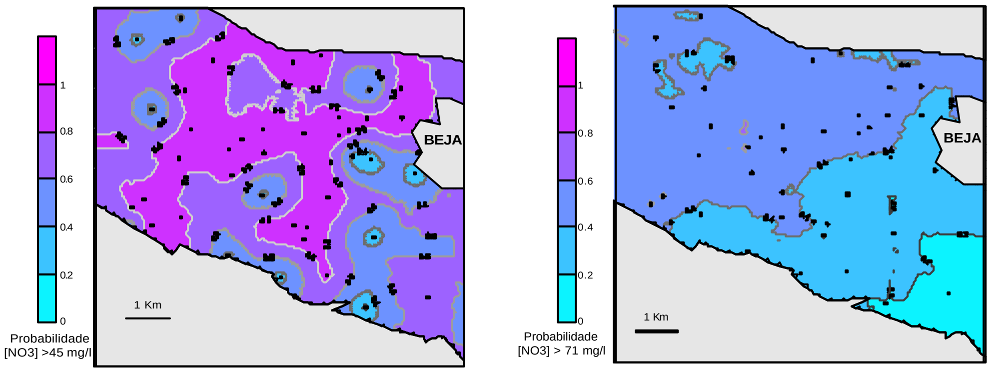


Figure 8 - Probability maps. Probability of exceeding 25% percentile (45 $mgNO_3/l$ - map A) and 60% percentile (71 $mgNO_3/l$ - map B).

CONCLUSIONS

Diffuse agricultural pollution is fairly widespread in Beja`s Gabbro-Aquifer but is more acute in the vicinity of Beja due to decades of excessive fertilization.

The current study shows space-time variability of groundwater nitrate content between July 1997 and July 2000 regarded agriculture practices and climate conditions. The intra-annual analysis has a large range variation reaching 100 mg/l and median range from 53 mg/l to 86 $mgNO_3/l$.

Spatial structural analysis of diffuse pollution was performed using geostatistcs technics namely Indicator Variography and Indicator Kriging. Probability maps of exceeding specific cut-off of 50 $mgNO_3/l$ represent stochastic simulations and therefor equally probable images of seasonal nitrate contamination useful in environmental management and municipal policies.

Assess diffuse pollution index based in the structure/de-structuration analysis of indicator variogram meaning continuity/non-continuity of contamination pattern shows that “maximum” diffuse pollution in July 99 is around 60 $mgNO_3/l$.

The unconfined shallow aquifer in the vicinities of Beja is very important for public supply but nitrate content often exceeds 50 $mgNO_3/l$. This situation must be changed according to the EU Nitrate Framework Directive and EC Water Framework Directive. Ministry of Agriculture and Ministry of Environment should mobilize funding to promote Best Agricultural Practices for Water Protection together with local farmers and an appropriate network to monitor trends in the quality of groundwater concerning diffuse pollution.

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