

About the Symmetry of the Upscaled Equivalent Transmissivity Tensor

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Abstract This paper provides a proof of the symmetry of the equivalent transmissivity tensor computed with a method based on the solution of the balance equation at the fine scale with integrated finite differences. The basic hypotheses are that the balance equation is solved on a block assigning Dirichlet boundary conditions that vary linearly with the space coordinates and the equivalent transmissivity tensor is computed as the linear tensor relating average flux and hydraulic gradient.

Keywords Upscaling · Equivalent transmissivity · Ground water · Integrated finite differences

Introduction

Numerical models that simulate water flow in geological formations are based on the discretization of the subsurface into grid-blocks for which homogeneous block-scale hydrodynamic parameters must be specified. In this paper we focus on the example of stationary water flow in a confined aquifer for which the assumption of 2D flow is assumed to be valid, so that the physical parameter to be considered is the aquifer transmissivity T . This allows us to keep the notation simple, but does not prevent from generalizing the results to the case of 3D flow, for which the relevant physical parameter is the hydraulic conductivity.

In real aquifers the local scale tensor T is heterogeneous within a block; therefore, it is necessary to find for each grid-block an equivalent transmissivity tensor $\tilde{T}$, that reproduces some average behavior of the T field at the fine scale.

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Commercial modelling packages usually assume that $\tilde{T}$ is symmetric or, even more restrictive, that the Cartesian axes coincide with the principal directions of this tensor. Theoretical studies show that the computation of $\tilde{T}$ with arbitrary boundary conditions might yield a non-symmetric tensor. Instead, Farmer (2002) states sufficient conditions in order to guarantee the symmetry of $\tilde{T}$ for a continuous domain.

The goal of this paper is to extend this theorem to a physically based conservative discrete model. Among the several numerical methods proposed in the literature, the integrated finite differences method has been chosen. It is worthwhile to recall some basic concepts about upscaling in order to fix the proper framework and relevance of our results. Different approaches have been used to transform a detailed description of the spatial variability of T to a coarser description; reviews and classifications of these methods can be found in Wen and Gómez-Hernández (1996), Renard and de Marsily (1997), Cushman et al. (2002), Nøtinger et al. (2005), and Sanchez-Vila et al. (2006).

A first distinction can be introduced between structural and functional hierarchy of scales (Cushman et al. 2002). Structural hierarchy implies that the structure of the porous medium can be modelled as a set of nested subunits; on the other hand, functional hierarchy implies that different flow and transport processes in the porous medium (and therefore different physico-mathematical equations) are relevant at different scales. Among the examples of the latter approach, we can mention the up-scaling from the Stokes equation at the microscopic (pores and grains) scale to the Darcy's law at the macroscopic (representative elementary volume) scale and the work by Hassanizadeh and Gray (1979) and their series of papers on equation averaging. In this paper we limit ourselves to consider a structural hierarchy, we assume that the Darcy's law is valid and we study the variation of the tensor T with scale length.

Another criterion of classification distinguishes between local and non-local methods (Renard and de Marsily 1997). In the local methods the equivalent block transmissivity is assumed to depend only on the local T values inside the block; in the non-local methods it depends on the whole T field, possibly through the source terms and the boundary conditions.

Then, upscaling methods can be analytical, i.e. based on algebraic averages of fine scale T , or numerical, i.e. based on the numerical solution of balance equations (Renard and de Marsily 1997). Analytical techniques assume that the block transmissivity tensor is an explicit function of the cell transmissivities, and they are often local methods. On the other hand, in numerical techniques the flow equation is solved at the fine scale, and the block transmissivity tensor is obtained after the computation of the block averaged flux $\langle \mathbf{q} \rangle$ and hydraulic gradient $\langle \mathbf{J} \rangle$. Numerical methods differ from each other in the extension of the area where the balance equation is solved at the fine scale and in the boundary conditions used for the solution. In particular, such methods can be either local, if the balance equation is solved on the block for which $\tilde{T}$ is computed, or non-local, if the balance equation is solved on the whole aquifer domain.

Here the focus is on numerical techniques; the spatially averaged flow through each block is computed from the solution of the flow problems at the fine scale, and the relationship between the total flow and the piezometric gradient at the faces of

the blocks permits to compute an upscaled transmissivity tensor for the coarse scale blocks.

The equivalent transmissivity tensor taken to represent the heterogeneous medium is defined according to a criterion of equality of flow, i.e. the flow at the boundaries of the domain must be the same for the heterogeneous medium and the equivalent homogeneous one, subjected to the same head gradient, or a criterion of equality of energy dissipated by the viscous forces in the heterogeneous and in the equivalent homogeneous medium (Renard and de Marsily 1997).

The geometrical regularity of heterogeneity at the fine scale, e.g. layering, yields anisotropy at the coarse scale; then the block transmissivity tensor is in general a non-diagonal tensor (White and Horne 1987). Moreover, $\tilde{T}$ is not an intrinsic property of the block, but depends on the boundary conditions, and in some cases it is not symmetric. The block transmissivity tensor could not admit principal directions of anisotropy if it is computed with methods that apply boundary conditions or considering heterogeneous media such that the symmetry of the tensor is not guaranteed. In other words, principal axes could not exist, i.e. a coordinate system in which the off-diagonal terms are equal to zero could not exist (White and Horne 1987; Zijl and Stam 1992). For non-symmetric tensors it is possible to perform a singular value decomposition, and two sets of principal directions, $V^{(q)} = \{\mathbf{e}_r^{(q)}, r = 1, 2\}$ and $V^{(J)} = \{\mathbf{e}_r^{(J)}, r = 1, 2\}$, are found. If the components of $\langle \mathbf{J} \rangle$ are evaluated with the $V^{(J)}$ orthonormal vectors and the components of $\langle \mathbf{q} \rangle$ with $V^{(q)}$ vectors, the relation between $\langle \mathbf{q} \rangle$ and $\langle \mathbf{J} \rangle$ involves only the principal components of $\tilde{T}$, with an expression similar to that applied when a symmetric tensor is expressed in the system of the principal directions (Zijl 1996). Nevertheless, it is impractical and therefore unusual to work with non-symmetric tensors.

From the physical point of view, the symmetry of T at the fine scale can be proven by means of thermodynamical arguments (Dagan 1989, p. 97).

The symmetry of the block transmissivity tensor is demonstrated with some assumptions by other authors. For instance, Durlofsky (1991) approach always yields symmetric and positive definite block conductivity tensors for a periodic medium. Furthermore, Trykozko et al. (2001) and Zijl and Trykozko (2001a) show nice properties of the equivalent tensor obtained by application of homogenization theory to periodic media. In particular, two alternative finite element methods permit to compute upper and lower bounds for the real upscaled tensor and to control the approximation error.

Farmer (2002) shows that the block scale tensor, computed as the coefficient of proportionality between the block averaged specific flux per unit length, $\langle \mathbf{q} \rangle$, and the block averaged hydraulic gradient $\langle \mathbf{J} \rangle$ is symmetric for any conductivity distribution and for any shape of the domain if $\langle \mathbf{q} \rangle$ is computed by solving forward problems with Dirichlet boundary conditions such that the prescribed head is a linear function of the space coordinates.

In this paper, we follow the proof of the symmetry of the upscaled transmissivity tensor given by Farmer (2002) and we demonstrate that even in the discrete case the result is strictly rigorous, provided that a physically based conservative numerical model is used. In particular, we consider the discretization of the balance equation with the integrated finite difference method (IFD). This

method was proposed in the ground water literature by Narasimhan and Witherspoon (1976) and has been applied by some authors to model regional flow (Fogg 1986; Vassena 2004). IFD can be useful to cope with heterogeneous fields for which sharp discontinuities can be recognized or to refine the grid in areas where a detailed description of the flow field is required. In the framework of upscaling studies, this method could be useful to model media which are the union of many zones, each of which characterized by a single hydrofacies. In fact, IFD permits the discretization of the discontinuities between different zones in a more accurate way than standard finite difference techniques which cannot handle non-rectangular grid cells. Nevertheless, the IFD method is based on a straightforward balance equation, which makes the physical interpretation of the results easy. Of course, other methods sharing the same properties can be applied, e.g. multipoint flux approximation models (Aavatsmark 2002) or finite element methods (Zijl 2005).

The Computation of the Equivalent Transmissivity Tensor

The aquifer under study is subdivided into coarse blocks, and each coarse block is subdivided into a fine grid of cells, so that at each fine cell the transmissivity takes a different value, obtained by direct measurements, interpolation or inversion procedures.

The block transmissivity tensor is computed with a local-numerical approach (local–local technique according to the classification of Farmer 2002). Virtual experiments are conducted on the block, solving the discrete balance equation on the fine grid for which the boundary conditions are assigned at the border of each block as prescribed heads that are linear functions of the space coordinates. Then the block averaged specific flux per unit length, $\langle \mathbf{q} \rangle$, is computed for each experiment. The block averaged hydraulic gradient $\langle \mathbf{J} \rangle$ is fixed from the boundary conditions and the equivalent transmissivity tensor $\tilde{T}$ is computed as

$$\langle \mathbf{q} \rangle = -\tilde{T} \langle \mathbf{J} \rangle. \quad (1)$$

The fine grid is constituted by a Voronoi diagram (de Marsily 1976, p. 353). Given a set of nodes, Voronoi polygons (Fig. 1) are built as the union of the mediators of each segment joining adjacent nodes. Each node will be denoted either by an integer index, e.g. j , or by its position vector, e.g. $\mathbf{x}_j = ((x_1)_j, (x_2)_j)$. Furthermore, any cell corresponding to the domain enclosed by a Voronoi polygon is labeled with the index of the node located at the center of the cell itself.

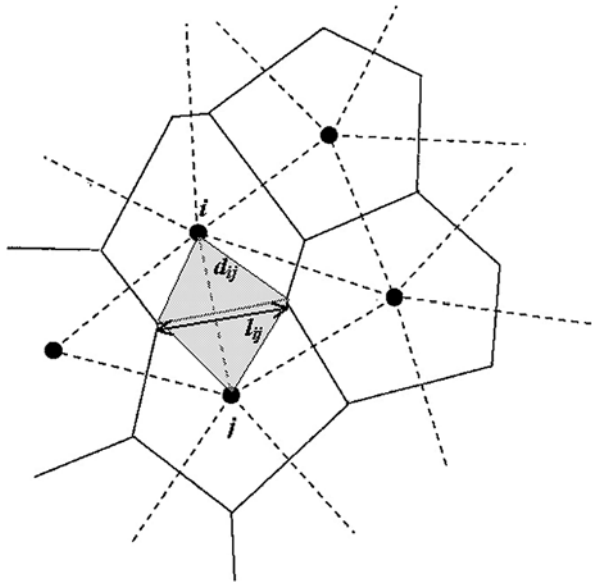
Let N be the set of nodes which belong to a coarse block, and let $N = N_0 \cup N_b$, where N_0 is the subset of nodes for which the balance equation can be written and N_b is the subset of the boundary nodes.

Let the boundary conditions on h assigned at the border of the coarse block be linear

$$h_i = \mathbf{x}_i \cdot \mathbf{a}, \quad i \in N_b, \quad (2)$$

where $\mathbf{a} = (a_1, a_2)$ is a fixed constant vector.

Fig. 1 Grid built with Voronoi polygons; $d_{i,j}$ is the length of the internode segment connecting nodes i and j ; $l_{i,j}$ is the length of the side separating the cells i and j ; the area of the gray region is $(d_{i,j}l_{i,j})/2$



The balance equation for any cell $j \in N_0$, assuming that the source terms are null, has the form

$$\frac{1}{A_j} \sum_{i \in S_j} T_{i,j} \frac{h_i - h_j}{d_{i,j}} l_{i,j} = 0, \quad (3)$$

where S_j is the subset of nodes connected to the j th node, A_j is the area of the j th cell, $T_{i,j}$ is the internode transmissivity, h_j is the piezometric head at the j th node, $d_{i,j} = \|\mathbf{x}_i - \mathbf{x}_j\|$ is the distance between the i th and j th nodes and $l_{i,j}$ is the length of the side separating the i th and j th cells.

Each of the terms $T_{i,j}(h_i - h_j)d_{i,j}^{-1}l_{i,j}$ appearing in the sum of (3) corresponds to the flux entering in the j th cell through the side separating it from the i th cell. Since this term involves the component of the discrete hydraulic gradient along the internode segment,

$$\frac{h_i - h_j}{d_{i,j}}, \quad (4)$$

it is implicitly assumed that the component of the hydraulic gradient parallel to the cell side does not contribute to the flow along the direction of the internode segment. In other words, the same discretisation can be applied for media which are isotropic at the fine scale or anisotropic, but such that the internode segments and the cell sides have the same directions as the principal axes of the local transmissivity tensor.

The use of Dirichlet boundary conditions could be questionable. In fact, the real head at the border of the block varies depending on the whole T field and on the source terms. However, a linear trend of piezometric head could be a reasonable approximation for distributed and weak source terms; on the other hand, Zijl and Trykozko (2001b) propose to scale the components of $\mathbf{q}$, $\mathbf{J}$ and T with powers of

the distance from the well, so that the fine-scale balance equation for cylindrical coordinates takes the same form as the balance equation for Cartesian coordinates and makes linear interpolation significant.

The Proof of the Symmetry of the Equivalent Transmissivity Tensor

Here we follow the same track of the proof given by Farmer (2002) in the continuous case. The gradients are substituted with the finite difference approximations, as in (4), and the integrals are substituted with sums over a given block.

Let φ be a nodal function vanishing on the boundary, i.e. $\varphi_j = 0$ for $j \in N_b$. First of all, (3) is multiplied by $\varphi_j A_j$ and summed over all internal nodes of the coarse block, obtaining

$$\sum_{j \in N_0} \varphi_j \sum_{i \in S_j} T_{i,j} \frac{h_i - h_j}{d_{i,j}} l_{i,j} = 0. \quad (5)$$

Using the property that φ vanishes on the boundary, it is

$$-\sum_{j \in N} \sum_{\substack{i \in S_j \\ i \leq j}} T_{i,j} \frac{h_i - h_j}{d_{i,j}} l_{i,j} (\varphi_i - \varphi_j) = 0. \quad (6)$$

Let

$$h_i^{(r)} = \mathbf{x}_i \cdot \mathbf{e}^{(r)}, \quad i \in N_b, \quad (7)$$

be the linear boundary conditions in the r th experiment, where

$$\mathbf{e}^{(1)} = (1, 0), \quad \mathbf{e}^{(2)} = (0, 1).$$

The piezometric head $h^{(r)}$ satisfies (3). Notice that in the rest of this paper the Einstein convention is adopted for indices $r, s \in \{1, 2\}$ so that they are assumed to be summed when repeated, while the sums over the indices belonging to N are written in the explicit form. If $\varphi = b_s h^{(s)} - \mathbf{b} \cdot \mathbf{x}$, where b_s is the s th component of an arbitrary constant vector $\mathbf{b}$, we obtain

$$\begin{aligned} & \sum_{j \in N} \sum_{\substack{i \in S_j \\ i \leq j}} T_{i,j} \frac{h_i^{(r)} - h_j^{(r)}}{d_{i,j}} l_{i,j} [b_1 (h_i^{(1)} - h_j^{(1)}) + b_2 (h_i^{(2)} - h_j^{(2)})] \\ &= \sum_{j \in N} \sum_{\substack{i \in S_j \\ i \leq j}} T_{i,j} \frac{h_i^{(r)} - h_j^{(r)}}{d_{i,j}} l_{i,j} [b_1 ((x_1)_i - (x_1)_j) + b_2 ((x_2)_i - (x_2)_j)]. \quad (8) \end{aligned}$$

For a general linear boundary condition assigned as in (2), the solution to (3) is given by $h = h^{(r)}a_r$, and the block averaged flux is given by

$$\langle q_s \rangle = \frac{1}{A} \sum_{j \in N} \sum_{\substack{i \in S_j \\ i \leq j}} T_{i,j} \frac{h_i^{(r)} - h_j^{(r)}}{d_{i,j}} a_r \frac{l_{i,j} d_{i,j}}{2} \frac{(x_s)_i - (x_s)_j}{d_{i,j}} \quad (9)$$

where

$$A = \sum_{j \in N} \sum_{i \in S_j, i \leq j} \frac{l_{i,j} d_{i,j}}{2}.$$

Notice that $l_{i,j} d_{i,j}/2$ is the surface of the gray area in Fig. 1.

Since $\mathbf{a}$ can be interpreted as $\langle \mathbf{J} \rangle$, from (1) the equivalent transmissivity of a coarse block is given by

$$\tilde{T}_{sr} = \frac{1}{A} \sum_{j \in N} \sum_{\substack{i \in S_j \\ i \leq j}} T_{i,j} \frac{h_i^{(r)} - h_j^{(r)}}{d_{i,j}} \frac{l_{i,j} d_{i,j}}{2} \frac{(x_s)_i - (x_s)_j}{d_{i,j}}. \quad (10)$$

The first index, s , refers to the direction of flow, whereas the second index, r , refers to the component of the hydraulic gradient.

If we introduce the quadratic form $\lambda(\mathbf{a}, \mathbf{b}) = \tilde{T}_{sr} a_r b_s$, where a_r and b_s are the components of arbitrary vectors $\mathbf{a}$ and $\mathbf{b}$, the elements of $\tilde{T}$ can be computed as

$$\tilde{T}_{sr} = \frac{\partial^2 \lambda}{\partial a_r \partial b_s}. \quad (11)$$

By (10), the quadratic form λ has the form

$$\lambda = \frac{1}{A} \sum_{j \in N} \sum_{\substack{i \in S_j \\ i \leq j}} T_{i,j} \frac{h_i^{(r)} - h_j^{(r)}}{d_{i,j}} \frac{l_{i,j} d_{i,j}}{2} a_r b_s \frac{(x_s)_i - (x_s)_j}{d_{i,j}}. \quad (12)$$

Using (8), we have

$$\lambda = \frac{1}{A} \sum_{j \in N} \sum_{\substack{i \in S_j \\ i \leq j}} T_{i,j} \frac{h_i^{(r)} - h_j^{(r)}}{d_{i,j}} \frac{l_{i,j}}{2} a_r b_s (h_i^{(s)} - h_j^{(s)}). \quad (13)$$

From (11) and (13) the following expression for the components of $\tilde{T}$ is obtained

$$\tilde{T}_{sr} = \frac{1}{A} \sum_{j \in N} \sum_{i \in S_j, i \leq j} T_{i,j} \frac{h_i^{(r)} - h_j^{(r)}}{d_{i,j}} \frac{h_i^{(s)} - h_j^{(s)}}{d_{i,j}} \frac{l_{i,j} d_{i,j}}{2}. \quad (14)$$

Equation (14) implies the symmetry of the equivalent transmissivity tensor at the coarse scale and completes the proof.

The Derivation of the Equivalent Transmissivity Tensor from the Energy Dissipation Criterion

An alternative way to compute $\tilde{T}$ is based on the equivalence between the dissipated energy averaged over a block, $-\langle \mathbf{q} \cdot \mathbf{J} \rangle$, and computed from block averaged quantities, $-\langle \mathbf{q} \rangle \cdot \langle \mathbf{J} \rangle$. In other words, the equivalent transmissivity tensor is obtained with the condition that

$$-\langle \mathbf{q} \cdot \mathbf{J} \rangle = -\langle \mathbf{q} \rangle \cdot \langle \mathbf{J} \rangle = \tilde{T}_{m,n} \langle J_m \rangle \langle J_n \rangle. \quad (15)$$

In order to apply (15), following the same line of previous sections, we have

$$\langle \mathbf{q} \cdot \mathbf{J} \rangle = \frac{1}{A} \sum_{j \in N} \sum_{i \in S_j, i \leq j} T_{i,j} \frac{h_i - h_j}{d_{i,j}} \frac{h_i - h_j}{d_{i,j}} \frac{l_{i,j} d_{i,j}}{2}. \quad (16)$$

We now recall that for linear boundary conditions as given by (2), the solution to (3) is obtained as $h = h^{(r)} a_r$, so that (16) can be written as

$$\langle \mathbf{q} \cdot \mathbf{J} \rangle = \frac{1}{A} \sum_{j \in N} \sum_{i \in S_j, i \leq j} T_{i,j} \frac{h_i^{(r)} - h_j^{(r)}}{d_{i,j}} a_r \frac{h_i^{(s)} - h_j^{(s)}}{d_{i,j}} a_s \frac{l_{i,j} d_{i,j}}{2}. \quad (17)$$

Inserting (17) into (15) and recalling that $\langle \mathbf{J} \rangle = \mathbf{a}$, we obtain (14) again. In other words, the block transmissivity tensors computed from the criteria of equivalence of flux and of energy dissipation coincide if fixed head boundary conditions that vary linearly in space are assigned.

Conclusions

We have proven the following theorem. Let the discrete balance equation (3) be valid over a Voronoi diagram, which is an IFD discretisation of a block. Let $h^{(r)}$ be the solution to (3) if Dirichlet boundary conditions are assigned so that the prescribed head is a linear function of the space coordinates, as given by (7). The block scale equivalent transmissivity tensor computed from (1) is symmetric for any transmissivity distribution and for any shape of the block.

This result has been obtained for the IFD method that is based on a balance equation and permits to approximate the (often irregular) discontinuities between different zones in a more accurate way than standard finite difference techniques. Moreover, the same discretization can be applied for media which are isotropic at the fine scale or anisotropic but such that the internode segments and the cell sides have the same direction as the principal axes of the local transmissivity tensor.

We have adopted a local numerical approach: the discrete balance equation is solved on the fine grid with boundary conditions assigned at the border of each block, and the equivalent transmissivity tensor is computed as the coefficient of proportionality between the block averaged flux and the block averaged hydraulic gradient. Furthermore, this tensor coincides with that computed from the equivalence of viscous energy dissipation.

The application of a local numerical method is not a strong limitation to the importance of our results. In fact, for a general flow situation, the balance equation (3) is solved over the whole domain with arbitrary boundary conditions and source terms, so that the right-hand side of (3) does not vanish but is equal to f_j , which is the sum of the source terms divided by A_j . Thus we cannot expect that (1) is still valid, but we can decompose $\langle \mathbf{q} \rangle$ as

$$\langle \mathbf{q} \rangle = -\tilde{T} \langle \mathbf{J} \rangle + \mathbf{q}_{nD},$$

where $\mathbf{q}_{nD}$ represents the non-Darcian block-averaged flow rate. The equivalent transmissivity tensor $\tilde{T}$, defined by (1) and computed by (10) or (14), is a local property of the medium at the coarse scale. Non-local effects are described by $\mathbf{q}_{nD}$, which depends on the whole transmissivity field, on the physical boundary conditions of the aquifer, and on the distribution of source terms.

In other words, we have proven the symmetry of the equivalent transmissivity tensor that controls the Darcian term of the block-averaged flux.

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