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

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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 45 m 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 multi-scale 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 km² (former Chimica Bianchi industrial area) to more than 11 km² (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 analyze 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 hydrodynamic 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
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 isophaetic 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
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) adopt-
ed in this work, a typical range of hydraulic conductivity coefficient
(LAMBE & WITMAN, 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 fol-
lowing procedure: a weighted mean of \( k_h \) has been assigned to each
stratigraphy log, multiplying the thickness of each recognized litho-
type for the relate range of \( k_h \) attributed to the same lithotype, accord-
ing to the concept of equivalent permeability (\( k_{eq} \)). This procedure of
\( k_h \) 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 transla-
tion into hydraulic conductivity ranges. The obtained data set of
hydraulic conductivity for each layer has been interpolated with geo-
statical methods (“kriging” with the SURFER software), in order to
provide maps of space variability of \( k_h \) 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 imperme-
able diaphragm, adopting constant-head conditions, in order to simu-
late 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 steady-
state condition; calibration of the model has been based on real inde-
pendent piezometric data, compared with the simulated ones, looking
for the \( k_h \) distribution giving the lower residuals (minimum mean
square deviations between the observed values and the measured
ones). The sensitivity analysis 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 compat-
ible with the reference conceptual model. Explicit attention has been

Fig. 4 - 3D map of geometrical relationships among shallow aquifer, aquitard and first aquifer. Grey: ground surface; red: shallow
aquifer bottom; blue: first aquifer top; cian: first aquifer bottom
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 its evaluation 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\(^3\)/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\(^2\) 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...
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 reliable 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 transmissivity. 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: 

$$k_{heq}(L_i) = \frac{\sum \text{[thickness}_{lithotype_i} \cdot k_h(\text{lithotype}_i)]}{\sum \text{thickness}_{lithotype}}.$$ 

To every lithotype a range of possible values has been attributed (generally spanning two orders of magnitude), on the basis of the USCS system previously mentioned; as a consequence it is possible 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 verify 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 homogenization 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 $k_{eq}$ available calculated values on a surface of 11 km$^2$). 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 $k_{hmed}$ and $k_{hmax}$ for L1 has been obtained. On this map (Fig. 7) $k_h$ 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 characterized by an average value of $k_{hmed}$ and $k_{hmax}$. In this case, the statistical approach does not evidence appraisable correlations, not allowing the estimation 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 homogenization 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 = $10^{-8}$ m/s; $k_h$ of L3 = $8\times10^{-4}$ m/s (for LSM) and $2\times10^{-4}$ m/s (for FSM).

**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
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 from the shallow to the first aquifer. This process has been taken 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 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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