# CONCEPTUAL MODEL AND FLOW NUMERICAL SIMULATION OF AQUIFER CONTAMINATED BY CHLORINATED SOLVENTS IN RHO (MI)

## FRANCESCA BOZZANO<sup>(\*)</sup>, MARCO PETITTA<sup>(\*)</sup>, ANDREA DEL BON<sup>(\*\*)</sup>, FABRIZIO NARDONI<sup>(\*\*)</sup> & EVA PACIONI<sup>(\*\*)</sup>

(\*) Sapienza Università di Roma - CERI Research Center - Piazza U. Pilozzi, 9 - 00038 Valmontone (RM), Italy

(\*\*) Sapienza Università di Roma - Department of Earth Sciences - Piazzale Aldo Moro, 5 - 00185 Roma, Italy

### ABSTRACT

The geological and hydrogeological characterization of a multilayer aquifer contaminated by organochlorinated compounds has been carried out in the industrial area of Rho (Milan, Italy). The hydrogeological setting is characterized by the presence of several aquifers overlying each other, separated by silty-clayey levels, whose presence and thickness tends to increase with depth. The "first aquifer", 35 m thick, is separated by a clayey level, located at 5-9 m below ground level varying in thickness between 0.5 and 2 m, from a perched aquifer of local interest, indicated as "shallow aquifer". Groundwater flows towards SSE in both shallow and deeper aquifer, with a mean 0.6% hydraulic gradient, showing highest values (+2 m) of the hydraulic head of the shallow aquifer, allowing possible seepage from the shallow aquifer to the deeper one, taking into account the small thickness of the aquitard.

Geological, hydrogeological and hydrogeochemical data have been included in a GIS and they have been used to interpolate geometry, thickness and piezometric surface of the shallow aquifer, of the aquitard and of the first aquifer. By scarcity of the experimental data, hydraulic coefficient evaluation has been integrated starting from grain size classes on single vertical boreholes. Space distribution of k has been derived by geostatistical tools, after validation of k classes referring to available investigation data.

Two groundwater flow mathematical models have been developed for the multilayer aquifer at different scales; a large scale model (LSM) and a fine scale one (FSM). After calibration and validation, the LSM sufficiently agrees with experimental data, offering the possibility to simulate regional flowpaths, both in shallow and first aquifer. Shallow aquifer heterogeneity appears significant in groundwater flow influence, allowing simulation of local flowpaths differently oriented from main groundwater flow direction. Heterogeneities in the first aquifer have not been reproduced in numerical models, assigning an average value of hydraulic conductivity to the layer, considered as an homogeneous aquifer for groundwater flow simulation.

At the FSM scale, a deeper characterization of the first aquifer it seems necessary, because simple uniform values of k cannot correctly simulate local water table variations and real flowpath directions. It can be inferred that this FSM can be used only to simulate shallow aquifer and seepage towards the first aquifer. Meanwhile, the FSM model cannot be used to assess final fate of the contaminant in the first aquifer.

Models support field data about the seepage from the shallow to the first aquifer, of both groundwater and dissolved contaminants, showing vertical transfer by particle tracking through the thin aquitard, which can explain high contaminant concentrations found in the first aquifer.

### **INTRODUCTION**

This paper is aimed at evaluating groundwater flow of industrial area Chimica Bianchi in Rho (Fig. 1), near Milan, being an example of multilayer heterogeneous aquifer. The characteristic of this aquifer is the superimposition of several layers with different permeability and consequently mutual interactions. The peculiarity of this systems respect to the water circulation and adjective transport of the contaminants are (GIERCZAK *et al.*, 2006; PARKER *et al.*, 2007): 1) the 3D geometry and the thickness of the aquifer layers and of the low permeability aquitards and 2) the lateral and vertical variations of the permeability coefficient, which both contribute to the heterogeneity of the system.

The methodology adopted in order to analyze groundwater flow in the aquifer of Rho is characterized by multiscale approach (BERETTA *et al.*, 2006), aimed to distinguish the regional influences on groundwater, from the ones which locally modify its characteristics, by using numerical simulation as a tool for analysis and validation.

### **STUDY AREA**

The Rho area (Fig. 1) is located in the Lombard plain some kilometers north of Milan; it is geologically characterized by alluvial and fluvioglacial quaternary sediments. The hydrogeological succession (Fig. 2) is given, in the upper part (up to around 50-60 m below ground level), by two overlapping aquifers (L1 and L3 in the following), separated by a fine grained level (aquitard, L2) (AVANZINI *et al.*, 1995; PROVINCIA DI MILANO, 1995; BERETTA *et al.*, 2003). The deepest of the two aquifer ("first aquifer" Auct., named L3) goes down to a depth of about 45m b.g.l.; it is in semi confined conditions and the average thickness of the saturated zone is 35 m. It is made up of coarse-grained soils with silt and clay levels. At a depth between 5 and 9 m b.g.l. a few meters thick clayey level (aquitard, named L2) is located; it supports a shallow aquifer (labelled L1 in Fig. 2) of local interest, made of gravel and sand with low silt and clay content. The piezometric level stands at around 6-7 m b.g.l. for L1, and at around 8.5 m for L3 in correspondence of the L2 aquitard. This setting allows for possible seepage from L1 towards L3 through L2 (BERETTA *et al.*, 2005).

Over the past years the shallow aquifer L1 has been deeply contaminated by chlorinated solvents (TeCA, TCE, PCE) (AULENTA *et al.*, 2005) inside the former industrial plant named "Chimica Bianchi". In a sector considered as being the contamination source area, an annular impermeable diaphragm has been realized some years ago (Figs. 3, 9) which is founded at a depth of around 9m b.g.l. in correspondence of the aquitard L2 level, aiming at limiting the migration of the contaminants and trying to isolate a portion of the shallow aquifer L1 containing the contaminants source.

## METHODOLOGICAL APPROACH

The analysis of the groundwater flow has been dealt with a multiscale approach. It is realized according to a first phase of enlargement of the two orders of magnitude of the study area, going from around 0.13 km<sup>2</sup> (former Chimica Bianchi industrial area) to more than 11 km<sup>2</sup> (Rho groundwater flow scale), lowering the observation scale (Fig. 1). The goal of this first phase has been to detect the main characteristics of the groundwater flow, surrounding the industrial site. In the second phase, starting from the groundwater conceptual model obtained from the first one, the analysis has been focused on the industrial site, increasing the observation scale in order to analize in a more detailed way the effects of the heterogeneity of the multilayer aquifer on groundwater flow. The local influences on groundwater flow have been considered, in order to obtain a detailed conceptual model of groundwater flow, which can be useful for building not only flow numerical models, but for mathematical models of contaminant transport too, including reactive models (AULENTA *et al.*, 2007).

Real data coming from the multilayer aquifer have been analysed, concerning lithological, piezometric and hydrodinamic data mainly pre-existing, coming from provincial and municipal archives and from literature (AVANZINI *et al.*, 1996; BERETTA *et al.*, 2003; CALLONI *et al.*, 1999; CIVITA *et al.*, 2002) and partly available from hydrogeological studies of the authors. The whole of these data has been gathered, adapted and rationalized in a database intentionally planned and carried out in ACCESS format. It contains hydrogeological and hydrogeochemical data referring in total to more than 300 verticals of studies developed in the Rho area, focusing mainly



Fig. 1 - Study area (dark grey), industrial site (red), Olona River (blue). Available data from boreholes and wells: U: location, D: depth, S: stratigraphy, I: image, P: piezometric level, F:screen, A: aquifer, Ca: hydraulic parameters, Ac: chemical analyses, Mp: multipacker



Fig.2 - Hydrogeological section showing relationships among the shallow aquifer, the aquitard and the "first aquifer". Codes refer to borehole available along the section

on the industrial site, where several piezometers of historical series of piezometric and hydrochemical data are available (Fig. 1).

The data concerning the geometry of the two recognized aquifer levels (L1, L3) and of the aquitard packed between them (L2) have been elaborated with geostatical methods ("kriging" with the SURFER software and geometrical analysis with AutoCAD MAP) in order to obtain in a GIS environment top and bottom surfaces of the aquitard level (Fig. 4), which represent the main elements influencing the hydrogeological setting, in order to solve the specific problem of the contaminant diffusion from the shallow aquifer (L1) to the semiconfined first aquifer (L3) through the aquitard (L2).

The data concerning the piezometric levels have been used as targets for calibration of the numerical flow model, implemented by MODFLOW code, ESI GROUNDWATER VISTAS 4.1 version. The piezometric data concerning the industrial area have been used to draw manually the isophreatic map of both shallow (L1) and first aquifer (L3) (Fig. 3).

The database also contains data referring to the hydraulic conductivity and to the transmissivity of the two aquifers resulting from site tests (pumping tests, slug tests). It results in only 14 data (Fig. 5). Considering the influence of this parameter on groundwater flow and the amplitude of the area, it has been necessary to increase hydrodynamic data set, using the lithological information related to the three



Fig. 3 - Piezometric map of the shallow aquifer (L1) and first aquifer (L3) of the industrial site. 1: isophreatic lines of the shallow aquifer; 2: isopiezometric lines of the first aquifer; 3: monitored piezometers; 4: contamination source area; 5: Olona River (October 2004 survey)



levels in the high number of boreholes distributed in the area. As known, it is possible to associate to the lithotype grain size, expressed through a classification system like the USCS (ASTM, 1987) adopted in this work, a typical range of hydraulic conductivity coefficient (LAMBE & WITHMAN, 1979). For every available stratigraphy log, the range of hydraulic conductivity coefficient which can be attributed to each aquifer or aquitard has been calculated (Fig. 6), adopting the following procedure: a weighted mean of kh has been assigned to each stratigraphy log, multiplying the thickness of each recognized lithotype for the relate range of kh attributed to the same lithotype, according to the concept of equivalent permeability  $(k_{eq})$ . This procedure of k<sub>b</sub> calculation has been verified through the comparison with the real available data previously mentioned (Fig. 5), in order to verify the reliability of the adopted procedure based on grain size class translation into hydraulic conductivity ranges. The obtained data set of hydraulic conductivity for each layer has been interpolated with geostatical methods ("kriging" with the SURFER software), in order to provide maps of space variability of kh inside the study area (Fig. 7) for shallow and first aquifers. The whole of these data, representing the conceptual model of groundwater flow in the studied multilayer aquifer, has been used for the flow numerical simulation, using the following softwares: MODFLOW, MODPATH e GROUNDWATER VISTAS (pre- and post-processor of the simulation softwares).

The numerical simulation has concerned the following models (Fig. 1):

 large Scale Model (LSM): domain dimensions 4000 m x 2500 m; grid orientation 0°; squared cells 100 m sized on three layers, to



represent groundwater flow in Rho area;

 fine Scale Model (FSM): domain dimensions 1330 m x 1260 m; grid orientation 340°; squared cells 10 m sized on three layers, to represent groundwater flow inside the industrial area.

The boundary conditions have been established as identical for the two aquifers, upstream and downstream of the annular impermeable diaphragm, adopting constant-head conditions, in order to simulate the hypothesis that the difference of water table levels between L1 and L3 can be attributed exclusively to the rainfall recharge from ground surface. Lateral boundaries of the model have been imposed as no-flow limit, because they are parallel to the flowpaths.

In the LSM the groundwater flow has been simulated in steadystate condition; calibration of the model has been based on real independent piezometric data, compared with the simulated ones, looking for the k<sub>h</sub> distribution giving the lower residuals (minimum mean square deviations between the observed values and the measured ones). The sensitivity analisys of the model has been carried out with respect to the hydraulic coefficient for L1 and L3, considering this parameter as liable to a large degree of incertitude, due to the aquifer heterogeneity and to the scarcity of available initial data. In the FSM the flow has been simulated in steady-state and transient conditions; pumping tests have been used for calibration of transient simulation. The comparison between LSM and FSM models with the measured piezometric maps has allowed to confirm the role and the influence on the groundwater flowpaths of the geometry of the layers, and to detect the values of the hydrodinamic parameters physically compatible with the reference conceptual model. Explicit attention has been



Fig. 5 - Comparison between hydraulic conductivity values (k) calculated by grain size classes and measured by field tests. Kmax: maximum calculated value; Kmed: medium calculated value; Kmin: minimum calculated value; Kmis: measured value

focused on the following elements: i) calculation procedure of  $k_{eq}$  starting from stratigraphies; ii) space interpolation through kriging of  $k_h$  range data; iii) boundary conditions of the numerical model; iv) representativeness of the obtained  $k_h$  distribution in order to simulate groundwater flow; v) adoption of the optimum value of  $k_h$  inside the range given by his evalutation by lithological base.

#### RESULTS

Figure 4 shows the geometry reconstructed for the Rho aquifer system. Figure 8 summarises the piezometric surfaces referred to the shallow and to the first aquifer as reconstructed through the LSM. Both groundwaters show a flow direction from NNW to SSE, in agreement with reconstruction on a regional scale proposed by the literature (PROVINCIA DI MILANO, 1995; CALLONI *et al.*, 1999).

In the here proposed reconstruction of the hydrogeological setting, the aquitard level L2 plays a fundamental role. Where the aquitard L2 is present (Fig. 4), an uncoupling condition of the groundwater is verified by the generation of the two aquifers: 1) the shallow and perched one (L1) characterised by phreatic conditions, water table located few meters below ground level and very limited thickness and 2) the semiconfined aquifer (L3) with a piezometric surface 1.5-2m deeper than the one of L1 (Figs. 2, 8). The aquitard disappears towards E-NE causing the coupling of the shallow aquifer with the first one (Fig. 8). Water seepages from L1 towards L3 are regulated by the aquitard L2 and modulated by its variations of thickness (Fig. 10) and by the local vertical hydraulic gradients.

In the area of the former Chimica Bianchi plant the two aquifers are separated. The reconstruction (Fig. 3) of the corresponding piezometric surfaces shows these groundwater flowpaths: from NNW to SSE for the shallow aquifer, in agreement with the results coming from the LSM (Fig. 8); from NNE to SSW for the first aquifer (BERETTA *et al.*, 2005) so that a difference with respect to the results of the LSM for a wider area (Fig. 8) exists.

A small hill shaped area characterises the piezometric surface of the shallow aquifer reported in Figure 3. It corresponds to the area enclosed by the above mentioned annular impermeable diaphragm that locally causes this anomaly of the piezometric head. It is reliable that in this area the shallow aquifer is only vertically recharged being isolated from the surrounding shallow aquifer. Figure 9 shows how the effect of the horizontal isolation of this part of the shallow aquifer and the consequent increase of the groundwater level inside the diaphragm area generated an increase of the vertical head, respect to the surrounding areas, causing a local increase of the seepage from L1 to L3 through L2. A total discharge of around 40 m<sup>3</sup>/year has been estimated with times of few years per meter of aquifer thickness (BOZZANO et al., 2006) inside the impermeable diaphragm area. It is derived that the L2 aquitard cannot guarantee a long term isolation of the aquifer L1 from L3, mainly because of its limited thickness.

The aquitard absence, reconstructed for a sector of some km<sup>2</sup> in the NE part of the area analyzed by the LSM (Fig. 4), determines on the other hand, the presence of a single aquifer (Fig. 8). The coupling of the piezometric surfaces referred to L1 and L3 takes place along the border of the aquitard itself and it is characterized by an increase of the L1 horizontal hydraulic gradient (Fig. 8).

The stratigraphy logs testify for the aquifers L1 and L3 a large



Fig. 6 - Hydraulic conductivity ranges assigned to aquifers (L1 and L3) and to the aquitard (L2) on the base of grain size classes. Borehole stratigraphies are classified by USCS method

lithological variability both towards the vertical and the horizontal directions. From a hydrogeological point of view the hydraulic conductivity coefficient can summarize these variations. So the attribution of  $k_h$  to the three levels L1, L2 and L3 and its spatial zonation were a crucial step to face the numerical simulation of the groundwater flow. In order to represent in a realiable way both the stratification and the lateral heterogeneity, the following methods have been adopted:

1) it has been assumed that in the two aquifers L1 e L3 the flow is mainly horizontal and that the hydrodynamic parameter which characterises groundwater flow is the trasmissivity. On this base, it has been calculated an "equivalent hydraulic conductivity coefficient", which is uniform along every vertical in each layer (L), as a function of  $k_h$  and of the thickness of every lithotype, according to the calculation method:  $k_{heq}$  (L<sub>i</sub>) = ( $\Sigma$ [thickness\_lithotype<sub>i</sub> \* $k_h$  (lithotype)<sub>i</sub>])/( $\Sigma$  thickness\_ lithotype). To every lithotype a range of possibile values has been attributed (generally spanning two orders of magnitude), on the basis of the USCS system previously mentioned; as a consequence it is possibile to attribute also a range of  $k_{eq}$  depending on the minimum or maximum values referred to every lithotype. However the comparison of the so derived range of  $k_{eq}$ with the  $k_h$  values derived from site tests (Fig. 5) allows to ver-



Fig. 7 - Map of hydraulic conductivity of the study area obtained by geostatistical analysis for both the shallow (a) and first (b) aquifer

ify that, using  $k_{hmin}$ ,  $k_{heq}$  is underestimated: the experimental value is generally placed between  $k_{hmed}$  and  $k_{hmax}$  as observed in Fig. 5. Nevertheless it is important to underline that even though  $k_{heq}$  seems to be efficient to simulate the groundwater flow, it cannot be considered appropriate to deal with transport and the possible temporary storage of contaminants. This is because the adoption of  $k_{heq}$  causes a homogeneization along the vertical direction overlooking the role of the levels with different  $k_h$ . As a consequence, the real vertical distribution of the contaminants in the aquifer layers cannot be inferred, neglecting the role of obstacle for the contamination diffusion, played by thin levels or lenses having low permeability.

2) Once it has been attributed a value of  $k_{eq}$  to every stratigraphy, its variation on space has been estimated by interpolation with geostatistical methods. In this specific case, the space distribution, thanks to the large number of available data, has been supported by structured variograms, only for L1 (198 k<sub>eq</sub> available calculated values on a surface of 11 km<sup>2</sup>). The interpolation has been carried out calculating weighted averages on logarithmical base (considering the exponent of the hydraulic conductivity coefficient). In this way a map of the space variability of k<sub>hmed</sub> and k<sub>hmax</sub> for L1 has been obtained. On this map (Fig. 7) k<sub>h</sub> has been considered uniform into the areas with the same order of magnitude. Differently L2 and L3, for which there are only 100 available data, have been considered layers laterally homoge-





neous, each caracterized by an average value of  $k_{hmed}$  and  $k_{hmax}$ . In this case, the statistical approach does not evidence appraisable correlations, not allowing the extimation of k in terms of lithological variability of L2 and L3, in spite of what had been done for L1. However, it can be seen that the homogeneization of  $k_h$  for L3 does not considerably reduce the simulation representativeness, as the considerable thickness of the aquifer allows to consider as neglectable the effects of local vertical heterogeneities for the groundwater flow model, assuming the transmissivity as main parameter influencing groundwater flow; viceversa, the zonation of the hydraulic coefficient is necessary to reproduce groundwater flowpaths in L1, as a function of his very limited thickness, in which minimum lithological variations determine major variations of  $k_h$ , as well as of transmissivity.

The sensitivity analysis of the numerical models has been carried out considering the average of the absolute values of the residues of piezometric levels, determined as the difference between estimated values and observed values in correspondence with 38 targets. It has indicated the following optimization values:  $k_h$  of L1 = 0.3 $k_{hmax}$  for each area with uniform  $k_h$  obtained by geostatistical interpolation;  $k_h$  of L2 = 10<sup>-8</sup> m/s;  $k_h$  of L3 = 8x10<sup>-4</sup>m/s (for LSM) and 2x10<sup>-4</sup> m/s (for FSM).



Fig. 9 - Scheme of the relationships between shallow and first aquifer in the confined source area with the impermeable wall. Water tables of the shallow aquifer (L1 in red) and of the first aquifer (L3 in blue)

#### CONCLUSIONS

The comparisons between the simulated piezometric maps and the ones drawn from the site data underline that the LSM can reproduce in a reliable way the regional groundwater flow, whereas the FSM, even though it was low residues (absolute residual mean of 0.2 m) and it can well reproduce the flowpath in the shallow aquifer, cannot reproduce for the first aquifer (L3), in the southern industrial area, the local flowpaths NE-SW oriented, respect to the main flowpaths direction NW-SE oriented (Fig. 3). This low reliability of FSM



Fig. 10 - Thickness of the aquitard in the industrial site and location of the confined source area with impermeable diaphragm (red)

can be attributed to the introduced simplification in hydraulic conductivity distribution, which has been simulated as homogeneous for L2 and L3, due to difficulties in zoning  $k_h$  and transmissivity for the first aquifer (L3), using the same method adopted for the shallow aquifer (L1). It can be explained by the larger thickness of L3 (10 x L1) and subsequent growing influence of transmissivity respect to the hydraulic conductivity, which evidently can not correctly estimated by grain size classes. Otherwise, in the shallow aquifer (L1) a reliable zonation of hydraulic conductivity coefficient has been obtained by the FSM (Fig. 7).

Being aware of this basic limit of FSM, the model has been further on implemented in order to verify the possibility of contaminant migration from the shallow to the first aquifer. This process depends on: a) thickness and permeability of the aquitard (L2); b) difference in the hydraulic heads between L1 and L3. Both parameters are well known by the conceptual model. As a consequence, as this analysis is not influenced by the distribution of k in L3 (which is the parameter not correctly simulated in the performed models), the results of the simulation can be considered as trustworthy for this aim.

Through the MODPATH code the flowpaths of hypothetical polluting particles integral with water molecules (passive transport) have been simulated, coming from a source of contamination in absence of the anular impermeable diaphragm. So only the advective transport of the contaminant has been take into account, neglecting diffusion/dispersion processes and the possible existence of NAPL too. It can be inferred that (Fig. 11) the pollutant particles released in L1 at the contamination source, within few meters downstream the source itself, are vehicled towards L3 seeping through the aquitard L2. The real flowpath of pollutant particles



Fig. 11 - Particle tracking by MODFLOW from contamination source area in the shallow aquifer. Industrial area in yellow; passive transport in shallow aquifer in red; passive transport in first aquifer in blue

cles once they have reached L3 is not shown by the FSM, because of the above mentioned unrepresentativeness of the model for L3. The simulation reliability of the contaminant transport from the source in the shallow aquifer through the aquitard, is supported by further independent data (historical distribution of contaminant concentrations; BOZZANO *et al.*, 2006). Final result of the study, in agreement with the piezometric maps, is the confirmation that the contaminant, starting from the same source in the shallow aquifer, can have reached the first aquifer downstream on the southwestern part of the industrial site, previously considered as not polluted.

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