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Modeling water flow and solute transport in alluvial sediments: scaling and hydrostratigraphy from the hydrological point of view

Modellazione del flusso idrico e del trasporto di soluti in sedimenti alluvionali: i passaggi di scala e l'idrostratigrafia dal punto di vista idrologico

GIUDICI M. (*)

ABSTRACT - The sustainable management and the protection and remediation of water resources often require that geoscientists study ground water flow and solute transport in alluvial aquifers. Modeling approaches differ according to the scales relevant for the specific practical problems and also the geological structures can be described with different approaches. The scales of interest can be identified with the horizontal and vertical domain lengths and resolutions. The scale lengths span a wide range from the dimension of water molecules to the typical size of sedimentary basins. Therefore the study of ground water flow and solute transport in alluvial sediments requires many different exploration and interpretation methods, including geochemistry, petrography, sedimentology, stratigraphy, geophysical prospecting, in order to map geological structures and to describe geological and physical processes at different scales. In this paper it is proposed a revised classification of the relevant scales, discussing the corresponding physical processes, flow and transport models, geological objects, investigation methods. In fact a proper characterization of alluvial sediments might help to correctly setup flow and transport numerical models.

KEY WORDS: alluvium aquifers, ground water, hydrology, mathematical models, prospecting, water resources.

RIASSUNTO - La gestione sostenibile, la protezione e la bonifica delle risorse idriche richiedono spesso lo studio del flusso idrico sotterraneo e del trasporto di soluti negli acquiferi alluvionali. Gli approcci modellistici si distinguono in base alle scale a cui vanno sviluppati per risolvere i problemi concreti e anche le strutture geologiche possono essere descritte con diversi approcci. Le scale di interesse possono essere identificate con le lunghezze caratteristiche dei domini e con le risoluzioni, che in generale sono diverse lungo le direzioni orizzontali e verticali. Queste scale coprono un ampio intervallo di dimensioni, da quelle delle molecole d'acqua a quelle dei bacini sedimentari. Pertanto lo studio del flusso idrico sotterraneo e del trasporto di soluti nei sedimenti alluvionali richiede l'applicazione di molte e diverse tecniche di esplorazione e interpretazione, tra le quali la geochimica, la petrografia, la sedimentologia, la stratigrafia, la geofisica applicata. In questo modo è possibile identificare le strutture geologiche e descrivere i processi geologici e fisici a diverse scale. In questo lavoro viene presentata una classificazione delle scale rilevanti, per le quali vengono discussi i principali processi fisici, i tipi di modelli di flusso e trasporto, gli oggetti geologici e le principali tecniche di indagine. Una caratterizzazione appropriata dei sedimenti alluvionali può aiutare a impostare in modo corretto i modelli numerici di flusso e trasporto.

PAROLE CHIAVE: acqua sotterranea, falda in alluvioni, idrologia, modelli matematici, prospezione, risorse idriche.

1. – INTRODUCTION

The sustainable management and the protection and remediation of water resources require decision support tools whose basic engines are numerical models of water flow and solute transport. In order to face practical problems, the development and application of numerical models should take into account the goals of the models, i.e. the actual problems to be solved, the relevant processes and the corresponding space and time scales (GIUDICI, 2001).

^(*) Università degli Studi di Milano, Dipartimento di Scienze della Terra "A. Desio", Sezione di Geofisica, via Cicognara 7, 20129 Milano, Mauro.Giudici@unimi.it

It is questionable to apply the same conceptual and mathematical model to compute water balance for ground water management policies at the basin scale and to study flow and transport at the local scale, e.g. for assessing the environmental impact of a landfill or for the remediation of a contaminated site. Different models should be used and different parameterisations of the geometry and of the heterogeneity of the subsurface are required: as a consequence, modelers need different types and details of geological information for different purposes.

The aim of this paper is to discuss the relationship between the geological information (hydrostratigraphy and aquifer sedimentology) and the ground water flow and solute transport models at different scales in alluvial aquifers. These sedimentological systems are considered in this paper because they host a lot of fresh water bodies exploited for drinkable purposes both in Italy and worldwide.

In the second section a brief review of scaling problems in modeling is given: it includes an improved characterization of the scales relevant for practical problems.

The classification scheme proposed in this paper is a revision of those proposed by HEINZ & EIGNER (2003) and by FALIVENE *et alii* (2007), whose work is mainly based on hierarchical dynamic stratigraphy; here the classification starts from hydrological aspects. In the third section the link between the hydrostratigraphic and the modeling approach to scaling is discussed.

In the last section some conclusive remarks are given.

All these topics are examined with examples taken from case studies of the Pleistocene sediments in the Po plain.

2. – THE SCALES AT WHICH GROUND WATER FLOW AND SOLUTE TRANSPORT ARE MODELLED

The goal of this section is to show how scaling issues arise from hydrological study to answer to practical questions related to the management and protection of water resources.

For instance, one of the questions that water management agencies, regional governments and local administrations pose to professionals is: which is the sustainable amount of water that can be extracted from an aquifer? In general this query is debatable (SOPHOCLEOUS, 1997; BEAR, 1979; ALLEY & LEAKE, 2004; SOPHOCLEOUS, 2005), but any tentative answer needs the identification of the terms of the water balance at the scale of an hydrographic basin. Therefore the study area could be larger than thousands of square kilometres and the typical horizontal length of the domain, H, could be greater than 10 km. At this scale hydrologists deal with the large scale aquifer structures down to depths of few hundred meters (V>100 m). Since the ratio H/V is very large and therefore vertical components of flow can be often neglected, the ground water flow is usually modeled with a 2D or quasi-3D approach. The relevant horizontal and vertical resolution lengths (h and v, respectively), i.e., the spacing of the grid used for numerical models, are h > 100 m, $\nu \approx 100$ m. At this scale the modelers consider the main aquifer groups, which are the result of the basin fill. In some cases it is necessary to map the horizontal and vertical continuity of the alternation of aquifers and aquitards produced by the climatic control on fluvio-glacial dynamics and deposition, in order to identify the capture zones of deep wells and to assess the degree of protection of deep water resources.

Of course these basin-scale models introduce strong simplifications of the geological complexity and some drastic approximations of processes occurring at finer scales. For instance the quantification of exchanges between ground and surface water bodies requires a finer resolution. This is also the case for models aimed at studying flow and transport in areas of limited extension, e.g. for the risk analysis of a contaminated site or the environmental impact assessment of a landfill. In these cases 100 m<H<1 km, 10 m<V<100 m, 1 m < b < 10 m, 0.1 m < v < 1 m and the vertical components of flow and transport cannot be neglected. Therefore, at this local scale, 3D flow and transport models require the distribution of permeable and poorly conductive sediments, in order to capture the effects of preferential flow paths or impermeable barriers. The heterogeneity at the local scale is controlled by the facies bodies created by the dynamics of the environmental system.

The hydrodynamic and hydrodispersive para-meters at the local scale depend upon the heterogeneity of the depositional elements and of the lithological strata for which the classical concept of representative elementary volume can be defined. Finer scales (the microscopic – pores and grains – scale and the molecular scale) are important for transport phenomena, because they are the proper scales at which hydrogeochemical processes take place. Notice that at these scales the horizontal and vertical resolution length can be identified with the size of the measurement support (CUSHMAN, 1986), i.e. the length over which physical quantities are averaged and assumed representative.

The synthetic description given above can be summarized in table 1, where a tentative ranking of scales is given. This is a refinement of the schemes originally proposed by HEINZ & EIGNER (2003) and by FALIVENE et alii (2007); the classifications proposed by these Authors were mainly based on the concept of hierarchical dynamic stratigraphy, whereas here the classification is mainly based on hydrological aspects, but the link between the two approaches is apparent in the sequel of this paper. Simplified schemes of scale classification have also been proposed, e.g., by DAGAN (1989), LUNATI et alii (2001), GIUDICI et alii (2007). The distinction between regional and local flow is given also in several textbooks, e.g., BEAR (1979) and FREEZE & CHERRY (1979).

3. – THE LINK BETWEEN HYDROSTRA-TIGRAPHY AND MODELLING OF FLOW AND TRANSPORT AT DIFFERENT SCALES

The different scales, at which flow and transport in alluvial sediments are studied, are now examined in more detail, with reference to the relevant physical quantities and processes. Moreover, the analytical methods, the sedimentary structures and the hydrological processes that are relevant at the different scales are listed.

It is important to stress that the classification

proposed here, like any classification scheme, could appear too rigid in specific cases. In fact there is no natural sharp distinction between different scales; in real world applications, professionals deal with a mixture of scales. However a classification scheme can be useful to fix ideas and concepts, to properly plan the investigation work and to identify the conceptual model.

3.1. - MOLECULAR SCALE

The finest scale at which a porous medium can be studied is the molecular scale ($h \cong v \cong 10^{-10}$ m). At this scale the relevant interactions are molecular forces, acting among the molecules constituting the fluid (liquid or gas) and the solid phases.

3.2. – Microscopic scale

At the characteristic scale considered in classical fluid dynamics, the relevant physical quantities (velocity, density, fluid pressure, solid stress, temperature, etc.) are averages of the physical quantities at the molecular scale over statistically significant volumes, that include a large number of molecules, but are nevertheless so small as to provide a point value. We refer to this scale as the microscopic scale (pore-grain scale, $10^{-5} \text{ m} \le h \cong v \le 10^{-3} \text{ m}$). The interactions between the pore fluid (water and solutes) and the porous matrix at this scale might be important to characterize some transport phe-

Scale	Scale length		Resolution			
	Horizontal	Vertical	Horizontal	Vertical	Objects	Hydrological models
Terascopic	10 ⁴ m	$10^2 \mathrm{m}$ to $10^3 \mathrm{m}$	$10^{2} \text{ m to} \\ 10^{3} \text{ m}$	$10 \text{ m to} \\ 10^2 \text{ m}$	Basins	2D or quasi-3D models
Gigascopic	$10^{3} \text{ m to} \\ 10^{4} \text{ m}$	$\begin{array}{c} 10 \text{ m to} \\ 10^2 \text{ m} \end{array}$	$10 \text{ m to} \\ 10^2 \text{ m}$	1 m to 10 m	Aquifer complexes	Quasi-3D models
Megascopic	10 m to 10 ³ m	$10 \text{ m to} \\ 10^2 \text{ m}$	1 m to 10 m	0.1 m to 10 m	Facies bodies	3D models
Macroscopic	1 m to 10 ² m	1 m to 10 ² m	10 ⁻² m to 1 m	10 ⁻² m to 1 m	Depositional elements	3D models
Mesoscopic			10 ⁻³ m to 10 ⁻¹ m	10 ⁻³ m to 10 ⁻¹ m	Strata, hydrofacies	Phenomenological (Darcy, Fick, Fourier) laws
Microscopic			10 ⁻⁵ m to 10 ⁻³ m	10 ⁻⁵ m to 10 ⁻³ m	Pores and grains	Classical continuum physics
Molecular			10 ⁻¹⁰ m	10 ⁻¹⁰ m	H ₂ O molecule, clay particles, minerals	

Tab. 1 - *Scale lengths at which ground water flow can be studied.* - Lunghezze di scala a cui può essere studiato il flusso idrico sotterraneo.

nomena (e.g., adsorption/desorption).

The characteristics of the porous medium at the microscopic scale are studied mainly with geochemistry and petrographical analyses. In particular the sediments petrography provides information on the grain minerals and therefore on the provenance and the origin of the sediments.

3.3. - Mesoscopic scale

A further step yields to the mesoscopic scale, the scale at which the representative elementary volume is defined $(10^{-3} \text{ m} \le h \ge v \le 10^{-1} \text{ m})$. At this scale the physical quantities (porosity, Darcy's velocity, solute concentration, volumetric water content, etc.) are representative of the physics of the porous medium, in the sense that they take into account the presence of several phases (gas, liquid, and solid phases) and possibly several constituents within each phase. This is the scale relevant for soil physics and for studies related to unsaturated flow and transport: this is the scale at which phenomenological laws (among which Darcy's, Fick's, Fourier's laws) are introduced and experimentally validated. The methods of investigation include laboratory experiments on samples and field tests involving small volumes.

The geological structures which are relevant at this scale are strata characterized by homogeneous features in terms of sedimentary properties (grainsize distribution, texture, fabric). These lithofacies are then differentiated according to sedimentary properties, which affect the hydrodynamic properties, namely the hydraulic conductivity. As a consequence, at this scale lithofacies can be grouped in hydrofacies, i.e. hydrogeological units which are relatively homogeneous, but possibly anisotropic (if the grains have an ellipsoidic shape or are deposited along preferential directions) with respect to the hydraulic conductivity. The sedimentological analysis of samples and of the outcropping sediments is one of the principal geological means of investigation at this scale.

3.4. – Macroscopic scale

The visual inspection of outcrops clearly shows that lithofacies types, and therefore hydrofacies, are organized in sedimentary bodies at a macroscopic scale characterised by $10^{-1} \text{ m} \le V < 10 \text{ m}$ and

 $1 \text{ m} \le H < 100 \text{ m}$. For sediments belonging to an alluvial depositional system, the individual architectural elements include channels, levees, floodplains, etc. The present day geometry of the depositional elements is the effect of their formation and evolution and determines the distribution

of the hydraulic conductivity, the correlation length and the connectivity of permeable units (see KNUDBY & CARRERA, 2005, and VASSENA et alii, 2009, for definitions and further references). The heterogeneity at mesoscale determines the effective hydrodynamic and hydrodispersive properties at the macroscopic scale. Moreover, the presence and the connectivity of permeable bodies introduces preferential flow paths, which are very important also for the fate of contaminant transport. This can be analysed with techniques of geostatistical simulation and three dimensional numerical modelling of flow and convective (possibly reactive) transport. In fact the link between meso- and macroscopic scales is sometimes performed with studies on aquifer analogues, i.e., outcropping sediments which are representative of the burden water reservoirs (see, e.g., JUSSEL et alii, 1994; RITZI et alii, 1995; WITTAKER & TEUTSCH, 1996; HUGGENBERGER & AIGNER, 1999; BERSEZIO et alii, 1999; ANDERSON et alii, 1999; ZAPPA et alii, 2006). The study at this scale is conducted not only with sedimentological analysis of samples and outcropping sediments, but also with geophysical exploration methods (e.g. ground penetrating radar) and with hydraulic field and laboratory tests (e.g., infiltration or permeametric tests).

The heterogeneous conductivity field, which is mapped at the macroscopic scale on the basis of the hydrofacies distribution, is upscaled to find equivalent parameters of the porous medium at the macro- or megascopic scale. Thorough reviews on upscaling are given by WEN & GÓMEZ-HERNÁNDEZ (1996), RENARD & MARSILY (1997), CUSHMAN *et alii* (2002), SÁNCHEZ-VILA *et alii* (2006).

The transition from the molecular scale to the microscopic and mesoscopic scales requires new physical quantities and physical laws (from molecular interactions to basic equations of fluid dynamics to Darcy's law). On the other hand, the upscaling from the meso- to the macroscale or to even larger scales (see section 3.5 below) is often performed in such a way that the same equations are applied, but the values of the physical parameters change. The geometrical regularity of the structures at the fine scales often yields anisotropy of the equivalent parameters at the coarser scales.

Also the meaning of some physical parameters is modified during the change of scale. For instance, the transport at the macroscopic scale is often modeled as purely convective and the irregularities of the flow field within pores are neglected or accounted for with small dispersivities. The transport at coarser scales is modeled with advective/dispersive equations which include the effects of the heterogeneity of the flow field related to the heterogeneity of the conductivity field at the macroscopic scale by means of the tensor of hy-

drodynamic dispersion. Examples of upscaling flow parameters from the meso- to the macroscopic or coarser scales in alluvial sediments of the Po plain are given by BERSEZIO et alii (1999), FELLETTI et alii (2006) and ZAPPA et alii (2006). The equivalent conductivity tensors have been computed from the distribution of the hydraulic conductivity at the mesoscopic scale. GIUDICI & VASSENA (2007) show that the method applied for this upscaling guarantees the symmetry of the equivalent conductivity tensor; furthermore VASSENA & GIUDICI (2007) show some effects of the discretisation on the computed equivalent conductivity tensor. In a recent work VASSENA et alii (2010) perform some numerical experiments of conservative transport on the blocks of sediments previously analyzed by ZAPPA et alii (2006) and they relate the hydrodispersive parameters to different types of connectivity indicators, namely: (1) the connectivity function (ALLARD & HERESIM GROUP, 1993; ALLARD, 1994; WESTERN et alii, 2001); (2) flow, transport and statistical connectivity indicators (KNUDBY & CARRERA, 2005); (3) original (intrinsic, normal and total) indicators of facies connectivity. VASSENA et alii (2010) show that some of these transport and statistical connectivity indicators are correlated with dispersivity and the joint analysis of the three indicators of facies connectivity permits to emphasize the fundamental geometrical features that control transport.

3.5. – Megascopic scale

Local field problems $(1 \le h \le 10 \le 0.1 \le v \le 1 \le n)$, $10 \le H \le 10^3 \le n$, $10 \le V \le 10^2 \le n)$ can be studied at the megascopic scale. This is the scale at which pumping tests are usually performed and analysed; it is also the typical scale at which 3D models of flow and transport are developed and applied for the characterization and remediation of contaminated sites or for environmental impact assessment during the design of landfills, buildings, dams, bridges, mines, etc.

From the sedimentological point of view at this scale the assemblage of depositional elements builds facies bodies and produces compartments within alluvial sediments. In fact, facies bodies can be characterised as permeable aquifer or less permeable aquitard structures, which influence both local and regional ground water flow and transport. Field tests are among the main investigation techniques at this scale, together with well log data. They are integrated with geophysical techniques, as DC electrical methods, electromagnetic methods (mainly in the frequency domain), refraction seismics or studies with surface waves.

Again upscaling studies are often conducted at this scale and are devoted, e.g., to the comprehension of the effect of connected permeable aquifer bodies on the results of well pumping tests and on the contaminant transport (FOGG, 1986; SCHAD & TEUTSCH, 1994; MEIER *et alii*, 1999; FERNÁNDEZ GARCIA *et alii*, 2002; CORTIS & KNUDBY, 2006; KNUDBY & CARRERA, 2005; MARTINEZ-LANDA & CARRERA, 2005; SÁNCHEZ-VILA *et alii*, 2006; FLECKENSTEIN & FOGG, 2008; TRINCHERO *et alii*, 2008; KERROU *et alii*, 2008).

Examples of analysis at this scale in restricted areas of the Po plain are given by BERSEZIO *et alii* (1999), who combine facies analysis and numerical modelling for a pro-glacial delta environment, and by BERSEZIO *et alii* (2007), who combine sedimento-logical and geophysical survey for a detailed 3D reconstruction of fluvial architectural elements.

3.6. – GIGA- AND TERASCOPIC SCALES

Finally, regional aquifer systems are studied at the giga- and terascopic scale ($10 \text{ m} \le h \le 10^3 \text{ m}$, $1 \text{ m} \le v \le 10^2 \text{ m}, 10^3 \text{ m} \le H \le 10^4 \text{ m}, 10 \text{ m} \le V \le 10^2 \text{ m}$), to develop engines of decision support tools for resource management and regional planning.

We refer to gigascale for the genetic sequences created by aquifer dynamics. In other words, we refer to the aquifer complexes which consist of aquifer/aquitard couples with a good lateral continuity and created by the alternation of different climatic conditions.

For these sequences the flow and transport processes are usually studied with quasi-3D models, i.e. assuming that the water flow is essentially horizontal in the aquifers and vertical in the aquitards.

Basin dynamics is instead controlled by longterm glacial and climatic cycles, as well as by tectonics. The assemblage of aquifer complexes yields aquifer groups, whose structure is characterised by basin-wide correlation of well data, interpolation of the results of well tests, geophysical prospecting (DC, TDEM and FDEM, reflection seismics). At this scale the thickness of the volume under study is much smaller than its horizontal extension, so that water flow can be approximated as two-dimensional.

4. – SUMMARY AND CONCLUSIONS

The answers to practical problems related to the management, protection and remediation of ground water resources require modelling water flow and transport at different scales. The numerical models should be simple enough to permit the numerical solution of the balance equations, the calibration and validation of the model. On the other hand they should be complex enough to describe the effects that heterogeneities at the fine scale can have on the processes occurring at the model scale.

From the point of view of a modeller, the physical parameters at the model coarse scale depend upon the heterogeneity at the finer scales, the link between the parameters at the fine and coarse scales is conceptually given by upscaling and the best values of the model parameters are often obtained with inverse methods (YEH, 1986; CARRERA, 1988; GINN & CUSHMAN, 1990; SUN, 1994; GIUDICI, 2001; CARRERA *et alii*, 2005).

Professionals can provide reliable forecasts of the behaviour of such heterogeneous natural systems as alluvial aquifers, if they clearly define the scale at which flow and transport are modelled, the types of sedimentary structures, the required data. The classification scheme proposed with this paper provides a revised description of the scales at which water flow and solute transport in alluvial aquifers are studied. Such scheme relates hydrological aspects to the structures studied with hierarchical dynamic stratigraphy and therefore is a contribution to the comprehension of the scaling issues and to the joint of the points of view of different experts: the geologists and the hydrologists, the sedimentologists and the modellers, the hydrogeologists and the geophysicists.

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