A hydrodynamic model of a contaminated fractured aquifer

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Abstract: - The study of contaminants propagation in fractured and karstic aquifers shows uncertainties caused by the conditions of anisotropy of the medium and by the presence of cavities and residual products that could make fluid flow and solute transport unforeseeable.

Therefore, in aquifers characterized by fissured and fractured solid matrix, in order to set up remediation strategies, it is necessary to represent the conditions of groundwater flow and contaminant propagation in such a way as to take into consideration the high heterogeneity connected to the presence of fractures and channels that act as preferential flow ways.

The study carried out in a specified site, located in the city of Bari, heavily contaminated by petroliferous substances allows to build a model able to simulate subterranean draining conditions that prove to be as near as possible to the real ones. This simulation could be helpful for the prevision of the dynamic behavior of the aquifer during the period of the treatment in order to allow optimizations on the technical and economical point of view and in order to check the effective functionality of the system in the presence of anthropic constraints.

Key-Words: - contaminant transport, fluid flow, Feflow, fractures, geostatistics, karst

1 Introduction

Previous studies carried out in the same area [1] have conducted simulations applying two distinct approaches: 1) the discrete fracture model (horizontal parallel set) [10], 2) stochastic fracture zone continuum model, through the use of Modflow [13]; in this approach the conditions of anisotropy of the medium are expressed by the hydraulic conductivities of the whole rock mass. Both the two simulations came to the construction of similar sceneries of contamination and therefore similar remediation strategies. Results that, without being in contrast with the previous simulations appear to be more coherent with the hydrodynamic conditions of the aquifer have been obtained considering a flow and transport model that, on the basis of the available stratigraphic data, takes into account the fracturing degree of the medium for significant depths as far as contaminant transport is concerned. Even for this model, the total phenols have been selected as contaminant indicator for the simulation, due to their conservative behavior during flow and transport into the studied subsoil. Biodegradation rates of total phenols and adsorption/desorption effects as well as the effects caused by seawater intrusion are neglected at this step.

2 Site Setting

The area of ex Gasometer (Fig. 1a) is located in the city centre of Bari, it extends for about 1.3 ha, is essentially flat, and has an elevation of 4m above sea level. The area is situated about 250 m far from the coastline.

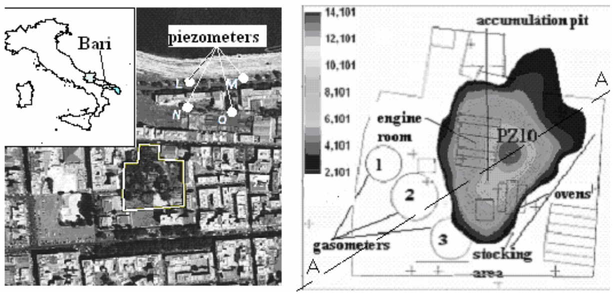

Fig.1a) Aerial photography of the territory of Bari with individuation of the study area; b) Distribution of phenols concentration (µg/l) in groundwater.

This area, starting from 1866 for about a century, has been occupied by installations for the production of town gas which made use of the controlled combustion of pit coal and successively of coke coal. In 1968 the installation has been reconverted in order to distribute methane. In 1975 any activity ended. Nowadays the area is devoid of constructions and is covered by a bed of gravel of about 15 cm thick. The study of the Plan of Characterization made in 2001 has shown the existence of a diffused contamination in the central part of the area that has interested soil and groundwater. The environmental investigations that have been carried out have shown a state of contamination of soil and groundwater which is typical of gas works. A more recent campaign of surveying on groundwater has been carried out in April 2004. The principal contamination caused by the activities of the installations is principally caused by the diffusion of organic aromatic compounds, both at light chain (BTX) and at longer chain (PAH) and phenols. On the whole, the pollutants characterized by longer chains are also the ones with higher persistence and refractoriness. In figure 1b are reported the distributions of the total phenols in groundwater. From this first reconstruction it is possible to emphasize a significant aspect: the presence of sharp hot spots, localized in the same area, well circumscribed and closed.

2.1 Geological and hydrogeological characters of the area

The area interested by the intervention of remediation lies in the coastal zone of the city of Bari, along the murgian adriatic margin of Apulia region.The stratigraphic sequence is characterized by a calcareous-dolomitic mesozoic bedrock on which marine carbonatic rocks and subordinately continental sediments have stratified in successive stages and in transgression. The geolithologic asset of the area is characterized, below a thin surficial layer of filling material, by a late-quaternary lithologic succession with interposition of terra rossa (red clay). The upper lithology of quaternary deposits is constituted by sandy-calcarenitic deposits of about 7m of thickness, frequently weathered, with rare well cemented levels, and more frequently with intercalations of markedly sandy levels [6]. The basal part of the quaternary formation is frequently less cemented, weathered and altered. This sandy-calcarenitic mass is below groundwater level and settles on a calcareous mesozoic bedrock constituted by micritic limestones locally dolomitic; in different parts is easy to find highly fractured and karstified levels with alternation of inclusions of terra rossa at different levels. Figure 2 shows the geologic section, whose sketch is reported in figure 1b.
In the study area an extended subterranean water circulation is localized, that is known as murgian groundwater, flowing in the cretaceous calcareous formations, which are permeable because of fissuration and karst phenomenon.

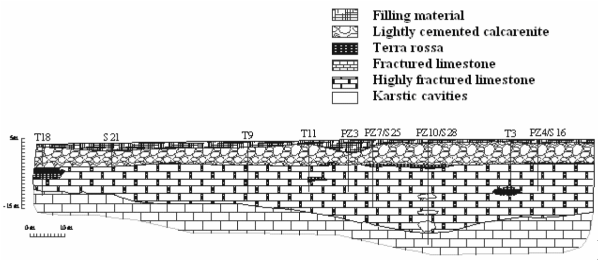

Fig.2 Geologic section A-A in which karstic cavities in correspondence of piezometer PZ10 are emphasized

This groundwater, floating on an underlying saltwater zone, flows locally in phreatic conditions. It has been involved by the process of seawater intrusion and shows concentrations of salt variable from 0.5 and 2.5 g/l. Due to the low distance to the sea, the piezometric level of groundwater is affected by oscillations caused by tides. During the Characterization of the site, discharge tests have been carried out (Lugeon) [5], and tracing tests with the point dilution method. From the above mentioned tests it has been possible to calculate the mean hydraulic conductivity value of the saturated thickness that is assumed equal to $0.8x10^{-3}$m/s, the storage coefficient, assumed equal to $5x10^{-3}$ and the specific discharge equal to 0.3-0.6 m/d.

2.2 Groundwater flow conditions

The complex system of fractures and the relevant expansion of karst phenomenon, create particular conditions of flow in the considered aquifer.
Actually, the grade of permeability of rocks, depending on their state of fissuration, produces high variations both horizontally, and vertically with the presence of fractured and karstified rocky levels at different stratigraphic heights that variously intersect. The characteristic of the examined aquifer is that downflow takes place not only in the existent fracture network, but also in the karstic draining system that has developed according to the geomorphologic evolution and to the structural geologic asset, therefore the anisotropy of the physical parameters determines different hydrodynamic conditions and temporal variability of the hydrochemical behavior. In these karstic aquifers flow takes place in a network of fractures that have a highly anisotropic hydraulic conductivity and depending on frequency, width and persistence of the single systems of fractures. The mesh of discontinuity is constituted by a

complex underground hydraulic network that is organized and structured in principal and secondary ramifications. The propagation of the contaminants follows the structure of discontinuities, partially penetrating into the rock-faces, characterized by extremely lower permeability compared to discontinuities. In those aquifers groundwater circulation could be conditioned by the existence of old erosive cracks placed on tectonic features. Those erosive grooves, located in proximity to mouths, in their round present altered lithozone, tectonized levels, concentrated and diffused karst phenomena, clogging of residual products and inclusions of debris and this is due to the drainage action operated in geologic times. Therefore, in these karstic aquifers it is necessary to set up specific interpretations of the methodologies of measurement and synthesis in order to achieve quantitative and qualitative evaluations of flow and propagation of the contamination [4].

3 Modeling approaches for flow in fractured and karstic aquifers

As far as flow in fractured an karstic aquifers is concerned, two basic approaches could be distinguished. The *discrete approach* considers the flow within individual fractures or conduits. In contrast, the *continuum approach* treats heterogeneities in terms of effective model parameters and their spatial distribution [9]. Several alternative model representations are available, that apply either the discrete or the continuum approach. These methods may be also combined [8]. Teutsch and Sauter [14] classified karst groundwater problems using the scale hierarchy approach (Fig.3); according to it five distributive approaches could be applied for the modeling of karst hydrodynamics:

- Discrete Fracture Network Approach (DFN)
- Discrete Channel Network Approach (DCN)
- Equivalent Porous Medium Approach (EPM)
- Double Continuum Approach (DC)
- Combined Discrete-Continuum Approach (CDC)

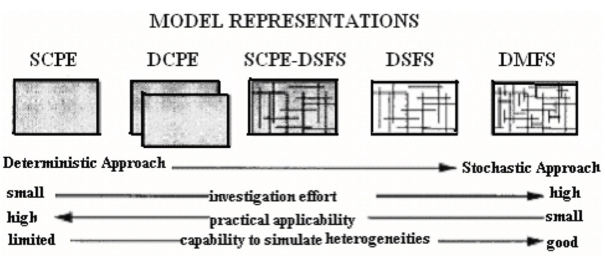

Fig 3. Classification of distributive methods applied to modeling of karst hydrodynamics.

4 The proposed model

In order to implement the hydrogeological model of the site, data obtained from the campaigns of investigation have been utilized. In particular a geostatistical analysis of geomechanical data coming from boreholes made in the area has been carried out.

The above mentioned investigations have concerned chemical analysis (of soil and groundwater), stratigraphical logs, discharge tests, analysis of the Rock Quality Designation (RQD) (in the first and in the second campaign) measures of piezometric head, soil top elevation etc. The top of limestone formation could be found at depth variable from -7 m and -9 m from the ground level. Nevertheless, in the points where the top of limestone is more superficial, the soil matrix appears to be extremely fractured and moreover full of terra rossa; therefore in those points it hasn't been possible to evaluate the Rock Quality Designation.

4.1 Geostatistical elaboration of RQD data

As far as the determination of the maximum depth at which to carry out the geostatistical analysis is concerned, it has been considered adequate to stop at – 15 m because until that depth there is a significant number of data. In reality in the integrative campaign of investigation, a depth equal to – 20 m has been reached just in few points but the RQD has been evaluated just in the last 3 meters of depth.

The absence of continuity in the information concerning this parameter (at -16 m and at – 17 m there is no presence of data) hasn't allowed to effectuate a complete reconstruction able to reproduce a representative model of the site, that would reach the depth of – 20m.

In order to obtain a study based on a higher number of data, the geostatistical analysis of the RQD values has been carried out, therefore, from – 8 m to – 15 m of depth from the ground level.

The distribution of the RQD values is characterized, for all boreholes, by high variability. It appears as a discrete variable, that is to say it doesn't assume all values among a specified interval, but either 0 or values included in a range from 10 to 60 (Fig. 4a). It is therefore possible to assimilate it to a binary variable, that could assume either a value equal to 0, in the case the solid matrix being so fractured that the thickness of the integer pieces is lower than 10 cm, (so the medium could be treated as an equivalent porous medium) or a distribution of values going from a minimum of 10 (found in some boreholes at specified depths) and a maximum of 60. In order to treat the RQD as a binary variable, it is necessary to subdivide it into two classes: the first one has RQD = 0, that could be assimilated to porous medium, and the second one is characterized by a distribution variable from 10 to 60. Anyway, in order to establish a correct subdivision into classes it has been necessary to carry out an accurate analysis of the boreholes so as to evaluate the threshold of belonging to each class; the aim of the procedure is that of defining which RQD value permits to consider the sample as constituted by fractured medium instead of equivalent porous medium; in fact, if it happens that for low values of RQD -for example 10- the limestone appears extremely fractured and with the presence of small cavities and vacuole from the stratigraphic analysis, the sample is considered belonging to the class of fractured medium. If those small cavities were full of terra rossa, the value RQD = 10 would be attributed to the first class and therefore the material will be considered as "porous medium". Through this approach it is possible to individuate two zones, one characterized by the presence of fractures and the other one by the presence of porous solid matrix.

The methodology of treating the RQD as a binary variable corresponds in geostatistical terms to the application of the Indicator Kriging (I_K). A value equal to 0 has been assigned to those points in which RQD<10 (that is to say the class having just the 0 value) and 1 to those values of RQD that are higher than or equal to 10. The Indicator in fact allows a better individuation and distinction of the zone in which the medium could be treated as fractured (I_K =0) from the zone in which it could be treated as (equivalent) porous (I_K =0). Anyway the RQD data have also been interpolated also through Ordinary Kriging in order to effectuate a comparison with the results of the Indicator Kriging. Once these zones are defined, for each depth the frequency of the fractures at each meter has been calculated, making use of the Priest and Hudson expression [12]:

$$RDQ= 100\, e^{-0.1\lambda}\, (0.1\lambda + 1) \qquad (1)$$

The Fig.4b shows the histogram of the distribution of fracture frequencies at -12m of depth.

As it is derived from the RQD parameter, also this variable could be treated as a binary variable: the first class is characterized by f=145, relating to RQD=0. The second class of values shows a distribution different from the gaussian one; nevertheless through the analysis of the Skewness parameter, it could be pointed out that it is characterized by very low values, close to 0; therefore there isn't any presence of tails neither on the right nor on the left.

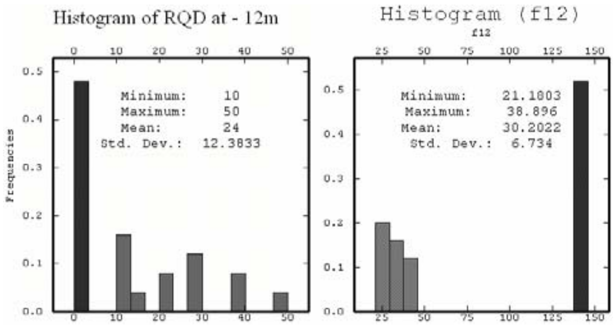

Fig. 4 Histogram of the distribution of RQD values at -12m of depth and of the distribution of fracture frequency per meter.

As far as the Kurtosis is concerned, it always shows values lower than three, just in some cases close to three. From this analysis it appears that, as the above mentioned parameters assume values close to the ones proper to a Gaussian distribution, it could be retained that, with a certain approximation, the mean value of the distribution of the frequency values is the more representative one. Once the mean value m of the above mentioned distribution relating to each meter of depth is calculated, the thickness b of the fractures at that depth will be equal to $1/m$. In Tab 1 are reported, for each depth, the mean values of the distribution of fracture frequencies and the relating thicknesses.

Depth	Mean value m	Thickness $b = 1/m$
-15m	22	0.045
-14m	27	0.037
-13m	28	0.036
-12m	30	0.034
-11m	25	0.04
-10m	29	0.0344
-9m	28	0.0357
-8m	31	0.032

Tab 1: Mean values of the frequencies of fractures and relating thicknesses.

4.2 The modeling approach used: the discrete feature approach

The proposed model makes use of the finite-element computer code Feflow 5.1 (Wasy) that is able to represent discrete elements in a porous matrix. In the discrete feature approach the three-dimensional geometry of the subsurface domain describing a porous matrix structure can be combined by interconnected one-dimensional and/or two-dimensional discrete feature elements in two and three dimensions [3]. Different laws of fluid motion can be defined within such discrete features, e.g., *Darcy*, *Hagen-Poiseuille* or *Manning-Strickler* laws.

4.3 Flow and transport modeling

On the basis of the analyses carried out in the two campaigns of investigations, it has been possible to effectuate a reconstruction of the soil top elevation: it has values variable from +4 m to +3 m above sea level. The model, coherently with the stratigraphical data, is made up of a superficial layer of porous material locally constituted by clay mixed with calcarenite, that crops out on the ground level and has got a thickness of about 8 m.

The presence of limestone has been modeled by inserting, starting from -8m until -15m, for each meter, a number of layers equal to the mean value of the fracture distribution relating to the examined depth, for a total of 215 layers. In each layer a fracture distribution has been assigned, that would follow the binary criterion of Indicator Kriging (I_K). In fact, once the Indicator Kriging has been performed, the above mentioned zoning operation has taken into account the values in the interpolated maps (Fig. 5).

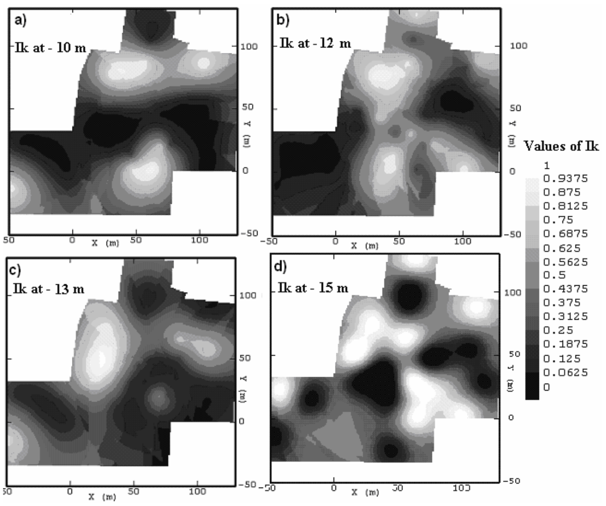

Fig.5 Map of the Indicator Kriging (Ik) at -10 m (a), -12 m (b), -13 m (c) and -15 m (d).

For some depths (for example – 15 m) the two macrozones could be clearly delineated, as there is a quite sharp change of I_K from 0 values to values equal to 1 or 95 (so with an error margin of 5%) Nevertheless some difficulties have been found for some other depths where either the scarce number of data at disposal or the extreme variability of them has generated in the interpolated maps intermediate zones where the variable I_K assumes values included in the range 0 -1. These maps have been compared with the ones obtained by the application of the Ordinary Kriging (Fig. 6) in such a way as to determine the values of RQD corresponding to those "intermediate" zones.

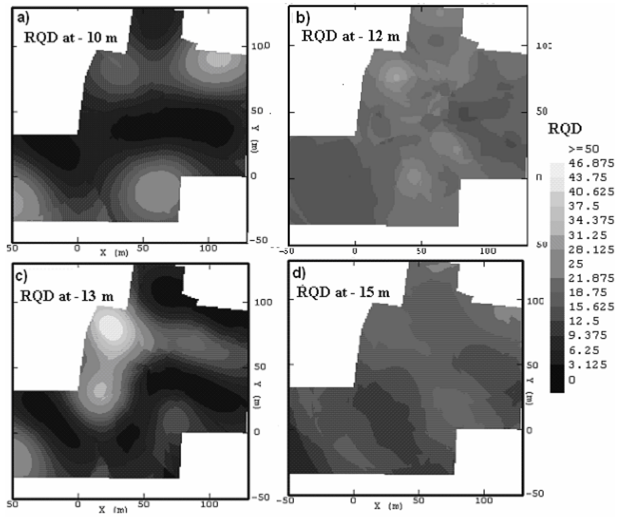

Fig. 6 Map of the RQD values at -10 m (a), -12 m (b), -13 m (c) and -15m (d).

In the zones characterized by values included in the range $0.75<I_K<1$, for which the RQD values are higher than 10 (10 has been chosen as the threshold for considering the matrix fractured), the fractures have been inserted. The maximum error margin results, therefore, at most equal to 25%. At each meter of depth there will be therefore a different distribution (Figure 7 a, b, c) and also a different thickness of the fractures, that could be obtained from the fracture frequency per meter. Once assigned the value of fractures thickness to the model, at each meter, it is necessary to calculate the hydraulic aperture *a*.

There are many indirect techniques to estimate the hydraulic aperture based on fluid flow through a rock mass. They are based on laboratory steady-state flow measurements and using in- situ tests. It is found from the literature that many researchers seem to be more comfortable with the equivalent cubic law aperture [7] based on hydraulic tests. Frequently, and for simplicity, the equivalent cubic law aperture is referred to as the hydraulic aperture or mean aperture. For laminar fluid flow through parallel joint walls, the equivalent cubic law aperture (a) is defined by:

$$a = \left[\frac{12q\mu}{b(dp/dx)} \right]^{1/3} \qquad (2)$$

Where: q = steady - state flow rate; b = width of the fracture; dp/dx = pressure gradient; μ = dynamic viscosity of the fluid. In the case study the calculated gradient is equal to 0.001.

Considering a value equal to 0.34 for the specific discharge of the aquifer (coming form the investigations carried out in the area), this will correspond for a 15 m thickness, to a discharge Q circulating through the model equal to 0.0213 m^3/sec. The same formula has been applied for the calculation of the hydraulic aperture of the vertical fractures, supposed having a distance of some meters from each other, with a thickness equal to 0.003 m.

Depth	q	b	i	a
15m	0.0213	0.045	0.001	0.017902
14m	0.0213	0.037	0.001	0.019109
13m	0.0213	0.036	0.001	0.019284
12m	0.0213	0.034	0.001	0.019655
11m	0.0213	0.04	0.001	0.018618
10m	0.0213	0.0344	0.001	0.019578
9m	0.0213	0.0357	0.001	0.019338
8m	0.0213	0.032	0.001	0.020056
Vert.fract	0.0213	0.003	0.001	0.044149
Cavities	0.0213	0.2	0.001	0.010888

Tab 2: calculation of fractures hydraulic apertures

The value of hydraulic conductivity assigned to the first layer is $1*10^{-5}$ m/sec, whereas for the lower layers 8 $*10^{-4}$, coming from the carried out investigations. The increase in hydraulic conductivity due to the presence of the fractures is taken into account by the standard hydraulic conductivity for the Hagen-Poiseuille law:

$$K = \frac{a^2 \rho_0 g}{12\mu_0} \qquad (3)$$

Where the following standard parameters are used here for water [3]:
$\rho_0 = 10^3$ kg m^{-3}, μ_0 = 1.3 Pa s, and g = 9.81 m^2 s^{-1}.It results a factor of $f_0 = \rho_0$ *and* g/μ_0 = 7.55 10^6 m^{-1} s^{-1}

Depth	a	K
15m	0.017902	201.6255
14m	0.019109	229.7309
13m	0.019284	233.9657
12m	0.019655	243.0531
11m	0.018618	218.0957
10m	0.019578	241.1653
9m	0.019338	235.2746
8m	0.020056	253.0777

Tab 3: increase of K values at each depth due to the presence of fractures

The value of the storage coefficient assigned to the model is 0.005 [2] coming from the carried out tests. The coefficients of longitudinal and transversal dispersivity, derived by the *channelling theory* suggested by Neretnieks [11], have been posed equal to D_L = 0.9 m^2/sec and D_T = 0.7 m^2/sec. As far as I type Boundary Conditions (Dirichlet) are concerned, in 49 piezometers hydraulic head values have been monitored. Constant head values on the upper and lower boundary have been assigned considering the interpolated hydraulic head values of 27 of those piezometers, the remaining 22 of have been used for calibration.

4.4 Cavities

On the basis of the available stratigraphical data, a reconstruction of the karstic cavities asset at each meter of depth, has been made, by means of Ordinary Kriging.

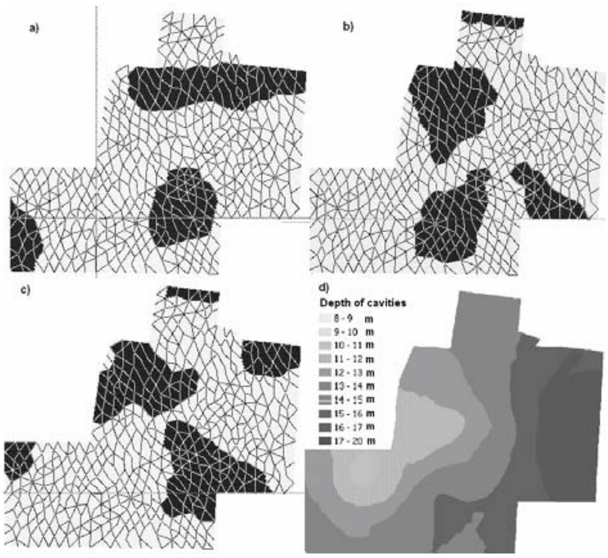

Fig. 7 Distribution of fractures at -10 m (a), -12 m (b) and -15 m (c); distribution of karstic cavities with depth.

In fact it emerges from the stratigraphies that at each point the cavities having relevant thickness are placed just at one specified depth, and this depth is almost always different for each point.

From the results of the interpolation (Fig 7c) it results that the cavities are intercommunicant, therefore there are preferential pathways of subterranean draining that are directed to the sea. In particular, from the analysis of the map, it emerges that the depths at which cavities are found are increasing from the left to the right side of the model.

The presence of the cavities has been simulated through the insertion, for each meter of depth and in the first layer representative of each meter of depth, of horizontal monodimensional tubular elements (channels) having a diameter equal to 20 cm, that corresponds to a cross sectional area equal to $\pi r^2 = 0.0314$. The value of the hydraulic aperture could be calculated by the thickness (20 cm) and is equal to 0.010888.

5 Results: Flow and transport

The piezometric heads derived from the flow simulation show, at each depth, a trend in the direction of downflow, going from SW to NE (Fig 8). The obtained results are coherent also with the map of hydraulic conductivities [1], being the flow channeled up to the zones at higher values of conductivity, that is to say the ones characterized by a higher degree of fissuration and karstic erosion.

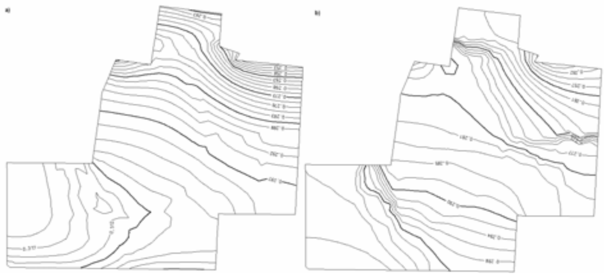

Fig. 8 Results of flow simulation at -7 m (a), -9 m (b)

The flow at – 7m depth assumes a quite homogeneous behavior; the more higher depths are reached, the more a certain degree of "disturb" could be observed in the trend of the piezometric heads.
As far as transport simulation is concerned, it has been chosen to investigate on the total phenols. In the description of the contaminant transport the advection, the dispersion and the diffusion have been considered, whereas retardation factors, biodegradations and processes of physical and chemical nature normally occurring in the subsoil have been neglected. At this step also the effects due to the different density caused by seawater intrusion are neglected. The results of transport simulation (Fig. 9) have shown a different behavior at each investigated depth. In the first modeled layer, ending where the top of limestone formation is reached, that is to say –7 m from the ground level, the contaminant plume, of modest dimensions, remains circumscribed in the central area, and doesn't propagate downstream from the area and moreover is not intercepted by the monitoring piezometers placed there. It is of particular relevance to emphasize that those piezometers just reach the depth of the top of limestone.
At –7 m the contaminant flow stops and intensifies in the areas characterized by higher underground draining, and there it remains immobilized in time. On the other hand at higher depths, a plume of broader dimensions starts delineating, and it is spread by the fissuration of the medium downstream from the industrial area. The dimensions of this plume increase with depth, and reach a maximum at about – 10 m from ground level, afterwards its values decrease with depth; at –15 m the peak of contamination, involving a volume of about 1.795 10^3 m^3, remains circumscribed in the area, although the plume propagates downstream from the site.

4 Conclusions

The obtained results delineate a scenery partly different from the one defined on the basis of the investigations previously carried out in the area [2].

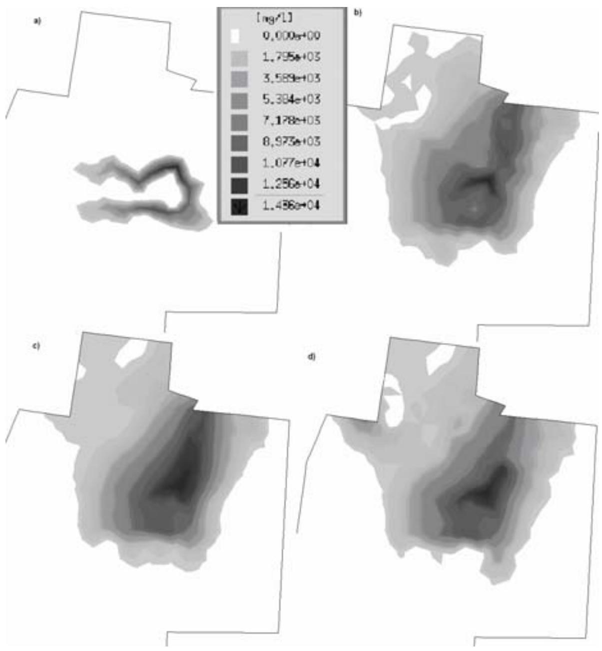

Fig. 9 Results of transport simulation at the top of groundwater level (a), at -7 m (b), -10 m (c) and -15 m (d)

The low concentration values found out in the external piezometers, even if shaping an encouraging setting, do not exclude the necessity to investigate on what happens at higher depths.
In fact the results of the flow and transport modeling in the area of the ex-Gasometer have shown a risk of contamination downstream from the site, in direction SW-NE, according to groundwater flow towards the sea.
Even if the major phenols contamination found in the aquifer appears to be circumscribed in the

industrial area, at depths higher than – 8 m the presence of a plume directed to the sea could be emphasized. In particular this plume shows broader dimensions at – 9 m and – 10 m of depth, then its values decrease with depth, even if it continues propagating downstream from the site.
It appears evident that it is necessary to carry out more accurate investigations and to realize further monitoring piezometers downstream from the site, that would reach higher depths in such a way as to be able to conduct investigations on the behavior of the plume in the fractured limestone.
The same criterion should be followed for the realization of any intervention of remediation on groundwater.

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