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Improved groundwater modeling by incorporating geological information from hydrogeological sections

Modellazione idraulica sotterranea migliorata tramite l'utilizzo di informazioni geologiche da sezioni idrogeologiche

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Riassunto

Le sezioni geologiche sono solitamente impiegate nella fase di concettualizzazione del modello idrogeologico, ma il loro utilizzo può non essere sfruttato appieno nelle successive fasi di modellazione. La distribuzione spaziale dei geomateriali (facies) lungo il tracciato di una sezione geologica può variare significativamente quando si utilizzano campi di facies casuali: questi ultimi potrebbero restituire distribuzioni di geomateriali fedeli alla concettualizzazione originale descritta dalla sezione geologica. Il presente lavoro offre una nuova metodologia per migliorare lo sviluppo di modelli numerici idrogeologici utilizzando le sezioni geologiche come una fonte quantitativa di informazioni. In particolare, la modifica nella distribuzione spaziale delle porosità viene trasferita dalla traccia della sezione ai punti circostanti del dominio attraverso un'opportuna procedura di *kriging* con una data scala di correlazione (R), che interpola le varianze delle porosità nello spazio con una struttura esponenziale. Questa procedura è testata utilizzando distribuzioni di porosità con diverse scale R, assegnando un valore di porosità a ciascuna facies, calcolando la relativa conducibilità idraulica associata a valori di porosità tramite formule empiriche, e informando diversi modelli numerici relativi a un caso studio reale (corpi acquiferi in provincia di Lecco, Nord Italia). La procedura proposta consente di migliorare significativamente la performance del precedente modello numerico calibrato. I risultati di questo studio mostrano che la scala R conveniente è compresa tra 2 e 5 chilometri, coerentemente con l'ampiezza della golena alluvionale e fluvio-glaciale che caratterizza in maniera più accurata l'acquifero in esame.

Abstract

Geological cross-sections are usually employed in the hydrogeological model conceptualization, but their usage may not be easily exploited in subsequent modeling phases. The spatial distribution of geological facies along a geological section's track may significantly vary when using random facies fields, and these may not be faithful to the original conceptualization described by the geological section. The present work offers a novel framework for improving available hydrogeological models using geological sections as a more quantitative source of information, hence by taking into account of information coming from a geological section. Then, this information given by the change in the distribution of porosities is transferred from the section's track to surrounding locations through a proper kriging procedure upon a chosen Correlation Scale (R), which is exponentially correlated in space. This procedure is tested by using porosity distributions upon several R, associating a conductivity value with each porosity one through empirical formulations, and informing several numerical models related to a real case study (an aquifer in the province of Lecco, Northern Italy). The proposed procedure enables to significantly outperform the former calibrated numerical model. Best-calibrated models show that the convenient R could be from 2 to 5 kilometers long, consistent with the width of the alluvial and fluvioglacial floodplain that characterizes the aquifer under examination.

Introduction

The sustainability of the groundwater resource passes from the comprehension of groundwater conceptual models and pathways. For this aim, understanding the hydrogeological setting of complex groundwater systems is as fundamental as a challenging task. From a stochastic viewpoint, several approaches can be adopted to employ suitable heterogeneous conductivity fields for modeling highly heterogeneous aquifer systems. To give some examples, Bianchi et al. (2015), in the way opened by Guadagnini et al. (2004), discussed two variogram-based methods to properly simulate (tri-dimensional) hydraulic conductivity fields (the Composite Medium and the Overlapping Continua approaches. Recently, Siena and Riva (2020) assessed the impact of different reconstructions of conductivity fields based on the MPS (Multiple Points Geostatistics) technique of Sequential Indicator Simulations (SISIM; see also Deutsch and Journel, 1997; Chiles and Delfiner, 2009) to estimate aquifers' connectivity metrics.

A very important issue in the proper modeling of (stochastic) geological facies, from which conductivity values can be inferred, is to faithfully adhere to the conceptual hydrogeological setup (if any) for the area under study. This means that, once one or more geological sections are available, the modeler should try to reproduce, even within a stochastic framework, a conductivity spatial distribution as similar as possible to geological section one, at least in the proximity of the section itself. This idea seems to be followed by one of the latest works in the field of facies reconstruction, proposed by Schorpp et al. (2022), where they proposed a framework to reconstruct facies boundaries and then to fill model layers with available facies units upon stratigraphic, geological and hydrogeological information sources. However, this approach requires (i) the prior knowledge of where facies boundaries are located for being interpolated throughout the whole domain, and this seems possible only along geological sections in the absence of further continuous data (e.g. ERTs techniques, Electrical resistivity tomography); (ii) it may lack in being faithful to the conceptual structure of the aquifer as well as informed by geological sections. Moreover, the idea of being more faithful to geological setups has been acknowledged by Jorreto-Zaguirre et al. (2020) when modeling a deltaic sedimentary domain.

The present work proposes to employ geological sections not only as qualitative but as more quantitative sources of information within a novel framework. Geological sections' information is employed to model bi-dimensional (estimated) porosity fields relying on facies data, on the way opened by Gueting et al. (2018). Conductivity fields to inform numerical models with are then deduced from porosity ones. This means that a porosity field can be informed by the geological section to adhere to its conceptual structure as much as possible. This task can be achieved by interpolating facies information through a proper kriging variogram-based procedure. This methodology is applied to a real case study area, located within the province of Lecco (Northern Lombardy, Italy), where a detailed geological section is available to test the present framework. The latter shows its effectiveness in significantly improving a previously calibrated heterogeneous numerical model.

Material and methods

Hydrogeological set-up and available data

The study area encompasses a fluvioglacial and alluvial plain within the province of Lecco (Northern Italy, see Figure 1 panel a) enclosed between river Lambro and Adda, tributaries of the Po River. The hydrogeological structure of the domain presents a surficial aquifer and a deeper one, which may locally be semi-confined and hence disconnected by the upper laying one. Large alluvial deposits can be assessed in the proximity of the river's riparian areas, especially for the Adda River, close to lakes in the Northern part of the domain, as well as in the Southern part of the domain (see Schiavo et al., 2022, and Schiavo, 2022, for further details). As in Schiavo et al. (2022), N=222 boreholes and wells are available for this study, providing valuable stratigraphic and geological information. Piezometers (12), all of those have filters located in both the phreatic and the confined aquifer, are used for calibrating the undifferentiated water table, and their locations on the map are highlighted by red diamonds. The analysis of stratigraphic information (see also Schiavo, 2023) allows for identifying a set of F = 5 main geomaterials, or facies, which constitute the geological setting of the aquifer system, identified as clay, sand, gravel, compact and fractured conglomerate, which volumetric fractions for all considered boreholes are reported in Figure 1, panel b. Each borehole is embedded with the type of facies having the highest volumetric ratio along the local aquifer system thickness, hence univocally characterizing the aquifer's local (overall) geological feature, as well as done in Schiavo (2022).

From geological facies to conductivity stochastic fields

Available boreholes are employed within a Sequential Indicator Simulations (SISIM) framework to obtain (conditional) stochastic fields of facies (Siena and Riva, 2020; Schiavo, 2023: see later Figure 2 for spatial structures' ranges). 2000 stochastic facies fields are simulated from the classification of facies illustrated in Figure 1, panel b. Thus, each i-th domain location is embedded by a value of F=1,5 upon the spatial modeling of facies correlation. The best-fitting indicator variogram model is achieved by a Maximum-Likelihood (ML) calibrated range (details not included), and Figure 1's panel c reports the description of employed boundary conditions in each numerical model run. Hydraulic conductivity (m/s) is assigned to each cell of the domain relying upon its local (total) porosity value, , evaluated by assigning literature-based values at each geomaterial (for details, Schiavo, 2023). The latter is evaluated through the Kozeny-Carman formulation (Kozeny, 1927; Carman, 1956) following the approach proposed by Riva et al. (2010) and later on by Schiavo (2023; details here not shown).

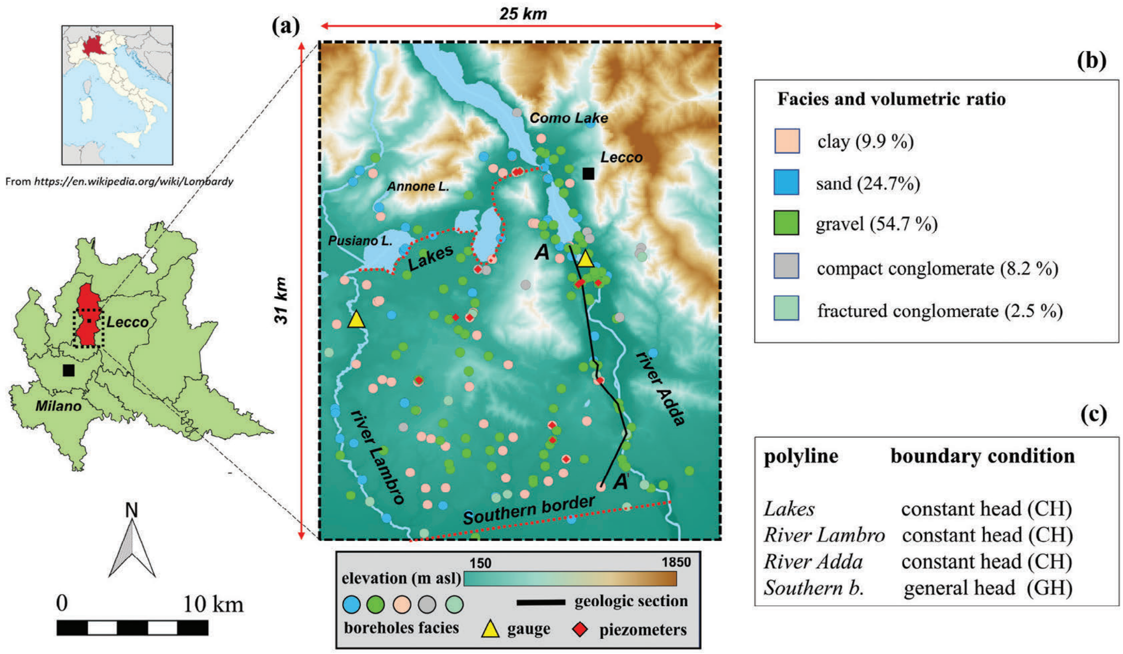

Fig. 1 - Sketch of the investigation domain and available data, (e.g. boreholes, piezometric head and geological section) (panel a). Geological facies volumetric ratios (b) and types of boundary conditions (c) are enclosed as well.

Fig. 1 - Rappresentazione del dominio e dei dati disponibili, ad esempio sondaggi, dati piezometrici, e relativi ad una sezione geologica (a). I rapporti volumetrici dei litotipi (b) e I tipi di condizioni al contorno (c) sono anch'essi forniti.

Affecting porosities upon geological sections' information

Geological facies are classified upon the classification offered in Figure 1 panel b, and an average porosity value taken from the literature (Freeze and Cherry, 1979) and coupled to each geomaterial as follows (as in Schiavo, 2023): clay=0.65, silty clay sand=0.45, gravel=0.35, rock/conglomerate=0.75, fractured rock/conglomerate=0.25. Let L be the total length of a geological section, discretized (as the inspection domain) in s=L/l cells of regular side l, each one identified by barycentric coordinates $\mathbf{x}_s=(x_s,y_s)$. Thus, facies $f_s=f(\mathbf{x}_s)$, with $f=1,\ F$ is assigned as prevalent in the s-th cell on the whole aquifer system thickness. The available geological section AA' is sketched in Figure 1, panel a, and is offered in detail in Figure 2 as well as each facies' range employed within the SISIM procedure, the latter highlighting the discretization of facies along the section's track.

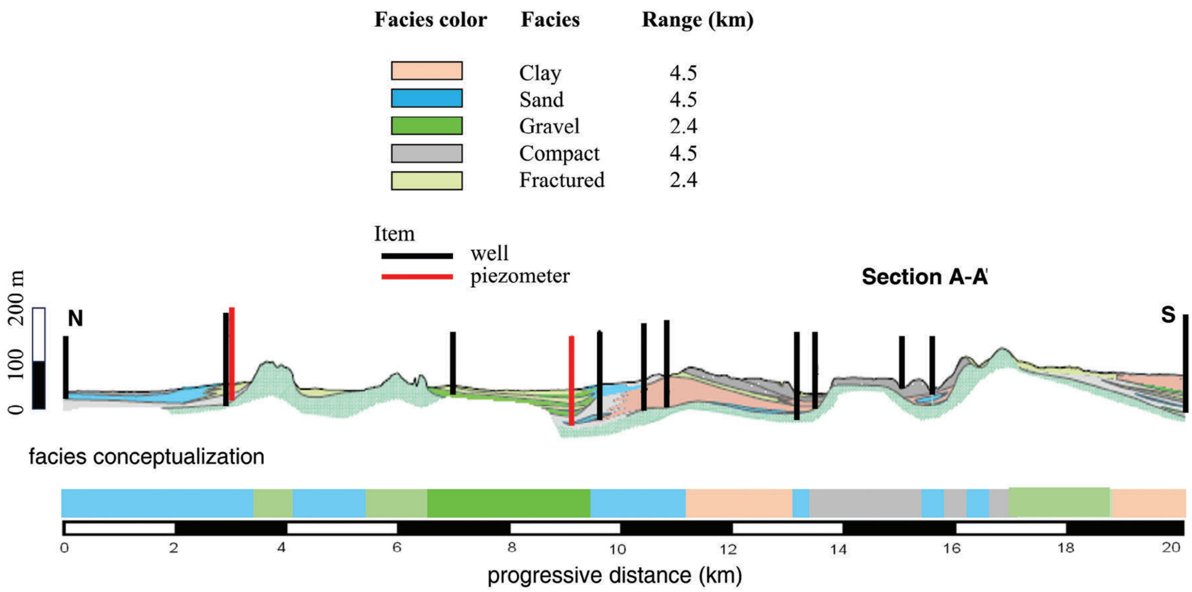

Fig. 2 - Geological Section AA' (see also Figure 1, panel a) and facies conceptualization.

Fig. 2 - Sezione geologica AA' (vedi anche Figura 1, pannello a) e concettualizzazione dei litotipi.

Spatial propagation of conductivity information

In general, local porosity values must be affected by the section's redistributed facies (hence porosities and later on conductivities) also outside of the geological section. In other words, the information of facies spatial organization, achieved along the section's track as described in previous paragraph, must be propagated in space to surrounding locations. Let now $\phi(x_i)= \phi_i$ be a generic conductivity cell i within the domain, available from a different (e.g. simulated) facies (hence conductivities) field, to be modified into a different ϕ'_i upon geological section proximity. Let be d={d} (m) a vector of distances between the i-th cell and those along the geological section. Moreover, let be R (m) a chosen Correlation Scale (R), expressing the correlation distance throughout the domain at which a generic i-th cell is influenced by the geological section's facies organization. This way, each vector's d entries may be of three types: (i) $d=0$ if the cell i is located along the geological section's track; (ii) $0<d<R$ if is located at a distance lower than the R from the section; (iii) $d\geq R$, if the distance is equal or longer than the R. For case (iii), the porosity value ϕ'_i remains equal to the original one, hence being $\phi'_i= \phi_i$, thus with the porosity embedding the cell i spatially not correlated to the geological section. For cases (i) and (ii), a mathematical function must be employed to model the spatial correlation between the cell i and the geological section.

Let ϕ'_i be a porosity value embedding cell i, located at a distance d from the section's furthest cell lower than the R. Therefore, ϕ'_i is conditioned upon d and r via an (isotropic) exponential variogram function:

$$\sigma^2_{i'-s}(d)= \sigma^2_{i'-s}[1\text{-exp}(-3d/R)] \qquad (1)$$

being $d=|x_i-x_z|$ the distance between two locations s and i, the former along the section and the latter a generic one; and $\sigma^2_{i'-z}(d)=\sigma^2_{i'-z}\ (\phi'_i- \phi_z)^2$ (m^2/s^2)the variance between the porosity values between locations s and i. The variance $\sigma^2_{i'-z}$ is the (spatial) variance between ϕ_i and ϕ_z. When $d=0$, $\sigma^2_{i'-s}= \sigma^2_{i-s}=0$ hence no difference exists between ϕ_i, ϕ'_i and ϕ_S values, and the porosity value "manually" evaluated at the geological section location is kept as it is, so $\phi'_i= \phi_S$. When $0<d<R$, if the distance between the i-th and the s-th locations is lower than a prescribed R, then the porosity value of the hydrogeological section rules above that of the preexistent simulated field being simulated as a function of distance d between the two locations. This is done through a simple kriging approach (Isaaks and Srivastava, 1989) via equation (1). In other words, as far as the distance d is within a certain R, then the kriged value of the local porosity inferred from the hydrogeological section, and this is done for each of the sites along the section. If $d>R$, the spatial influence of the geological section ends and the local porosity value is that of the preexistent simulated field, hence $\phi'_i= \phi_i$.

Results and Discussion

Performance analysis applied to a Groundwater Flow Model

The well-known code MODFLOW-2005 (Harbaugh, 2005) is employed to simulate steady-state groundwater flow within the domain. Aquifer's recharge is given by infiltration from average (uniform) annual precipitation rate, locally injected on the saturated water table. The latter is calculated upon a steady (calibrated) infiltration coefficient, taken as uniform throughout the domain because of the presence of sparse and limited urbanized areas (and previously calibrated within a preliminary model tun). Constant Head boundary conditions (CH, Figure 1 panels a and c) are set along the major rivers of the area (the Lambro and the Adda rivers, respectively), this choice relies on available stratigraphic and hydrogeological data and other studies (Cavallin et al., 1983; Fontana et al., 2014; Schiavo et al., 2022; and Schiavo, 2023a), showing that both two rivers are directly connected with the phreatic groundwater system. This peculiar condition can be interpreted as a one-directional drain directed from the aquifer to the system, not dependent on the river stage (hence CH is the most appropriate type of boundary condition). River water stages have been deduced upon mean annual water levels, available in one section for each river, and linearly interpolated along rivers' tracks parallel to the local depths of the riverbed, available in several cross-sections (about the riverbed and banks dimensions). Generalized Head boundary conditions (GH) are set along the Northern and Southern boundaries of the model according to previous hydrogeological studies available for the province of Lecco (Cavallin et al., 1983; Beretta et al., 1984). GHB local values have been obtained by interpolating available piezometric levels through an Ordinary Kriging (OK) procedure, without considering local variances of the (estimated) water table, and the same procedure has been applied to retrieve the aquifer bottom surface upon borehole data (details about the water table are not shown, butcan be found in Schiavo et al., 2022). The area simulated via numerical models is a portion of the whole domain, encompassed between the two CH and the two GH contours. Stochastic (bi-dimensional) facies fields inform numerical models. A collection of 2000 Monte Carlo (MC) stochastic facies realizations (from now on, fields) are available in each i-th domain location and are vertically extended for the whole thickness of the aquifer system.

The spatial influence of the geological section information

An example of porosity fields that can be obtained by porosity ones after being affected by the geological section as source of information is illustrated in Figure 3, where spatially-distributed porosity values obtained before (panels a-d) the redistribution procedure are offered. Porosity values, as the output of SISIM-based simulation of geomaterials (categorical variables), are depth-averaged across the whole aquifer depth.

The redistribution procedure is then applied to each stochastic porosity field, as well as to Figure 3' panels

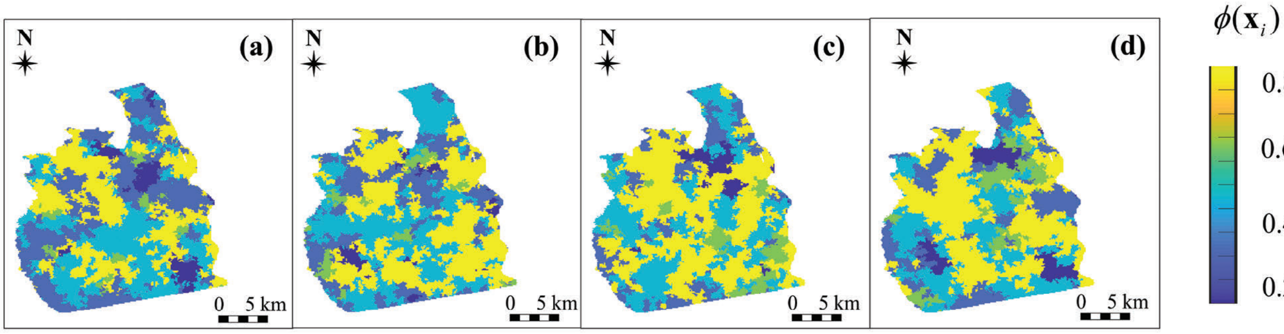

Fig. 3 - Exemplary porosity fields (panels a-d) are illustrated as original porosity fields from whose conductivity fields are retrieved.

Fig. 3 - Campi di porosità esemplificativi (pannelli a-d) originati da simulazioni geostatistiche, usati per ottenere i relativi campi di conducibilità idraulica.

a-d, to propagate the information due to the porosities along section AA' to surrounding locations. Considering Figure 3's panel a porosity field, modified porosity fields that can be obtained, are illustrated in Figure 4 panels' a-e upon different correlation lengths, i.e.R = 1, 2, 5, 10, and 15 km in panels a-e, respectively. The higher the R, the longer is the range of sensitivity of local (corrected) facies (hence conductivity) to the change along section AA'. Similar results can be obtained starting from any other simulated facies field. At the end, the procedure returns as the output of the redistributed procedure conductivity fields different both from the original ones, and from the raw kriged ones, rather than porosity fields whose local porosity values Φ_i are determined depending on the distance from each hydrogeological section's pixel. The following Figure 5 and panels therein illustrate the final porosity fields, to be employed in subsequent computations, after the redistribution procedure upon varying correlation scales, R. Porosity fields illustrated in Figure 5's panels have been obtained by applying the redistribution procedure to the MC-averaged porosity fields (i.e. the fields of porosities obtained as the local mean values across the whole ensamble of MC simulations), hence affecting the MC-averages porosities upon the porosity values appraised from the hydrogeological section (see Figure 2).

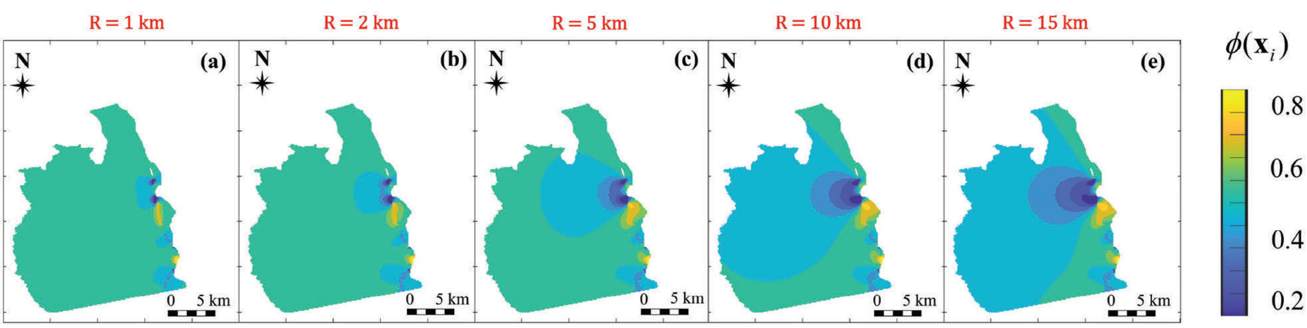

Fig. 4 - An example of porosity fields interpolated upon a simple kriging procedure for different correlation scales, R.

Fig. 4 - Esempio di campo di porosità interpolate tramite Simple Kriging per diverse scale di correlazione R.

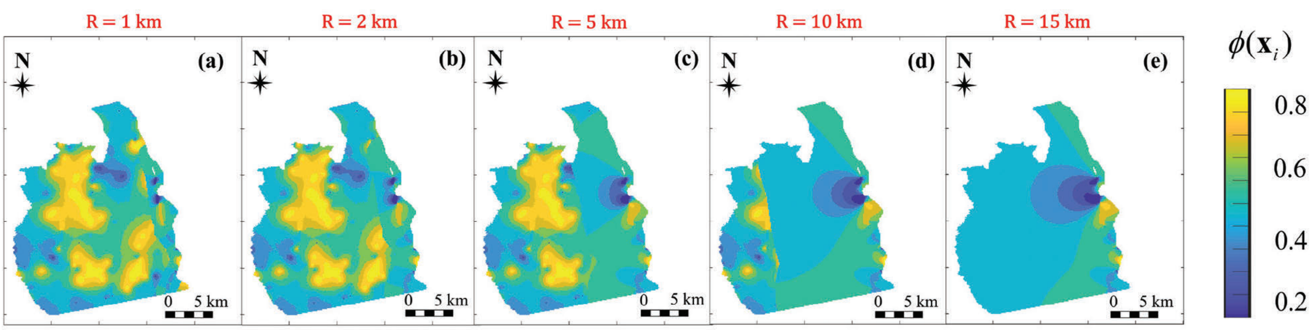

Fig. 5 - Final porosity fields at the end of the redistribution procedure upon varying correlation scales of R=1, 2, 5, 10, and 15 km (panels a, b, c, d, and e, respectively).

Fig. 5 - Campo definitivo di porosità al termine della procedura di redistribuzione tramite diverse scale di correlazione: R=1, 2, 5, 10, e 15 km (pannelli a-e).

The performance of affecting conductivity fields via geological section information on a calibrated Groundwater Flow Model

Each employed R is applied within equation (1) to inform a pre-existent (stochastic) spatial field of conductivities. Each modified spatial field of conductivities, as those illustrated in Figure 5 and its panels, is employed within a MODFLOW groundwater model. As an example of the results that can be achieved, the calibrated piezometric level by using the stochastic field of conductivities illustrated in Figure 5 panel a is offered in the following Figure 6's panels. The original model (i.e. the model with not redistributed porosities, hence conductivities) is informed by conducitivity values obtained by MC_average porosity fields (see Figure 3's panels). While panel a represents the model run for the original conductivity field (i.e. not redistributed upon the procedure) deduced from one simulated porosity field (from SISIM, as in Schiavo, 2023), panels from b to f illustrates the same conductivity field affected for R of 1, 2, 5, 10, and 15 km.

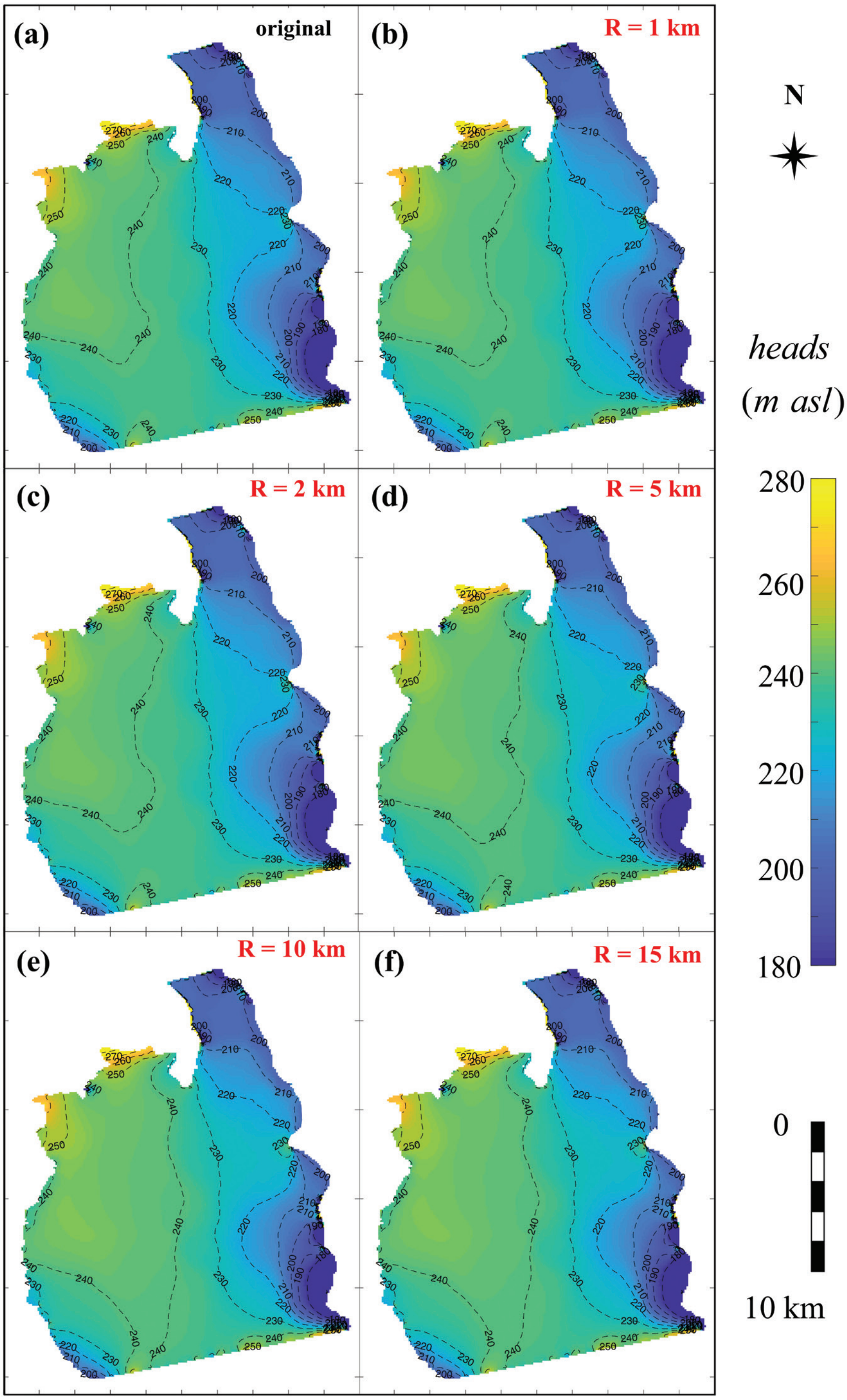

Fig. 6 - Piezometric levels for the domain of investigation simulated upon different conductivity fields.

Fig. 6 - Livelli piezometrici per il dominio studiato simulate in ambiente MODFLOW 2005 per differenti campi di conducibilità idraulica.

Water table levels show clear variations between panels a (uncorrected case), b, c, and d (R of 1, 2 and 5 km, respectively) and panels e and f (R of 10 and 15 km, respectively). The water levels tend to increase at the increase of the employed R, as highlighted by level contoursand their westward shift for large correlation scales. However, most of the calibration piezometers are located within the alluvial valley on the righter side of the river Adda, and therefore the following Table 1 is needed for a deeper inspect the impact of the R on models results.

Table 1's left column reports the employed R, and the righter ones the statistical indices. The Sum of Square Residuals (SSR) is evaluated upon calibration piezometers residuals. The lowest SSR are those for R of 2 and 5 km, while R=10, 15 km returns the highest values of SSR. Moreover, the ratio between each SSR, depending on a different correlation scale, and the original value appraised for the uncorrected model reveals the percentage change of SSR: the highest (positive) value of SSR/SSR0 is that for R=5km. Furthermore, the lowest value of Mean Absolute Error (MAE) in piezometric (simulated) heads is achieved by using a 5-km-R, which also returns the highest value of Nash-Sutcliffe Index of Efficiency evaluated between observed and simulated piezometers heads. After all, the best choice for R is a 5-km-R, although good results also seem achievable with 2 < R < 5 km. Moreover, there is a clear difference when employing a certain range of Correlation Scales.

Tab. 1 - Numerical models' statistics, divided upon different employed Correlation Scales, R. Table 1 reports, for each model run, the Sum of Residuals (SSR); the ratio between SSR of the original model and further runs; the Mean Absolute Error (MAE) between simulated and observed heads; the Root Mean Square Error (RMSE) and the efficiency index of Nash-Sutcliffe (NSE).

Tab. 1 - Statistiche dei modelli numerici, divisi per diverse scale di correlazione R. La tabella 1 riporta, per ogni simulazione, la somma dei residui (SSR); il rapporto tra SSR del modello originale e per le simulazioni successive; l'errore medio assoluto (MAE) tra livelli piezometrici osservati e simulati; l'errore quadratico medio (RMSE) e l'indice di efficienza di Nash-Sutcliffe (NSE).

model	SSR (m^2)	SSR ratio	MAE (m)	RMSE (m)	NSE (-)
original	237.8	-	3.9	4.45	0.90
R=1 km	233.9	1.6	3.8	4.41	0.93
R=2 km	218.8	8.0	3.7	4.27	0.93
R=5 km	186.9	21.4	3.1	3.95	0.94
R=10 km	477.4	-100.8	5.5	6.31	0.84
R=15 km	480.0	-101.0	5.5	6.31	0.84

A short correlation scale (e.g. R=1 km), returns numerical models' results that are not different from the original case (Figure 5 panel a). Long correlation scales seem to significantly alter the simulated water table, giving results far from (and worse than) the original (calibrated) model. Thus, for the present application, an improvement of the groundwater model efficiency can be achieved if a R between 2 and 5 km is employed. The choice of R=5km, for example, let the original (calibrated) model be further improved by a reduction of 21% of the original SSR (see the SSR ratio column), and a reduction of MAE of about 20%, with an improved NSE efficiency of 0.94. Results of the same kind, i.e. indicating that R between 2 and 5 km can effectively improve calibrated models, can be obtained for other employed porosity (hence conductivity) fields.

Hydrogeological consistency of employed Correlation Scales

The optimal choice of a R between 2 and 5 km is not casual in the present application but retains a precise hydrogeological signature. The latter can be appraised at least by considering two issues. The first one is given by the best-fitted ranges for isotropic variograms simulating facies (see Schiavo, 2023). As one can appraise, all the modeled facies ranges are within the 2-5 km interval, suggesting that this range for employing a R is a proper choice to capture the spatial patterns of facies distribution, hence, to propagate geological information upon their use to surrounding locations. The second issue to sustain this choice for R is the spatial width of the alluvial aquifer on the river Adda's righter side. The latter can be (semi-quantitatively) appraised by several cross sections performed across a geological chart (see Data Source Section for details), available for the province of Lecco, to locally estimate the range of alluvial and fluvioglacial sediments fan. The alluvial fan widths with the highest empirical probability density are those between 2.5 and 3 km, being calculated for one side of the river Adda alluvial valley (see the following Figure 7, panel a), which is within half of the R's range of 2-5 km (Figure 7, panel b) indicated as the most suitable to improve the original groundwater model.

R longer than 5km, such as 10 and 15 km employed ones, seem to perform worse than the original calibrated model, hence their usage seems not appropriate, at least for the present numerical application. This consideration might lead toward asking if a prior measure of the average width of alluvial sediments fan could directly inform the propagation procedure here proposed. This proposal seems reasonable, at least for the hydrogeological setting of the present study area, because the spatial distribution of sediments inferred from a geological section is likely to be within the same geological environment, i.e. within the same alluvial and fluvioglacial area. In this sense, more investigations are needed for different case studies, but the present work proposes novel and interesting tools to improve the hydrogeological modeling of complex aquifer systems.

Conclusions

Hydrogeological (calibrated) models, which employ stochastic conductivity fields, can be further improved by a more faithful mimic of the spatial distributions of geomaterials along geological sections. The spatial distribution inferred from the geological section must be adapted propagated through a proper correlation distance. The latter as a key factor of the redistributed conductivity field has been revealed to be potentially highly impacting on further model calibration. The proper correlation scale interprets the hydrogeological nature of the aquifer system under investigation since has a

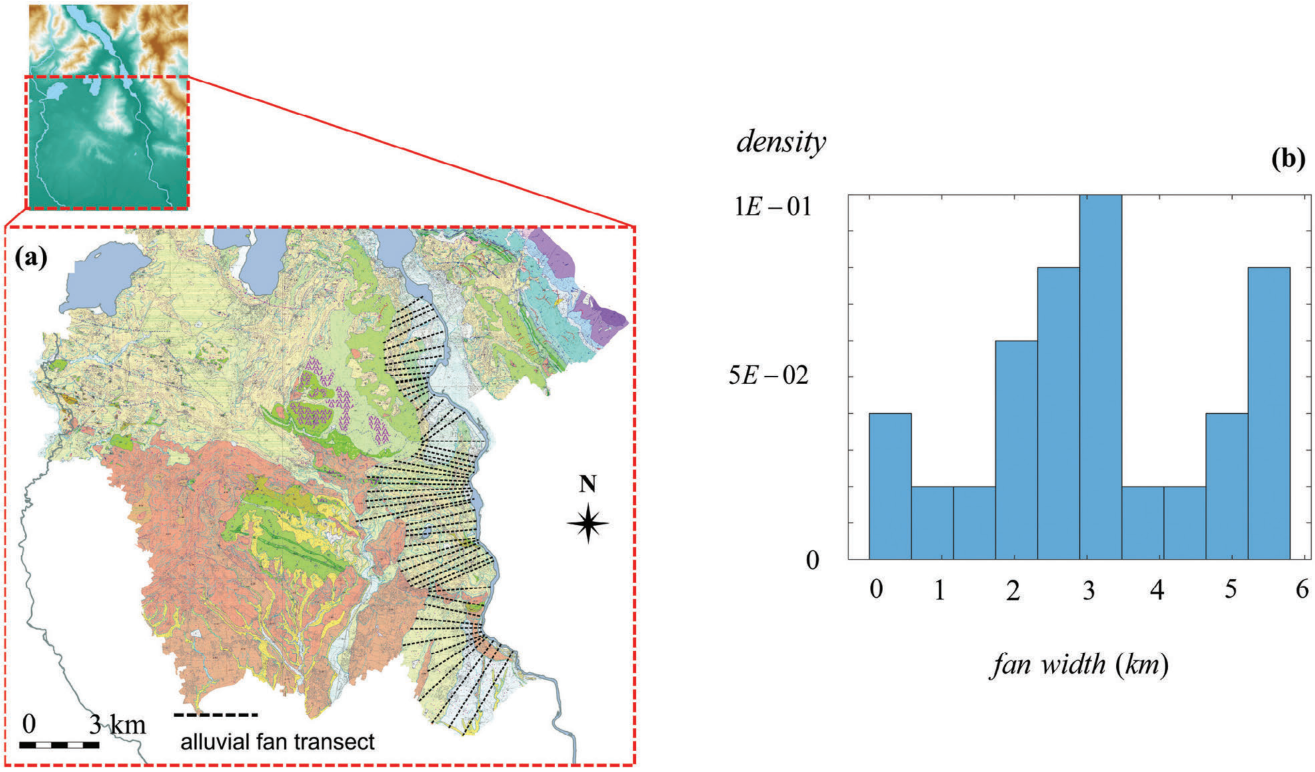

Fig. 7 - Transects across the river Adda alluvial valley (panel a), depicted via geological chart, can inform about the probable width of alluvial (greenly yellow) and fluvioglacial (light blue) sediments (panel b).

Fig. 7 - Transetto lungo la valle alluvionale del fiume Adda (pannello a), rappresentata tramite carta geologica, avvisa riguardo la probabile ampiezza dei sedimenti alluvionali (in giallo-verde chiaro) e fluvio-glaciali (in azzurro, pannello b).

value comparable (i) to that of the range employed to simulate geological facies, and (ii) consistent with the most frequent width of the alluvial sediments fan, where the geological information is propagated. The employment of correlation scales between 2 and 5 km has improved the performance of simulated heads, leading toward a lower SSR and a higher NSE index. Conversely, a very long R (i.e. 10-15 km) seems to be not recommendable, since the numerical models' statistics appraised by employing this kind of conductivity fields are worse than both the uncorrected models, and those obtained by using shorter R. A R of 5 km seems the best choice for the domain under investigation because of its hydrogeological consistency with other kinds of data.

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Data sources

All data used within the present work can be found in the Lombardy Regional repository (https://www.geoportale.regione.lombardia.it/) or in the ARPA Lombardia one (https://www.arpalombardia.it/Pages/ARPA_Home_Page.aspx) upon request.

Competing interest

All authors, the corresponding author states that there is no conflict of interest.

Author contributions

Massimiliano Schiavo: conceptualization, Methodology, Formal analysis, Investigation, Data curation, Writing, Visualization, Supervision. The author has read and agreed to the final version of the manuscript.

Additional information

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