Upscaling and dispersion for transport in heterogeneous media

2004 J. Phys. A: Math. Gen. 37 9587

(http://iopscience.iop.org/0305-4470/37/40/018)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **37** (2004) 9587–9602 PII: S0305-4470(04)82121-8

Upscaling and dispersion for transport in heterogeneous media

Jens Eberhard

Interdisciplinary Center for Scientific Computing, University of Heidelberg,
Im Neuenheimer Feld 368, D-69120 Heidelberg, Germany

E-mail: jens.eberhard@iwr.uni-heidelberg.de

Received 11 June 2004, in final form 17 August 2004
Published 22 September 2004
Online at stacks.iop.org/JPhysA/37/9587
doi:10.1088/0305-4470/37/40/018

Abstract

This paper focuses on upscaling of the transport equation for heterogeneous porous media with random flow. We consider the local flow field being a stationary random field and develop an upscaling by the recently developed coarse graining method which is based on filtering procedures in Fourier space. The coarse graining method is used to obtain an upscaled dispersion tensor which depends on the given length scale of the upscaling. We give explicit results for the scale-dependent dispersion coefficient in lowest-order perturbation theory. For finite length scales the upscaled dispersion models the effect of the unresolved subscale flow fluctuations, and for a global upscaling the upscaled value agrees with the well-known macrodispersion coefficient, which is, however, nearly approached for length scales larger than tenfold of the correlation length.

PACS numbers: 05.10.Gg, 47.55.Mh

1. Introduction

Solute transport in porous media is usually dominated by the flow which involves multiple scales due to the heterogeneities of the media. To analyse the transport of dissolved pollutants in saturated aquifers stochastic models have become an invaluable tool, see [7, 12, 4]. In the stochastic approach the strong heterogeneities of the medium are modelled as a time-independent random field with given statistical properties. The characteristic large-scale behaviour then follows from appropriately defined averages over the ensemble of all possible aquifer realizations. The approach has been used in the past to determine ensemble-averaged dispersion coefficients as well as effective dispersion coefficients for the macroscopic scale behaviour, see e.g. [14, 13, 7, 12, 9]. However, the study of scale-dependent dispersion coefficients for transient transport with the help of the stochastic approach was rarely focused.

Besides the works [15, 16, 2], in which block-effective dispersion coefficients are formulated for transport simulations, there have been only small efforts to obtain upscaled dispersion coefficients that explicitly depend on the given length scale and, therefore, predict the scale transition from micro to macro scale. Since experimental results of macroscopic dispersion coefficients crucially depend on the resolution scale at which the measurements are done it is also important to study the impact of the resolution scale on the transport of a solute concentration distribution [6]. It is clear that in cases of upscaling to infinite length scales an appropriately defined scale-dependent dispersion coefficient should coincide with the ensemble-averaged dispersion coefficient given as the large-scale transport parameter, which is called macrodispersion, in the stochastic framework, see e.g. [9]. The importance of understanding how the transport equation depends on the resolution scale also becomes apparent when constructing numerical models with coarser resolution. Here, upscaling methods can be utilized to incorporate subgrid-scale information into the transport parameters of numerical models on coarser grids, see e.g. [11].

For the case of upscaling of fine-scale hydraulic conductivity fields there are innumerable works to determine effective conductivity coefficients on larger scales, see e.g. [18] for an overview. In that particular case the recently developed coarse graining method proved very useful, see [5, 3, 10]. This method was introduced for upscaling the hydraulic conductivity of porous media and succeeded in describing the flow equation on coarser resolution scales. As shown in [10], the method predicts the scale-dependent transition for the effective conductivity tensor correctly. Further, the method is very successful when applied in numerical methods and applications like multigrid methods, see [11].

For the present study we use the theoretical concept given by the coarse graining method to scale up the time-dependent transport process given by the convection–diffusion equation. We utilize the method for upscaling the heterogeneous flow fluctuations and focus on scale-dependent dispersion coefficients which arise from the upscaling of the heterogeneous flow in the case of transient transport in saturated media. For finite length scales the resulting upscaled dispersion coefficient models the effect of the unresolved subscale flow fluctuations, and for an infinite length scale, also termed global upscaling, the upscaled value agrees with the well-known macrodispersion coefficient from the literature.

The paper is organized as follows. The next section is devoted to the transport model and the stochastic modelling. In section 3 we describe the coarse graining method and derive the upscaled transport equation. Section 4 gives explicit results for the upscaled dispersion tensor by a perturbation theory, and it comprises the discussion of the results. The last section concludes with a summary.

2. The model

2.1. Transport equation

The steady-state process of a solute in a heterogeneous porous medium is given by a convection–diffusion equation (see, e.g. [7, 12])

$$\frac{\partial}{\partial t}c(x,t) + \nabla \cdot (u(x)c(x,t)) - \nabla \cdot D\nabla c(x,t) = \rho(x)\delta(t) \qquad (1)$$

where $c(x,t)$ is the spatial concentration of the mobile solute. Because of spatial fluctuations in the local hydraulic conductivity of the medium the flow velocity $u(x)$ varies locally as given by Darcy's law. However, as a consequence of the incompressibility of the fluid, it fulfils $\nabla \cdot u(x) = 0$. The tensor D is the local diffusion tensor which includes all dispersion effects due to fluctuations on microscopic scales. Its general structure is discussed in [17]. Due to its dependence on the flow, D is a spatially fluctuating quantity. However, the consideration of this dependence only yields negligible contributions to the transport parameters, see e.g. [13]. We assume a constant local diffusion tensor which is of diagonal form, $D_{ij} = D_{ii}\delta_{ij}$. The right-hand side $\rho(x)$ of equation (1) is a source or sink term.

In the framework of the second-order perturbation theory used to obtain explicit results, the dispersion coefficient is completely determined by the mean value and the two-point correlation function of the random flow field.

2.2. Correlation function

In the stochastic approach the spatially inhomogeneous distribution $u(x)$ in the given aquifer is identified with one single realization of a spatial stochastic process defined by the ensemble of all possible realizations. We assume this process to be statistically translation invariant in space. It implies that the ensemble average $\overline{u(x)}$ does not depend on the spatial position x. The over-bar always stands for the average over the ensemble. We split the flow field into a deterministic and a random contribution,

$$u(x) = \overline{u} - w(x) \tag{2}$$

where $\overline{u} = \overline{u(x)}$ is the constant averaged flow velocity and $w(x)$ is the random fluctuation field about the mean value. Without loss of generality the mean flow is aligned with the x_1-direction, that is, $\overline{u}_i = u_0\delta_{1i}$.

For a Gaussian random field the flow contribution $w_i(x)$ is a random function with zero mean. Following [13] we define

$$\overline{\hat{w}_i(k)\hat{w}_j(k')} = (2\pi)^d\delta(k+k')u_0^2 p_i(k)p_j(k)\hat{C}(k), \tag{3}$$

where the Fourier transform is defined by $\hat{g}(k,t) = \int \exp(-\mathrm{i}k\cdot x)g(x,t)\,\mathrm{d}^d x$ and $g(x,t) = \int_k \mathrm{e}^{\mathrm{i}k\cdot x}\hat{g}(k,t)$. As a convenient shorthand notation we use $\int_k \ldots \equiv (2\pi)^{-d}\int \mathrm{d}^d k \ldots$.

The function $\hat{C}(k)$ in (3) is the autocorrelation spectrum of the log-hydraulic conductivity of the heterogeneous media. The approach is mathematically well-defined subject to some additional requirements for C that can be found e.g. in [12]. The particular functional form of C is to some extent arbitrary. Reflecting the situation in a heterogeneous aquifer it should drop to zero sharply for lengths larger than the correlation length scales l_i. We choose a Gauss-shaped function for C. Thus the autocorrelation spectrum $\hat{C}(k)$ is given by

$$\hat{C}(k) = q_0(2\pi)^{d/2}\prod_{i=1}^{d} l_i \exp\left(-\frac{k_i^2 l_i^2}{2}\right). \tag{4}$$

The variance q_0 measures the strength of the heterogeneities, and l_i, $i = 1,\ldots,d$, denotes the correlation length of the field in the direction of x_i. In the anisotropic case two or more correlation lengths are unequal. For an isotropically correlated field the lengths l_i are equally denoted by l_0. In that case, the correlation function merely depends on the distance $|x - x'|$ of the two points.

The functions $p_i(k)$ in (3) are projectors which ensure the incompressibility of the fluid. In a d-dimensional system ($d \geqslant 2$), they are given by $p_i(k) = \delta_{1i} - k_1k_i/k^2$, $i = 1,\ldots,d$, see [13]. The autocorrelation functions of the components of the flow field then read according to [13]

$$\overline{w_i(x)w_j(x')} = u_0^2\int_k \exp(\mathrm{i}k\cdot(x-x'))p_i(k)p_j(k)\hat{C}(k).$$

3. The coarse graining method

In the following we develop the upscaling for the transport equation using the coarse graining technique. The coarse graining method was developed and applied in [3, 10] to scale up the flow equation with a given heterogeneous hydraulic conductivity field. The upscaling is based on filtering in Fourier space, i.e. high oscillatory modes are eliminated by cutting off the function values of the Fourier transform for large wave vectors.

In the case of upscaling the transport process the coarse graining method results in an upscaled transport equation on larger scales starting from the transport process with the fine-scale flow. The method does not model the fine-scale heterogeneity up to a given length scale λ explicitly, but models the influences of the subscale fluctuations by a scale-dependent upscaled dispersion coefficient. The upscaled coefficient incorporates the impact of the unresolved fine-scale flow fluctuations. In the following, we denote the coarser length scale by λ and apply Einstein's sum convention.

3.1. Coarse graining for the transport equation

The starting point of the coarse graining method is the transport equation (1) that in Fourier space reads

$$\frac{\partial}{\partial t}\hat{c}(k,t) + (\mathrm{i}\overline{u}_j + k_m D_{mj})k_j\hat{c}(k,t) = \delta(t)\hat{\rho}(k) + \int_{k'} \hat{W}(k,k-k')\hat{c}(k',t), \tag{5}$$

using the definition $\hat{W}(k,k') := \mathrm{i}k_j\hat{w}_j(k')$ and applying $\sum_{j=1}^{d} k_j\hat{w}_j(k) = 0$ due to the incompressibility. For $\hat{w}(k) \equiv 0$ and a point-like injection, that is $\hat{\rho}(k) = 1$, the solution of (5) denoted by $\hat{c}^0$ reads

$$\hat{c}^0(k,t) = \Theta(t)\exp(-k_m D_{mj}k_j t - \mathrm{i}k_j\overline{u}_j t)$$

where $\Theta(t)$ denotes the Heaviside step function, see [1]. Due to its variations the flow field $u : \mathbb{R}^d \to \mathbb{R}^d, x \mapsto u_i(x), i = 1,\ldots,d$, is assumed to be a realization of a scalar random field with mean $\overline{u}_i$ and fluctuations $w_i(x)$ as given by (2). As boundary conditions we choose zero boundary conditions at infinity.

Equation (5) is transformed for an arbitrary $\hat{\rho}$ into the equivalent integral equation,

$$\hat{c}(k,t) = \hat{c}^0(k,t)\hat{\rho}(k) + \int_{-\infty}^{\infty}\mathrm{d}t'\hat{c}^0(k,t-t')\int_{k'}\hat{W}(k,k-k')\hat{c}(k',t'). \tag{6}$$

Definition 1. *We introduce projections P^+ and P^- for cutting off low and high frequency modes in Fourier space:*

$$P^+_{\lambda,k}(\hat{c}(k,t)) := \begin{cases}\hat{c}(k,t) & \text{if } |k_i| > a_s/\lambda \text{ for an } i \in \{1,\ldots,d\}\\ 0 & \text{otherwise,}\end{cases}$$

$$P^-_{\lambda,k}(\hat{c}(k,t)) := \begin{cases}\hat{c}(k,t) & \text{if } |k_i| \leqslant a_s/\lambda \text{ for all } i \in \{1,\ldots,d\}\\ 0 & \text{otherwise,}\end{cases}$$

where $P^+_{\lambda,k}\big(P^+_{\lambda,k}(\hat{c}(k,t))\big) = P^+_{\lambda,k}(\hat{c}(k,t))$, and for $P^-_{\lambda,k}$ analogously. The parameter $a_s \geqslant 1$ is a constant. If it is possible we will omit the index λ respectively k in the following, and use $P^+_{\lambda,k,k'}(\hat{g}(k,k',t))$ instead of $P^+_{\lambda,k}\big(P^+_{\lambda,k'}(\hat{g}(k,k',t))\big)$ for a function $\hat{g}$ that depends on two Fourier variables.

Definition 2. *We define an integral operator $\mathcal{A}(k,t)$ by*

$$\mathcal{A}(k,t)[f(k,t)] := \int_{-\infty}^{\infty}\hat{c}^0(k,t-t')f(k,t')\,\mathrm{d}t'.$$

So we immediately obtain for the solution $\hat{c}(k,t)$ due to (6):

$$\hat{c}(k,t) = \mathcal{A}(k,t)[\delta(t)\hat{\rho}(k)] + \mathcal{A}(k,t)\left[\int_{k'} \hat{W}(k, k-k')\hat{c}(k',t)\right].$$

The inverse operator of $\mathcal{A}(k,t)$ is therefore given by $(\mathcal{A}(k,t))^{-1} = \partial/\partial t + (\mathrm{i}\overline{u}_j + k_m D_{mj})k_j$ which yields due to the transport equation

$$(\mathcal{A}(k,t))^{-1}[\hat{c}(k,t)] = \delta(t)\hat{\rho}(k) + \int_{k'} \hat{W}(k, k-k')\hat{c}(k',t). \tag{7}$$

Due to the definition of the projections P_k^+ and P_k^-, the integral operator $\mathcal{A}(k,t)$ and its inverse operator commutate both with P_k^+ and P_k^-, respectively. That means that the equality

$$P_k^+(\mathcal{A}(k,t)[f(k)]) - \mathcal{A}(k,t)\big[P_k^+(f(k))\big] = 0$$

and the corresponding equality for P_k^- holds true. Using the defined projections we easily get

$$P_{\lambda,k}^+(\hat{c}(k,t)) = P_{\lambda,k}^+(\mathcal{A}(k,t)[\delta(t)\hat{\rho}(k)]) + P_{\lambda,k}^+\left(\mathcal{A}(k,t)\left[\int_{k'} \hat{W}(k, k-k')\hat{c}(k',t)\right]\right) \tag{8}$$

and the analogous expression for $P_{\lambda,k}^-(\hat{c}(k,t))$. We split the Fourier transform of c by the projections, that is, $\hat{c}(k,t) = P_\lambda^-(\hat{c}(k,t)) + P_\lambda^+(\hat{c}(k,t))$. Inserting this identity into the integral of (8) the expression for $P_\lambda^-(\hat{c}(k,t))$ and $P_\lambda^+(\hat{c}(k,t))$ are coupled with each other. Now, the idea is to derive a closed expression for $P_\lambda^-(\hat{c}(k,t))$ involving merely the low frequency components. This can be achieved by substituting $P_\lambda^+(\hat{c}(k,t))$ in the analogous expression to (8) for $P_\lambda^-(\hat{c}(k,t))$. Therefore, we define operators $\mathcal{L}$ and $\mathcal{R}$ by

Definition 3.

$$\begin{aligned}
\mathcal{L}\hat{c} &:= \int L(k,k',t)\hat{c}(k',t)\,\mathrm{d}^d k' \\
&:= \int ((\mathcal{A}(k',t))^{-1}[\delta(k-k')] - \hat{W}(k, k-k'))\hat{c}(k',t)\,\mathrm{d}^d k' \\
\mathcal{R}\hat{c} &:= \int \hat{W}(k, k-k')\hat{c}(k',t)\,\mathrm{d}^d k'.
\end{aligned}$$

With the aid of equation (6), we have $\hat{c}(k,t) = \mathcal{A}(k,t)[\delta(t)\hat{\rho}(k) + \mathcal{R}\hat{c}(k,t)]$ and $\mathcal{L}\hat{c} = \hat{\rho}(k)\delta(t)$ which both lead to

$$\mathcal{L}\hat{c} = (\mathcal{A}(k,t))^{-1}[\hat{c}(k,t)] - \mathcal{R}\hat{c}(k,t). \tag{9}$$

Furthermore, we obtain for $P^-(\hat{c})$ and $P^+(\hat{c})$:

$$\begin{aligned}
P^-(\hat{c}) &= P^-(\mathcal{A}(k,t)[\delta(t)\hat{\rho}(k)] + \mathcal{A}(k,t)[\mathcal{R}\hat{c}(k,t)]) \\
&= P^-(\mathcal{A}(k,t)[\delta(t)\hat{\rho}(k)] + \mathcal{A}(k,t)[\mathcal{R}(P^-(\hat{c}(k,t)) + P^+(\hat{c}(k,t)))]),
\end{aligned} \tag{10}$$

$$P^+(\hat{c}) = P^+(\mathcal{A}(k,t)[\delta(t)\hat{\rho}(k)] + \mathcal{A}(k,t)[\mathcal{R}(P^-(\hat{c}(k,t)) + P^+(\hat{c}(k,t)))]). \tag{11}$$

Further we assume that Green's function $\hat{G}(k,k',t,t')$ of the transport equation in Fourier space exists. Due to the definition of $(\mathcal{A}(k,t))^{-1}$ and (7), $\hat{G}(k,k',t,t')$ fulfils the integral equation

$$\int ((\mathcal{A}(k'',t))^{-1}[\delta(k-k'')] - \hat{W}(k, k-k''))\hat{G}(k'',k',t,t')\,\mathrm{d}^d k'' = \delta(k+k')\delta(t-t'). \tag{12}$$

As a result $\hat{G}(k, k', t, t')$ is merely a function of $t - t'$, and for vanishing flow fluctuations $\hat{w} \equiv 0$, that is $\hat{W} \equiv 0$, $\hat{G}$ is simply given by $\hat{G}(k, k', t - t') = \delta(k + k')\hat{c}^0(k, t - t')$. Consequently, we get for the function $L(k, k'', t)$ given by definition 3 using (12)

$$\int L(k, k'', t)\hat{G}(k'', k', t' - t'')\, \mathrm{d}^d k'' \mathrm{d}t'' = \delta(k + k')\delta(t - t'). \tag{13}$$

Thus the inverse of L, which fulfils (13) with right-hand side $(2\pi)^{-2d}\delta(k - k')\delta(t)$, can be written as $L^{-1}(k, k', t) := (2\pi)^{-2d}\hat{G}(k, -k', t)$. Further, Green's function, $P^+_{\lambda,k'}(\hat{G}(k, k', t - t'))$, of the transport equation in Fourier space projected on high frequencies solves due to (12):

$$\int P^+_{\lambda,k}((\mathcal{A}(k'', t))^{-1}[\delta(k - k'')] - \hat{W}(k, k - k''))P^+_{\lambda,k'}(\hat{G}(k'', k', t - t'))\, \mathrm{d}^d k''$$
$$= P^+_{\lambda,k,k'}(\delta(k + k'))\delta(t - t').$$

Thus, the definition of L yields

$$\int P^+_{\lambda,k}(L(k, k'', t))P^+_{\lambda,k'}(\hat{G}(k'', k', t' - t''))\, \mathrm{d}^d k''\, \mathrm{d}t'' = P^+_{\lambda,k,k'}(\delta(k + k'))\delta(t - t'),$$

and the inverse of $P^+_{\lambda,k}(L(k, k'', t))$ is given by

$$\left(P^+_{\lambda,k'}(L(k'', k', t))\right)^{-1} := (2\pi)^{-2d} P^+_{\lambda,k'}(\hat{G}(k'', -k', t - t')).$$

By that we define the operator $(P^+\mathcal{L})^{-1}$.

Definition 4.

$$(P^+\mathcal{L})^{-1}\hat{c} := \int \left(P^+_{\lambda,k'}(L(k, k', t))\right)^{-1}\hat{c}(k', t')\, \mathrm{d}^d k'\, \mathrm{d}t'$$
$$= (2\pi)^{-2d}\int_0^t \mathrm{d}t' \int P^+_{\lambda,k'}(\hat{G}(k, -k', t - t'))\hat{c}(k', t')\, \mathrm{d}^d k'.$$

Now, equation (11) leads to

$$P^+((\mathcal{A}(k, t))^{-1}[\hat{c}]) = P^+(\delta(t)\hat{\rho}(k)) + P^+(\mathcal{R}(P^-(\hat{c}(k, t)) + P^+(\hat{c}(k, t))))$$

and, applying the operator $\mathcal{L}$ and equation (9), to

$$P^+(\mathcal{L}P^+(\hat{c})) = P^+((\mathcal{A}(k, t))^{-1}[P^+(\hat{c})] - \mathcal{R}P^+(\hat{c}))$$
$$= P^+(\delta(t)\hat{\rho}(k)) + P^+(\mathcal{R}(P^-(\hat{c}(k, t)))). \tag{14}$$

With the inverse operator $(P^+\mathcal{L})^{-1}$ and (14) we can rewrite the solution $P^+(\hat{c})$ of the transport equation as

$$P^+(\hat{c}(k, t)) = P^+((P^+\mathcal{L})^{-1}P^+(\delta(t)\hat{\rho}(k)) + (P^+\mathcal{L})^{-1}P^+(\mathcal{R}P^-(\hat{c}(k, t)))).$$

Hence, we suceeded in formulating $P^+(\hat{c})$ in terms of the solution $P^-(\hat{c})$. $P^+(\hat{c})$ can be substituted into (10) to obtain a closed expression for $P^-(\hat{c})$:

$$P^-(\hat{c}) = P^-(\mathcal{A}(k, t)[\delta(t)\hat{\rho}(k)]) + P^-(\mathcal{A}(k, t)[\mathcal{R}(P^-(\hat{c}(k, t)))])$$
$$+ P^-(\mathcal{A}(k, t)[\mathcal{R}(P^+(\hat{c}(k, t)))])$$
$$= P^-(\mathcal{A}(k, t)[\delta(t)\hat{\rho}(k)] + \mathcal{A}(k, t)[\mathcal{R}(P^-(\hat{c}(k, t)))])$$
$$+ P^-(\mathcal{A}(k, t)[\mathcal{R}P^+((P^+\mathcal{L})^{-1}P^+(\delta(t)\hat{\rho}(k)))])$$
$$+ P^-(\mathcal{A}(k, t)[\mathcal{R}P^+((P^+\mathcal{L})^{-1}P^+(\mathcal{R}P^-(\hat{c}(k, t))))]). \tag{15}$$

According to the last equation in (15) we can split the solution $P^-(\hat{c})$ into two parts:

$$P^-_k(\hat{c}(k, t)) = \mathcal{A}(k, t)[S(k, t)] + \mathcal{A}(k, t)[Q(k, t)] \tag{16}$$

where

$$S(k,t) := P_k^-\left(\delta(t)\hat{\rho}(k) + \int_{k'} \hat{W}(k,k-k')P_{k'}^-(\hat{c}(k',t))\right),$$

and $Q(k,t) := Q_1(k,t) + Q_2(k,t)$, with the functions

$$\begin{aligned} Q_1(k,t) &:= P_k^-\left(\int R(k,k')P_{k'}^+\left(\int \left(P_{k''}^+(L(k',k''))\right)^{-1} P_{k''}^+(\hat{\rho}(k''))\,\mathrm{d}^d k''\right)\mathrm{d}^d k'\right) \\ &= (2\pi)^{-2d} P_k^-\left(\int \hat{W}(k,k-k')P_{k'}^+\left(\int\int_0^t \mathrm{d}t'\,P_{k''}^+(\hat{G}(k',-k'',t-t'))\right.\right. \\ &\quad \left.\left.\times\,\hat{\rho}(k'')\delta(t')\,\mathrm{d}^d k''\right)\mathrm{d}^d k'\right) \end{aligned} \tag{17}$$

and

$$\begin{aligned} Q_2(k,t) &:= P_k^-\left(\int R(k,k')P_{k'}^+\left(\int \left(P_{k''}^+(L(k',k''))\right)^{-1}\right.\right. \\ &\quad \left.\left.\times\,P_{k''}^+\left(\int R(k'',k''')P_{k'''}^-(\hat{c}(k'''))\,\mathrm{d}^d k'''\right)\mathrm{d}^d k''\right)\mathrm{d}^d k'\right) \\ &= (2\pi)^{-2d} P_k^-\left(\int \hat{W}(k,k-k')P_{k'}^+\left(\int\int_0^t \mathrm{d}t'\,P_{k''}^+(\hat{G}(k',-k'',t-t'))\right.\right. \\ &\quad \left.\left.\times\int \hat{W}(k'',k''-k''')P_{k'''}^-(\hat{c}(k''',t'))\,\mathrm{d}^d k'''\,\mathrm{d}^d k''\right)\mathrm{d}^d k'\right). \end{aligned}$$

The function $S(k,t)$ in (16) results from the influence of small wave vectors k. Whereas $Q(k,t)$ incorporates the influence of the high frequency components.

The function $Q_1(k,t)$ vanishes if the source fulfils $\hat{\rho}(k) \equiv 0$. Further, it vanishes in the cases of source terms $\rho(x)$ which do not include any short wave components. As the source term is usually given by experiments it normally includes only contributions varying on scales larger than λ. Thus, the condition

$$\hat{\rho}(k) := P_{\lambda,k}^-(F(k)) \tag{18}$$

is reasonable where $F(k)$ is a suitable function. We assume that $\hat{\rho}$ fulfils (18) in the following. Inserting $P_{k''}^+(\hat{\rho}(k'')) \equiv 0$ into (17) we obtain $Q_1(k,t) \equiv 0$.

For further simplification we assume that the influence of subscale fluctuations given by $Q(k,t)$ is well approximated by the ensemble average of Q. Hence, $Q(k,t)$ is given by the mean $\overline{Q_2(k,t)}$ and (16) can be reduced to

$$P_k^-((\mathcal{A}(k,t))^{-1}[\hat{c}(k,t)]) = S(k,t) + \overline{Q_2(k,t)}, \tag{19}$$

where $\overline{Q_2(k,t)}$ is given by

$$\begin{aligned} \overline{Q_2(k,t)} &= (2\pi)^{-2d} P_k^-\left(\int_0^t \mathrm{d}t'\right. \\ &\quad \left.\times\int \overline{\mathrm{i}k_j\hat{w}_j(k-k')P_{k',k''}^+(\hat{G}(k',-k'',t-t'))\mathrm{i}k_m\hat{w}_m(k''-k)P_k^-(\hat{c}(k,t'))}\,\mathrm{d}^d k''\,\mathrm{d}^d k'\right) \end{aligned}$$

using $\hat{W}(k,k') = \mathrm{i}k_j\hat{w}_j(k')$ and the translation invariance in Fourier space, $k - k''' = 0$, induced by the ensemble average. Further, we approximate $\hat{c}(k,t')$ in $\overline{Q_2(k,t)}$ by the leading-order term given by a Taylor expansion in time. $\overline{Q_2(k,t)}$ is thus approximately given by

$$\begin{aligned} \overline{Q_2(k,t)} &= (2\pi)^{-2d} P_k^-\left(\mathrm{i}k_j\int_0^t \mathrm{d}t'\right. \\ &\quad \left.\times\int \overline{\hat{w}_j(k-k')P_{k',k''}^+(\hat{G}(k',-k'',t-t'))\hat{w}_m(k''-k)}\,\mathrm{d}^d k''\,\mathrm{d}^d k'\,\mathrm{i}k_m\hat{c}(k,t)\right). \end{aligned}$$

With the following definition of $\delta D^*_{jm}(k, t, \lambda)$,

$$\delta D^*_{jm}(k, t, \lambda) := \frac{1}{(2\pi)^{2d}} \int_0^t \mathrm{d}t' \times \int \overline{\hat{w}_j(k - k') P^+_{k',k''}(\hat{G}(k', -k'', t - t'))\hat{w}_m(k'' - k)}\, \mathrm{d}^d k''\, \mathrm{d}^d k',$$

the function $\overline{Q_2(k,t)}$ can now be rewritten in the form

$$\overline{Q_2(k,t)} = P_k^-(\mathrm{i}k_i \delta D^*_{ij}(k, t, \lambda)\mathrm{i}k_j \hat{c}(k, t)). \tag{20}$$

The so-defined $\delta D^*(k, t, \lambda)$ can be understood as a scale-dependent upscaled dispersion tensor. It is induced by subscale heterogeneities varying on length scales smaller than λ. Finally, we obtain due to (19) and (20)

$$P_k^-((\mathcal{A}(k,t))^{-1}[\hat{c}(k,t)]) = P_k^-\left(\delta(t)\hat{\rho}(k) + \int_{k'} \hat{W}(k, k - k') P_{k'}^-(\hat{c}(k', t))\right) + P_k^-(\mathrm{i}k_i \delta D^*_{ij}(k, t, \lambda)\mathrm{i}k_j \hat{c}(k, t)), \tag{21}$$

therein $\delta D^*(k, t, \lambda)$ corresponds to a non-local term in real space. It can be localized by setting $k = 0$. An approximation such as $\delta D^*(k) \approx \delta D^*(k = 0)$ improves for increasing λ due to the projection $P^-_{\lambda,k}$ in (21). For a global upscaling, i.e. $\lambda \to \infty$, the localization becomes exact. Thus we approximate $\delta D^*(k, t, \lambda)$ in $P_k^-(\mathrm{i}k_i \delta D^*_{ij}(k, t, \lambda)\mathrm{i}k_j \hat{c}(k, t))$ by its value for $k = 0$, and we neglect the correction terms arising from $\delta D^*(k) - \delta D^*(k = 0)$. It turns out an upscaled transport equation for the given length scale λ

$$\frac{\partial}{\partial t} P_k^-(\hat{c}(k,t)) + (\mathrm{i}\overline{u}_j + k_m D^*_{mj}(t, \lambda))k_j P_k^-(\hat{c}(k,t)) = \delta(t) P_k^-(\hat{\rho}(k)) + P_k^-\left(\int_{k'} \hat{W}(k, k - k') P_{k'}^-(\hat{c}(k', t))\right) \tag{22}$$

which includes an upscaled dispersion tensor:

Definition 5 (Upscaled dispersion tensor)**.**

$$D^*_{ij}(t, \lambda) := D_{ij} + \delta D^*_{ij}(0, t, \lambda) = D_{ij} + \frac{1}{(2\pi)^{2d}} \int_0^t \mathrm{d}t' \times \int \overline{\hat{w}_i(-k') P^+_{\lambda,k'}\left(P^+_{\lambda,k''}(\hat{G}(k', -k'', t'))\hat{w}_j(k'')\right)}\, \mathrm{d}^d k''\, \mathrm{d}^d k'. \tag{23}$$

3.2. Upscaled transport equation

The upscaled transport equation derived by (22) for the scale λ yields in real space

$$\frac{\partial}{\partial t} c_\lambda(x,t) + \nabla \cdot ((\overline{u} - w(x)|_\lambda) c_\lambda(x,t)) - \nabla \cdot D^*(t,\lambda)\nabla c_\lambda(x,t) = \rho(x)|_\lambda \delta(t),$$

where $w(x)|_\lambda$ and $\rho(x)|_\lambda$ are the inverse Fourier transforms of the filtered quantities $P^-_{\lambda,k}(\hat{w}(k))$ and $P^-_{\lambda,k}(\hat{\rho}(k))$, and $c_\lambda(x,t)$ is the solution on the length scale λ.

The upscaled transport equation and the upscaled dispersion tensor D^* are the main results of the coarse graining method. Further, equation (22) equals the original equation (5) in Fourier space for $\lambda = 0$. In this case, $Q(k,t) \equiv 0$ is valid due to the projectors P^+ in $Q(k,t)$. Thus we have $P_k^-(\mathcal{A}(k,t)^{-1}[\hat{c}(k,t)]) = S(k,t)$ and $D^*(t, 0) = D$. Even in the hyperbolic case where the local diffusion tensor vanishes, $D = 0$, i.e. the convection solely governs the transport of the plume, the coarse graining method yields a finite upscaled dispersion $D^*(t, \lambda)$.

The result for $D^*(t, \lambda)$ given by the coarse graining method can be compared with the block-effective macrodispersion coefficient derived by a subgrid variability approach in the recent works of Rubin *et al* [16, 15]. Unlike the coarse graining method their approach is guided by the idea of upscaling homogenized areas or numerical grid blocks to fulfil the demand for such blocks by numerical models. The corresponding expression for the scale-dependent dispersion tensor in [16], cf equations (37) and (38), agrees with the coarse graining result when considering the time-dependent leading-order approximation of the Green's function $\hat{G}$. The length scale λ corresponds to the block or grid spacing used in these studies. Rubin *et al* only give analytical results for the case of planar flow defined by an exponential log-conductivity covariance. Whereas we derive analytical expressions for the upscaled dispersion coefficient also for a general anisotropic model in d space dimensions.

4. Results for the upscaled dispersion coefficient

4.1. Results for a smooth cut-off function

Explicit results for $D^*(t, \lambda)$ can be obtained using a perturbative expansion for Green's function $\hat{G}$ in equation (23). We calculate $D^*(t, \lambda)$ in lowest-order perturbation theory for a smooth cut-off function instead of the sharp projection of definition 1, as often done in the literature, see for instance [3, 5].

Definition 6. *We define the integration*

$$\int P^+_{\lambda,k}(f(k))\,\mathrm{d}^d k \quad by \quad \int \left(1 - \exp\left(-\tfrac{k^2\lambda^2}{2a_w^2}\right)\right) f(k)\,\mathrm{d}^d k,$$

with a constant $a_w \geqslant 1$.

4.2. Lowest-order perturbation theory

Here, we consider the general case of full anisotropy in d spatial dimensions and calculate the diagonal components of $D^*(t, \lambda)$. In lowest-order perturbation theory we obtain for Green's function

$$\hat{G}(k, -k', t) = \delta(k - k')\Theta(t)\exp(-k_m D_{mj} k_j t - \mathrm{i} k_j \overline{u}_j t)$$

with summing up over the indices j and m. As shown in appendix A, the expressions of the dispersion coefficients can be rewritten for the smooth projector P^+ as given by definition 6 in the form

$$D^*_{ii}(t, \lambda) = D_{ii} + u_0 l_1 M_i(t/\tau_u; 0, \ldots, 0) - u_0 l_1 M_i\left(t/\tau_u; \frac{\lambda^2}{2a_w l_1^2}, \ldots, \frac{\lambda^2}{2a_w l_d^2}\right). \tag{24}$$

For a d-dimensional system the functions M_i are defined by

$$M_i(T; b_1, \ldots, b_d) := \left(\prod_{n=1}^{d} l_n^{-1}\right) \int_\kappa \int_0^T \mathrm{d}\tau \exp\left(-\sum_{n=1}^{d} \kappa_n^2 b_n\right) \times \exp\left(-\sum_{n=1}^{d} \epsilon_n \kappa_n^2 \tau - \mathrm{i}\kappa_1 \tau\right) p_i^2\left(\frac{\kappa_1}{l_1}, \ldots, \frac{\kappa_d}{l_d}\right) \hat{C}\left(\frac{\kappa_1}{l_1}, \ldots, \frac{\kappa_d}{l_d}\right), \tag{25}$$

with $\kappa_i = l_i k_i$ and inverse Peclet numbers $\epsilon_i := \frac{D_{ii}}{u_0 l_i}\frac{l_1}{l_i}$, $i = 1, \ldots, d$. The functions M_i can be found in the theoretical study of Dentz *et al* [9] for the macrodispersion coefficient. The constant $\tau_u := l_1/u_0$ defines the characteristic advective timescale. Due to (24) it holds $D^*_{ii}(t, \lambda) = D_{ii}$ for $\lambda = 0$.

From Dentz *et al* we already know the second-order perturbative result for the ensemble-averaged macrodispersion coefficient denoted by $D^{\mathrm{ens}}(t)$, see [9], cf equation (45):

$$D_{ii}^{\mathrm{ens}}(t) = D_{ii} + u_0 l_1 M_i(t/\tau_u; 0, \ldots, 0).$$

The result for the upscaled dispersion coefficient agrees with the macrodispersion in the limit of upscaling to infinite length scales as shown in appendix A, that is,

$$\lim_{\lambda\to\infty} D_{ii}^*(t, \lambda) = D_{ii}^{\mathrm{ens}}(t).$$

In the case of stationary transport, the upscaled dispersion tensor is given by $\lim_{t\to\infty} D^*(t, \lambda)$ which can be simplified for the isotropic model, see below.

4.3. Isotropic model

We start with the result for the simplified case of a model with an isotropic disorder correlation function as well as an isotropic local dispersion tensor, that is, $l_1 = l_2 = \cdots = l_d = l_0$ in (4) and $D_{ij} = D\delta_{ij}$. As a result, one has two different characteristic timescales: the advective one, $\tau_u = l_0/u_0$, and a dispersive timescale $\tau_D := l_0^2 \big/ D$, as discussed e.g. in [4]. The ratio between the advective and the dispersive timescales defines the inverse Peclet number $\epsilon = \tau_u/\tau_D = D/u_0 l_0$. For a realistic situation one expects $\epsilon \ll 1$ [13], so the two scales are well separated, $\tau_D \gg \tau_u$.

For a Gauss-shaped disorder correlation function all integral expressions generated by the second-order expansion can be evaluated explicitly in space dimension $d = 3$. As shown in the following, the $d = 3$ result simplifies considerably in the limiting case of a finite but small inverse Peclet number, $\epsilon \ll 1$, which is the most relevant case for all practical purposes [12, 9], and times $t/\tau_u \gg 1$.

The fact that it is possible to evaluate the perturbation theory integral expressions in closed form actually is a lucky but nongeneric situation. For the given Gauss-shaped disorder correlation function it is possible only for the case of odd space dimensions. For $d = 2$ the expressions do not reduce to standard integrals at all. However, it is still possible to extract the leading behaviour in the small-ϵ case in the more general situations where it is no longer possible to evaluate the integrations completely, see appendix C.

4.3.1. Temporal and scale-dependent behaviour. In the advective time regime $t < \tau_u$ the ensemble-averaged quantity has a restricted meaning with respect to properties found in one given realization as the behaviour depends sensitively on the particular microscopic structure of this aquifer, see e.g. [9]. We therefore concentrate on the more relevant time regime $t \gtrsim \tau_u$.

Figure 1 shows the temporal behaviour of the upscaled dispersion coefficient for times $t \geqslant 0.1\tau_u$ for different values of the length scale λ. The plot follows from the explicit second-order results for M_i for $d = 3$ in the isotropic model given in appendix B. It shows that the upscaled dispersion coefficients tend to the macrodispersion result D^{ens} for increasing length scales λ. For finite length scales the upscaled dispersion stays below the global upscaled result since the low frequency parts of the flow fluctuations are still modelled explicitly, compare figure 1. However, D^* approaches the macrodispersion coefficient D^{ens}, and for $\lambda/l_0 = 10$ the relative deviation between the quantities is less than 1.1%.

In figure 2 the scale-dependent behaviour of $D_{11}^*(\lambda)$ is depicted for various time steps t/τ_u and isotropic correlation. It clearly demonstrates the increase of D_{11}^* with growing length scale and travel time t. For very large times the upscaled dispersion coefficient again tends to the macrodispersion coefficent D^{ens}.

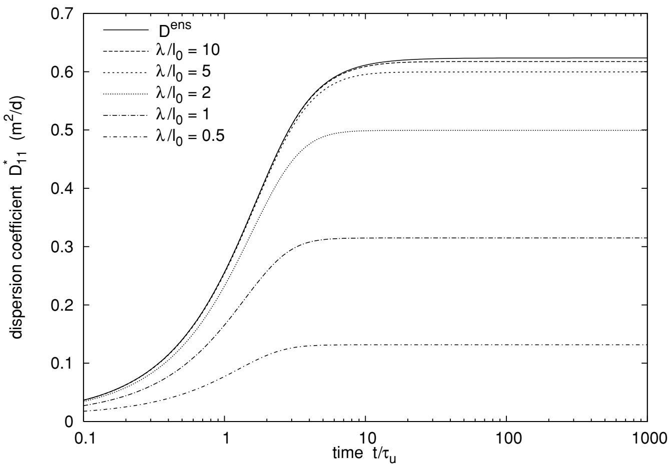

Figure 1. Temporal behaviour of the longitudinal upscaled dispersion coefficient $D^*_{11}(t, \lambda)$ as given by the explicit second-order result for $\epsilon = \tau_u/\tau_D = 0.01$ with variance $q_0 = 0.5$ in the isotropic case. The length scale λ/l_0 varies from 0.5 to 10 ($u_0 = 1m/d, l_0 = 1m$). D^{ens} denotes the longitudinal macrodispersion coefficient.

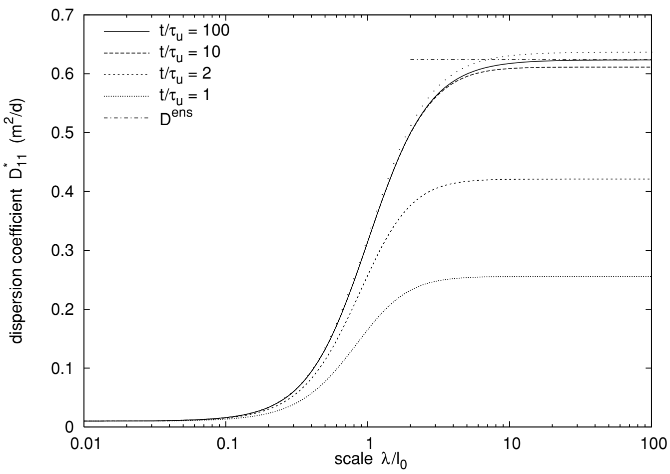

Figure 2. Scale-dependent behaviour of the longitudinal dispersion coefficient $D^*_{11}(t, \lambda)$ given by the result of the second-order perturbation theory for $\epsilon = 0.01$ and variance $q_0 = 0.5$ for the isotropic model. The dotted line shows the corresponding behaviour of the upscaled dispersion coefficient derived from the small-ϵ approximation for $t/\tau_u \gg 1$ discussed in the text. D^{ens} indicates the macrodispersion result for $t/\tau_u = 100$.

In the given second-order approach one finds for the upscaled dispersion in the stationary case

$$D_{ii} + u_0 l_0 \lim_{t\to\infty} M_i(t/\tau_u; 0, 0, 0) - u_0 l_0 \lim_{t\to\infty} M_i\left(t/\tau_u; \frac{\lambda^2}{2a_w l_0^2}, \frac{\lambda^2}{2a_w l_0^2}, \frac{\lambda^2}{2a_w l_0^2}\right)$$

where the explicit expressions of the functions $\lim_{T\to\infty} M_i(T; b, b, b)$ can be found in appendix B. Further, we find for the isotropic model in the given second-order approach for $\lambda \to \infty$:

$$\lim_{\lambda\to\infty}\lim_{t\to\infty} D^*_{11}(t,\lambda) = D + q_0u_0l_0\sqrt{\frac{\pi}{2}}\left(1 - 8\epsilon^4 \exp\left(\frac{1}{2\epsilon^2}\right)\operatorname{erfc}\left(\frac{1}{\sqrt{2\epsilon^2}}\right)\right.$$
$$\left. + 8\epsilon^4 - \epsilon^3\frac{16}{\sqrt{2\pi}} + 4\epsilon^2 - \epsilon\frac{16}{3\sqrt{2\pi}}\right),$$

where $\operatorname{erfc}(x)$ denotes the error function as defined by [1]. It agrees with the result for the macrodispersion coefficient for $t \to \infty$, $\lim_{t\to\infty} D^{\rm ens}_{11}(t)$, see [9] equation (50). In the limiting case of a vanishing inverse Peclet number, that is, $\epsilon = 0$ (i.e., $D = 0$), it reduces to the standard result given by Gelhar and Axness [13] and Dagan [8] for the global upscaling,

$$\lim_{\epsilon\to 0}\lim_{\lambda\to\infty}\lim_{t\to\infty} D^*_{11}(\lambda) = D + q_0u_0l_0\sqrt{\pi/2}.$$

4.3.2. Asymptotic expansion for small inverse Peclet numbers. The explicit result given in appendix B for the dispersion coefficients in a three-dimensional model can be simplified considerably in the limit of a small inverse Peclet number. In that limiting case it is also possible to derive the leading behaviour of the perturbation theory expression in the case of arbitrary space dimensions where a full explicit evaluation of the integral expression is no longer possible. For a d-dimensional model we find for times $t \gg \tau_u$ and for small $\epsilon_i \ll 1$

$$M_1(t/\tau_u; b_1, \ldots, b_d) = q_0\sqrt{\pi/2}\prod_{j>1}^{d}(1+2b_j)^{-1/2} + \cdots, \qquad (26)$$

see appendix C.

To illustrate the quality of the approximation, we included the leading small-ϵ result for $d = 3$ to the plot in figure 2. The dotted line shows the leading small-ϵ approximation result for $D^*_{11}(t,\lambda)$ as given by (26). As figure 2 demonstrates, the asymptotic expansion used to evaluate the leading behaviour is not only valid in a mathematically asymptotic sense, it also yields quantitatively reliable results for $t/\tau_u \gg 1$ in the relevant parameter range for realistic values of λ.

4.4. Anisotropic case

In the anisotropic case the functions M_i which define the upscaled dispersion coefficient $D^*(\lambda)$ no longer reduce to standard functions. In the practically most relevant case of small $\epsilon_i \ll 1$ we obtain (26) as an asymptotic result for the function M_1 in a d-dimensional system for the case $t/\tau_u \gg 1$. Using this asymptotic evaluation of the perturbation theory expression, we are able to derive the temporal behaviour of the transport coefficients for anisotropic models.

In figure 3 the result for $D^*_{11}(t,\lambda)$ is plotted for cases of different correlation lengths. The plot shows that the larger the ratio l_2/l_1 of the correlation lengths, the more delayed the increase of the upscaled dispersion coefficient. This is due to the stronger longitudinal mixing caused by the flow heterogeneities which results in a weaker upscaling of the subscale fluctuations for a given length scale. Accordingly, the increase of the longitudinal upscaled dispersion coefficient is shifted to larger scales.

5. Summary

The study aims at developing a new upscaling method for solute transport in heterogeneous porous media. Upscaling for the transient transport process reveals the temporal and scale-dependent behaviour of the transport parameters.

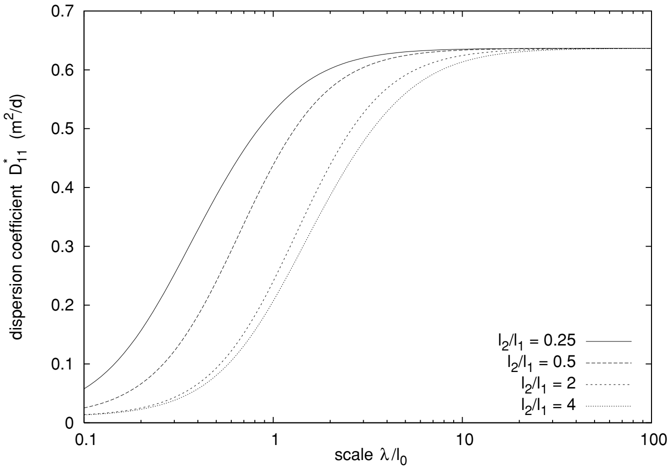

Figure 3. Scale-dependent behaviour of the upscaled longitudinal dispersion coefficient $D^*_{11}(t, \lambda)$ for different anisotropies with variance $q_0 = 0.5$ $(t/\tau_u = 100, u_0 = 1m/d, l_1 = l_3 = 1m)$.

We introduce the coarse graining method for upscaling the flow field which varies over many length scales induced by the heterogeneities of the hydraulic conductivity. The coarse graining method scales the flow fluctuations on an arbitrary length scale λ by introducing an upscaled dispersion tensor $D^*(t, \lambda)$ in the transport equation. The upscaled dispersion incorporates the impact of the subscale fluctuations which are not resolved. The method relies on a stochastic modelling for the flow field. For a global upscaling, that is, $\lambda \to \infty$, the resulting dispersion coefficient agrees with the known result for the macrodispersion D^{ens} given by the second-order perturbation expansion. For finite scales the upscaled coefficient models the effect of the unresolved subscale flow fluctuations and remains below D^{ens}. However, D^{ens} is almost nearly approached by D^* for length scales $\lambda/l_0 \geqslant 10$.

On the basis of the result for the upscaled dispersion tensor given by the coarse graining it might be possible to develop a numerical method for a local upscaling of the flow fluctuations. This could be done similar to the numerical upscaling in the case of the flow equation as done in [10]. Therein the numerically upscaled coefficient is obtained by the solution of an auxiliary partial differential equation similar to the flow equation.

Appendix A. Result for the upscaled dispersion tensor

The result for the upscaled dispersion coefficient $\delta D^*(0, t, \lambda)$ of a d-dimensional system with diagonal local diffusion D is given by the coarse graining method as

$$\delta D^*_{ii}(0, t, \lambda) = (2\pi)^{-2d} \int_0^t \mathrm{d}t' \int \overline{\hat{w}_i(-k)\hat{w}_i(k') P^+_{k,k'}(\hat{G}(k, -k', t'))}\, \mathrm{d}^d k'\, \mathrm{d}^d k$$

$$= (2\pi)^{-d/2} u_0^2 q_0 \int_0^t \mathrm{d}t' \int \mathrm{d}^d k (p_i(k))^2 \left(\prod_{m=1}^{d} l_m \exp\left(-\frac{1}{2} k_m^2 l_m^2\right)\right)$$

$$\times P^+_{k,\lambda} \left(\exp\left(-t' \sum_{m=1}^{d} \left(\mathrm{i}\overline{u}_m k_m + \sum_{n=1}^{d} k_m D_{mn} k_n \right)\right)\right)$$

$$= (2\pi)^{-d/2} u_0^2 q_0 \int_0^t \mathrm{d}t' \int \mathrm{d}^d k (p_i(k))^2 \left(\prod_{m=1}^{d} l_m \exp\left(-\frac{1}{2} k_m^2 l_m^2 \right) \right)$$
$$\times \left(1 - \exp\left(-\frac{k^2 \lambda^2}{2a_w} \right) \right) \exp\left(-t' \sum_{m=1}^{d} \left(\mathrm{i}\overline{u}_m k_m + \sum_{n=1}^{d} k_m D_{mn} k_n \right) \right)$$
$$= (2\pi)^{-d/2} q_0 u_0 l_1 \int_0^{t/\tau_u} \mathrm{d}t' \int \mathrm{d}^d k \left(p_i \left(\tfrac{k_1}{l_1}, \ldots, \tfrac{k_d}{l_d} \right) \right)^2 \exp\left(-\frac{1}{2} \sum_{m=1}^{d} k_m^2 \right)$$
$$\times \left(1 - \exp\left(-\frac{\lambda^2}{2a_w} \sum_{m=1}^{d} \frac{k_m^2}{l_m^2} \right) \right) \exp\left(-\mathrm{i}t' k_1 - \sum_{m=1}^{d} t' \epsilon_m k_m^2 \right)$$
$$= u_0 l_1 M_i(t/\tau_u; 0, \ldots, 0) - u_0 l_1 M_i \left(t/\tau_u; \frac{\lambda^2}{2a_w l_1^2}, \ldots, \frac{\lambda^2}{2a_w l_d^2} \right).$$

The functions M_i are defined by (25).

For infinite length scale λ the projectors vanish in the integration for δD^*. Thus, $\lim_{\lambda\to\infty} \delta D_{ii}^*(0, t, \lambda)$ is given by

$$\lim_{\lambda\to\infty} \delta D_{ii}^*(0, t, \lambda) = (2\pi)^{-d/2} u_0^2 q_0 \int_0^t \mathrm{d}t' \int \mathrm{d}^d k (p_i(k))^2 \left(\prod_{m=1}^{d} l_m \exp\left(-\frac{1}{2} k_m^2 l_m^2 \right) \right)$$
$$\times \exp\left(-t' \sum_{m=1}^{d} \left(\mathrm{i}\overline{u}_m k_m + \sum_{n=1}^{d} k_m D_{mn} k_n \right) \right)$$
$$= (2\pi)^{-d/2} q_0 u_0 l_1 \int_0^{t/\tau_u} \mathrm{d}t' \int \mathrm{d}^d k \left(p_i \left(\tfrac{k_1}{l_1}, \ldots, \tfrac{k_d}{l_d} \right) \right)^2$$
$$\times \exp\left(-\frac{1}{2} \sum_{m=1}^{d} k_m^2 \right) \exp\left(-\mathrm{i}t' k_1 - \sum_{m=1}^{d} t' \epsilon_m k_m^2 \right)$$
$$= u_0 l_1 M_i(t/\tau_u; 0, \ldots, 0).$$

Appendix B. Explicit results for $d = 3$

In the case of an isotropic velocity spectrum, that is, $l_1 = l_2 = l_3 = l_0$ in (4), and an isotropic local diffusion tensor D, the perturbation theory expression (24) for the dispersion coefficient can be evaluated explicitly, see also [9]. The functions M_i given by (25), which determine the final result (with $b_1 = b_2 = b_3 = b$ in the isotropic case), read

$$M_1(T; b, b, b) = q_0 \sqrt{\pi/2} (1 + 2b)^{-1} \left(\operatorname{erf}(g(T)) + \frac{1}{\sqrt{\pi}} \exp(-g^2(T)) \right.$$
$$\times \left(\frac{1}{g(T)} + 4\Lambda^2 \frac{f(T)}{g^2(T)} - \frac{3}{2} \frac{1}{g^3(T)} \right) + \operatorname{erf}(g(T))$$
$$\times \left(4\Lambda^2 \frac{f(T)}{g(T)} - \frac{1}{g^2(T)} + \frac{3}{4} \frac{1}{g^4(T)} - 2\Lambda^2 \frac{f(T)}{g^3(T)} + 8\Lambda^4 \frac{f(T)}{g(T)} \right)$$
$$\left. - 8\Lambda^4 \exp\left(\frac{1}{2\Lambda^2} \right) \left(\operatorname{erfc}\left(\frac{1}{\sqrt{2}\Lambda} \right) - \operatorname{erfc}(f(T)) \right) - \frac{4\sqrt{8}}{3\sqrt{\pi}} \Lambda - \frac{4\sqrt{8}}{\sqrt{\pi}} \Lambda^3 \right),$$

$$M_2(T;b,b,b) = M_3(T;b,b,b) = q_0\sqrt{\pi/8}(1+2b)^{-1}$$
$$\times\left(\frac{1}{2\sqrt{\pi}}\exp(-g^2(T))\left(\frac{3}{g^3(T)} - \frac{8\Lambda^2 f(T)}{g^2(T)}\right) + \mathrm{erf}(g(T))\left(\frac{1}{2g^2(T)}\right.\right.$$
$$\left.\left. - \frac{2\Lambda^2 f(T)}{g(T)} - \frac{3}{4g^4(T)} - \frac{8\Lambda^4 f(T)}{g(T)} + \frac{2\Lambda^2 f(T)}{g^3(T)}\right) - \exp\left(\frac{1}{2\Lambda^2}\right)\right.$$
$$\left.\times\left(\mathrm{erfc}(f(T)) - \mathrm{erfc}\left(\frac{1}{\sqrt{2}\Lambda}\right)\right)(8\Lambda^4 - 2\Lambda^2) + \frac{\sqrt{8}\Lambda}{3\sqrt{\pi}} + \frac{4\sqrt{8}\Lambda^3}{\sqrt{\pi}}\right),$$

with $\Lambda = \epsilon(1+2b)^{-1/2}$ and

$$f(t) = \frac{1}{\sqrt{2}}\frac{(1+2b)\epsilon^{-1} + t/\tau_u}{\sqrt{(1+2b)+2t/\tau_D}}, \qquad g(t) = \frac{1}{\sqrt{2}}\frac{t/\tau_u}{\sqrt{(1+2b)+2t/\tau_D}}$$

where $\tau_u = l_0/u_0$ and $\tau_D = l_0^2/D$. The explicit results for M_i are already given by Dentz *et al* [9], see for $M_i^-(T;b,b,b)$ therein.

For the case of $T\to\infty$ in the stationary case, we obtain the expressions

$$\lim_{T\to\infty} M_1(T;b,b,b) = q_0\sqrt{\pi/2}(1+2b)^{-1}$$
$$\times\left(1 + 4\Lambda^2 + 8\Lambda^4 - 8\Lambda^4\exp\left(\frac{1}{2\Lambda^2}\right)\mathrm{erfc}\left(\frac{1}{\sqrt{2}\Lambda}\right) - \frac{4\sqrt{8}}{3\sqrt{\pi}}\Lambda - \frac{4\sqrt{8}}{\sqrt{\pi}}\Lambda^3\right)$$

and

$$\lim_{T\to\infty} M_2(T;b,b,b) = \lim_{T\to\infty} M_3(T;b,b,b) = q_0\sqrt{\pi/8}(1+2b)^{-1}$$
$$\times\left(-2\Lambda^2 - 8\Lambda^4 + \exp\left(\frac{1}{2\Lambda^2}\right)\mathrm{erfc}\left(\frac{1}{\sqrt{2}\Lambda}\right)(8\Lambda^4 - 2\Lambda^2) + \frac{\sqrt{8}\Lambda}{3\sqrt{\pi}} + \frac{4\sqrt{8}\Lambda^3}{\sqrt{\pi}}\right).$$

Appendix C. Leading behaviour for small inverse Peclet numbers

For two spatial dimensions, $d = 2$, or a model with anisotropic local diffusion tensor and disorder correlation function, the integrations which define the upscaled dispersion coefficients in the second-order perturbation theory no longer reduce to standard functions. Nevertheless it is possible to evaluate their leading behaviour in the practically most relevant case of small inverse Peclet numbers ϵ_i for times $t \gg \tau_u$, using the Gaussian correlation spectrum. The upscaled dispersion D^* is determined by the functions $M_i(T;b_1,\ldots,b_d)$ given by (25). To evaluate these functions further, we expand the exponential function $\exp\left(-\sum_{n=1}^d \epsilon_n\kappa_n^2\tau\right)$ in the integrand of (25) into its power series,

$$M_i(T;b_1,\ldots,b_d) = q_0(2\pi)^{d/2}\int_0^T \mathrm{d}\tau\int_\kappa\left(1 - \sum_{n=1}^d \epsilon_n\kappa_n^2\tau + \cdots\right)$$
$$\times\exp\left(-\sum_{n=1}^d (b_n + 1/2)\kappa_n^2\right)\exp(\mathrm{i}\kappa_1\tau)p_i^2\left(\frac{\kappa_1}{l_1},\ldots,\frac{\kappa_d}{l_d}\right).$$

The resulting expressions can be evaluated further for $t \gg \tau_u$. As shown in [9] a detailed investigation for the case of widely separated scales, i.e. $\epsilon_n \ll 1$, yields for $t \gg \tau_u$ and $i = 1$ the leading part of the auxiliary function M_1 to be

$$M_1(t/\tau_u;b_1,\ldots,b_d) = q_0\sqrt{\pi/2}\prod_{j>1}^d (1+2b_j)^{-1/2} + \cdots,$$

where the dots indicate subleading corrections which are of the order of $O(\epsilon)$ and of the order of $O((t/\tau_u)^{-(d-1)})$ or which are already exponentially small on the advective timescale. The result yields $M_1(t/\tau_u; 0, \ldots, 0) = q_0\sqrt{\pi/2} + \cdots$.

For $i = 2, \ldots, d$, that is, for the contributions to the transversal dispersion coefficient, one finds that the remaining integral is of the order of $(t/\tau_u)^{-(d-1)}$ because of the special form of the projectors p_i in this case. For $t \gg \tau_u$ one gets only negligibly small corrections to the transversal dispersion coefficient in this time regime. As is well-known from the literature, this is a general feature of a second-order treatment for the transversal dispersion coefficient.

References

[1] Abramowitz M 1972 *Handbook of Mathematical Functions* (New York: Dover)

[2] Ahmadi A, Aigueperse A and Quintard M 2001 Calculation of the effective properties describing active dispersion in porous media: from simple to complex unit cells. *Adv. Water Res.* **24** 423–38

[3] Attinger S 2003 Generalized coarse graining procedures for flow in porous media *Comput. Geosci.* **7** 253–73

[4] Attinger S, Dentz M, Kinzelbach H and Kinzelbach W 1999 Temporal behaviour of a solute cloud in a chemically heterogeneous porous medium *J. Fluid Mech.* **386** 77–104

[5] Attinger S, Eberhard J and Neuss N 2002 Filtering procedures for flow in heterogeneous porous media: numerical results *Comput. Visual. Sci.* **5** 67–72

[6] Beckie R 2001 A comparison of methods to determine measurement support volumes *Water Resour. Res.* **37** 925–36

[7] Dagan G 1989 *Flow and Transport in Porous Formations* (Berlin: Springer)

[8] Dagan G 1994 An exact nonlinear correction to transverse macrodispersivity for transport in heterogeneous formations *Water Resour. Res.* **30** 2699–705

[9] Dentz M, Kinzelbach H, Attinger S and Kinzelbach W 2000 Temporal behavior of a solute cloud in a heterogeneous porous medium: 1. Point-like injection *Water Resour. Res.* **36** 3591–604

[10] Eberhard J, Attinger S and Wittum G 2004 Coarse graining for upscaling of flow in heterogeneous porous media *Multiscale Model. Simul.* **2** 269–301

[11] Eberhard J and Wittum G 2004 A coarsening multigrid method for flow in heterogeneous porous media *Multiscale Methods in Science and Engineering (Lecture Notes in Computational Science and Engineering)* ed B Engquist and P Lötstedt (Heidelberg: Springer)

[12] Gelhar L W 1993 *Stochastic Subsurface Hydrology* (Englewood Cliffs, NJ: Prentice-Hall)

[13] Gelhar L W and Axness C L 1983 Three-dimensional stochastic analysis of macrodispersion in aquifers *Water Resources Res.* **19** 161–80

[14] Gelhar L W, Gutjahr A L and Naff R L 1979 Stochastic analysis of macrodispersion in a stratified aquifer *Water Resources Res.* **15** 1387–97

[15] Rubin Y, Bellin A and Lawrence A E 2003 On the use of block-effective macrodispersion for numerical simulations of transport in heterogeneous formations *Water Resources Res.* **39** 4.1–4.10

[16] Rubin Y, Sun A, Maxwell R and Bellin A 1999 The concept of block-effective macrodispersivity and a unified approach for grid-scale- and plume-scale-dependent transport *J. Fluid Mech.* **395** 161–80

[17] Scheidegger A E 1961 General theory of dispersion in porous media *J. Geophys. Res.* **66** 3273–8

[18] Wen X-H and Gomez-Hernandez J J 1996 Upscaling hydraulic conductivities in heterogeneous media: an overview *J. Hydrol.* **183** ix–xxxii