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NUMERICAL SIMULATION ON THE GROUNDWATER CONTAMINATION EVOLUTION IN INDUSTRIAL SETTINGS

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EXTENDED ABSTRACT

La modellazione idrogeologica gioca un ruolo cruciale nello studio delle acque sotterranee e soprattutto nella relativa gestione e protezione. La realizzazione di modelli numerici di flusso delle acque sotterranee e di trasporto di contaminanti permette di ricostruire e comprendere dinamiche sotterranee più o meno complesse. Ottenere un modello numerico delle acque sotterranee assume notevole importanza soprattutto nei casi di contaminazione ambientale, dove la modellazione permette di riscostruire i meccanismi di trasporto dei contaminanti all'interno dei sistemi idrogeologici. L'obiettivo del presente lavoro è quello di studiare il flusso sotterraneo nell'ambito di un acquifero sotteso ad una zona altamente industrializzata, dove il possibile sversamento di contaminanti nel sottosuolo rappresenta un rischio per le numerose opere di captazione presenti, per valutare il trend di trasporto di una ipotetica contaminazione in fase disciolta e la relativa interazione con pozzi in emungimento.

L'area di studio ricade nella piana alluvionale del fiume Simeto, a sud della città di Catania, che rappresenta la porzione orientale del bacino idrografico più esteso della Sicilia. Nello specifico, questo si estende tra il margine settentrionale dell'Altopiano Ibleo e le propaggini meridionali dell'Etna ed è caratterizzato dalla presenza di tre principali corpi idrici che la solcano in direzione E-W, ossia i fiumi Simeto, Dittaino e Gornalunga. L'acquifero alluvionale della Piana di Catania è un acquifero assai complesso ed eterogeneo, sede di corpi idrici in parte separati ed in parte interconnessi con caratteristiche di falde libere o semi-confinate. L'alimentazione di tale acquifero deriva principalmente dagli apporti del Simeto che, a sua volta, riceve il contributo dei deflussi sotterranei derivanti dal versante occidentale dell'Etna. La direzione generale dei deflussi sotterranei è da ovest verso est, parallelamente al reticolo idrografico. In questo scenario si inserisce l'intensa presenza antropica della zona industriale di Catania. Questa zona è ricca di attività commerciali ed industriali che possono senza dubbio aumentare la vulnerabilità dell'acquifero, che è sfruttato in maniera intensa. Ciò comporta locali condizioni di accentuata depressione delle falde, con conseguenze sul regime idrodinamico e sulla qualità delle risorse idriche. In questo studio, al fine di modellare l'evoluzione di un possibile scenario di contaminazione ambientale, si è ipotizzato lo sversamento accidentale di un contaminante oleoso a bassa densità. Sulla base di un dettagliato modello concettuale geologico ed idrogeologico sono stati impostati sia un modello di flusso, sia un modello di trasporto della fase disciolta della contaminazione.

I risultati mostrano che l'andamento delle acque sotterranee, e nello specifico di un potenziale plume di contaminazione, sono fortemente influenzati dai parametri idrodinamici dell'acquifero, dalla concentrazione del contaminante e dalla presenza di prelievi antropici. Il modello di flusso mostra che l'andamento delle acque sotterranee in condizioni statiche prosegue da ovest verso la costa orientale della Sicilia; il modello di trasporto ha permesso di definire il trend di un potenziale contaminante, in base alle caratteristiche idrodinamiche dell'acquifero ed all'interazione con diverse opere di captazione ipotizzate. Queste ultime, da una parte accelerano il deflusso della contaminazione e, dall'altra, ne determinano una maggiore incidenza in corrispondenza di campi di pozzi in emungimento. I risultati conseguiti evidenziano l'efficacia dell'approccio adoperato nel fornire una valutazione su larga scala del flusso delle acque e del trasporto di un contaminante.

Nonostante si tratti di scenari ipotetici, l'approccio è generalizzabile a diversi contesti geologici. In questo caso studio la modellazione numerica è servita per identificare, su un'area significativamente estesa, potenziali zone a rischio di inquinamento (campi pozzi) e conseguentemente sospettare una potenziale intrusione salina nell'area costiera.

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ABSTRACT

The hydrogeological numerical simulation represents a tool for the protection of aquifers and for modeling the groundwater flow and transport. This study aims to build numerical models of a porous aquifer located in the alluvial plain of Catania (eastern Sicily, Italy), to evaluate groundwater flow and hypothetical contamination plume trends, even in interaction with pumping activity. To implement the flow and transport simulations, geological and hydrogeological conceptual models were defined using borehole and well data. The studied aquifer is semi-confined, with the presence of alluvial sediments mixed with sandy clays and silts. Because of the presence of anthropic activities in the area, the accidental spill of a contaminant would represent a social problem in the frame of the environmental and health risk. In this regard, we carried out numerical simulations that consider the hydrodynamic parameters of the aquifer, the contaminant concentration, and the presence of pumping wells. The model shows that groundwater flow is directed towards east, and that the presence of wells locally affects it. The transport model shows that a hypothetical dissolved contamination plume mainly follows the groundwater flow path, and that the presence of pumping well accelerates its flow towards elements at risk.

Keywords: *numerical model, groundwater, aquifer, environmental pollution.*

INTRODUCTION

Groundwater is a precious natural resource used for various purposes such as domestic, agricultural, and industrial. Numerical modeling of groundwater is useful for simulating different flow scenarios, especially in highly industrialized areas, and for taking corrective measures for the sustainable use of water resources. Several studies have been conducted on this topic in the past, investigating the impact of pumping activities on groundwater exploitation using MODFLOW (Onta & Gupta, 1995; Zume & Tarhule, 2008; Al-Salamah *et alii*, 2011; Gaur *et alii*, 2011). This work aims to study the impact that pumping activities have on groundwater flow and dissolved contamination transport in a porous medium through numerical simulations. In particular, the modeled aquifer represents one of the most important hydrogeological units in eastern Sicily (Italy) and falls within the Simeto River basin. The study area is characterized by the presence of numerous commercial and industrial activities that may represent a risk for water resources in case a contamination occurs. Considering stratigraphic and borehole data, conceptual geological and hydrogeological models were designed and used to define numerical models. In detail, the accidental release of a contaminant was hypothesized and, through the simulation of different scenarios, flow and transport models were built. These were run by considering both the absence of withdrawal activities and the effects of pumping wells, which were placed throughout the area both as isolated wells and as clusters. In fact, it is known in literature that pumping wells can alter groundwater flow, accelerating or slowing the spread of pollutants (Mustafa *et alii*, 2016, 2020; Ahmadi *et alii*, 2021, Mineo *et alii*, 2022).

To build the models, the QGIS platform (https://qgis.org/) and the FREEWAT plugin (Rossetto *et alii*, 2018) were used. The approach of this study, based on a hypothetical contamination scenario, can be used as a reference to be applied to different case studies, e.g., to assess the impact of withdrawals, formulate sustainable water resource management strategies, and provide risk mitigation plans.

GEOLOGICAL AND HYDROGEOLOGICAL CONCEPTUAL MODELS

The study area falls within the Simeto River basin, located in the central-eastern part of Sicily. It is a 430 km^2 wide alluvial plain (Catania Plain) that represents an important element from both the geomorphological and hydrogeological points of view. It is bounded by the sedimentary rock outcrops of the Hyblaean Foreland to the south, by the Etna volcano to the north, by the outcrops of the Apennine-Maghrebid Chain to the west, and by the Ionian Sea to the east (Labaume *et alii*, 1990; Grasso, 1993). The thick alluvial cover gives the Plain a generally flat or sub-flat morphology, that is interrupted to the south by NE-SW trending rocky outcrops. The stratigraphic setting of Catania Plain is characterized by four main units (Torelli *et alii*, 1998; Longhitano & Colella, 2002; Guastaldi *et alii*, 2014), described as follows from bottom to top (Fig. 1):

- bluish marly clay consisting of marine sediments (Lower Pleistocene);
- sands and gravel of the San Giorgio Formation (Middle Pleistocene), cropping out at the northern edge of the Plain;
- polygenic gravels and conglomerates of the Monti Tiritì Formation (Pleistocene middle – upper Pleistocene);
- recent alluvial sediments: silts and sands evolving in organic clay eastwards (Holocene).

To define a conceptual hydrogeological model, these lithological units were grouped into three main hydrogeological complexes (Costa, 2008):

- marly clays complex characterized by a very low permeability (10^{-11} m/s) and representing the aquiclude (U3);
- sands and gravels complex characterized by a medium-high permeability (10^{-3} m/s) (U2);
- silty-clayey and silty-sandy complexes consisting of sediments with a medium-low permeability (medium-low permeability (10^{-4} - 10^{-6} m/s) (U1).

In detail, the studied aquifer is represented by the hydrogeological unit U3. According to available data (Ferrara, 1998) the groundwater table depth is about 6 m b.g.l. at the northwestern sector of the study area, while it approaches the sea level at the coastal sector.

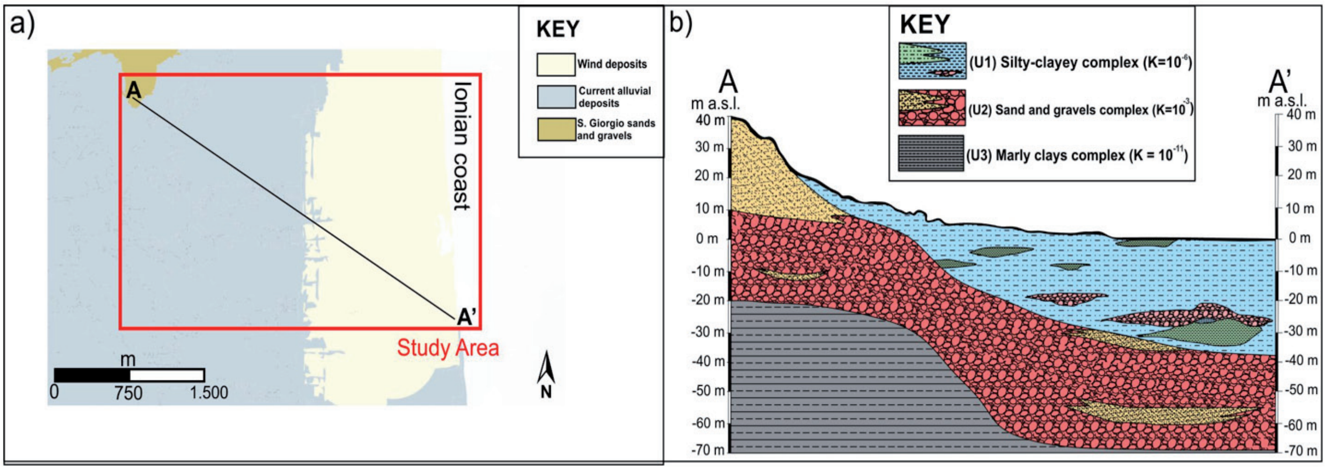

Fig. 1 - a) Geological map of the study area with trace of the hydrogeological section shown in inset b1.b; b) hydrogeological section of the studied aquifer. Hydraulic conductivities (K) are expressed in m/s

METHODOLOGICAL APPROACH AND MODEL SETTING

The methodological approach followed in this study is based on the collection of borehole and well data, used to define the geological and hydrogeological conceptual models, which represent the basis for the numerical simulation. The numerical flow and transport models were built in QGIS 2.18 environment through the FREEWAT 1.2.0 plug-in (Rossetto *et alii*, 2018), MODFLOW-2005 (Harbaugh Aw, 2005) and MT3DMS (Zheng & Wang, 1999) modelling codes. The active domain of the models is 800×580 m large, divided into 1,160 squared cells, each having a 20 m side. The aquifer system was divided into three layers (model depth 37 m), defined according to the hydrogeological conceptual model:

- model layer 1: 4 meters-thick silty clay level (hydraulic conductivity in the range of 10^{-6} to 10^{-5} m/s; this layer belongs to the U1 silty-clay complex);
- model layer 2: 3 meters-thick silty sandy layer (hydraulic conductivity around 10-4 m/s; this layer belongs to the U1 silty-sandy complex);
- model layer 3: it is the sandy-gravel aquifer (hydraulic conductivity of 10^{-3} m/s) with a surveyed thickness of about 30 m (U2).

In detail, model layer 1 and model layer 2 are overlapped and represent the same hydrogeological unit U1. Specifically, the first one represents the clay-silty part, with a lower hydraulic conductivity, while the sandy-silty model layer 2 has a higher conductivity. Below unit U1, the aquifer is represented by unit U2. The temporal discretization of the model was based on Stress Periods (SP), namely time intervals with constant boundary conditions and sink/source terms. Five SP were set to discretize a cumulative simulated period of 365 days. The first SP refers to a 1-day simulation, to observe the short-term flow behavior, while the remaining four SP were set to 91 days. A no flow condition was imposed to the cells along the northern and southern edges of the domain, while at the eastern and western edges the Constant Head (CHD) package was used to simulate head boundaries. Recharge to the water table was implemented by means of the Recharge (RCH) package, and it was kept constants for all the SP. Finally, we used the WEL package to simulate the presence of numerous wells in the area, which were randomly placed as both isolated wells and two well fields. These, referred to as WF1 and WF2, were placed about 1 km and 4 km away from the source of contamination, respectively. A pumping rate of 1,000 m^3/day was assigned to each well, in accordance with the local pumping rates. For the transport model, the same characteristics of the flow model layers were used. The USB (Unsaturated Solute Balance) package was used to simulate the dissolved low-density oil-like pollutant transport within the aquifer, with a constant pollutant concentration of 700 kg/m^3. The hydrodynamic parameters assigned to the three model layers, for both the flow and transport models, are summarized in Tables 1 and 2.

RESULTS

Flow model

The first scenario simulation (Fig. 2a) is aimed at showing the groundwater flow direction with no effects played by well pumping, and it is the result of one-day simulation (first SP). Results show that the groundwater flows towards the coastline, from west to east. The groundwater table lays between 6 m a.s.l. and the sea level to the west and east, respectively. In the second scenario (Fig. 2b), simulated with activated wells, the

Model Layer	Kx	Ky	Kz	SS	SY
1	0.0864	0.0864	0.00864	5e-05	0.15
2	8.64	8.64	0.864	8e-05	0.2
3	86.4	86.4	8.6	0.001	0.35

Tab. 1 - Hydraulic parameters of each layer used for the numerical simulation; Kx, Ky and Kz are the hydraulic conductivity values expressed in m/day; SS is the specific storage coefficient expressed in 1/m; SY is the specific yield (dimensionless). (Costa, 2008)

Model Layer	a_L	a_{TH}	a_{TV}	D_M	N_E
1	20	6	1	10^{-10}	0.15
2	20	6	1	10^{-10}	0.2
3	20	6	1	10^{-10}	0.35

Tab. 2 - Parameters used for the transport model. aL, is the longitudinal dispersivity (m); aTH and aTV are the ratio of the horizontal and vertical transverse dispersivity to the longitudinal dispersivity, respectively (dimensionless); DM is the molecular diffusion coefficient (m2/day); NE is the effective porosity (dimensionless) (APAT, 2008; Pickens & Grisak, 1981; Spitz & Moreno, 1996)

groundwater flow keeps a general trend due east, although it is influenced by the pumping. Isolated wells produce only local effects on the flow, while WFs produce a greater recall effect along with a local variation of the main outflow pathway. The water table is lowered, with a maximum rate of about 2 meters at WF1. At WF2, the groundwater level contours show that the water table lays slightly below the sea level. This suggests a possible seawater intrusion, which is a known phenomenon occurring in the study area. (Ferrara & Pappalardo, 2004; Ferrara *et alii*, 2007).

Transport model

For transport simulation, the contaminant release from a hypothesized underground tank, buried at about 2 m b.g.l. in the northwest part of the modeling area, was simulated with the same SPs (Fig. 3). In the no-pumping scenario, the contamination plume has a shape elongated towards ESE with a certain dispersion rate southward. After 365 days, the plume has traveled 4.6 km from the contamination source, and the lowest concentration near the coastline is around 0.5 kg/m^3. This suggests that the sea represents an element at risk for potential contamination arising from the study area. By considering the action of pumping wells, the plume trend keeps the same orientation, but a change in its velocity is outlined. In particular, after 92 days the plume reaches WF1 (Fig. 3a); after 183 days, the plume is approaching some individual wells located about 2 km eastward from the source (Fig. 3b). In these two cases, the plume progression towards the coastline is faster when pumping is considered. Nevertheless, at the end of the third SP (274 days from the spill beginning, Fig. 3c), the contamination levels of both the simulated scenarios almost overlap. This may be explained by a recall rate by WF1 wells, which delay the flow towards the coast. At the end of the 365 days simulation (Fig.3d), the plume approaches WF2, with a concentration of 0.5 kg/m^3, after having traveled about 4 km from the contamination source.

DISCUSSIONS AND CONCLUSIONS

The results of this study shed light on the groundwater trends through a porous medium in an industrialized area, and on the propagation of a hypothetical dissolved contamination plume over time. Pumping well activity proved influencing the direction of groundwater flow and the water table depth, according to the

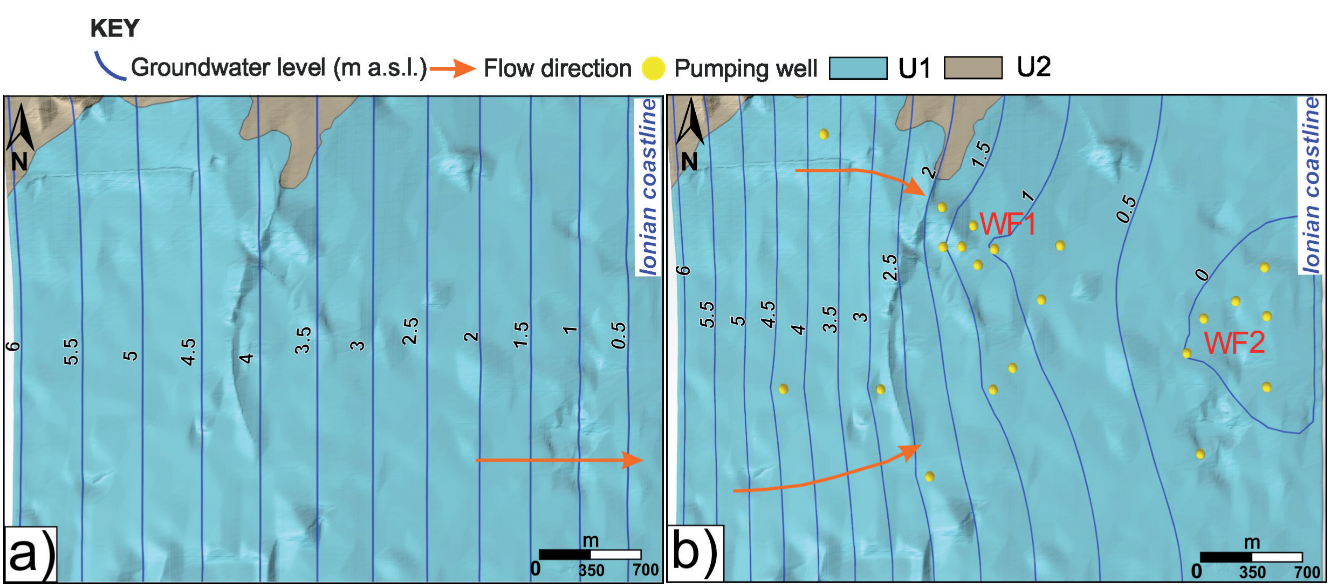

Fig. 2 - Results of the numerical simulations of the groundwater flow (one-day simulation, SP1) with no pumping action (a) and under pumping

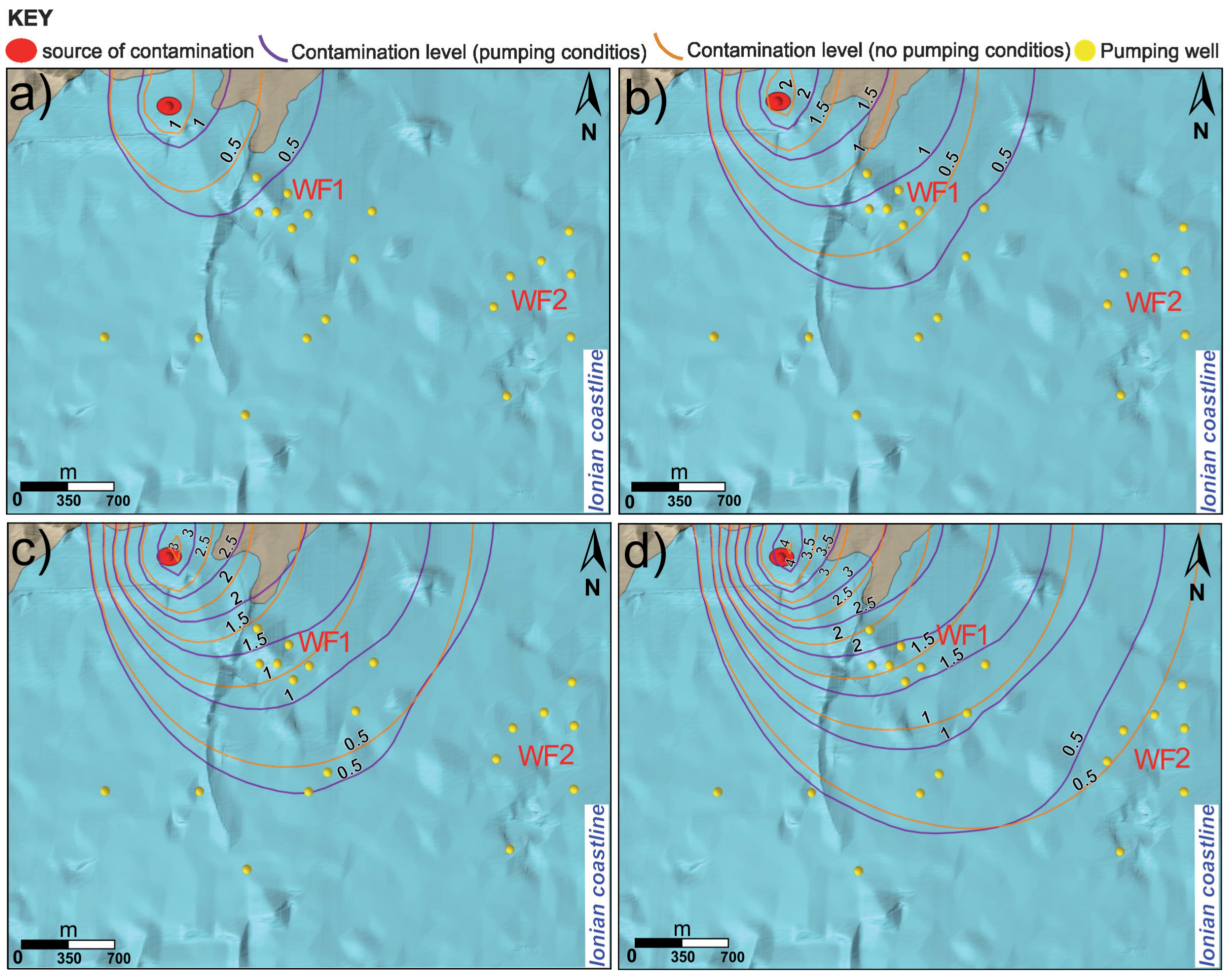

Fig. 3 - Results of the numerical simulations of contaminant transport after a) 91 days (SP2); b) 183 days (SP3); c) 274 days (SP4); d) 365 days (SP5)

literature knowledge (e.g. Barackman & Brusseau, 2002). The major effects were observed at the well fields, where the groundwater table is lowered of about 0.5-2 meters. The highest lowering rate was observed at WF1, whereas at the coastline (WF2) the fluctuation is less evident, although all the wells were simulated with the same pumping rate. Single wells, on the other hand, produce only local effects of capture (Fig. 2). The dissolved contamination transport model shows how the presence of a potential contaminant can travel considerable distances from the source, first of all because of the hydraulic characteristics of the aquifer (Fig. 3). In fact, it is shown that the contamination level approaches the coastline after 365 days from the spilling if no pumping is considered. In this case, the plume shape is quite uniform, and its direction matches with the groundwater flow trend. This behavior is justified by the assumed homogeneity of the modelled medium, which was set free of geological heterogeneities, such as lenses with different hydraulic conductivity. In facts, the presence of spatial heterogeneity is a common cause of uncertainty in hydrogeology and contamination modelling (e.g. De Marsily *et alii*, 2005; Zhang *et alii*, 2019a, 2019b; Mineo, 2023). When pumping is introduced in the simulation, some differences are outlined. It was observed that WF1 represents the main controlling transport element, being the capture zone closest to the contamination source, as well as an element at risk itself (Fig. 3). In fact, after 91 days of simulation, the dissolved contamination 0.5 kg/m^3 isocone reaches WF1, with an approximate rate of 10 m/day. By comparing this result with the corresponding scenario in no pumping conditions, the same distance is covered with a rate of about 6.5 m/day (Fig. 3a). Therefore, WF1 provides an acceleration to the upstream plume path. On the other hand, an inverse behavior was observed when the contamination goes beyond WF1. In fact, by considering the plume trend downstream the well field, a slowing action played by WF1 is suggested. After 365 days of simulation (Fig. 3d), the 0.5 kg/m^3 isocone approaches WF2 with a 6.7 m/day rate, which is lowered than its initial velocity. At the end of the simulation, the contaminant concentration is about 2 kg/m^3 near WF1 and 0.5 kg/m^3 near WF2. Besides being considered elements affecting the plume propagation, wells represent an element at risk for the environment and human health, which is a debated issue worldwide. In this frame, the results obtained from this study gain wide scientific relevance, since the numerical modelling proved a useful tool to understand the dynamics of an aquifer system, in accordance with literature (e.g. Velasco & Capilla, 2019; Vallejos *et alii*, 2020; Benyoussef *et alii*, 2021; Mineo, 2023). Moreover, the numerical simulation allowed establishing different evolution scenarios based on field data. While these are hypothetical herein, the approach used for this study can be applied to different cases and geological contexts worldwide. In fact, the approach allowed us to identify areas at risk of potential contamination (WF1 and WF2) and to focus attention on other issues, such as the possible seawater intrusion near shorelines. This establishes the basis for future studies applied to land use planning, groundwater exploitation, groundwater remediation strategies, and environmental risk prevention plans.

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