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Effective parameters for flow in saturated heterogeneous porous media

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Abstract

Effective parameters for flow in saturated porous media are obtained via Taylor–Aris–Brenner moment analysis considering both periodic as well as stationary porous medium properties. It is assumed that a slug is instantaneously introduced into an unbounded, anisotropic porous medium having a compressible matrix, and that the correlation length of the local hydraulic conductivity and specific storage fluctuations is smaller than the correlation length of hydraulic head fluctuations (gradually varying flow). It is shown that the effective specific storage is equal to its volume average. The effective hydraulic conductivity is derived by a small-perturbation analysis and it is shown to consist of its volume average and of a second term which accounts for the 'small' local conductivity fluctuations.

1. Introduction

The study of heterogeneity in subsurface systems has captured the attention of many researchers. The reasons for this interest are not hard to perceive. Heterogeneity is impossible to ignore because it is so evident whenever field observations are analyzed. For instance, measurements of hydraulic conductivity, through core samples or borehole flowmeters, indicate that conductivity may vary by orders of magnitude over short distances. All properties which affect the rates of groundwater flow and transport have been shown to be highly spatially variable. Although hydrogeologists have always been aware of the heterogeneity in their systems, they have not been reluctant to use the classical prediction tools of hydrogeology which assume some form of spatial uniformity in formation parameters. Analytical approaches practically always assume homogeneous formations. Finite-element methods are less confined but must still subdivide the flow domain into a conglomeration of homogeneous blocks; however, in practice, these blocks are much larger than the

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Notation

$\boldsymbol{b}$, $\boldsymbol{d}$	vectors of integers (wavenumbers): $\boldsymbol{b} = (b_1, b_2, b_3)^T$
$\grave{\boldsymbol{b}}$, $\grave{\boldsymbol{d}}$	normalized vectors: $\grave{\boldsymbol{b}} = (b_1/l_1, b_2/l_2, b_3/l_3)^T$
$\mathrm{d}s$	infinitesimal area on ∂V_o
$\mathrm{d}^3\boldsymbol{x}$	differential volume within a unit element
$\boldsymbol{D}$	'diffusion' coefficient, equal to $\boldsymbol{K}/S$ (L^2/t)
$E[\ ]$	expected value
$\boldsymbol{F}$	arbitrary global or local function
G_{ij}	constant
H_{ij}	function of local coordinates
j	imaginary number unit: $j = (-1)^{1/2}$
$\boldsymbol{k}_i$	column of the hydraulic conductivity coefficient tensor: $\boldsymbol{k}_2 = (K_{12}, K_{22}, K_{32})^T$
K_{ij}	hydraulic conductivity coefficient (L/t)
$\boldsymbol{K}$	hydraulic conductivity coefficient tensor
l_i	characteristic linear dimension of a unit element (L)
$\boldsymbol{l}_i$	basic vectors which define a unit element
$\boldsymbol{m}_\mathrm{p}$	liquid-phase local moments
$\boldsymbol{M}_\mathrm{p}$	continuous and discrete representation of liquid-phase global moments
$\boldsymbol{n}_s$	outer unit vector normal to ∂V_o
O	order of magnitude
$P_{k_i'k_j'}$	discrete power spectrum, a dyadic
$\boldsymbol{r}$	separation vector
$R_{k_i'k_j'}$	and covariance function
$s_{\pm i}$	faces of the unit element
S	specific storage coefficient (L^{-1})
t	time (t)
V_o	domain of a unit element: $V_o = l_1 l_2 l_3$
V_w	volume of water introduced into the porous formation (L^3)
∂V_o	external surface of a unit element
x_i	local Cartesian coordinates (L)
$\boldsymbol{x}$	local position vector within a unit element
$\partial \boldsymbol{x}_i$	interface of a unit element
X_i	global Cartesian coordinates (L)
$\boldsymbol{X}$	discrete position vector of a general point
$\boldsymbol{X}_{\boldsymbol{n}}$	discrete position vector locating the origin of the $\boldsymbol{n}$th unit element
Greek letters	
$\delta()$	Dirac delta function
δ_{ij}	Kronecker delta
ϵ	mathematical artifice, scalar
κ, μ	Fourier coefficients (defined in (A4) and (19), respectively)
ϕ	head above background piezometric head (L)
ϕ_o	background piezometric head (L)
Subscripts	
i, j, k	direction of principal axes: $i, j, k = x, y, z$
$\boldsymbol{n}$	$\boldsymbol{n}$th unit element: $\{\boldsymbol{n}\} = \{n_1, n_2, n_3\}$
1, 2, 3	principal directions of a Cartesian coordinate system (x, y, z)
Superscripts	
T	transpose
$\Diamond$	effective global coefficient
$'$	indicates the value of a function minus its average over the volume of a unit element
$\dagger$	complex conjugate

scale of variability of the properties. Thus, finite-element and similar numerical methods are successful in handling large-scale variability but not small-scale variability.

Despite the concern that homogeneous media represented by analytical and finite-element models are not realistic, these models have been applied widely to study actual systems and to engineer solutions to problems. The use of these models has been justified on practical grounds (they are available, usable, and widely accepted) but also on the assumption that a heterogeneous medium macroscopically behaves like a homogeneous medium with properly chosen effective (or macroscopic) parameters.

The concept of effective conductivity was questioned in the pioneering studies of Warren and Price (1961), Matheron (1967), and Freeze (1975), as well as more recent works. These analyses have motivated the introduction to hydrogeology of large-scale effective parameters which account for the effect of small-scale spatially variable hydrogeologic properties. Several methods have been applied to determine the effective conductivity in a medium where the conductivity fluctuates about a mean. Gelhar (1977), Gutjahr et al. (1978), and Dagan (1982) used a stochastic small-perturbation approach. Dagan (1979, 1981) applied the embedding matrix approach. Sáez et al. (1989) employed the homogenization approach and Kitanidis (1990) the method of moments. The most popular method, however, for the study of statistical variability in parameters is Monte Carlo simulations coupled with numerical groundwater flow models (i.e. Freeze, 1975; Smith and Freeze, 1979; Desbarats, 1987; Durlofsky, 1991, to mention a few).

The impact of heterogeneity in the specific storage coefficient has not been explored except in the work of Dagan (1982), who used stochastic small-perturbation analysis to demonstrate that the effective storage coefficient in gradually varying flow is approximately equal to the arithmetic average of the locally variable storage coefficient. This work complements Dagan's research by investigating the effect of spatially variable hydraulic conductivity and specific storage coefficient in gradually varying flow using a different approach. The method employed in this work is based on volume averaging whereas Dagan's method uses stochastic random functions; furthermore, the effective parameters are defined by the method of moments whereas Dagan's definition is based on a macroscopic form of Darcy's equation. It should be noted that this analysis is based on the generalized Taylor–Aris–Brenner method of moments.

2. Problem formulation

Let us consider a three-dimensional porous formation with spatially periodic hydraulic conductivity and specific storage coefficient in all three directions. The need for periodic parameters is imposed by the Taylor–Aris–Brenner method of analysis employed in this study; however, as will be discussed in a subsequent section, the results can be extended to the more general case of stationary random porous media. A definition sketch is provided in Fig. 1. Assuming that all periodic

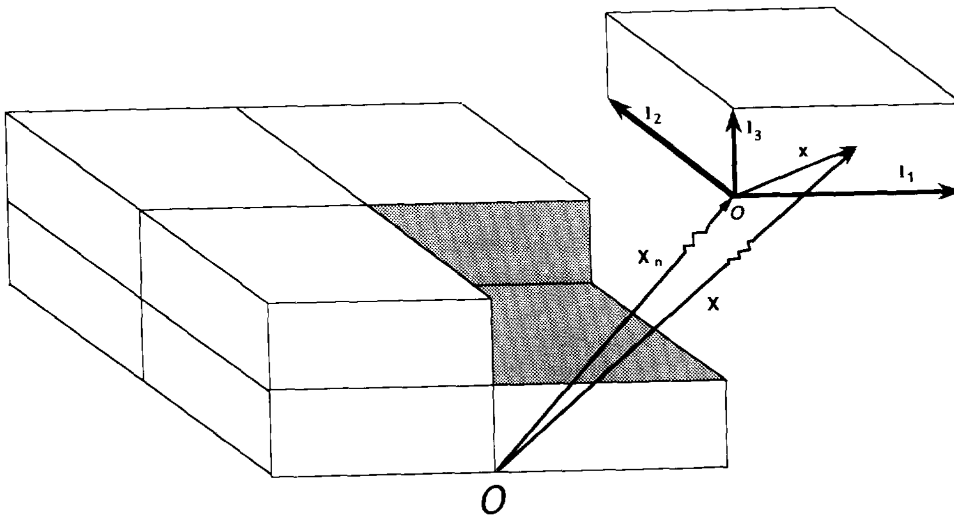

Fig. 1. Schematic representation of a periodic formation and associated bounded/unbounded spatial coordinates (O and o indicate the origin of the global and a local regular Cartesian coordinate system, respectively).

parameters vary in each principal direction of a regular Cartesian coordinate system with spatial intervals l_1, l_2, and l_3, respectively, the porous formation may be divided into identical rectangular parallelepiped elements ('unit' elements) with edges defined by the vectors $\boldsymbol{l}_1$, $\boldsymbol{l}_2$, and $\boldsymbol{l}_3$ (e.g. $\boldsymbol{l}_2 = (0, l_2, 0)^T$). A vector of spatial coordinates $\boldsymbol{X}$ may be written as the sum of an unbounded global variable $\boldsymbol{X}_n$ and a bounded local variable $\boldsymbol{x}$ (Brenner, 1980b), i.e. $\boldsymbol{X} = \boldsymbol{X}_n + \boldsymbol{x}$, where $\boldsymbol{X}_n = (X_1, X_2, X_3)^T = (n_1 l_1, n_2 l_2, n_3 l_3)^T$ ($n_i = 0, \pm 1, \pm 2, \ldots$; $i = 1, 2, 3$) locates the origin of the $\boldsymbol{n}$th unit element which is defined by the triplet of integers: $\{\boldsymbol{n}\} = \{n_1, n_2, n_3\}$, and $\boldsymbol{x} = (x_1, x_2, x_3)^T$ ($0 \leqslant x_i \leqslant l_i$) specifies a local point within the $\boldsymbol{n}$th unit element.

The unsteady flow through a confined, three-dimensional, heterogeneous, anisotropic formation of compressible matrix, in the absence of sources or sinks, is governed by the following partial differential equation:

$$S(\boldsymbol{X}) \frac{\partial \phi_o(t, \boldsymbol{X})}{\partial t} = \nabla \cdot [\boldsymbol{K}(\boldsymbol{X}) \cdot \nabla \phi_o(t, \boldsymbol{X})] \tag{1}$$

where $\phi_o(t, \boldsymbol{X})$, which can also be written as $\phi_0(t, \boldsymbol{X}_n, \boldsymbol{x})$, is the piezometric head (in this work it will be referred to as 'background' piezometric head), $\boldsymbol{K}(\boldsymbol{X})$ is a symmetric second-order tensor (dyadic) of the hydraulic conductivity coefficients, $S(\boldsymbol{X})$ is the specific storage coefficient, t is time, ∇ is the vector gradient operator with respect to the local coordinates ($\nabla = [\partial/\partial x_1, \partial/\partial x_2, \partial/\partial x_3]^T$), and $\nabla \cdot$ denotes divergence ($\nabla \cdot \boldsymbol{F} = \partial F_1/\partial x_1 + \partial F_2/\partial x_2 + \partial F_3/\partial x_3$, where $\boldsymbol{F}$ is an arbitrary three-dimensional vector function of local coordinates).

For an unbounded porous formation in which a slug of water is instantaneously introduced or withdrawn, leading to a 'unit' increase/decrease in the piezometric head, at $t = 0$ at an arbitrarily chosen point $\boldsymbol{X}^0 = \boldsymbol{X}_{\boldsymbol{n}^0} + \boldsymbol{x}^0$, where superscript 0 associates the corresponding flow conditions with the location of the slug introduction/withdrawal, the appropriate initial condition is

$$\phi(0, \boldsymbol{X}) = \pm\delta(\boldsymbol{X} - \boldsymbol{X}^0) = \pm\delta_{\boldsymbol{nn}^0}\delta(\boldsymbol{x} - \boldsymbol{x}^0) \tag{2}$$

and the boundary condition is

$$\lim_{\|\boldsymbol{X}-\boldsymbol{X}^0\|\to\infty} \phi(t, \boldsymbol{X}) = \lim_{\|\boldsymbol{X}_{\boldsymbol{n}}-\boldsymbol{X}_{\boldsymbol{n}^0}\|\to\infty} \phi(t, \boldsymbol{X}) = 0 \tag{3}$$

where $\phi(t, \boldsymbol{X})$ is the head change above/below background piezometric head; $\delta_{\boldsymbol{nn}^0}$ is the Kronecker delta for unit elements $\boldsymbol{n}$ and $\boldsymbol{n}^0$ ($\delta_{\boldsymbol{nn}^0} = \delta_{n_1 n_1^0}\delta_{n_2 n_2^0}\delta_{n_3 n_3^0}$), which is used to identify the correct macroscopic element where the slug occurs; $\delta(\boldsymbol{x} - \boldsymbol{x}^0)$ is a Dirac delta function, which is used to identify the point of slug introduction/withdrawal within the element. It should be noted that $\delta_{\boldsymbol{nn}^0}\delta(\boldsymbol{x} - \boldsymbol{x}^0) = \delta(\boldsymbol{X} - \boldsymbol{X}^0)$. The initial condition (2) implies that at time zero a volume of water is introduced/withdrawn at $\boldsymbol{X}^0$ which yields a 'unit' change in head above/below background piezometric head $\phi(0, \boldsymbol{X})$. This change in piezometric head begins inducing changes in the flow field within the formation. An illustration of ϕ_0 and ϕ for a hypothetical aquifer is shown in Fig. 2. The first equality in condition (3) holds, because $\|\boldsymbol{x} - \boldsymbol{x}^0\| = O(l_i)$; so the local coordinates are not needed at large distances.

Hereafter, it is assumed that $\phi(t, \boldsymbol{X})$ refers to head above $\phi_0(t, \boldsymbol{X})$, and for notational convenience it is assumed that $\boldsymbol{X}_{\boldsymbol{n}^0} = \boldsymbol{0}$ and $\boldsymbol{x}^0 = \boldsymbol{0}$, where $\boldsymbol{0}$ is the null vector and indicates that the origin of the coordinate system is at the origin of the unit element defined by $\{\boldsymbol{n}^0\} = \{0, 0, 0\}$. Furthermore, it is imposed that $\phi(t, \boldsymbol{X})$ and its derivatives with respect to the local coordinates are continuous on each interface of a unit element.

In the present analysis, the hydraulic conductivity and the specific storage coefficient are modeled as periodic with the same directional spatial intervals l_1, l_2, and l_3; which means that they depend only on local coordinates. Furthermore, $S(\boldsymbol{x})$ and $\boldsymbol{K}(\boldsymbol{x})$, as well as their derivatives with respect to the local coordinates, are also continuous at any point on the six faces of each parallelepiped unit element.

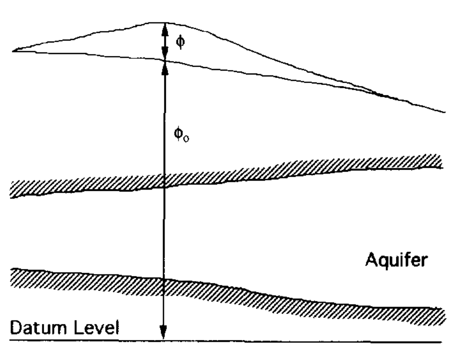

Fig. 2. Illustration of the background piezometric head, ϕ_0, and the change in piezometric head above background, ϕ, following an injection of a slug of water into an aquifer.

3. Taylor–Aris–Brenner spatial moments

Assuming that the distribution of the head above background piezometric head, $\phi(t, \boldsymbol{X})$, can be characterized by spatial moments, an expression for the asymptotic effective hydraulic conductivity coefficients can be obtained via a generalized version (Brenner, 1980a, 1982a,b; Frankel and Brenner, 1989) to earlier theoretical work on moment analysis (Taylor, 1953, 1954; Aris, 1956). In the context of the generalized Taylor–Aris–Brenner theory, the local spatial moments of the head above background piezometric head are defined as

$$\boldsymbol{m}_p(t, \boldsymbol{x}) = \sum_{\boldsymbol{n}} \boldsymbol{X_n}^p \phi(t, \boldsymbol{X_n}, \boldsymbol{x}) \qquad (p = 0, 1, 2, \ldots,) \tag{4}$$

where $\sum_{\boldsymbol{n}}$ denotes the triple summation $\sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} \sum_{n_3=-\infty}^{\infty}$, and $\boldsymbol{X_n}^p = \boldsymbol{X_n} \ldots \boldsymbol{X_n}$ (p times) is known as a p-adic. For example, for $p = 0$, $\boldsymbol{X_n}^0 = 1$ is a scalar; for $p = 1$, $\boldsymbol{X_n}^1 = \boldsymbol{X_n} = (n_1 l_1, n_2 l_2, n_3 l_3)^T$ is a three-dimensional vector of global coordinates indicating the origin of the $\boldsymbol{n}$th unit element; for $p = 2$, $\boldsymbol{X_n}^2$ is the second-order tensor or dyadic whose ijth element is the product of the i and j element of $\boldsymbol{X_n}$, and so on. The zero-order local moment, $m_0'(t, \boldsymbol{x})$, is a scalar and represents the sum of head above background piezometric head at all points of the domain with local coordinates $\boldsymbol{x}$. The first-order local moment, $\boldsymbol{m}_1(t, \boldsymbol{x})$, is a three-dimensional vector whose ith element is $m_{1(i)}(t, \boldsymbol{x}) = \sum_{\boldsymbol{n}} (n_i l_i) \phi(t, \boldsymbol{X_n}, \boldsymbol{x})$. The second-order local moment is a 3×3 symmetric matrix whose ijth element is $m_{2(ij)}(t, \boldsymbol{x}) = \sum_{\boldsymbol{n}} (n_i l_i)(n_j l_j) \phi(t, \boldsymbol{X_n}, \boldsymbol{x})$. The global moments of $\phi(t, \boldsymbol{X})$ are defined from the integral of local moments over the local coordinates as

$$\boldsymbol{M}_p(t) = \int_{V_o} \boldsymbol{m}_p(t, \boldsymbol{x}) \mathrm{d}^3\boldsymbol{x} \qquad (p = 0, 1, 2, \ldots,) \tag{5}$$

where V_o is the domain of a unit element and $\mathrm{d}^3\boldsymbol{x}$ is a differential volume within a unit element.

For the derivation of the effective parameters of the porous formation considered in this study only the zero-, first-, and second-order global moments are required by the selected method of analysis. It should be noted that the change in piezometric head, ϕ, is related to the volume of water injected, V_w, the volume of the porous medium where the water injection occurs, V_o, and the specific storage coefiicient, S, by the following expression: $\phi = V_w / V_o S$ (Bear, 1979, p. 86). Therefore, the distribution of ϕ is proportional to the distribution of the water volume injected. The zeroth global moment (M_0) is a scalar and represents the total change in head above background piezometric head, which is proportional to the volume of water introduced into the porous formation; the first moment ($\boldsymbol{M}_1$) is a vector and $\boldsymbol{M}_1 / M_0$ indicates the position of the center of the distribution of ϕ, or equivalently the center of the water mass injected; the second moment ($\boldsymbol{M}_2$) is a dyadic and $\boldsymbol{M}_2 / M_0$ measures the mean square displacement of the distribution, after averaging the piezometric head within each element, about the origin of the $\boldsymbol{n}^0$th unit element where the slug of water was introduced instantaneously as a point source.

4. Equations satisfied by the local moments

The rate of change of the local moments of $\phi(t, \boldsymbol{X})$ is obtained by rewriting Eq. (1) in terms of local coordinates, substituting ϕ for ϕ_o, multiplying the resulting equation by $\boldsymbol{X}_n^{\mathrm{P}}$ and then summing over all unit elements. Explicitly,

$$\sum_n \boldsymbol{X}_n^p \left\{ S(\boldsymbol{x}) \frac{\partial \phi(t, \boldsymbol{X}_n, \boldsymbol{x})}{\partial t} - \nabla \cdot [\boldsymbol{K}(\boldsymbol{x}) \cdot \nabla \phi(t, \boldsymbol{X}_n; \boldsymbol{x})] \right\} = 0 \tag{6}$$

As $S(\boldsymbol{x})$ and $\boldsymbol{K}(\boldsymbol{x})$ are independent of $\boldsymbol{n}$, in view of the definition of the local spatial moments (4), Eq. (6) may be written as

$$S(\boldsymbol{x}) \frac{\partial \boldsymbol{m}_p(t, \boldsymbol{x})}{\partial t} = \nabla \cdot [\boldsymbol{K}(\boldsymbol{x}) \cdot \nabla \boldsymbol{m}_p(t, \boldsymbol{x})] \tag{7}$$

The preceding equation is a partial differential equation in terms of the local moments $\boldsymbol{m}_{\mathrm{p}}(t, \boldsymbol{x})$. In addition to Eq. (7), the local moments satisfy the following boundary conditions imposed at the unit-element surfaces which are expressed in terms of 'local jumps' (Brenner, 1980b):

$$[\![m_0]\!] = 0, \qquad [\![\nabla m_0]\!] = 0 \tag{8a,b}$$

$$[\![\boldsymbol{m}_1]\!] = -[\![\boldsymbol{x} m_0]\!], \qquad [\![\nabla \boldsymbol{m}_1]\!] = -[\![\nabla(\boldsymbol{x} m_0)]\!] \tag{9a,b}$$

$$[\![\boldsymbol{m}_2]\!] = \left[\!\!\left[\frac{\boldsymbol{m}_1 \boldsymbol{m}_1}{m_0}\right]\!\!\right], \qquad [\![\nabla \boldsymbol{m}_2]\!] = \left[\!\!\left[\nabla\left(\frac{\boldsymbol{m}_1 \boldsymbol{m}_1}{m_0}\right)\right]\!\!\right] \tag{10a,b}$$

Local jumps are denoted by double brackets $[\![\ ]\!]$ and indicate the difference between the values of the function within the brackets at equivalent points on opposite faces of a unit element; for example, $[\![\boldsymbol{F}(\boldsymbol{x})]\!] = \boldsymbol{F}(\boldsymbol{x} - \boldsymbol{l}_i) - \boldsymbol{F}(\boldsymbol{x})$ for $\boldsymbol{x} \in \partial \boldsymbol{x}_{\mathrm{i}}$, where $\partial \boldsymbol{x}_{\mathrm{i}}$ indicates the ith interface of a unit element.

Integrating both sides of Eq. (7) over the domain of a unit element and employing Gauss's theorem, which let us convert a volume integral over the enclosed region of a unit element to a closed surface integral, leads to

$$\int_{V_o} S(\boldsymbol{x}) \frac{\partial \boldsymbol{m}_p}{\partial t} \mathrm{d}^3 \boldsymbol{x} = \int_{\partial V_o} [\boldsymbol{K}(\boldsymbol{x}) \cdot \nabla \boldsymbol{m}_p] \cdot \boldsymbol{n}_s \mathrm{d}s = \sum_i \int_{s_{+i}} [\![\boldsymbol{K}(\boldsymbol{x}) \cdot \nabla \boldsymbol{m}_p]\!] \cdot \boldsymbol{n}_s \mathrm{d}s \tag{11}$$

where ∂V_{o} is the external surface area of a unit element, $\boldsymbol{n}_{\mathrm{s}}$ is the outer unit vector normal to ∂V_{o} and $\mathrm{d}s$ is an infinitesimal surface area on ∂V_{o}, and $s_{\pm i}$ denotes the faces of the unit element, where the plus or minus sign permits identification of equivalent but opposite faces. For example, s_{+1} is the downstream face of a unit element on the x_2–x_3 plane, and s_{-1} is the opposite face. Because the unit element is a parallelepiped, $s_{+i} = s_{-i}$. The latter formulation in the preceding equation is the consequence of allowing the surface integral over the area of a unit element to be written in terms of local jumps (Brenner, 1980b).

5. Large-time behavior

In this section the expressions for the zero-, first- and second-order global moments are obtained with the methods of Chrysikopoulos et al. (1992a,b). At large values of time when the slug of water injected extends over several unit elements, for $p = 0$ (zero-order moments), the solution to Eq. (7) subject to jump boundary conditions (8a,b) is by inspection deduced to be

$$m_0 = \text{const.} \tag{12}$$

The preceding equation indicates that a steady state has been reached for m_0, and certainly does not mean that $\phi(t, \boldsymbol{X})$ has reached steady state. At large time, $\phi(t, \boldsymbol{X})$ is uniformly distributed over the domain of each unit element. The assumption made here is that the flow is gradually varying, which implies that the correlation length of the local hydraulic conductivity and specific storage fluctuations is smaller than the correlation length of hydraulic head fluctuations. The assumption of gradually varying flow has also been employed by Dagan (1982) and Kitanidis (1990). Because at large values of time m_0 is a position-independent constant, one can verify that

$$m_0 = \frac{1}{l_1 l_2 l_3} = \frac{1}{V_o} \tag{13}$$

and, consequently, integrating m_0 over the volume of a unit element yields the zero-order global moment

$$M_0 = 1 \tag{14}$$

The value of M_0 is one at all times because it was assumed that a 'unit' change in head above background piezometric head is caused by the slug of water injected into the formation (see initial condition (2)).

For $p = 1$ (first-order moments), Eq. (11) can be written as

$$\int_{V_o} S(\boldsymbol{x}) \frac{\partial \boldsymbol{m}_1}{\partial t} \mathrm{d}^3 \boldsymbol{x} = -\sum_i \int_{S_{+i}} [\![\boldsymbol{K}(\boldsymbol{x}) \cdot \nabla(\boldsymbol{x} m_0)]\!] \cdot \boldsymbol{n}_s \mathrm{d}s = 0 \tag{15}$$

where the local unit-element boundary condition (9b) has been employed. The second equality in (15) holds because the term $[\![\boldsymbol{K}(\boldsymbol{x}) \cdot \nabla(\boldsymbol{x} m_0)]\!] = m_0 [\![\boldsymbol{K}(\boldsymbol{x}) \cdot \nabla \boldsymbol{x}]\!] = m_0 [\![K(\boldsymbol{x})]\!]$ is equal to zero. We recall that $\boldsymbol{K}(\boldsymbol{x})$ is periodic, i.e. $\boldsymbol{K}(\boldsymbol{x}) = \boldsymbol{K}(\boldsymbol{x} + \boldsymbol{l}_i)$. The boundary conditions (9a) and 9(b) and Eq. (15) suggest that for large times a trial solution for $m_{1(i)}$, where the subscript in parentheses indicates the appropriate element of the vector $\boldsymbol{m}_1$, is of the form

$$m_{1(i)} = [-x_i + \Phi_i(\boldsymbol{x})] \frac{1}{V_o} \qquad (i = 1, 2, 3) \tag{16}$$

where $\Phi_i(\boldsymbol{x})$ is a function of the local coordinates with symmetric values on the boundary of the unit element; this function should be determined so that Eq. (15)

subject to conditions (9a) and 9(b) is satisfied. Employing Eqs. (5) and (16) yields the expression for the elements of the first global moment

$$M_{1(i)} = \left[-\frac{l_i}{2} + \overline{\Phi}_i \right] \tag{17}$$

where the overline indicates an average over the volume of a unit element.

To obtain the description of the first-order local moments, $\Phi_i(\boldsymbol{x})$ must be determined. As $\Phi_i(\boldsymbol{x})$ is periodic, it can be expanded into the following Fourier series:

$$\Phi_i(\boldsymbol{x}) = \overline{\Phi}_i + \Phi_i'(\boldsymbol{x}) = \overline{\Phi}_i + \sum_{\substack{\boldsymbol{b} \\ \boldsymbol{b}\neq \boldsymbol{0}}} \mu_i(\boldsymbol{b}) \exp[j2\pi \boldsymbol{x}\cdot\grave{\boldsymbol{b}}] \tag{18}$$

where the prime signifies fluctuations about the mean value, $j = (-1)^{1/2}$, $\boldsymbol{b}$ is a three-dimensional vector of integers, $\grave{\boldsymbol{b}} = (\grave{b}_1, \grave{b}_2, \grave{b}_3)^T = (b_1/l_1, b_2/l_2, b_3/l_3)^T$ and $\mu_i(\boldsymbol{b})$ is a scalar (Fourier coefficients) derived in Appendix A by the method of small perturbations or first-order approximation

$$\mu_i(\boldsymbol{b}) = \frac{-j}{2\pi} \left[\frac{\kappa_i(\boldsymbol{b})\cdot\grave{\boldsymbol{b}}}{\grave{\boldsymbol{b}}\cdot\overline{\boldsymbol{K}}\cdot\grave{\boldsymbol{b}}} \right] \tag{19}$$

$\kappa(\boldsymbol{b})$ is a symmetric dyadic of known coefficients of the Fourier series expansion of $\boldsymbol{K}(\boldsymbol{x})$ defined in (A4), and $\kappa_i(\boldsymbol{b})$ is the ith column of $\kappa(\boldsymbol{b})$. It should be noted that $\mu_i(\boldsymbol{b})$ is independent of the variability of the specific storage. Thus, $m_{1(i)}$ and $M_{1(i)}$ are also independent of the fluctuations of the specific storage and, as will be shown in the following section, the variability of the specific storage does not affect the effective hydraulic conductivity.

For $p = 2$ (second-order moments), Eq. (11) can be written as

$$\int_{V_o} S(\boldsymbol{x}) \frac{\partial \boldsymbol{m}_2}{\partial t} \mathrm{d}^3\boldsymbol{x} = \sum_i \int_{s_{+i}} \left[\!\left[\boldsymbol{K}(\boldsymbol{x})\cdot\nabla\left(\frac{\boldsymbol{m}_1\boldsymbol{m}_1}{m_0}\right) \right]\!\right] \cdot\boldsymbol{n}_s \mathrm{d}s \tag{20}$$

where the local unit-element jump boundary condition (10b) has been used. For the element $m_{2(ij)}$, where the double subscripts in parentheses indicate the corresponding element of the dyadic $\boldsymbol{m}_2$, Eq. (20) can be written as

$$\int_{V_o} S(\boldsymbol{x}) \frac{\partial m_{2(ij)}}{\partial t} \mathrm{d}^3\boldsymbol{x} = \int_{\partial V_o} \left[\boldsymbol{K}(\boldsymbol{x})\cdot\nabla\left(\frac{m_{1(i)}m_{1(j)}}{m_0}\right) \right] \cdot\boldsymbol{n}_s \mathrm{d}s$$

$$= [2\overline{K}_{ij} + \Theta_{ij} + \Theta_{ji}] \tag{21}$$

where the last formulation in the preceding equation is the consequence of employing (16) and (18) followed by integral evaluations,

$$\Theta_{ij} = -j2\pi \sum_{\substack{\boldsymbol{b} \\ \boldsymbol{b}\neq \boldsymbol{0}}} [\kappa_i^\dagger(\boldsymbol{b})\cdot\grave{\boldsymbol{b}}] \mu_j(\boldsymbol{b}) \tag{22}$$

and the exponent † denotes complex conjugation.

To determine the second global moment, we assume a trial solution for the $m_{2(ij)}$ entry of the dyadic $\boldsymbol{m}_2$ of the form

$$m_{2(ij)} = [G_{ij}t + H_{ij}(\boldsymbol{x})]\frac{1}{V_o} \tag{23}$$

where G_{ij} is a constant to be determined and $H_{ij}(\boldsymbol{x})$ is a function of the local coordinates. As will be shown in the next section, $H_{ij}(\boldsymbol{x})$ has no influence on the time derivative of $M_{2(ij)}$; thus, its exact form is not required for the determination of the desired effective parameters. The necessary term of the second local moment is evaluated by substitution of (23) into (21):

$$G_{ij} = \frac{1}{\overline{S}}[2\overline{K}_{ij} + \Theta_{ij} + \Theta_{ji}] \tag{24}$$

Therefore, the second global moment can be written as

$$M_{2(ij)} = \left[\frac{2\overline{K}_{ij}t}{\overline{S}} + (\Theta_{ij} + \Theta_{ji})\frac{t}{\overline{S}} + \overline{H}_{ij}\right] \tag{25}$$

where substitution of (24) into (23) followed by integration over the volume of a unit element have been employed. Now that the expressions for the zero-, first- and second-order global moments have been derived, the effective parameters for gradually varying flow in saturated porous media with spatially periodic hydraulic conductivity and specific storage can be obtained.

6. Effective parameters

Following the work of Brenner (1980a,b), one can show that the effective or macroscopic expression for the 'diffusion' dyadic $\boldsymbol{D}(\boldsymbol{x}) = \boldsymbol{K}(\boldsymbol{x})/S(\boldsymbol{x})$ can be defined as

$$\begin{aligned}\boldsymbol{D}^{\diamond} &= \frac{1}{2}\lim_{t\to\infty}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\boldsymbol{M}_2}{M_0} - \frac{\boldsymbol{M}_1\boldsymbol{M}_1}{M_0^2}\right)\\ &= \frac{1}{\overline{S}}\begin{pmatrix} K^{\bullet}_{xx} & K^{\bullet}_{xy} & K^{\bullet}_{xz}\\ K^{\bullet}_{yx} & K^{\bullet}_{yy} & K^{\bullet}_{yz}\\ K^{\bullet}_{zx} & K^{\bullet}_{zy} & K^{\bullet}_{zy}\end{pmatrix}\\ &= \frac{\boldsymbol{K}^{\diamond}}{S^{\diamond}}\end{aligned} \tag{26}$$

where the superscript diamond denotes an effective parameter and

$$\begin{aligned} K_{ij}^{\bullet} &= \overline{K}_{ij} + \frac{1}{2}(\Theta_{ij} + \Theta_{ji}) \\ &= \overline{K}_{ij} - \sum_{\substack{b \\ b \neq 0}} \frac{Re([\kappa_i^{\dagger}(\boldsymbol{b})\cdot\grave{\boldsymbol{b}}][\kappa_j^{\dagger}(\boldsymbol{b})\cdot\grave{\boldsymbol{b}}])}{\grave{\boldsymbol{b}}\cdot\overline{\boldsymbol{K}}\cdot\grave{\boldsymbol{b}}} \end{aligned} \tag{27}$$

where Re indicates the real part of a complex variable. It should be noted that the latter formulation in (26) is a consequence of employing (14), (17) and (25), whereas the latter expression in (27) is a consequence of employing (19), (22) and the identity $z_1^{\dagger}z_2 + z_2^{\dagger}z_1 = 2\mathrm{Re}(z_1^{\dagger}z_2)$, where z_1 and z_2 are complex variables. The coefficients $K_{ij}^{\bullet}$ consist of two terms: the first term is the average hydraulic conductivity coefficient, and the second term, which accounts for the local-scale variability, appears as a result of the homogenization or of averaging the spatially periodic hydraulic conductivity coefficient over the volume of a unit element. This second term incorporates known coefficients ($\kappa_i(\boldsymbol{b})$, the ith column of the dyadic $\kappa(\boldsymbol{b})$) of the Fourier expansion of the hydraulic conductivity fluctuations (see Eq. (A3)) and the matrix $\overline{\boldsymbol{K}}$. In view of (27), it is clear that $K_{ij}^{\bullet}$ is independent of the variability of the specific storage. Therefore, it is evident that the effective hydraulic conductivity coefficients are $K_{ij}^{\diamond} = K_{ij}^{\bullet}$ and the effective specific storage is $S^{\diamond} = \overline{S}$. These effective parameters are easily evaluated assuming that the hydraulic conductivity and specific storage of a saturated heterogeneous subsurface formation are deterministically known and periodic. It should be noted, however, that (27) is applicable to cases where the variability scales of the hydraulic conductivity are smaller than the periodicity. Furthermore, the effective parameters can be used in the macroscopic flow equation with constant coefficients to describe field-scale hydraulic head distributions.

The major assumptions associated with the derivation of (27) are that the subsurface formation is periodic and the exact variability in the periodic parameters is known. The spatially periodic model for heterogeneous subsurface formations employed in this investigation allows averaging of the local-scale variability, and is no more unrealistic than the frequently used infinite or semi-infinite models of porous formations (Van Genuchten et al., 1984; Goltz and Roberts, 1986; Chrysikopoulos et al., 1990). The assumption of exact knowledge of the variability may seem unrealistic, as such information is hardly ever available.

However, for the case of 'small' variance these assumptions can be relaxed and the previously derived results can be extended to stationary random porous media by the procedures of Van Lent and Kitanidis (1989). The stationary assumption is most suitable for stochastic functions characterized by the absence of well-defined trends and resembles the superposition of many waves of variable wavelength and displacement. Such processes are best described through spectra, which measure the amplitude and phase of the waves that form the variable parameter versus the wavelength. To obtain expressions for the effective hydraulic conductivity coefficients of a stationary porous formation, first, we define a covariance function of two columns of the matrix of hydraulic conductivity fluctuations, $\boldsymbol{k}_i'(\boldsymbol{x})$ and $\boldsymbol{k}_j'(\boldsymbol{x}+\boldsymbol{r})$, where

$\boldsymbol{k}_i'(\boldsymbol{x}) = [K_{1i}'(\boldsymbol{x}), K_{2i}'(\boldsymbol{x}), K_{3i}'(\boldsymbol{x})]^T$ and $\boldsymbol{r}$ is the separation vector, as

$$\begin{aligned} R_{k_i'k_j'}(\boldsymbol{r}) &= E[\boldsymbol{k}_i'(\boldsymbol{x})\boldsymbol{k}_j'(\boldsymbol{x}+\boldsymbol{r})] \\ &= \frac{1}{V_o}\int_{V_o} \sum_{\substack{\boldsymbol{d} \\ \boldsymbol{d}\neq\boldsymbol{0}}} \kappa_i(\boldsymbol{d}) \exp[j2\pi\boldsymbol{x}\cdot\grave{\boldsymbol{d}}] \sum_{\substack{\boldsymbol{b} \\ \boldsymbol{b}\neq\boldsymbol{0}}} \kappa_j(\boldsymbol{b}) \exp[j2\pi(\boldsymbol{x}+\boldsymbol{r})\cdot\grave{\boldsymbol{b}}]\mathrm{d}^3\boldsymbol{x} \\ &= \sum_{\substack{\boldsymbol{b} \\ \boldsymbol{b}\neq\boldsymbol{0}}} \kappa_i(-\boldsymbol{b})\kappa_j(\boldsymbol{b}) \exp[j2\pi\boldsymbol{r}\cdot\grave{\boldsymbol{b}}] \\ &= \sum_{\substack{\boldsymbol{b} \\ \boldsymbol{b}\neq\boldsymbol{0}}} \kappa_i^{\dagger}(\boldsymbol{b})\kappa_j(\boldsymbol{b}) \exp[j2\pi\boldsymbol{r}\cdot\grave{\boldsymbol{b}}] \end{aligned} \tag{28}$$

where $E[\ ]$ signifies ensemble mean or expected value, and the following identity was employed:

$$\frac{1}{V_o}\int_{V_o} \exp[j2\pi\boldsymbol{x}\cdot(\grave{\boldsymbol{b}}+\grave{\boldsymbol{d}})]\mathrm{d}^3\boldsymbol{x} = \begin{cases} 1 & \boldsymbol{b} = -\boldsymbol{d} \\ 0 & \boldsymbol{b} \neq -\boldsymbol{d} \end{cases} \tag{29}$$

It should be noted that $\kappa(\boldsymbol{b}) = \kappa^{\dagger}(-\boldsymbol{b})$. The latter formulation in (28) indicates that the derived covariance function is independent of the local spatial coordinates. Furthermore, by inspection we can deduce that the volume integral of a column of the matrix of the hydraulic conductivity fluctuations, expanded into an infinite series of complex exponentials, is equal to zero ($E[\boldsymbol{k}_i'(\boldsymbol{x})] = 0$) and $E[\boldsymbol{k}_i'(\boldsymbol{x})\boldsymbol{k}_j'(\boldsymbol{x}+\boldsymbol{r})] = R_{k_i'k_j'}(r)$. As $\boldsymbol{k}_i'(\boldsymbol{x})$ is a zero-mean function and its covariance depends only on the separation vector and not the actual spatial location, $\boldsymbol{k}_i'(\boldsymbol{x})$ is a stationary function. The covariance function $R_{k_i'k_j'}$ is periodic (see Eq. (28)); therefore, the discrete power spectrum of $\boldsymbol{k}_i'(\boldsymbol{x})$ and $\boldsymbol{k}_j'(\boldsymbol{x})$ is given by

$$\begin{aligned} P_{k_i'k_j'}(\boldsymbol{b}) &= \kappa_i^{\dagger}(\boldsymbol{b})\kappa_j(\boldsymbol{b}) \\ &= \frac{1}{V_o}\int_{V_o} R_{k_i'k_j'}(\boldsymbol{r}) \exp[-j2\pi\boldsymbol{r}\cdot\grave{\boldsymbol{b}}]\mathrm{d}^3\boldsymbol{r} \qquad (\boldsymbol{b} \neq 0) \end{aligned} \tag{30}$$

It should be noted that the discrete power spectrum $P_{k_i'k_j'}(\boldsymbol{b})$ is a dyadic, and $R_{k_i'k_j'}(\boldsymbol{r})$ and $P_{k_i'k_j'}(\boldsymbol{b})$ are a Fourier transform pair. Then, in view of (27) and (30), the ijth element of the effective hydraulic conductivity matrix is written as

$$K_{ij}^{\Diamond} = \overline{K}_{ij} - \sum_{\substack{\boldsymbol{b} \\ \boldsymbol{b}\neq\boldsymbol{0}}} \frac{\mathrm{Re}(\grave{\boldsymbol{b}}\cdot P_{k_i'k_j'}\cdot\grave{\boldsymbol{b}})}{\grave{\boldsymbol{b}}\cdot\overline{\boldsymbol{K}}\cdot\grave{\boldsymbol{b}}} \tag{31}$$

The advantage of the preceding formulation is that the effective hydraulic conductivity coefficients can be evaluated from the covariance function of the fluctuations of the hydraulic conductivity, which does not require the hydraulic conductivity matrix to be deterministically known, because there is an infinite number of functions with identical covariance functions.

Borrowing from the classical development of stochastic processes, where infinite domain solutions are obtained by first assuming a periodic system, and then taking the limit as period approaches infinity (Priestley, 1981), the results derived for the stationary but periodic hydraulic conductivity (Eq. (31)) can be extended to incorporate the case of stationary non-periodic or random subsurface formations. For this case, in the limit as the size of the unit element is increased without bound, the summations are replaced by an integral, and the variable $\boldsymbol{b}$ is no longer a discrete variable but a continuous variable. This is an important result, because the original and somewhat restrictive assumption of a periodic porous medium is relaxed.

7. Discussion

In this work, an expression for the effective diffusion coefficients $D_{ij}^{\Diamond}$ is derived (see Eq. (26)). Initially, it is assumed that the hydraulic conductivity and specific storage are deterministically known and periodic. Subsequently, expressions for the effective parameters are derived for the more general case of stationary periodic porous formations.

For the case where the hydraulic conductivity coefficient tensor is periodic in all three directions and can be expanded into a Fourier series (A3), it is shown that the effective specific storage is equal to its volume average $S^{\Diamond} = \overline{S}$ (26), and the effective hydraulic conductivity ($K_{ij}^{\Diamond} = K_{ij}^{\bullet}$) is equal to its volume average with an additional term accounting for the local-scale fluctuations within the unit element (27). Furthermore, it is concluded that the effective hydraulic conductivity is independent of the variability of the specific storage ($K_{ij}^{\bullet}$ defined in (27) is independent of S). This result is in general agreement with that of of Dagan (1982), who has employed small-perturbation analysis to show that the effective storage coefficient is equal to the arithmetic mean of the locally variable specific storage. For the special case where $S(\boldsymbol{x}) = \overline{S}$, the results of this work can be reduced to those presented by Kitanidis (1990), who has employed moment analysis to derive an integral form of the effective hydraulic conductivity, suitable for numerical approximations. For stationaryperiodic porous formations, the effective hydraulic conductivity is evaluated from the covariance function of the fluctuations of the hydraulic conductivity (31). This extension for the effective parameters is relatively important because the requirement for the hydraulic conductivity matrix to be deterministically known is relaxed.

The effective parameters derived in this work are valid for saturated, heterogeneous, three-dimensional periodic porous formations of compressible matrix, assuming that the fluctuations in hydraulic conductivity are 'small' with no restrictions on the variability of the specific storage coefficient. The range of applicability of the results remains to be explored.

Assuming that a heterogeneous subsurface formation macroscopically behaves like a homogeneous medium, the effective parameters derived in this work can be useful in describing the field (macroscopic) scale distribution of the hydraulic head. Thus, the governing macroscopic flow equation with constant coefficients is

$$S^{\diamond}\frac{\partial\bar{\phi}(t,\boldsymbol{X}_n)}{\partial t}=\nabla\cdot[\boldsymbol{K}^{\diamond}\cdot\nabla\bar{\phi}(t,\boldsymbol{X}_n)] \tag{32}$$

where $\bar{\phi}$ is the hydraulic head averaged over the volume of the unit element. The hydraulic head in the macroscopic flow equation is no longer a function of local coordinates. It should be noted that this issue can easily be overlooked and lead to a macroscopic flow equation with incorrect representation of the hydraulic head. Obviously, the variability of the hydraulic head at the local scale cannot be captured by the preceding effective flow equation.

8. Summary

Expressions for the effective specific storage and hydraulic conductivity dyadic were derived via Taylor–Aris–Brenner moment analysis. A three-dimensional heterogeneous porous medium with spatially periodic specific storage and hydraulic conductivity was considered. The periodic parameters were assumed to possess identical spatial periods in each principal direction of a Cartesian coordinate system. The domain was divided into rectangular unit elements with identical properties. Furthermore, the correlation length of the fluctuations of specific storage and hydraulic conductivity was assumed to be smaller than the correlation length of the hydraulic head, representing a gradually varying flow. It was shown that the effective specific storage is equal to its volume average, and the effective hydraulic conductivity is equal to its volume average plus a term expressing the effect of the locally variable hydraulic conductivity. No restrictions were imposed on the variability of the specific storage coefficient. The fluctuations of the hydraulic conductivity were assumed 'small' because of the perturbation method employed. It was shown that the spatial variability of the specific storage does not influence the effective hydraulic conductivity. This result is in agreement with that of Dagan (1982). The expression for the effective hydraulic conductivity was modified accordingly so that the case of stationary porous formations can also be included. For this important situation, instead of a deterministic knowledge of the variability of hydraulic conductivity, only its covariance function is required. This work complements the research by Dagan (1982), who has employed a stochastic approach, as well as the research by Kitanidis (1990), who has assumed a constant specific storage coefficient and focused on numerical techiques for the determination of the effective hydraulic conductivity.

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Appendix: derivation of the Fourier coefficients $\mu_i(\boldsymbol{b})$

Substituting (16) into (7), (9a) and 9(b) leads to the following set of partial differential equation and local jump conditions:

$$\nabla\cdot[\boldsymbol{K}(\boldsymbol{x})\cdot\nabla\Phi_i(\boldsymbol{x})] - \nabla\cdot\boldsymbol{k}_i(\boldsymbol{x}) = \boldsymbol{0} \tag{A1}$$

$$[\![\Phi_x(\boldsymbol{x})]\!] = 0, \qquad [\![\nabla\Phi_x(\boldsymbol{x})]\!] = 0 \tag{A2a,b}$$

where $\boldsymbol{k}_i(\boldsymbol{x})$ is the first column of the hydraulic conductivity coefficient tensor. As $\boldsymbol{K}(\boldsymbol{x})$ is periodic in all three directions, it can be expanded into the following Fourier series:

$$\boldsymbol{K}(\boldsymbol{x}) = \overline{\boldsymbol{K}} + \boldsymbol{K}'(\boldsymbol{x}) = \overline{\boldsymbol{K}} + \sum_{\substack{\boldsymbol{b}\\ \boldsymbol{b}\neq\boldsymbol{0}}} \kappa(\boldsymbol{b})\exp[j2\pi\boldsymbol{x}\cdot\grave{\boldsymbol{b}}] \tag{A3}$$

where the prime signifies fluctuations, $j = (-1)^{1/2}$, and $\kappa(\boldsymbol{b})$ is a symmetric matrix of known coefficients, given by

$$\kappa(\boldsymbol{b}) = \frac{1}{V_o}\int_{V_o} \boldsymbol{K}(\boldsymbol{x})\exp[-j2\pi\boldsymbol{x}\cdot\grave{\boldsymbol{b}}]\mathrm{d}^3\boldsymbol{x} \tag{A4}$$

It should be noted that $\kappa(\boldsymbol{b}) = \kappa^{\dagger}(-\boldsymbol{b})$.The solution of (A1) which satisfies (A2a) and (A2b) is

$$\Phi_i(\boldsymbol{x}) = \overline{\Phi}_i + \Phi_i'(\boldsymbol{x}) = \overline{\Phi}_i + \sum_{\substack{\boldsymbol{b}\\ \boldsymbol{b}\neq\boldsymbol{0}}} \mu_i(\boldsymbol{b})\exp[j2\pi\boldsymbol{x}\cdot\grave{\boldsymbol{b}}] \tag{A5}$$

where $\mu(\boldsymbol{b})$ is unknown. We can rewrite Eqs. (A3) and (A5) as

$$\boldsymbol{K}(\boldsymbol{x}) = \epsilon^0\overline{\boldsymbol{K}} + \epsilon^1\boldsymbol{K}'(\boldsymbol{x}), \qquad \Phi_i(\boldsymbol{x}) = \epsilon^0\overline{\Phi}_i + \epsilon^1\Phi_i'(\boldsymbol{x}) \tag{A6a,b}$$

where the superscript zero indicates zero-order terms, and the superscript one designates first-order terms. It should be noted that the introduction of ϵ is solely a mathematical artifice which permits separation of the 'small' high-order terms from the larger low-order terms, and bookkeeping of terms of the same order. Substituting (A6a) and (A6b) into the governing equation (A1) leads to

$$\nabla\cdot[(\epsilon^0\overline{\boldsymbol{K}} + \epsilon^1\boldsymbol{K}\prime(\boldsymbol{x}))\cdot\nabla(\epsilon^0\overline{\Phi}_i + \epsilon^1\Phi_i'(\boldsymbol{x}))] - \nabla\cdot(\epsilon^0\overline{\boldsymbol{k}}_i + \epsilon^1\boldsymbol{k}_i'(\boldsymbol{x})) = 0 \tag{A7}$$

This equation must be satisfied separately for terms of each order. Equating coefficients of ϵ^0 into Eq. (A7) yields

$$\nabla[\overline{\boldsymbol{K}}\cdot\nabla\overline{\Phi}_i] = 0 \tag{A8}$$

By inspection we can deduce that the preceding equation is satisfied, as $\overline{\Phi}_i$ is a constant. Equating coefficients of ϵ^1 into Eq. (A7) yields

$$\nabla\cdot[\overline{\boldsymbol{K}}\cdot\nabla\Phi_i'(\boldsymbol{x})] - \nabla\cdot\boldsymbol{k}_i'(\boldsymbol{x}) = 0 \tag{A9}$$

Employing Eqs. (A3) and (A5) in (A9) yields

$$\sum_{\substack{\boldsymbol{b}\\ \boldsymbol{b}\neq 0}}\{-[4\pi^2\grave{\boldsymbol{b}}\cdot\overline{\boldsymbol{K}}\cdot\grave{\boldsymbol{b}}]\mu_i(\boldsymbol{b}) - j2\pi\kappa_i(\boldsymbol{b})\cdot\grave{\boldsymbol{b}}\}\exp[j2\pi\boldsymbol{x}\cdot\grave{\boldsymbol{b}}] = 0 \tag{A10}$$

where $\kappa_i(\boldsymbol{b})$ is the ith column of the coefficient matrix $\kappa(\boldsymbol{b})$. As the complex exponentials form a complete orthogonal basis, the bracketed expressions in the previous equation must be zero for every $\boldsymbol{b} \neq 0$. Hence, it follows that

$$\mu_i(\boldsymbol{b}) = \frac{-j}{2\pi}\left(\frac{\kappa_i(\boldsymbol{b})\cdot\grave{\boldsymbol{b}}}{\grave{\boldsymbol{b}}\cdot\overline{\boldsymbol{K}}\cdot\grave{\boldsymbol{b}}}\right) \qquad (\boldsymbol{b}\neq 0) \tag{A11}$$

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