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Transient flow in bounded randomly heterogeneous domains
1. Exact conditional moment equations and recursive approximations

Daniel M. Tartakovsky[1] and Shlomo P. Neuman

Department of Hydrology and Water Resources, The University of Arizona, Tucson

Abstract. We consider the effect of measuring randomly varying local hydraulic conductivities $K(\mathbf{x})$ on one's ability to predict transient flow within bounded domains, driven by random sources, initial head, and boundary conditions. Our aim is to allow optimum unbiased prediction of local hydraulic heads $h(\mathbf{x}, t)$ and Darcy fluxes $\mathbf{q}(\mathbf{x}, t)$ by means of their ensemble moments, $\langle h(\mathbf{x}, t)\rangle_c$ and $\langle \mathbf{q}(\mathbf{x}, t)\rangle_c$, conditioned on measurements of $K(\mathbf{x})$. We show that these predictors satisfy a compact deterministic flow equation which contains a space-time integrodifferential "residual flux" term. This term renders $\langle \mathbf{q}(\mathbf{x}, t)\rangle_c$ nonlocal and non-Darcian so that the concept of effective hydraulic conductivity looses meaning in all but a few special cases. Instead, the residual flux contains kernels that constitute nonlocal parameters in space-time that are additionally conditional on hydraulic conductivity data and thus nonunique. The kernels include symmetric and nonsymmetric second-rank tensors as well as vectors. We also develop nonlocal equations for second conditional moments of head and flux which constitute measures of predictive uncertainty. The nonlocal expressions cannot be evaluated directly without either a closure approximation or high-resolution conditional Monte Carlo simulation. To render our theory workable, we develop recursive closure approximations for the moment equations through expansion in powers of a small parameter which represents the standard estimation error of natural log $K(\mathbf{x})$. These approximations are valid to arbitrary order for either mildly heterogeneous or well-conditioned strongly heterogeneous media. They allow, in principle, evaluating the conditional moments numerically on relatively coarse grids, without upscaling, by standard methods such as finite elements.

1. Introduction

Neuman and Orr [1993] and *Neuman et al.* [1996] developed an exact nonlocal formalism for the prediction of steady state flow in randomly heterogeneous geologic media by conditional moments under the action of uncertain forcing terms (sources and boundary conditions). They started from the premise that Darcy's law applies locally, at some support scale ω, which need not constitute a representative elementary volume (REV) in any traditional sense of the term. Their only requirement was that all quantities of interest (volume flux, hydraulic gradient, hydraulic conductivity, and forcing terms) be measurable in principle, directly or indirectly, on the scale ω at each point in the flow domain. They further postulated that given measurements of the local hydraulic conductivity $K(\mathbf{x})$ at a sufficiently large number of points $\mathbf{x}$ in space, one should be able to obtain an optimum unbiased estimate of its spatial distribution throughout the domain of interest by evaluating geostatistically its conditional ensemble mean (expectation) function $\langle K(\mathbf{x})\rangle_c$, as well as the conditional variance-covariance of the associated estimation error. To render corresponding predictions of hydraulic head $h(\mathbf{x})$ and Darcy flux $\mathbf{q}(\mathbf{x})$ on the scale ω, one option is to conduct numerical Monte Carlo simulations on a fine computational grid with cells of size ω (so as to resolve spatial fluctuations of correspondingly high frequencies) and then average the results so as to obtain the conditional ensemble mean functions $\langle h(\mathbf{x})\rangle_c$ and $\langle \mathbf{q}(\mathbf{x})\rangle_c$ of head and flux on the scale ω, as well as the conditional variance-covariance of the associated prediction errors. Another option is to compute these optimum ω-scale predictors of head and flux and to assess their prediction error variance-covariance directly. To allow this, Neuman and Orr derived an integrodifferential equation that is satisfied exactly by the predictors $\langle h(\mathbf{x})\rangle_c$ and $\langle \mathbf{q}(\mathbf{x})\rangle_c$, and explicit expressions for the corresponding second conditional moments. Their conditional mean flow equation contains a residual flux term which is nonlocal and therefore non-Darcian. To evaluate this term without high-resolution conditional Monte Carlo simulation requires a closure approximation; the same is true about the explicit second moment expressions. Neuman and Orr explored the conditions under which a local ensemble mean form of Darcy's law would hold, so as to allow defining a corresponding effective hydraulic conductivity, and proposed a weak approximation to deal with the more general nonlocal problem of predicting flow. The purpose of this paper is to present (1) a complementary nonlocal theoretical framework for transient flow, (2) implicit equations for the second conditional ensemble moment of hydraulic heads, which we show have an advantage over explicit equations of the kind developed for

[1]Now at Geoanalysis Group, Earth and Environmental Sciences Division, Los Alamos National Laboratory, Los Alamos, New Mexico.

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steady state by Neuman and Orr, and (3) an alternative to the weak approximation proposed by these authors.

Our aim is to allow optimum unbiased prediction of local hydraulic heads $h(\mathbf{x}, t)$ and Darcy fluxes $\mathbf{q}(\mathbf{x}, t)$ by means of their ensemble moments, $\langle h(\mathbf{x}, t)\rangle_c$ and $\langle \mathbf{q}(\mathbf{x}, t)\rangle_c$, conditioned on measurements of $K(\mathbf{x})$. We show below that these predictors satisfy a deterministic flow equation which contains a space-time integrodifferential residual flux term that renders $\langle \mathbf{q}(\mathbf{x}, t)\rangle_c$ nonlocal and non-Darcian. We also develop nonlocal equations for second conditional moments of head and flux so as to allow assessment of predictive uncertainty. After exploring the properties of integral kernels which enter into these equations, we present recursive closure approximations for the moment equations in terms of a small parameter that corresponds to the standard estimation error of natural log $K(\mathbf{x})$. These approximations allow, in principle, evaluating the conditional moments numerically on relatively coarse grids, without upscaling, by standard methods such as finite elements.

The space-time nonlocal nature of (unconditional) mean transient flow has been recognized by others, most notably *Hu and Cushman* [1994] and *Indelman* [1996]. Our work is most closely related to that of *Indelman* [1996], who used perturbation analysis to formulate an effective Darcy's law, and corresponding effective hydraulic conductivity, valid far from boundaries in Fourier-Laplace (FL) space. The inverse FL transform yields a mean flux term that is nonlocal, forming a convolution integral in space-time of a kernel with the mean head gradient. This kernel is the inverse FL transform of the effective conductivity tensor as defined in FL space. Since we are interested primarily in bounded domains and conditional hydraulic conductivity fields that are statistically nonhomogeneous, we cannot generally apply Fourier but only Laplace transform to our expressions; this is explored by *Tartakovsky and Neuman* [this issue (a)]. We show there that in the special case of flow in an infinite statistically homogeneous conductivity field, our theory becomes fully compatible with that of *Indelman* [1996].

2. Statement of Problem

Following *Neuman and Orr* [1993], we start from the premise that Darcy's law,

$$\mathbf{q}(\mathbf{x}, t) = -K(\mathbf{x})\nabla h(\mathbf{x}, t), \tag{1}$$

applies at any time t when the flux $\mathbf{q}$, the hydraulic conductivity K, and the hydraulic gradient ∇h are representative of a bulk support volume ω centered about a point $\mathbf{x}$, such that ω is small compared to the flow domain Ω but is sufficiently large for (1) to apply locally. Like *Neuman and Orr* [1993], we do not require that ω constitute an REV in any traditional sense of this term, but only that each of the above quantities be, in principle, amenable to direct or indirect measurement at each point $\mathbf{x}$ in Ω and on its boundary Γ. We further take h to satisfy locally the transient continuity equation

$$S(\mathbf{x})\,\frac{\partial h}{\partial t} = -\nabla\cdot\mathbf{q}(\mathbf{x}, t) + f(\mathbf{x}, t) \qquad \mathbf{x}\in\Omega \tag{2}$$

subject to the initial and boundary conditions

$$h(\mathbf{x}, 0) = H_0(\mathbf{x}) \qquad \mathbf{x}\in\Omega \tag{3}$$

$$h(\mathbf{x}, t) = H(\mathbf{x}, t) \qquad \mathbf{x}\in\Gamma_D \tag{4}$$

$$-\mathbf{q}(\mathbf{x}, t)\cdot\mathbf{n}(\mathbf{x}) = Q(\mathbf{x}, t) \qquad \mathbf{x}\in\Gamma_N. \tag{5}$$

Here $S(\mathbf{x})$ is specific storage, $f(\mathbf{x}, t)$ is a random source function, $H_0(\mathbf{x})$ is a random initial head distribution, $H(\mathbf{x}, t)$ is random head on Dirichlet boundary segments Γ_D, $Q(\mathbf{x}, t)$ is random flux across Neumann boundary segments Γ_N, and $\mathbf{n}(\mathbf{x})$ is a unit outward normal to the boundary Γ, which in turn forms the union of Γ_D and Γ_N. It is common among hydrologists to prescribe source and boundary values in a manner that is statistically independent of hydraulic conductivities. Though our theory does not require it, we assume for simplicity only that the random functions $f(\mathbf{x}, t)$, $H_0(\mathbf{x})$, $H(\mathbf{x}, t)$, and $Q(\mathbf{x}, t)$ are uncorrelated with each other and with $K(\mathbf{x}, t)$.

As $K(\mathbf{x})$ is usually much more variable than $S(\mathbf{x})$, we treat the former as a random field and the latter as a deterministic function [e.g., *Indelman*, 1996]. Let $\langle K(\mathbf{x})\rangle_c$ be the ensemble mean of $K(\mathbf{x})$ conditioned on a discrete number of measurements in space. As such, it constitutes a relatively smooth optimum unbiased estimate of $K(\mathbf{x})$ and is commonly determined by geostatistical methods such as kriging. The unknown hydraulic conductivity $K(\mathbf{x})$ differs from its known estimate $\langle K(\mathbf{x})\rangle_c$ by a randomly fluctuating estimation error $K'(\mathbf{x})$,

$$K(\mathbf{x}) \equiv \langle K(\mathbf{x})\rangle_c + K'(\mathbf{x}) \qquad \langle K'(\mathbf{x})\rangle_c \equiv 0. \tag{6}$$

Whereas $K'(\mathbf{x})$ is generally unknown, its conditional mean is by definition zero and we assume that its spatial covariance can be inferred geostatistically from the data [*Neuman and Orr*, 1993]. By the same token, we represent the unknown random functions $h(\mathbf{x}, t)$ and $\mathbf{q}(\mathbf{x}, t)$ in terms of their conditional ensemble means, and random fluctuations about these means, via

$$h(\mathbf{x}, t) \equiv \langle h(\mathbf{x}, t)\rangle_c + h'(\mathbf{x}, t) \qquad \langle h'(\mathbf{x}, t)\rangle_c \equiv 0 \tag{7}$$

$$\mathbf{q}(\mathbf{x}, t) \equiv \langle \mathbf{q}(\mathbf{x}, t)\rangle_c + \mathbf{q}'(\mathbf{x}, t) \qquad \langle \mathbf{q}'(\mathbf{x}, t)\rangle_c \equiv 0 \tag{8}$$

where the subscript c indicates conditioning on the same hydraulic data used to obtain $\langle K(\mathbf{x})\rangle_c$. Taking the conditional ensemble mean of (2)–(5) yields

$$S(\mathbf{x})\,\frac{\partial\langle h(\mathbf{x}, t)\rangle_c}{\partial t} = -\nabla\cdot\langle \mathbf{q}(\mathbf{x}, t)\rangle_c + \langle f(\mathbf{x}, t)\rangle \qquad \mathbf{x}\in\Omega \tag{9}$$

$$\langle h(\mathbf{x}, 0)\rangle_c = \langle H_0(\mathbf{x})\rangle \qquad \mathbf{x}\in\Omega \tag{10}$$

$$\langle h(\mathbf{x}, t)\rangle_c = \langle H(\mathbf{x}, t)\rangle \qquad \mathbf{x}\in\Gamma_D \tag{11}$$

$$-\langle \mathbf{q}(\mathbf{x}, t)\rangle_c\cdot\mathbf{n}(\mathbf{x}) = \langle Q(\mathbf{x}, t)\rangle \qquad \mathbf{x}\in\Gamma_N \tag{12}$$

where $\langle f(\mathbf{x}, t)\rangle$, $\langle H_0(\mathbf{x})\rangle$, $\langle H(\mathbf{x}, t)\rangle$, and $\langle Q(\mathbf{x}, t)\rangle$ are prescribed unconditional ensemble means of the statistically independent random source, initial, and boundary functions $f(\mathbf{x}, t)$, $H_0(\mathbf{x})$, $H(\mathbf{x}, t)$, and $Q(\mathbf{x}, t)$, respectively. This is a standard continuity equation driven by ensemble mean forcing terms. The conditional mean flux $\langle \mathbf{q}(\mathbf{x}, t)\rangle_c$ is obtained by taking the conditional ensemble mean of (1) while considering (6)–(8),

$$\begin{aligned}\langle \mathbf{q}(\mathbf{x}, t)\rangle_c &= -\langle K(\mathbf{x})\rangle_c\nabla\langle h(\mathbf{x}, t)\rangle_c + \mathbf{r}_c(\mathbf{x}, t)\\ \mathbf{r}_c(\mathbf{x}, t) &= -\langle K'(\mathbf{x})\nabla h'(\mathbf{x}, t)\rangle_c.\end{aligned} \tag{13}$$

Here $\mathbf{r}_c(\mathbf{x}, t)$ is a residual flux arising from the product of random fluctuations in hydraulic conductivity and gradient about their respective conditional mean values. It has been traditional in some of the stochastic subsurface hydrology literature [e.g., *Bakr et al.*, 1978; *Mizell et al.*, 1982; *Sun and Yeh*, 1992; *Gracham and Tankersley*, 1994] to disregard products of random fluctuations so as to render the mathematics tractable. However, we know that the residual flux may sometimes be a major contributor to effective hydraulic conductivity [e.g., *Neuman and Orr*, 1993; *Paleologos et al.*, 1996] and therefore must not be disregarded in (13). That terms involving the products of fluctuations are not always small has also been demonstrated by *Loaicigia and Mariño* [1990]. Therefore we devote a good part of this paper to the development of exact formal, and approximate working, expressions for $\mathbf{r}_c(\mathbf{x}, t)$ in terms of deterministic head gradients and boundary fluxes as done earlier by *Neuman and Orr* [1993] and *Neuman et al.* [1996] for steady state flow and by *Neuman* [1993] and *Zhang and Neuman* [1996] for transport.

3. Exact Conditional Mean Flow Expressions

Let $G(\mathbf{y}, \mathbf{x}, t - \tau)$ be a random Green's function representing the solution of (1)–(5), subject to homogeneous initial and boundary conditions, due to an instantaneous point source $f(\mathbf{x}, t) = \delta(\mathbf{x} - \mathbf{y})\delta(t - \tau)$ of unit strength at $(\mathbf{y}, \tau)$ where δ is the Dirac delta function. The function G depends on the original boundary configuration but not on the boundary values H and Q. Equation (A9) (Appendix A) expresses the random head distribution $h(\mathbf{x}, t)$ in terms of the random Green's function $G(\mathbf{y}, \mathbf{x}, t - \tau)$. Taking the conditional mean of (A9) gives

$$\begin{aligned}\langle h(\mathbf{x}, t)\rangle_c = &\int_0^t \int_\Omega \langle f(\mathbf{y}, \tau)\rangle \langle G(\mathbf{y}, \mathbf{x}, t - \tau)\rangle_c \, d\mathbf{y}\, d\tau \\ &- \int_0^t \int_{\Gamma_D} \langle H(\mathbf{y}, \tau)\rangle \langle K(\mathbf{y}) \nabla_y G(\mathbf{y}, \mathbf{x}, t - \tau)\rangle_c \cdot \mathbf{n}(\mathbf{y})\, d\mathbf{y}\, d\tau \\ &+ \int_0^t \int_{\Gamma_N} \langle Q(\mathbf{y}, \tau)\rangle \langle G(\mathbf{y}, \mathbf{x}, t - \tau)\rangle_c \, d\mathbf{y}\, d\tau \\ &+ \int_\Omega S(\mathbf{y}) \langle H_0(\mathbf{y})\rangle \langle G(\mathbf{y}, \mathbf{x}, t)\rangle_c \, d\mathbf{y}. \end{aligned} \tag{14}$$

This is an explicit expression for $\langle h(\mathbf{x}, t)\rangle_c$ in terms of mean initial and forcing functions as well as conditional moments involving a random Green's function which is independent of these initial and forcing terms. The expression is formal in that these moments are unknown and cannot be evaluated without either high-resolution Monte Carlo simulation or approximation. Reliance on a Green's function is nevertheless useful because once its moments have been evaluated, they can be used to generate deterministically conditional mean solutions corresponding to arbitrary initial and forcing functions.

We shall see later that evaluating $\langle h(\mathbf{x}, t)\rangle_c$ implicitly by solving (9)–(13) is preferred over evaluating it explicitly by means of (14). This is so because an explicit evaluation to a given order of accuracy requires approximating the Green's functions to higher orders than does an implicit evaluation. We therefore do not pursue explicit expressions for head moments any further in this paper. Instead, we seek expressions for the residual flux in (9)–(13) that render these equations formally solvable.

In Appendix A we employ (A9) to derive exactly an explicit compact integral expression for the residual flux,

$$\begin{aligned}\mathbf{r}_c(\mathbf{x}, t) = &\int_0^t \int_\Omega \mathbf{a}_c(\mathbf{y}, \mathbf{x}, t - \tau) \nabla_y h_c(\mathbf{y}, \tau)\, d\mathbf{y}\, d\tau \\ &+ \int_0^t \int_{\Gamma_N} \mathbf{b}_c(\mathbf{y}, \mathbf{x}, t - \tau) \langle Q(\mathbf{y}, \tau)\rangle \, d\mathbf{y}\, d\tau \\ &+ \int_\Omega \int_{\Gamma_N} \int_0^t \int_0^\tau \mathbf{c}_c(\mathbf{z}, \mathbf{y}, \mathbf{x}, t - \tau, \tau - \tau_1) \\ &\cdot \langle Q(z, \tau_1)\rangle \, d\tau_1\, d\tau\, dz\, d\mathbf{y} \end{aligned} \tag{15}$$

where the kernels of the integrals are given formally by

$$\mathbf{a}_c(\mathbf{y}, \mathbf{x}, t - \tau) = \langle K'(\mathbf{y}) K'(\mathbf{x}) \nabla_x \nabla_y^T G(\mathbf{y}, \mathbf{x}, t - \tau)\rangle_c \tag{16}$$

$$\begin{aligned}\mathbf{b}_c(\mathbf{y}, \mathbf{x}, t - \tau) = &-\langle K'(\mathbf{x}) K^{-1}(\mathbf{y})\rangle_c \langle K(\mathbf{y})\rangle_c \nabla_x G_c(\mathbf{y}, \mathbf{x}, t - \tau) \\ &- \langle K'(\mathbf{x}) K'(\mathbf{y}) \nabla_x G(\mathbf{y}, \mathbf{x}, t - \tau)\rangle_c \langle K(\mathbf{y})\rangle_c^{-1} \end{aligned} \tag{17}$$

$$\begin{aligned}\mathbf{c}_c(\mathbf{z}, \mathbf{y}, \mathbf{x}, t - \tau, \tau - \tau_1) = &\langle K'(\mathbf{x}) \nabla_x G(\mathbf{y}, \mathbf{x}, t - \tau) \\ &\nabla_y \cdot [K'(\mathbf{y}) \nabla_y G_c(\mathbf{z}, \mathbf{y}, \tau - \tau_1)] \\ &\cdot [\langle K(\mathbf{z})\rangle_c K^{-1}(\mathbf{z}) - 1]\rangle_c \end{aligned} \tag{18}$$

$h_c(\mathbf{x}, t)$ is the solution of the deterministic flow problem

$$S(\mathbf{x}) \frac{\partial h_c(\mathbf{x}, t)}{\partial t} = \nabla \cdot [\langle K(\mathbf{x})\rangle_c \nabla h_c(\mathbf{x}, t)] + \langle f(\mathbf{x}, t)\rangle \qquad \mathbf{x} \in \Omega \tag{19}$$

$$h_c(\mathbf{x}, 0) = \langle H_0(\mathbf{x})\rangle \qquad \mathbf{x} \in \Omega \tag{20}$$

$$h_c(\mathbf{x}, t) = \langle H(\mathbf{x}, t)\rangle \qquad \mathbf{x} \in \Gamma_D \tag{21}$$

$$\langle K(\mathbf{x})\rangle_c \nabla h_c(\mathbf{x}, t) \cdot \mathbf{n}(\mathbf{x}) = \langle Q(\mathbf{x}, t)\rangle \qquad \mathbf{x} \in \Gamma_N \tag{22}$$

and G_c is a corresponding Green's function, that is, the solution of (19)–(22) due to a mean instantaneous point source $\langle f(\mathbf{x}, t)\rangle = \delta(\mathbf{x} - \mathbf{y})\delta(t - \tau)$ subject to homogeneous initial and boundary conditions. Alternatively, one can express the residual flux implicitly as (Appendix B)

$$\begin{aligned}\mathbf{r}_c(\mathbf{x}, t) = &\int_0^t \int_\Omega \mathbf{a}_c(\mathbf{y}, \mathbf{x}, t - \tau) \nabla_y \langle h(\mathbf{y}, \tau)\rangle_c \, d\mathbf{y}\, d\tau \\ &+ \int_0^t \int_\Omega \mathbf{d}_c(\mathbf{y}, \mathbf{x}, t - \tau) \mathbf{r}_c(\mathbf{y}, \tau)\, d\mathbf{y}\, d\tau \end{aligned} \tag{23}$$

where the kernel $\mathbf{d}_c(\mathbf{y}, \mathbf{x}, t - \tau)$ is given formally by

$$\mathbf{d}_c(\mathbf{y}, \mathbf{x}, t - \tau) = \langle K'(\mathbf{x}) \nabla_x \nabla_y^T G(\mathbf{y}, \mathbf{x}, t - \tau)\rangle_c. \tag{24}$$

It is evident from (15)–(24) that all four residual flux kernels are nonlocal (depend on more than one point) in space-time. Their space-time "memory" reflects the fact that predictions made under uncertainty at one point are correlated with (dependent on) information at other points. This dependence of the kernels on information content (scale, quantity, and quality of measurements) renders these nonlocal parameters conditional on measured data and thereby nonunique; the same is true about the local parameter $\langle K(\mathbf{x})\rangle_c$. As these local and nonlocal quantities are additionally independent of sources as well as initial and boundary values (though they do depend on boundary configuration), they constitute information-dependent (and thus nonunique) system parameters. Since Green's functions are symmetric in space and $\mathbf{a}_c(\mathbf{y}, \mathbf{x}, t - \tau)$ is a quadratic form in space, the latter parameter forms a time-dependent, symmetric, positive semidefinite second-rank tensor (dyadic). On the other hand, $\mathbf{d}_c(\mathbf{y}, \mathbf{x}, t - \tau)$ forms a nonsymmetric tensor while $\mathbf{b}_c(\mathbf{y}, \mathbf{x}, t - \tau)$ and $\mathbf{c}_c(\mathbf{z}, \mathbf{y}, \mathbf{x}, t - \tau, \tau - \tau_1)$ are vectors. The residual flux $\mathbf{r}_c(\mathbf{x}, t)$ is generally not proportional to the local hydraulic gradient and is therefore non-Darcian. The same is true about the flux predictor $\langle \mathbf{q}(\mathbf{x}, t)\rangle_c$ so that the notion of effective hydraulic conductivity loses meaning in the conditional ensemble mean context in all but a few special cases.

As information content (data quantity and quality) increases, the magnitude of the residual flux generally diminishes. The same happens to the estimation error associated with $\langle K(\mathbf{x})\rangle_c$ and to the prediction errors associated with $\langle h(\mathbf{x}, t)\rangle_c$ and $\langle \mathbf{q}(\mathbf{x}, t)\rangle_c$. In the hypothetical limit where perfect and complete hydraulic conductivity data become available, the corresponding estimation error and residual flux vanish. If additionally all sources as well as initial and boundary conditions are specified with certainty, there is no prediction error and the flow problem becomes deterministic at the local, Darcian level.

In the special case where all Neumann boundary conditions are of the mean no-flow type, $\langle Q(\mathbf{x}, t)\rangle \equiv 0$, the last two integral terms in (15) vanish. If additionally $\nabla h_c \equiv \langle \nabla h\rangle_c \equiv$ constant, then this term can be taken outside the remaining integral in (15), rendering the mean (residual and total) flux Darcian and the associated effective hydraulic conductivity tensor symmetric (we devote a separate paper [*Tartakovsky and Neuman*, this issue (b)] to the evaluation of this tensor in a box-shaped domain). In the more general case where $\langle Q(\mathbf{x}, t)\rangle \not\equiv 0$, one can force the last two terms in (15) to vanish by moving Γ_N a small distance ε outward, defining it as a mean no-flow boundary and then formally absorbing Q along the original Neumann boundary (just inside the newly defined mean no-flow boundary) into the interior source term f [*Neuman et al.*, 1996]. This simplification is especially well suited for numerical solutions of the conditional mean flow equations. The last two terms in (15) also drop out in the special case where $K(\mathbf{x})$ along Γ_N is deterministic (known with certainty) so that $K'(\mathbf{x}) = 0$.

In the limit as $t \to \infty$, Green's functions associated with transient flow problems tend asymptotically to those associated with corresponding steady state flow problems. It follows that our transient nonlocal expressions reduce to those developed by *Neuman and Orr* [1993] and *Neuman et al*, [1996] for steady state flow.

4. Recursive Conditional Mean Flow Approximations

To render the above formal conditional mean flow expressions workable, we expand them below in a small parameter σ_Y representing a measure of the standard deviation of $Y'(\mathbf{x}) = Y(\mathbf{x}) - \langle Y(\mathbf{x})\rangle_c$ where $Y(\mathbf{x}) = \ln K(\mathbf{x})$; this nominally limits our approximation either to mildly heterogeneous or to well-conditioned strongly heterogeneous media with $\sigma_Y < 1$. Expanding h, K, and G within (14) in powers of $Y'(\mathbf{x})$ and collecting terms of like powers of σ_Y yields the following zeroth- and ith-order approximations for $\langle h\rangle_c$, respectively,

$$\begin{aligned}\langle h^{(0)}(\mathbf{x}, t)\rangle_c = &\int_0^t \int_\Omega \langle f(\mathbf{y}, \tau)\rangle \langle G^{(0)}(\mathbf{y}, \mathbf{x}, t-\tau)\rangle_c \, d\mathbf{y}\, d\tau \\ &- \int_0^t \int_{\Gamma_D} \langle H(\mathbf{y}, \tau)\rangle K_G(\mathbf{y}) \nabla_y \langle G^{(0)}(\mathbf{y}, \mathbf{x}, t-\tau)\rangle_c \\ &\cdot \mathbf{n}(\mathbf{y})\, d\mathbf{y}\, d\tau + \int_0^t \int_{\Gamma_N} \langle Q(\mathbf{y}, \tau)\rangle \langle G^{(0)}(\mathbf{y}, \mathbf{x}, t-\tau)\rangle_c \, d\mathbf{y}\, d\tau \\ &+ \int_\Omega S(\mathbf{y}) \langle H_0(\mathbf{y})\rangle \langle G^{(0)}(\mathbf{y}, \mathbf{x}, t)\rangle_c \, d\mathbf{y}\end{aligned} \tag{25}$$

and

$$\begin{aligned}\langle h^{(i)}(\mathbf{x}, t)\rangle_c = &\int_0^t \int_\Omega \langle f(\mathbf{y}, \tau)\rangle \langle G^{(i)}(\mathbf{y}, \mathbf{x}, t-\tau)\rangle_c \, d\mathbf{y}\, d\tau \\ &- \int_0^t \int_{\Gamma_D} \langle H(\mathbf{y}, \tau)\rangle K_G(\mathbf{y}) \sum_{n=0}^{i} \frac{\langle Y'(\mathbf{y})^n\rangle_c}{n!} \nabla_y \langle G^{(i-n)}(\mathbf{y}, \mathbf{x}, t-\tau)\rangle_c \\ &\cdot \mathbf{n}(\mathbf{y})\, d\mathbf{y}\, d\tau + \int_0^t \int_{\Gamma_N} \langle Q(\mathbf{y}, \tau)\rangle \langle G^{(i)}(\mathbf{y}, \mathbf{x}, t-\tau)\rangle_c \, d\mathbf{y}\, d\tau \\ &+ \int_\Omega S(\mathbf{y}) \langle H_0(\mathbf{y})\rangle \langle G^{(i)}(\mathbf{y}, \mathbf{x}, t)\rangle_c \, d\mathbf{y}.\end{aligned} \tag{26}$$

Here the superscript (i) indicates terms of ith order in σ_Y, $K_G(\mathbf{x}) = \exp\langle Y(\mathbf{x})\rangle_c$, $\langle Y'(\mathbf{x})\rangle_c \equiv 0$, and all higher-order odd moments of $Y'(\mathbf{x})$ vanish in the special case where the hydraulic conductivity is lognormal. Even though $h^{(0)}$ and $G^{(0)}$ are deterministic functions, we write them as $\langle h^{(0)}\rangle_c$ and $\langle G^{(0)}\rangle_c$ so as to emphasize their conditional nature. Note that using (25) and (26) to evaluate $\langle h\rangle_c$ to a given order of approximation requires that one first evaluate $\langle G\rangle_c$ to this and all lower orders. We derive below a set of recursive equations for $\langle G^{(i)}\rangle_c$ that allows doing so to any order i.

A perturbation expansion of (15) leads to the following ith-order approximation for the residual flux,

$$\begin{aligned}\mathbf{r}_c^{(i)}(\mathbf{x}, t) = &\int_0^t \int_\Omega \sum_{n=0}^{i} \mathbf{a}_c^{(n)}(\mathbf{y}, \mathbf{x}, t-\tau) \nabla_y h_c^{(i-n)}(\mathbf{y}, \tau)\, d\mathbf{y}\, d\tau \\ &+ \int_0^t \int_{\Gamma_N} \mathbf{b}_c^{(i)}(\mathbf{y}, \mathbf{x}, t-\tau) \langle Q(\mathbf{y}, \tau)\rangle \, d\mathbf{y}\, d\tau \\ &+ \int_\Omega \int_{\Gamma_N} \int_0^t \int_0^\tau \mathbf{c}_c^{(i)}(\mathbf{z}, \mathbf{y}, \mathbf{x}, t-\tau, \tau-\tau_1) \\ &\cdot \langle Q(\mathbf{z}, \tau_1)\rangle \, d\tau_1\, d\tau\, d\mathbf{z}\, d\mathbf{y}.\end{aligned} \tag{27}$$

Here $h_c^{(i)}$ is the ith-order solution of (19)–(22), that is, the solution of

$$S(\mathbf{x})\,\frac{\partial h_c^{(0)}(\mathbf{x},t)}{\partial t} = -\nabla\cdot\mathbf{q}_c^{(0)}(\mathbf{x},t) + \langle f(\mathbf{x},t)\rangle$$

$$\mathbf{q}_c^{(0)}(\mathbf{x},t) = -K_G(\mathbf{x})\nabla h_c^{(0)}(\mathbf{x},t) \qquad (28)$$

$$S(\mathbf{x})\,\frac{\partial h_c^{(i)}(\mathbf{x},t)}{\partial t} = -\nabla\cdot\mathbf{q}_c^{(i)}(\mathbf{x},t)$$

$$\mathbf{q}_c^{(i)}(\mathbf{x},t) = -K_G(\mathbf{x})\sum_{n=0}^{i}\frac{\langle Y'^n\rangle_c}{n!}\nabla h_c^{(i-n)}(\mathbf{x},t) \qquad i\ge 1$$

subject to the initial and boundary conditions

$$h_c^{(0)}(\mathbf{x},0) = \langle H_0(\mathbf{x})\rangle \qquad \mathbf{x}\in\Omega \qquad (29)$$

$$h_c^{(0)}(\mathbf{x},t) = \langle H(\mathbf{x},t)\rangle \qquad \mathbf{x}\in\Gamma_D \qquad (30)$$

$$-\mathbf{q}_c^{(0)}(\mathbf{x},t)\cdot\mathbf{n}(\mathbf{x}) = \langle Q(\mathbf{x},t)\rangle \qquad \mathbf{x}\in\Gamma_N \qquad (31)$$

and, for $i \ge 1$,

$$h_c^{(i)}(\mathbf{x},0) = 0 \qquad \mathbf{x}\in\Omega \qquad (32)$$

$$h_c^{(i)}(\mathbf{x},t) = 0 \qquad \mathbf{x}\in\Gamma_D \qquad (33)$$

$$-\mathbf{q}_c^{(i)}(\mathbf{x},t)\cdot\mathbf{n}(\mathbf{x}) = 0 \qquad \mathbf{x}\in\Gamma_N. \qquad (34)$$

We show in Appendix C that

$$\mathbf{a}_c^{(0)} = \mathbf{a}_c^{(1)} = 0$$

$$\mathbf{a}_c^{(2)}(\mathbf{y},\mathbf{x},t-\tau) = K_G(\mathbf{x})K_G(\mathbf{y})\langle Y'(\mathbf{x})Y'(\mathbf{y})\rangle_c\nabla_x\nabla_y^T \cdot\langle G^{(0)}(\mathbf{y},\mathbf{x},t-\tau)\rangle_c \qquad (35)$$

$$\mathbf{b}_c^{(0)} = \mathbf{b}_c^{(1)} = \mathbf{b}_c^{(2)} = 0$$
$$\mathbf{c}_c^{(0)} = \mathbf{c}_c^{(1)} = \mathbf{c}_c^{(2)} = 0. \qquad (36)$$

It then follows that

$$\mathbf{r}_c^{(0)}(\mathbf{x},t) = \mathbf{r}_c^{(1)}(\mathbf{x},t) = 0 \qquad (37)$$

and

$$\mathbf{r}_c^{(2)}(\mathbf{x},t) = \int_0^t\int_\Omega \mathbf{a}_c^{(2)}(\mathbf{y},\mathbf{x},t-\tau)\nabla_y h_c^{(0)}(\mathbf{y},\tau)\,d\mathbf{y}\,d\tau. \qquad (38)$$

Approximating the residual flux on the left-hand side of the implicit expression (23) to ith order renders this expression explicit. This is so because $\mathbf{d}_c$ is at least of order 1 owing to the presence of K', so that $\mathbf{r}_c$ on the right-hand side of (23) cannot be of order higher than $i - 1$. Hence approximating (23) to second order yields the same expression as (38) but with $\nabla\langle h^{(0)}\rangle_c$ instead of $\nabla h_c^{(0)}$. Clearly, these two gradient terms must be the same. This is indeed seen from the following recursive conditional mean flow equations:

$$S(\mathbf{x})\,\frac{\partial\langle h^{(0)}(\mathbf{x},t)\rangle_c}{\partial t} = -\nabla\cdot\langle\mathbf{q}^{(0)}(\mathbf{x},t)\rangle_c + \langle f(\mathbf{x},t)\rangle$$
$$S(\mathbf{x})\,\frac{\partial\langle h^{(i)}(\mathbf{x},t)\rangle_c}{\partial t} = -\nabla\cdot\langle\mathbf{q}^{(i)}(\mathbf{x},t)\rangle_c \qquad i\ge 1 \qquad (39)$$

where $\mathbf{q}^{(0)}$ is deterministic but written as $\langle\mathbf{q}^{(0)}\rangle_c$ to emphasize its conditional nature, the fluxes are given by

$$\langle\mathbf{q}^{(0)}(\mathbf{x},t)\rangle_c = -K_G(\mathbf{x})\nabla\langle h^{(0)}(\mathbf{x},t)\rangle_c$$
$$\langle\mathbf{q}^{(1)}(\mathbf{x},t)\rangle_c = -K_G(\mathbf{x})\nabla\langle h^{(1)}(\mathbf{x},t)\rangle_c \equiv 0$$
$$\langle\mathbf{q}^{(2)}(\mathbf{x},t)\rangle_c = -K_G(\mathbf{x})\left[\nabla\langle h^{(2)}(\mathbf{x},t)\rangle_c + \frac{\sigma_Y^2(\mathbf{x})}{2}\nabla\langle h^{(0)}(\mathbf{x},t)\rangle_c\right] + \mathbf{r}_c^{(2)}(\mathbf{x},t) \qquad (40)$$
$$\langle\mathbf{q}^{(i)}(\mathbf{x},t)\rangle_c = -K_G(\mathbf{x})\sum_{n=0}^{i}\frac{\langle Y'^n\rangle_c}{n!}\nabla\langle h^{(i-n)}(\mathbf{x},t)\rangle_c + \mathbf{r}_c^{(i)}(\mathbf{x},t) \qquad i\ge 0$$

subject to the initial and boundary conditions

$$\langle h^{(0)}(\mathbf{x},0)\rangle_c = \langle H_0(\mathbf{x})\rangle \qquad \mathbf{x}\in\Omega \qquad (41)$$

$$\langle h^{(0)}(\mathbf{x},t)\rangle_c = \langle H(\mathbf{x},t)\rangle \qquad \mathbf{x}\in\Gamma_D \qquad (42)$$

$$-\langle\mathbf{q}^{(0)}(\mathbf{x},t)\rangle_c\cdot\mathbf{n}(\mathbf{x}) = \langle Q(\mathbf{x},t)\rangle \qquad \mathbf{x}\in\Gamma_N \qquad (43)$$

and, for $i \ge 1$,

$$\langle h^{(i)}(\mathbf{x},0)\rangle_c = 0 \qquad \mathbf{x}\in\Omega \qquad (44)$$

$$\langle h^{(i)}(\mathbf{x},t)\rangle_c = 0 \qquad \mathbf{x}\in\Gamma_D \qquad (45)$$

$$-\langle\mathbf{q}^{(i)}(\mathbf{x},t)\rangle_c\cdot\mathbf{n}(\mathbf{x}) = 0 \qquad \mathbf{x}\in\Gamma_N. \qquad (46)$$

The zeroth-order conditional mean head expressions in (39)–(43) are the same as (28)–(31) which demonstrates that $h_c^{(0)} \equiv \langle h^{(0)}\rangle_c$.

We saw that to evaluate the residual flux $\mathbf{r}_c$ one needs to evaluate the conditional mean Green's function $\langle G\rangle_c$. Let $\boldsymbol{\rho}_c(\mathbf{y},\mathbf{x},t-\tau) = \langle K'(\mathbf{x})\nabla_x G'(\mathbf{y},\mathbf{x},t-\tau)\rangle_c$ be a residual flux associated with G. One can obtain $\langle G\rangle_c$ to arbitrary orders of approximation by solving a modified version of (39)–(46) in which $\langle f\rangle$ is replaced by the delta function, $\mathbf{r}_c$ is replaced by $\boldsymbol{\rho}_c$, and all initial and boundary functions are set identically equal to zero. Since G satisfies homogeneous initial and boundary conditions we can write, in analogy to (27) and in accord with (B7),

$$\boldsymbol{\rho}_c^{(i)}(\mathbf{y},\mathbf{x},t-\tau) = \int_0^t\int_\Omega\sum_{n=0}^{i}\mathbf{a}_c^{(n)}(\mathbf{y},\mathbf{z},t-\tau)\,\nabla_z G_c^{(i-n)}(\mathbf{z},\mathbf{x},t-\tau)\,d\mathbf{z}\,d\tau. \qquad (47)$$

One can likewise obtain G_c to arbitrary orders of approximation by solving a modified version of (28)–(34) in which $\langle f\rangle$ is replaced by the delta function and all initial and boundary functions are set identically equal to zero; these equations do not involve a residual flux.

Equations (40) show that flux approximations to any order higher than 1 are nonlocal and thus non-Darcian. This notwithstanding, all of the above flow equations contain relatively smooth deterministic quantities which allows solving them by standard numerical methods, such as finite elements, on grids with cell sizes much larger than the support scale ω, without upscaling.

5. Exact Conditional Second Moment Expressions

Let $C_{hc}(\mathbf{x}, \mathbf{y}, t, s) = \langle h'(\mathbf{x}, t)h'(\mathbf{y}, s)\rangle_c$ be the conditional covariance of hydraulic head predictions and $\mathbf{C}_{qc}(\mathbf{x}, \mathbf{y}, t, s) = \langle \mathbf{q}'(\mathbf{x}, t)\mathbf{q}'^T(\mathbf{y}, s)\rangle_c$ be the conditional covariance tensor of flux predictions, where the superscript T indicates transpose. It is possible by means of (B5) and (B13) to derive an explicit expression for C_{hc} as was done for steady state flow by *Neuman and Orr* [1993]. We pointed out earlier, however, that it is advantageous to work instead with implicit conditional moment equations, and we therefore pursue this latter approach below. For simplicity, we do so for the case where all forcing terms have 0 variance. We show in Appendix B that then C_{hc} satisfies

$$S(\mathbf{x}) \frac{\partial C_{hc}(\mathbf{x}, \mathbf{y}, t, s)}{\partial t} = \nabla_x \cdot [\langle K(\mathbf{x})\rangle_c \nabla_x C_{hc}(\mathbf{x}, \mathbf{y}, t, s) + \mathbf{p}_c(\mathbf{x}, \mathbf{y}, t, s) + u_c(\mathbf{x}, \mathbf{y}, s)\nabla_x\langle h(\mathbf{x}, t)\rangle_c] \tag{48}$$

subject to the homogeneous initial and boundary conditions

$$C_{hc}(\mathbf{x}, \mathbf{y}, t, s) = 0 \qquad t = 0 \qquad \mathbf{x} \in \Omega \tag{49}$$

$$C_{hc}(\mathbf{x}, \mathbf{y}, t, s) = 0 \qquad \mathbf{x} \in \Gamma_D \tag{50}$$

$$[\langle K(\mathbf{x})\rangle_c \nabla_x C_{hc}(\mathbf{x}, \mathbf{y}, t, s) + \mathbf{p}_c(\mathbf{x}, \mathbf{y}, t, s) + u_c(\mathbf{x}, \mathbf{y}, s)\nabla_x\langle h(\mathbf{x}, t)\rangle_c] \cdot \mathbf{n}(\mathbf{x}) = 0 \qquad \mathbf{x} \in \Gamma_N. \tag{51}$$

Here

$$\mathbf{p}_c(\mathbf{x}, \mathbf{y}, t, s) = \langle K'(\mathbf{x})\nabla_x h'(\mathbf{x}, t)h'(\mathbf{y}, s)\rangle_c = \int_0^s \int_\Omega \mathbf{r}_c^T(\mathbf{z}, \tau)\nabla_z\langle G(\mathbf{z}, \mathbf{y}, s-\tau)K'(\mathbf{x})\nabla_x^T h'(\mathbf{x}, t)\rangle_c \, d\mathbf{z}\, d\tau - \int_0^s \int_\Omega \nabla_z^T\langle h(\mathbf{z}, \tau)\rangle_c \cdot \langle K'(\mathbf{z})\nabla_z G(\mathbf{z}, \mathbf{y}, s-\tau)K'(\mathbf{x})\nabla_x^T h'(\mathbf{x}, t)\rangle_c \, d\mathbf{z}\, d\tau \tag{52}$$

and

$$u_c(\mathbf{x}, \mathbf{y}, s) = \langle K'(\mathbf{x})h'(\mathbf{y}, s)\rangle_c = \int_0^s \int_\Omega \mathbf{r}_c(\mathbf{z}, \tau) \cdot \nabla_z\langle G(\mathbf{z}, \mathbf{y}, s-\tau)K'(\mathbf{x})\rangle_c \, d\mathbf{z}\, d\tau - \int_0^s \int_\Omega \nabla_z\langle h(\mathbf{z}, \tau)\rangle_c \cdot \langle K'(\mathbf{z})\nabla_z G(\mathbf{z}, \mathbf{y}, s-\tau)K'(\mathbf{x})\rangle_c \, d\mathbf{z}\, d\tau. \tag{53}$$

It is shown in Appendix B that $\mathbf{C}_{qc}$ can be found from the following relationship:

$$\begin{aligned}\mathbf{C}_{qc}(\mathbf{x}, \mathbf{y}, t, s) &= \langle \mathbf{q}'(\mathbf{x}, t)\mathbf{q}'^T(\mathbf{y}, s)\rangle_c = -\mathbf{r}_c(\mathbf{x}, s)\mathbf{r}_c^T(\mathbf{y}, s) \\ &+ \langle K(\mathbf{x})\rangle_c \nabla_x\nabla_y^T C_{hc}(\mathbf{x}, \mathbf{y}, t, s)\langle K(\mathbf{y})\rangle_c \\ &+ \nabla_x\langle h(\mathbf{x}, t)\rangle_c\langle K'(\mathbf{x})K'(\mathbf{y})\rangle_c\nabla_y^T\langle h(\mathbf{y}, s)\rangle_c \\ &+ \nabla_x\langle h(\mathbf{x}, t)\rangle_c\langle K'(\mathbf{x})\nabla_y^T h'(\mathbf{y}, s)\rangle_c\langle K(\mathbf{y})\rangle_c \\ &+ \langle K(\mathbf{x})\rangle_c\langle K'(\mathbf{y})\nabla_x h'(\mathbf{x}, t)\rangle_c\nabla_y^T\langle h(\mathbf{y}, s)\rangle_c \\ &+ \langle K'(\mathbf{x})\nabla_x h'(\mathbf{x}, t)\nabla_y^T h'(\mathbf{y}, s)\rangle_c\langle K(\mathbf{y})\rangle_c \\ &+ \langle K(\mathbf{x})\rangle_c\langle K'(\mathbf{y})\nabla_x h'(\mathbf{x}, t)\nabla_y^T h'(\mathbf{y}, s)\rangle_c \\ &+ \langle K'(\mathbf{y})K'(\mathbf{x})\nabla_x h'(\mathbf{x}, t)\rangle_c\nabla_y^T\langle h(\mathbf{y}, s)\rangle_c \\ &+ \nabla_x\langle h(\mathbf{x}, t)\rangle_c\langle K'(\mathbf{x})K'(\mathbf{y})\nabla_y^T h'(\mathbf{y}, s)\rangle_c \\ &+ \langle K'(\mathbf{x})\nabla_x h'(\mathbf{x}, t)K'(\mathbf{y})\nabla_y^T h'(\mathbf{y}, s)\rangle_c.\end{aligned} \tag{54}$$

Recursive conditional approximations for C_{hc} and $\mathbf{C}_{qc}$ are derived in Appendix D.

6. Conclusions

Our analysis leads to the following major conclusions:

1. The steady state nonlocal formalism of *Neuman and Orr* [1993] can be extended to transient flow. Starting from the premise that Darcy's law applies locally with a random hydraulic conductivity field on a support scale ω, one can render optimum unbiased predictions of system behavior on the same scale by means of conditional ensemble average hydraulic heads and fluxes. The support scale ω need not constitute an REV in any traditional sense of the term. The optimum predictors satisfy exactly a compact space-time nonlocal conditional ensemble mean flow equation in which the flux predictor is generally non-Darcian. Hence the notion of effective hydraulic conductivity loses meaning in all but a few special cases. The conditional mean flow equation contains local and nonlocal parameters that depend on data and are therefore nonunique. The nonlocal parameters take on the forms of symmetric and nonsymmetric second rank tensors (dyadics) as well as vectors.

2. To estimate nonlocal mean flow parameters on the basis of measured hydraulic conductivities requires either high-resolution (ω-scale) conditional Monte Carlo simulation or approximation. We showed how these parameters can be approximated to arbitrary order in a small parameter σ_Y that represents the standard conditional error of natural log hydraulic conductivity. Such approximations are nominally valid either for mildly heterogeneous media or for well-conditioned strongly heterogeneous media. We also presented recursive conditional mean flow equations to arbitrary orders of approximation in σ_Y.

3. Under favorable conditions it should be possible in principle to estimate both local and nonlocal parameters of the conditional mean flow equation by inverse methods based on ω-scale measurements not only of hydraulic conductivity but also of heads and/or fluxes. This is tantamount to conditioning the mean flow equations, and their parameters, on an expanded database. Since the parameters are data-dependent, the very act of altering the database alters their values. This implies that inverse methods, applied to deterministic equations of flow in randomly heterogeneous media, can never yield a unique set of deterministic flow parameters. It explains why in many practical applications of inverse methods to deterministic flow problems, the computed parameters keep changing as the database expands.

4. Second conditional ensemble moments of head and flux constitute ω-scale measures of predictive uncertainty. We developed compact nonlocal equations that are satisfied exactly by these moments. To render these equations workable, we presented recursive approximations that are valid to fourth order in σ_Y.

5. Although conditional mean heads and fluxes provide optimum predictions of actual heads and fluxes on the scale ω, they nevertheless tend to vary much more smoothly in space than do their ω-scale random counterparts. Whereas resolving

spatial fluctuations in the latter requires a computational grid with cells of size ω, resolving spatial fluctuations in the former may often be accomplished with a much coarser grid without any need for upscaling. To the extent that upscaling is desired (say, to compute average flow rates across interior or boundary surfaces on scales larger than ω), this can be accomplished a posteriori by spatial integration of predicted ω-scale quantities.

Appendix A

Upon combining (1) and (2), the resultant equation can be recast in operational form as

$$\mathcal{L}_{t,x}h(\mathbf{x}, t) + f(\mathbf{x}, t) = 0 \tag{A1}$$

where

$$\begin{aligned} \mathcal{L}_{t,x} &\equiv -S(\mathbf{x})\frac{\partial}{\partial t} + \nabla\cdot[K(\mathbf{x})\nabla] = L_{t,x} + \Re_{t,x}, \\ \Re_{t,x} &\equiv \Re_x \equiv \nabla\cdot[K'(\mathbf{x})\nabla],\ \langle\Re_x\rangle_c = 0, \\ L_{t,x} &= -S(\mathbf{x})\frac{\partial}{\partial t} + \nabla\cdot[\langle K(\mathbf{x})\rangle_c\nabla]. \end{aligned} \tag{A2}$$

Here and in the rest of Appendix A, $\mathcal{L}$ and $\Re$ are stochastic operators and L is the deterministic operator. From $L_{t,x}h = f - \Re_{t,x}h$ it follows that

$$h = L_{t,x}^{-1}f - L_{t,x}^{-1}\Re_{t,x}h + \hat{h} \tag{A3}$$

where

$$L_{t,x}^{-1}f(\mathbf{x}, t) = -\int_\Omega\int_0^t f(\mathbf{y}, \tau)G_c(\mathbf{y}, \mathbf{x}, t, \tau)\, d\tau\, d\mathbf{y} \tag{A4}$$

and $\hat{h}$ satisfies $L\hat{h} = 0$ subject to (3)–(5). Here $G_c(\mathbf{y}, \mathbf{x}, t - \tau)$ is the deterministic Green's function that satisfies (20)–(23) with $\langle f(\mathbf{x}, t)\rangle$ replaced by $\delta(\mathbf{x} - \mathbf{y})\delta(t - \tau)$, subject to $\langle H_0(\mathbf{x})\rangle \equiv \langle H(\mathbf{x}, t)\rangle \equiv \langle Q(\mathbf{x}, t)\rangle \equiv 0$. Since $L_{t,x}^{-1}$ is purely an integral operator, one has $LL^{-1} = L^{-1}L = I$ where I is the identity operator. Set $h_0 = L_{t,x}^{-1}f + \hat{h}$ and note from (A3) that

$$h = h_0 - L_{t,x}^{-1}\Re_{t,x}h. \tag{A5}$$

Omitting a series of intermediate manipulations identical to those of *Neuman et al.* [1996] one has, similar to their (A10),

$$h = (1 - \mathcal{L}_{t,x}^{-1}\Re_{t,x})h_0 \tag{A6}$$

where

$$\mathcal{L}_{t,x}^{-1}f(\mathbf{x}, t) = \int_\Omega\int_0^t f(\mathbf{y}, \tau)G(\mathbf{y}, \mathbf{x}, t - \tau)\, d\tau\, d\mathbf{y}. \tag{A7}$$

Operating on (A6) with $K'\nabla_x$ and taking conditional ensemble mean gives

$$\langle K'(\mathbf{x})\nabla_x h\rangle_c = \langle K'(\mathbf{x})\nabla_x h_0\rangle_c - \langle K'(\mathbf{x})\nabla_x\mathcal{L}_{t,x}^{-1}\Re_x h_0\rangle_c. \tag{A8}$$

Expressing (1)–(5) in terms of $\mathbf{y}$ and τ, substituting (1) into (2), multiplying by $G(\mathbf{y}, \mathbf{x}, t - \tau)$, integrating in time from 0 to t and in space over Ω, applying Green's identity twice to the resulting divergence integral, and then integrating the left-hand side with respect to τ yields, considering (4) and (5), the following formal expression for the hydraulic head:

$$\begin{aligned} h(\mathbf{x}, t) = &\int_0^t\int_\Omega f(\mathbf{y}, \tau)G(\mathbf{y}, \mathbf{x}, t - \tau)\, d\mathbf{y}\, d\tau \\ &- \int_0^t\int_{\Gamma_D} K(\mathbf{y})H(\mathbf{y}, \tau)\nabla_y G(\mathbf{y}, \mathbf{x}, t - \tau)\cdot\mathbf{n}(\mathbf{y})\, d\mathbf{y}\, d\tau \\ &+ \int_0^t\int_{\Gamma_N} Q(\mathbf{y}, \tau)G(\mathbf{y}, \mathbf{x}, t - \tau)\, d\mathbf{y}\, d\tau \\ &+ \int_\Omega S(\mathbf{y})H_0(\mathbf{y})G(\mathbf{y}, \mathbf{x}, t)\, d\mathbf{y}. \end{aligned} \tag{A9}$$

Multiplying (A6) by $G_c(\mathbf{y}, \mathbf{x}, t - \tau)$, and applying Green's formula yields, in analogy to (A9),

$$\begin{aligned} h_0(\mathbf{x}, t) = &\int_0^t\int_\Omega f(\mathbf{y}, \tau)G_c(\mathbf{y}, \mathbf{x}, t - \tau)\, d\mathbf{y}\, d\tau \\ &- \int_0^t\int_{\Gamma_D} \langle K(\mathbf{y})\rangle_c H(\mathbf{y}, \tau)\nabla_y G_c(\mathbf{y}, \mathbf{x}, t - \tau)\cdot\mathbf{n}(\mathbf{y})\, d\mathbf{y}\, d\tau \\ &+ \int_0^t\int_{\Gamma_N} \langle K(\mathbf{y})\rangle_c K^{-1}(\mathbf{y})Q(\mathbf{y}, \tau)G_c(\mathbf{y}, \mathbf{x}, t - \tau)\, d\mathbf{y}\, d\tau \\ &+ \int_\Omega S(\mathbf{y})H_0(\mathbf{y})G_c(\mathbf{y}, \mathbf{x}, t)\, d\mathbf{y} = L_{t,x}^{-1}f + \hat{h}. \end{aligned} \tag{A10}$$

Here $L_{t,x}^{-1}f$ represents the first integral on the right-hand side, as defined in (A4), and $\hat{h}$, first defined in (A3), represents the remaining integrals in (A10). Writing in analogy to h in (A9) the deterministic function h_c defined in (19)–(22) as

$$\begin{aligned} h_c(\mathbf{x}, t) = &\int_0^t\int_\Omega \langle f(\mathbf{y}, \tau)\rangle G_c(\mathbf{y}, \mathbf{x}, t - \tau)\, d\mathbf{y}\, d\tau \\ &- \int_0^t\int_{\Gamma_D} \langle K(\mathbf{y})\rangle_c\langle H(\mathbf{y}, \tau)\rangle\nabla_y G_c(\mathbf{y}, \mathbf{x}, t - \tau)\cdot\mathbf{n}(\mathbf{y})\, d\mathbf{y}\, d\tau \\ &+ \int_0^t\int_{\Gamma_N} \langle Q(\mathbf{y}, \tau)\rangle G_c(\mathbf{y}, \mathbf{x}, t - \tau)\, d\mathbf{y}\, d\tau \\ &+ \int_\Omega S(\mathbf{y})\langle H_0(\mathbf{y})\rangle G_c(\mathbf{y}, \mathbf{x}, t)\, d\mathbf{y} \end{aligned} \tag{A11}$$

leads to

$$\begin{aligned} h_0(\mathbf{x}, t) = h_c(\mathbf{x}, t) + &\int_0^t\int_\Omega f'(\mathbf{y}, \tau)G_c(\mathbf{y}, \mathbf{x}, t - \tau)\, d\mathbf{y}\, d\tau \\ &- \int_0^t\int_{\Gamma_D} \langle K(\mathbf{y})\rangle_c H'(\mathbf{y}, \tau)\nabla_y G_c(\mathbf{y}, \mathbf{x}, t - \tau)\cdot\mathbf{n}(\mathbf{y})\, d\mathbf{y}\, d\tau \\ &+ \int_0^t\int_{\Gamma_N} Q'(\mathbf{y}, \tau)G_c(\mathbf{y}, \mathbf{x}, t - \tau)\, d\mathbf{y}\, d\tau \\ &+ \int_\Omega S(\mathbf{y})H_0'(\mathbf{y})G_c(\mathbf{y}, \mathbf{x}, t)\, d\mathbf{y} + \int_0^t\int_{\Gamma_N} [\langle K(\mathbf{y})\rangle_c K^{-1}(\mathbf{y}) \end{aligned} \tag{A12}$$

$$- 1]Q(\mathbf{y}, \tau)G_c(\mathbf{y}, \mathbf{x}, t - \tau)\, d\mathbf{y}\, d\tau.$$

Substituting (A12) into (A8) gives

$$\begin{aligned}\langle K'(\mathbf{x})\nabla_x h\rangle_c = &\int_0^t \int_{\Gamma_N} \langle K'(\mathbf{x})[\langle K(\mathbf{y})\rangle_c K^{-1}(\mathbf{y}) - 1]\rangle_c \\ &\langle Q(\mathbf{y}, \tau)\rangle \nabla_x G_c(\mathbf{y}, \mathbf{x}, t - \tau)\, d\mathbf{y}\, d\tau \\ &+ \int_\Omega \int_0^t \langle K'(\mathbf{x})\nabla_x G(\mathbf{y}, \mathbf{x}, t - \tau) \\ &\nabla_y \cdot [K'(\mathbf{y})\nabla_y h_c(\mathbf{y}, \tau)]\rangle_c\, d\tau\, d\mathbf{y} \\ &- \int_\Omega \int_0^t \langle K'(\mathbf{x})\nabla_x G(\mathbf{y}, \mathbf{x}, t - \tau) \\ &\nabla_y \cdot \left[K'(\mathbf{y})\nabla_y \left\{ \int_0^\tau \int_{\Gamma_N} (\langle K(\mathbf{z})\rangle_c K^{-1}(\mathbf{z}) - 1) \right.\right. \\ &\left.\left. \langle Q(\mathbf{z}, \tau_1)\rangle G_c(\mathbf{z}, \mathbf{y}, \tau - \tau_1)\, d\mathbf{z}\, d\tau_1 \right\}\right]\rangle_c\, d\tau\, d\mathbf{y}.\end{aligned} \tag{A13}$$

Applying Green's identity to the first domain integral yields

$$\begin{aligned}\langle K'(\mathbf{x})\nabla_x h\rangle_c = &\\ &\int_0^t \int_{\Gamma_N} \langle K'(\mathbf{x})K^{-1}(\mathbf{y})\rangle_c \langle K(\mathbf{y})\rangle_c \langle Q(\mathbf{y}, \tau)\rangle \nabla_x G_c(\mathbf{y}, \mathbf{x}, t - \tau) \\ &d\mathbf{y}\, d\tau - \int_\Omega \int_0^t \langle K'(\mathbf{x})K'(\mathbf{y})\nabla_x \nabla_y^T G(\mathbf{y}, \mathbf{x}, t - \tau)\rangle_c \\ &\nabla_y h_c(\mathbf{y}, \tau)\, d\tau\, d\mathbf{y} + \int_0^t \int_{\Gamma_N} \langle K'(\mathbf{x})K'(\mathbf{y}) \\ &\nabla_x G(\mathbf{y}, \mathbf{x}, t - \tau)\rangle_c \langle K(\mathbf{y})\rangle_c^{-1} \langle Q(\mathbf{y}, \tau)\rangle\, d\mathbf{y}\, d\tau \\ &- \int_\Omega \int_0^t \langle K'(\mathbf{x})\nabla_x G(\mathbf{y}, \mathbf{x}, t - \tau) \\ &\nabla_y \cdot \left[K'(\mathbf{y})\nabla_y \left\{ \int_0^\tau \int_{\Gamma_N} (\langle K(\mathbf{z})\rangle_c K^{-1}(\mathbf{z}) - 1) \right.\right. \\ &\left.\left.\left. \langle Q(\mathbf{z}, \tau_1)\rangle G_c(\mathbf{z}, \mathbf{y}, \tau - \tau_1)\, d\mathbf{z}\, d\tau_1 \right\}\right]\right\rangle_c d\tau\, d\mathbf{y}.\end{aligned} \tag{A14}$$

Considering that by virtue of (13), $\mathbf{r}_c = -\langle K'\nabla h'\rangle_c = -\langle K'\nabla h\rangle_c$ leads directly to (15)–(18).

Appendix B

Substituting (6)–(8) into (1)–(5), taking conditional ensemble mean, and subtracting the latter from the former leads to

$$\nabla \cdot [K(\mathbf{x})\nabla h'(\mathbf{x}, t)] + \nabla \cdot [K'(\mathbf{x})\nabla \langle h(\mathbf{x}, t)\rangle_c]$$

$$- \nabla \cdot \langle K'(\mathbf{x})\nabla h'(\mathbf{x}, t)\rangle_c + f'(\mathbf{x}, t) = S(\mathbf{x})\, \frac{\partial h'(\mathbf{x}, t)}{\partial t} \tag{B1}$$

subject to

$$\begin{gathered} h'(\mathbf{x}, 0) = H'_0(\mathbf{x}) \qquad \mathbf{x} \in \Omega \\ h'(\mathbf{x}, t) = H'(\mathbf{x}, t) \qquad \mathbf{x} \in \Gamma_D \end{gathered} \tag{B2}$$

$$[K(\mathbf{x})\nabla h'(\mathbf{x}, t) + K'(\mathbf{x})\nabla \langle h(\mathbf{x}, t)\rangle_c - \langle K'(\mathbf{x})\nabla h'(\mathbf{x}, t)\rangle_c] \cdot \mathbf{n}(\mathbf{x}) = Q'(\mathbf{x}, t) \qquad \mathbf{x} \in \Gamma_N.$$

Expressing (B1) in terms of $\mathbf{y}$ and τ, multiplying by $G(\mathbf{y}, \mathbf{x}, t - \tau)$, and integrating over Ω and time gives

$$\begin{aligned}&\int_0^t \int_\Omega \nabla_y \cdot [K(\mathbf{y})\nabla_y h'(\mathbf{y}, \tau)]G(\mathbf{y}, \mathbf{x}, t - \tau)\, d\mathbf{y}\, d\tau \\ &\quad + \int_0^t \int_\Omega \nabla_y \cdot [K'(\mathbf{y})\nabla_y \langle h(\mathbf{y}, \tau)\rangle_c]G(\mathbf{y}, \mathbf{x}, t - \tau)\, d\mathbf{y}\, d\tau \\ &\quad - \int_0^t \int_\Omega \nabla_y \cdot [\langle K'(\mathbf{y})\nabla_y h'(\mathbf{y}, \tau)\rangle_c]G(\mathbf{y}, \mathbf{x}, t - \tau)\, d\mathbf{y}\, d\tau \\ &\quad + \int_0^t \int_\Omega f'(\mathbf{y}, \tau)G(\mathbf{y}, \mathbf{x}, t - \tau)\, d\mathbf{y}\, d\tau \\ &\quad = \int_0^t \int_\Omega S(\mathbf{y})\, \frac{\partial h'(\mathbf{y}, \tau)}{\partial \tau}\, G(\mathbf{y}, \mathbf{x}, t - \tau)\, d\mathbf{y}\, d\tau.\end{aligned} \tag{B3}$$

Applying Green's formula to the first integral, integrating by parts the last integral, and recalling the definition of $G(\mathbf{y}, \mathbf{x}, t - \tau)$ yields

$$\begin{aligned}h'(\mathbf{x}, t) = &-\int_0^t \int_{\Gamma_D} H'(\mathbf{y}, \tau)K(\mathbf{y})\nabla_y G(\mathbf{y}, \mathbf{x}, t - \tau) \\ &\cdot \mathbf{n}(\mathbf{y})\, d\mathbf{y}\, d\tau + \int_0^t \int_{\Gamma_N} G(\mathbf{y}, \mathbf{x}, t - \tau) \\ &K(\mathbf{y})\nabla_y h'(\mathbf{y}, \tau) \cdot \mathbf{n}(\mathbf{y})\, d\mathbf{y}\, d\tau \\ &+ \int_0^t \int_\Omega \nabla_y \cdot [K'(\mathbf{y})\nabla_y \langle h(\mathbf{y}, \tau)\rangle_c]G(\mathbf{y}, \mathbf{x}, t - \tau)\, d\mathbf{y}\, d\tau \\ &- \int_0^t \int_\Omega \nabla_y \cdot [\langle K'(\mathbf{y})\nabla_y h'(\mathbf{y}, \tau)\rangle_c]G(\mathbf{y}, \mathbf{x}, t - \tau)\, d\mathbf{y}\, d\tau \\ &+ \int_0^t \int_\Omega f'(\mathbf{y}, \tau)G(\mathbf{y}, \mathbf{x}, t - \tau)\, d\mathbf{y}\, d\tau \\ &+ \int_\Omega S(\mathbf{y})H'_0(\mathbf{y})G(\mathbf{y}, \mathbf{x}, t)\, d\mathbf{y}.\end{aligned} \tag{B4}$$

Applying Green's identity to divergence integrals and taking into account the last equation in (B2) gives

$$
\begin{aligned}
h'(\mathbf{x}, t) &= \int_0^t \int_\Omega \langle K'(\mathbf{y}) \nabla_y h'(\mathbf{y}, \tau)\rangle_c \cdot \nabla_y G(\mathbf{y}, \mathbf{x}, t-\tau)\, d\mathbf{y}\, d\tau \\
&- \int_0^t \int_\Omega K'(\mathbf{y}) \nabla_y \langle h(\mathbf{y}, \tau)\rangle_c \cdot \nabla_y G(\mathbf{y}, \mathbf{x}, t-\tau)\, d\mathbf{y}\, d\tau \\
&+ \int_0^t \int_\Omega f'(\mathbf{y}, \tau) G(\mathbf{y}, \mathbf{x}, t-\tau)\, d\mathbf{y}\, d\tau \\
&+ \int_\Omega S(\mathbf{y}) H_0'(\mathbf{y}) G(\mathbf{y}, \mathbf{x}, t)\, d\mathbf{y} \\
&- \int_0^t \int_{\Gamma_D} H'(\mathbf{y}, \tau) K(\mathbf{y}) \nabla_y G(\mathbf{y}, \mathbf{x}, t-\tau) \cdot \mathbf{n}(\mathbf{y})\, d\mathbf{y}\, d\tau \\
&+ \int_0^t \int_{\Gamma_N} G(\mathbf{y}, \mathbf{x}, t-\tau) Q'(\mathbf{y}, \tau)\, d\mathbf{y}\, d\tau.
\end{aligned} \tag{B5}
$$

Operating with $K'(\mathbf{x})\nabla_x$ on (B5) and taking conditional ensemble mean leads directly to (23).

Taking the conditional ensemble mean of (B5) yields the following formal relationship:

$$
\begin{aligned}
&\int_0^t \int_\Omega \mathbf{r}_c(\mathbf{y}, \tau) \cdot \nabla_y \langle G(\mathbf{y}, \mathbf{x}, t-\tau)\rangle_c\, d\mathbf{y}\, d\tau \\
&\quad = \int_0^t \int_\Omega \boldsymbol{\rho}_c(\mathbf{y}, \mathbf{x}, t-\tau) \cdot \nabla_y \langle h(\mathbf{y}, \tau)\rangle_c\, d\mathbf{y}\, d\tau
\end{aligned} \tag{B6}
$$

where $\boldsymbol{\rho}_c(\mathbf{y}, \mathbf{x}, t-\tau) = -\langle K'(\mathbf{y})\nabla_y G'(\mathbf{y}, \mathbf{x}, t-\tau)\rangle_c$ is a residual flux corresponding to Green's function. In analogy to (15), and because of the homogeneous boundary conditions satisfied by $G_c(\mathbf{y}, \mathbf{x}, t-\tau)$,

$$
\begin{aligned}
\boldsymbol{\rho}_c(\mathbf{y}, \mathbf{x}, t-\tau) &= \int_0^t \int_\Omega \mathbf{a}_c(\mathbf{y}, \mathbf{z}, t-\tau) \\
&\quad \nabla_z G_c(\mathbf{z}, \mathbf{x}, t-\tau)\, d\mathbf{z}\, d\tau
\end{aligned} \tag{B7}
$$

where $\mathbf{a}_c$ is given by (16).

Multiplying (B1) by $h'(\mathbf{y}, s)$ and taking conditional ensemble mean leads directly to (48). Multiplying (B5) by $K'(\mathbf{x})\nabla_x h'(\mathbf{x}, t)$ and $K'(\mathbf{x})$, respectively, then taking the conditional ensemble mean, leads directly to (52) and (53).

Rewriting (B1) in terms of $(\mathbf{y}, s)$, postmultiplying by $K'(\mathbf{x})\nabla_x^T h'(\mathbf{x}, t)$, and taking conditional ensemble mean leads to the following equation for $\mathbf{p}_c(\mathbf{x}, \mathbf{y}, t, s)$,

$$
\begin{aligned}
&\nabla_y^T[\langle K(\mathbf{y})\rangle_c \nabla_y \mathbf{p}_c^T(\mathbf{x}, \mathbf{y}, t, s)] + \nabla_y^T \boldsymbol{\alpha}_c(\mathbf{x}, \mathbf{y}, t, s) \\
&\quad + \nabla_y^T[\nabla_y \langle h(\mathbf{y}, s)\rangle_c \boldsymbol{\beta}_c^T(\mathbf{y}, \mathbf{x}, t)] - \nabla_y^T \mathbf{r}_c(\mathbf{y}, s) \mathbf{r}_c^T(\mathbf{x}, t) \\
&\quad = S(\mathbf{y}) \frac{\partial \mathbf{p}_c^T(\mathbf{x}, \mathbf{y}, t, s)}{\partial s}.
\end{aligned} \tag{B8}
$$

Here $\boldsymbol{\alpha}_c(\mathbf{x}, \mathbf{y}, t, s) = \langle K'(\mathbf{x}) K'(\mathbf{y}) \nabla_y h'(\mathbf{y}, s) \nabla_x^T h'(\mathbf{x}, t)\rangle_c$ is obtained by operating with $K'(\mathbf{x}) K'(\mathbf{y}) \nabla_x h'(\mathbf{x}, t) \nabla_y^T$ on (B5) after replacing $(\mathbf{x}, t)$ by $(\mathbf{y}, s)$ and taking conditional ensemble mean,

$$
\begin{aligned}
\boldsymbol{\alpha}_c(\mathbf{x}, \mathbf{y}, t, s) &= \int_0^s \int_\Omega \langle K'(\mathbf{x}) K'(\mathbf{y}) \nabla_y \nabla_z^T G(\mathbf{z}, \mathbf{y}, s-\tau) \\
&\quad \mathbf{r}_c(\mathbf{z}, \tau) \nabla_x^T h'(\mathbf{x}, t)\rangle_c\, d\mathbf{z}\, d\tau \\
&- \int_0^s \int_\Omega \langle K'(\mathbf{x}) K'(\mathbf{y}) K'(\mathbf{z}) \nabla_y \nabla_z^T G(\mathbf{z}, \mathbf{y}, s-\tau) \\
&\quad \nabla_z \langle h(\mathbf{z}, \tau)\rangle_c \nabla_x^T h'(\mathbf{x}, t)\rangle_c\, d\mathbf{z}\, d\tau.
\end{aligned} \tag{B9}
$$

The fourth order approximation of (B9) contains the term $\boldsymbol{\alpha}_{1c}(\boldsymbol{\xi}, \mathbf{x}, \mathbf{y}, t, s) = \langle K'(\boldsymbol{\xi}) K'(\mathbf{x}) K'(\mathbf{y}) \nabla_x h'(\mathbf{x}, t)\rangle_c$. Similar to $\boldsymbol{\alpha}_c$, this term is obtained by operating on (B5) with $K'(\boldsymbol{\xi}) K'(\mathbf{x}) K'(\mathbf{y}) \nabla_x$ and taking conditional ensemble mean. The fourth-order approximation of the resulting expression is given by (D11).

An equation satisfied by $u_c(\mathbf{y}, \mathbf{x}, t) = \langle K'(\mathbf{y}) h'(\mathbf{x}, t)\rangle_c$ is derived upon multiplying (B1) by $K'(\mathbf{y})$ and taking conditional ensemble mean,

$$
\begin{aligned}
&\nabla_x \cdot [\langle K(\mathbf{x})\rangle_c \nabla_x u_c(\mathbf{y}, \mathbf{x}, t)] + \nabla_x \cdot \boldsymbol{\beta}_c(\mathbf{y}, \mathbf{x}, t) \\
&\quad + \nabla_x \cdot [\langle K'(\mathbf{x}) K'(\mathbf{y})\rangle_c \nabla_x \langle h(\mathbf{x}, t)\rangle_c] = S(\mathbf{x}) \frac{\partial u_c(\mathbf{y}, \mathbf{x}, t)}{\partial t}.
\end{aligned} \tag{B10}
$$

Here an explicit expression for $\boldsymbol{\beta}_c(\mathbf{y}, \mathbf{x}, t) = \langle K'(\mathbf{x}) K'(\mathbf{y}) \nabla_x h'(\mathbf{x}, t)\rangle_c$ is derived by operating with $K'(\mathbf{x}) K'(\mathbf{y}) \nabla_x$ on (B5) and taking conditional ensemble mean,

$$
\begin{aligned}
&\boldsymbol{\beta}_c(\mathbf{y}, \mathbf{x}, t) = \\
&\quad \int_0^t \int_\Omega \langle K'(\mathbf{x}) K'(\mathbf{y}) \nabla_x \nabla_z^T G(\mathbf{z}, \mathbf{x}, t-\tau)\rangle_c \mathbf{r}_c(\mathbf{z}, \tau)\, d\mathbf{z}\, d\tau \\
&\quad - \int_0^t \int_\Omega \langle K'(\mathbf{x}) K'(\mathbf{y}) K'(\mathbf{z})\rangle_c \nabla_x \nabla_z^T \langle G(\mathbf{z}, \mathbf{x}, t-\tau)\rangle_c \\
&\quad \nabla_z \langle h(\mathbf{z}, \tau)\rangle_c\, d\mathbf{z}\, d\tau \\
&\quad - \int_0^t \int_\Omega \langle K'(\mathbf{x}) K'(\mathbf{y}) K'(\mathbf{z}) \nabla_x \nabla_z^T G'(\mathbf{z}, \mathbf{x}, t-\tau)\rangle_c \\
&\quad \nabla_z \langle h(\mathbf{z}, \tau)\rangle_c\, d\mathbf{z}\, d\tau.
\end{aligned} \tag{B11}
$$

To derive an explicit expression for $\boldsymbol{\beta}_{1c} = \langle K'(\mathbf{x}) K'(\mathbf{y}) K'(\mathbf{z}) \nabla_x \nabla_z^T G'(\mathbf{z}, \mathbf{x}, t-\tau)\rangle_c$ we note that in analogy to (B5),

$$
\begin{aligned}
G'(\mathbf{z}, \mathbf{x}, t-\tau) &= \int_0^t \int_\Omega \langle K'(\mathbf{y}) \nabla_y G'(\mathbf{z}, \mathbf{y}, t-\tau)\rangle_c \\
&\quad \cdot \nabla_y G(\mathbf{y}, \mathbf{x}, t-\tau)\, d\mathbf{y}\, d\tau \\
&- \int_0^t \int_\Omega K'(\mathbf{y}) \nabla_y \langle G(\mathbf{z}, \mathbf{y}, t-\tau)_c \\
&\quad \cdot \nabla_y G(\mathbf{y}, \mathbf{x}, t-\tau)\, d\mathbf{y}\, d\tau.
\end{aligned} \tag{B12}
$$

Operating with $K'(\mathbf{x}) K'(\mathbf{y}) K'(\mathbf{z}) \nabla_x \nabla_z^T$ on (B12) and taking conditional ensemble mean leads to an expression for $\boldsymbol{\beta}_{1c}$. A fourth-order approximation of this expression is given by (D14).

Substituting (6)–(8) into (13) gives

$$\mathbf{q}'(\mathbf{x}, t) = -\mathbf{r}_c(\mathbf{x}, t) - \langle K(\mathbf{x})\rangle_c \nabla h'(\mathbf{x}, t) - K'(\mathbf{x})\nabla\langle h(\mathbf{x}, t)\rangle_c - K'(\mathbf{x})\nabla h'(\mathbf{x}, t). \tag{B13}$$

Hence the second conditional moment of $\mathbf{q}'(\mathbf{x}, t)$ is given by (54).

Appendix C

Consider $Y(\mathbf{x}) = \langle Y(\mathbf{x})\rangle + Y'(\mathbf{x})$ with $\langle [Y'(\mathbf{x})]^2\rangle_c = \sigma_Y^2(\mathbf{x})$. Then

$$K(\mathbf{x}) = e^{Y(\mathbf{x})} = e^{\langle Y(\mathbf{x})\rangle_c + Y'(\mathbf{x})} = K_G(\mathbf{x}) e^{Y'(\mathbf{x})} \tag{C1}$$

where $K_G(\mathbf{x}) = e^{\langle Y(\mathbf{x})\rangle_c}$. Taking conditional ensemble mean yields

$$\langle K(\mathbf{x})\rangle_c = K_G(\mathbf{x}) \langle e^{Y'(\mathbf{x})}\rangle_c \tag{C2}$$

and hence

$$K'(\mathbf{x}) = K(\mathbf{x}) - \langle K(\mathbf{x})\rangle_c = K_G(\mathbf{x})[e^{Y'(\mathbf{x})} - \langle e^{Y'(\mathbf{x})}\rangle_c]. \tag{C3}$$

Substituting (C3) into the first equation of (16), expanding the exponents in powers of Y', and collecting terms of same power shows that the three leading-order approximations (in σ_Y) of $\mathbf{a}_c$ are given by (35).

Expanding $\langle K(\mathbf{y})\rangle_c$ and $\langle K(\mathbf{y})\rangle_c^{-1}$ and collecting terms of same power in σ_Y yields, upon noting that expansion of the second term in (17) is similar to that of (16) as given by (35), $\mathbf{b}_c^{(0)}(\mathbf{y}, \mathbf{x}, t-\tau) = \mathbf{b}_c^{(1)}(\mathbf{y}, \mathbf{x}, t-\tau) = 0$ and

$$\mathbf{b}_c^{(2)}(\mathbf{y}, \mathbf{x}, t-\tau) = -K_G(\mathbf{x})\langle Y'(\mathbf{x})Y'(\mathbf{y})\rangle_c [\nabla_x G_c^{(0)}(\mathbf{y}, \mathbf{x}, t-\tau) - \nabla_x \langle G^{(0)}(\mathbf{y}, \mathbf{x}, t-\tau)\rangle_c]. \tag{C4}$$

Since $\langle G^{(0)}\rangle_c = G_c^{(0)}$, $\mathbf{b}_c^{(2)}(\mathbf{y}, \mathbf{x}, t-\tau) = 0$ as indicated by (36). By the same token, it follows from (18) that $\mathbf{c}_c^{(0)}(\mathbf{z}, \mathbf{y}, \mathbf{x}, t-\tau, \tau-\tau_1) = \mathbf{c}_c^{(1)}(\mathbf{z}, \mathbf{y}, \mathbf{x}, t-\tau, \tau-\tau_1)$. To obtain a second-order approximation for $\mathbf{c}_c$, we rewrite (18) as

$$\begin{aligned}\mathbf{c}_c(\mathbf{z}, \mathbf{y}, \mathbf{x}, t-\tau, \tau-\tau_1) &= \langle K'(\mathbf{x})\nabla_x G(\mathbf{y}, \mathbf{x}, t-\tau) \nabla_y \cdot [K'(\mathbf{y})\nabla_y G_c(\mathbf{z}, \mathbf{y}, t-\tau_1)]\rangle_c \\ &\quad - \langle K'(\mathbf{x})\nabla_x G(\mathbf{y}, \mathbf{x}, t-\tau)\nabla_y \cdot [K'(\mathbf{y})\nabla_y G_c(\mathbf{z}, \mathbf{y}, t-\tau_1)]K^{-1}(\mathbf{z})\rangle_c \langle K(\mathbf{z})\rangle_c.\end{aligned} \tag{C5}$$

Expanding the first term to second order gives

$$\begin{aligned}&\langle K'(\mathbf{x})\nabla_x G(\mathbf{y}, \mathbf{x}, t-\tau)\nabla_y \cdot [K'(\mathbf{y})\nabla_y G_c(\mathbf{z}, \mathbf{y}, t-\tau_1)]\rangle_c \\ &\quad = \langle K_G(\mathbf{x}) Y'(\mathbf{x}) \nabla_x \langle G^{(0)}(\mathbf{y}, \mathbf{x}, t-\tau)\rangle_c \nabla_y \cdot [K_G(\mathbf{y})Y'(\mathbf{y})\nabla_y G_c^{(0)}(\mathbf{y}, \mathbf{x}, t-\tau)\rangle_c + O(\sigma_Y^3) \\ &\quad = K_G(\mathbf{x})\nabla_x \langle G^{(0)}(\mathbf{y}, \mathbf{x}, t-\tau)\rangle_c \nabla_y \cdot [K_G(\mathbf{y}) \langle Y'(\mathbf{x})Y'(\mathbf{y})\rangle_c \nabla_y G_c^{(0)}(\mathbf{y}, \mathbf{x}, t-\tau)] + O(\sigma_Y^3).\end{aligned} \tag{C6}$$

Expanding the second term in (C5) yields, to second order,

$$\begin{aligned}&\langle K'(\mathbf{x})\nabla_x G(\mathbf{y}, \mathbf{x}, t-\tau)\nabla_y \cdot [K'(\mathbf{y})\nabla_y G_c(\mathbf{z}, \mathbf{y}, t-\tau_1)] K^{-1}(\mathbf{z})\rangle_c \langle K(\mathbf{z})\rangle_c = K_G(\mathbf{x})\nabla_x \langle G^{(0)}(\mathbf{y}, \mathbf{x}, t-\tau)\rangle_c \\ &\quad \nabla_y \cdot [K_G(\mathbf{y})\langle Y'(\mathbf{x})Y'(\mathbf{y})\rangle_c \nabla_y G_c^{(0)}(\mathbf{y}, \mathbf{x}, t-\tau)] + O(\sigma_Y^3).\end{aligned} \tag{C7}$$

Substituting (C6) and (C7) into (C5) leads to (36).

Appendix D

A perturbation expansion of (48)–(53) leads to the following ith-order approximation ($i \geq 2$) for $C_{hc}(\mathbf{x}, \mathbf{y}, t, s)$:

$$\begin{aligned}S(\mathbf{x}) \frac{\partial C_{hc}^{(i)}(\mathbf{x}, \mathbf{y}, t, s)}{\partial t} &= \nabla_x \cdot \Bigg[K_G(\mathbf{x}) \sum_{n=0}^{i} \frac{1}{n!} \langle Y'^n(\mathbf{x})\rangle_c \nabla_x C_{hc}^{(i-n)}(\mathbf{x}, \mathbf{y}, t, s) + \mathbf{p}_c^{(i)}(\mathbf{x}, \mathbf{y}, t, s) \\ &\quad + \sum_{n=0}^{i} u_c^{(n)}(\mathbf{x}, \mathbf{y}, s) \nabla_x \langle h^{(i-n)}(\mathbf{x}, t)\rangle_c \Bigg]\end{aligned} \tag{D1}$$

subject to

$$C_{hc}^{(i)}(\mathbf{x}, \mathbf{y}, t, s) = 0 \qquad t = 0 \qquad \mathbf{x} \in \Omega \tag{D2}$$

$$C_{hc}^{(i)}(\mathbf{x}, \mathbf{y}, t, s) = 0 \qquad \mathbf{x} \in \Gamma_D \tag{D3}$$

$$\Bigg[K_G(\mathbf{x}) \sum_{n=0}^{i} \frac{1}{n!} \langle Y'^n(\mathbf{x})\rangle_c \nabla_x C_{hc}^{(i-n)}(\mathbf{x}, \mathbf{y}, t, s) + \mathbf{p}_c^{(i)}(\mathbf{x}, \mathbf{y}, t, s) + \sum_{n=0}^{i} u_c^{(n)}(\mathbf{x}, \mathbf{y}, s) \nabla_x \langle h^{(i-n)}(\mathbf{x}, t)\rangle_c \Bigg] \cdot \mathbf{n}(\mathbf{x}) = 0 \qquad \mathbf{x} \in \Gamma_N. \tag{D4}$$

The three leading terms in the perturbation expansion of $\mathbf{p}_c$ and u in (52) and (53) are given by

$$u_c^{(0)}(\mathbf{x}, \mathbf{y}, s) = u_c^{(1)}(\mathbf{x}, \mathbf{y}, s) = 0 \tag{D5}$$

$$u_c^{(2)}(\mathbf{x}, \mathbf{y}, s) = -K_G(\mathbf{x}) \int_0^s \int_\Omega \nabla_z \langle h^{(0)}(\mathbf{z}, \tau)\rangle_c \cdot \nabla_z \langle G^{(0)}(\mathbf{z}, \mathbf{y}, s-\tau)\rangle_c K_G(\mathbf{z}) \langle Y'(\mathbf{z})Y'(\mathbf{x})\rangle_c \, d\mathbf{z}\, d\tau \tag{D6}$$

$$\mathbf{p}_c^{(0)}(\mathbf{x}, \mathbf{y}, t, s) = \mathbf{p}_c^{(1)}(\mathbf{x}, \mathbf{y}, t, s) = \mathbf{p}_c^{(2)}(\mathbf{x}, \mathbf{y}, t, s) = 0. \tag{D7}$$

Thus second-order approximation of the conditional covariance of hydraulic head predictions, $C_{hc}^{(2)}(\mathbf{x}, \mathbf{y}, t, s)$, can be obtained by solving (D1)–(D7) with $i = 2$. Evaluating $C_{hc}^{(4)}(\mathbf{x}, \mathbf{y}, t, s)$ requires third- and fourth-order approximations of $\mathbf{p}_c$ and u_c. It is easy to see that these approximations contain moments of cross products of K', h', and/or G', which renders them unsuitable for numerical evaluation without Monte Carlo simulation. An implicit alternative to the explicit expressions (52) and (53) is given by (B8)–(B11). Perturbation expansion of (B8), (B9), and (B11) yields the following equations for $\mathbf{p}_c^{(3)}$ and $\mathbf{p}_c^{(4)}$:

$$\nabla_y^T [K_G(\mathbf{y})\nabla_y \mathbf{p}_c^{(3)T}(\mathbf{x}, \mathbf{y}, t, s)] + \nabla_y^T [\nabla_y \langle h^{(0)}(\mathbf{y}, s)\rangle_c \boldsymbol{\beta}_c^{(3)T}(\mathbf{x}, \mathbf{y}, t)] = S(\mathbf{y}) \frac{\partial \mathbf{p}_c^{(3)T}(\mathbf{x}, \mathbf{y}, t, s)}{\partial s} \tag{D8}$$

$$\begin{aligned}&\nabla_y^T [K_G(\mathbf{y})\nabla_y \mathbf{p}_c^{(4)T}(\mathbf{x}, \mathbf{y}, t, s)] + \nabla_y^T \boldsymbol{\alpha}_c^{(4)T}(\mathbf{x}, \mathbf{y}, t, s) + \nabla_y^T [\nabla_y \langle h^{(0)}(\mathbf{y}, s)\rangle_c \boldsymbol{\beta}_c^{(4)T}(\mathbf{x}, \mathbf{y}, t)] \\ &\quad + \nabla_y^T [\nabla_y \langle h^{(1)}(\mathbf{y}, s)\rangle_c \boldsymbol{\beta}_c^{(3)T}(\mathbf{x}, \mathbf{y}, t)] - \nabla_y^T \mathbf{r}_c^{(2)}(\mathbf{y}, s)\mathbf{r}_c^{(2)T}(\mathbf{x}, t) = S(\mathbf{y}) \frac{\partial \mathbf{p}_c^{(4)T}(\mathbf{x}, \mathbf{y}, t, s)}{\partial s}\end{aligned} \tag{D9}$$

where

$$\boldsymbol{\alpha}_c^{(4)}(\mathbf{x}, \mathbf{y}, t, s) = -\int_0^s \int_\Omega \nabla_y \nabla_z^T \langle G^{(0)}(\mathbf{z}, \mathbf{y}, s-\tau)\rangle_c \nabla_z \langle h^{(0)}(\mathbf{z}, \tau)\rangle_c \boldsymbol{\alpha}_{1c}^{(4)T}(\mathbf{z}, \mathbf{x}, \mathbf{y}, t)\, d\mathbf{z}\, d\tau, \tag{D10}$$

$$\boldsymbol{\alpha}_{1c}^{(4)}(\mathbf{x}, \mathbf{y}, \mathbf{z}, t) = -K_G(\mathbf{x})K_G(\mathbf{y})K_G(\mathbf{z}) \int_0^t \int_\Omega K_G(\boldsymbol{\xi}) \langle Y'(\boldsymbol{\xi})Y'(\mathbf{x})Y'(\mathbf{y})Y'(\mathbf{z})\rangle_c \nabla_x \nabla_\xi^T \langle h^{(0)}(\boldsymbol{\xi}, \tau)\rangle_c \nabla_\xi \langle G^{(0)}(\boldsymbol{\xi}, \mathbf{x}, t-\tau)\rangle_c\, d\boldsymbol{\xi}\, d\tau, \tag{D11}$$

and

$$\boldsymbol{\beta}_c^{(3)}(\mathbf{y}, \mathbf{x}, t) = -K_G(\mathbf{x})K_G(\mathbf{y}) \int_0^t \int_\Omega K_G(\mathbf{z}) \langle Y'(\mathbf{x})Y'(\mathbf{y})Y'(\mathbf{z})\rangle_c \nabla_x \nabla_z^T \langle G^{(0)}(\mathbf{z}, \mathbf{x}, t-\tau)\rangle_c \nabla_z \langle h^{(0)}(\mathbf{z}, \tau)\rangle_c\, d\mathbf{z}\, d\tau \tag{D12}$$

$$\begin{aligned}\boldsymbol{\beta}_c^{(4)}(\mathbf{y}, \mathbf{x}, t) = {}& K_G(\mathbf{x})K_G(\mathbf{y})\langle Y'(\mathbf{x})Y'(\mathbf{y})\rangle_c \int_0^t \int_\Omega \nabla_x \nabla_z^T \langle G^{(0)}(\mathbf{z}, \mathbf{x}, t-\tau)\rangle_c \mathbf{r}_c^{(2)}(\mathbf{z}, \tau)\, d\mathbf{z}\, d\tau \\ & - K_G(\mathbf{x})K_G(\mathbf{y}) \int_0^t \int_\Omega K_G(\mathbf{z}) \langle Y'(\mathbf{x})Y'(\mathbf{y})Y'(\mathbf{z})\rangle_c \{\nabla_x \nabla_z^T \langle G^{(0)}(\mathbf{z}, \mathbf{x}, t-\tau)\rangle_c \\ & \nabla_z \langle h^{(1)}(\mathbf{z}, \tau)\rangle_c + \nabla_x \nabla_z^T \langle G^{(1)}(\mathbf{z}, \mathbf{x}, t-\tau)\rangle_c \\ & \nabla_z \langle h^{(0)}(\mathbf{z}, \tau)\rangle_c\}\, d\mathbf{z}\, d\tau - \int_0^t \int_\Omega \boldsymbol{\beta}_{1c}^{(4)}(\mathbf{z}, \mathbf{y}, \mathbf{x}, t) \nabla_z \langle h^{(0)}(\mathbf{z}, \tau)\rangle_c\, d\mathbf{z}\, d\tau\end{aligned} \tag{D13}$$

where

$$\beta_{1c}^{(4)}(\mathbf{z}, \mathbf{x}, \mathbf{y}, t) = -K_G(\mathbf{x})K_G(\mathbf{y})K_G(\mathbf{z}) \int_0^t \int_\Omega K_G(\boldsymbol{\xi}) \langle Y'(\boldsymbol{\xi})Y'(\mathbf{x})Y'(\mathbf{y})Y'(\mathbf{z})\rangle_c \nabla_x \nabla_z^T [\nabla_\xi^T \langle G^{(0)}(\boldsymbol{\xi}, \mathbf{z}, t-\tau)\rangle_c \nabla_\xi \langle G^{(0)}(\boldsymbol{\xi}, \mathbf{x}, t-\tau)\rangle_c]\, d\boldsymbol{\xi}\, d\tau. \tag{D14}$$

Similarly, perturbation expansion of (B10) yields the following equations for $u_c^{(3)}$ and $u_c^{(4)}$

$$\begin{aligned}&\nabla_x \cdot [K_G(\mathbf{x})\nabla_x u_c^{(3)}(\mathbf{y}, \mathbf{x}, t)] + \nabla_x \boldsymbol{\beta}_c^{(3)}(\mathbf{y}, \mathbf{x}, t) \\ &\quad + \frac{1}{2} K_G(\mathbf{y})\nabla_x \cdot [K_G(\mathbf{x})\{\langle Y'^2(\mathbf{x})Y'(\mathbf{y})\rangle_c \\ &\quad + \langle Y'(\mathbf{x})Y'^2(\mathbf{y})\rangle_c\}\nabla_x \langle h^{(0)}(\mathbf{x}, t)\rangle_c] + K_G(\mathbf{y})\nabla_x \\ &\quad \cdot [K_G(\mathbf{x})\langle Y'(\mathbf{x})Y'(\mathbf{y})\rangle_c \nabla_x \langle h^{(1)}(\mathbf{x}, t)\rangle_c] \\ &\quad = S(\mathbf{x}) \frac{\partial u_c^{(3)}(\mathbf{y}, \mathbf{x}, t)}{\partial t}\end{aligned} \tag{D15}$$

$$\begin{aligned}&\nabla_x \cdot [K_G(\mathbf{x})\nabla_x u_c^{(4)}(\mathbf{y}, \mathbf{x}, t)] + \frac{1}{2}\nabla_x \\ &\quad \cdot [K_G(\mathbf{x})\sigma_Y^2(\mathbf{x})\nabla_x u_c^{(2)}(\mathbf{y}, \mathbf{x}, t)] + \nabla_x \cdot \boldsymbol{\beta}_c^{(4)}(\mathbf{y}, \mathbf{x}, t) \\ &\quad + K_G(\mathbf{y})\nabla_x \cdot \left[K_G(\mathbf{y})\left\{\frac{\langle Y'(\mathbf{x})Y'^3(\mathbf{y})\rangle_c + \langle Y'^3(\mathbf{x})Y'(\mathbf{y})\rangle_c}{6}\right.\right. \\ &\quad \left.\left. + \frac{\langle Y'^2(\mathbf{x})Y'^2(\mathbf{y})\rangle_c - \sigma_Y^2(\mathbf{x})\sigma_Y^2(\mathbf{y})}{4}\right\}\nabla_x \langle h^{(0)}(\mathbf{x}, t)\rangle_c\right] \\ &\quad + \frac{1}{2} K_G(\mathbf{y})\nabla_x \cdot [K_G(\mathbf{x})\{\langle Y'^2(\mathbf{x})Y'(\mathbf{y})\rangle_c \\ &\quad + \langle Y'(\mathbf{x})Y'^2(\mathbf{y})\rangle_c\}\nabla_x h^{(1)}(\mathbf{x}, t)] + K_G(\mathbf{y}) \\ &\quad \nabla_x \cdot [K_G(\mathbf{x})\langle Y'(\mathbf{x})Y'(\mathbf{y})\rangle_c \nabla_x \langle h^{(2)}(\mathbf{x}, t)\rangle_c] \\ &\quad = S(\mathbf{x}) \frac{\partial u_c^{(4)}(\mathbf{y}, \mathbf{x}, t)}{\partial t}.\end{aligned} \tag{D16}$$

One can easily verify that the three leading terms in the perturbation expansion of $\mathbf{C}_{qc}$ in (54) are

$$\begin{aligned}\frac{\mathbf{C}_{qc}^{(2)}(\mathbf{x}, \mathbf{y}, t, s)}{K_G(\mathbf{x})K_G(\mathbf{y})} = {}& \nabla_x \nabla_y^T C_{hc}^{(2)}(\mathbf{x}, \mathbf{y}, t, s) + \nabla_x \langle h^{(0)}(\mathbf{x}, t)\rangle_c \\ & \nabla_y^T \langle h^{(0)}(\mathbf{y}, s)\rangle_c \langle Y'(\mathbf{x})Y'(\mathbf{y})\rangle_c \\ & + \frac{1}{K_G(\mathbf{x})}\nabla_x \langle h^{(0)}(\mathbf{x}, t)\rangle_c \\ & \nabla_y^T u_c^{(2)}(\mathbf{x}, \mathbf{y}, s) + \frac{1}{K_G(\mathbf{y})}\nabla_x u_c^{(2)}(\mathbf{y}, \mathbf{x}, t)\nabla_y^T \langle h^{(0)}(\mathbf{y}, s)\rangle_c\end{aligned} \tag{D17}$$

$$\begin{aligned}\frac{\mathbf{C}_{qc}^{(3)}(\mathbf{x}, \mathbf{y}, t, s)}{K_G(\mathbf{x})K_G(\mathbf{y})} = {}& \nabla_x \nabla_y^T C_{hc}^{(3)}(\mathbf{x}, \mathbf{y}, t, s) \\ & + \frac{\langle Y'(\mathbf{x})Y'^2(\mathbf{y})\rangle_c + \langle Y'^2(\mathbf{x})Y'(\mathbf{y})\rangle_c}{2}\nabla_x \langle h^{(0)}(\mathbf{x}, t)\rangle_c \\ & \nabla_y^T \langle h^{(0)}(\mathbf{y}, s)\rangle_c + [\nabla_x \langle h^{(1)}(\mathbf{x}, t)\rangle_c \nabla_y^T \langle h^{(0)}(\mathbf{y}, s)\rangle_c \\ & + \nabla_x \langle h^{(0)}(\mathbf{x}, t)\rangle_c \nabla_y^T \langle h^{(1)}(\mathbf{y}, s)\rangle_c]\langle Y'(\mathbf{x})Y'(\mathbf{y})\rangle_c \\ & + \frac{1}{K_G(\mathbf{x})}[\nabla_x \langle h^{(1)}(\mathbf{x}, t)\rangle_c \nabla_y^T u_c^{(2)}(\mathbf{x}, \mathbf{y}, s) \\ & + \nabla_x \langle h^{(0)}(\mathbf{x}, t)\rangle_c \nabla_y^T u_c^{(3)}(\mathbf{x}, \mathbf{y}, s)] + \frac{1}{K_G(\mathbf{y})}[\nabla_x u_c^{(2)}(\mathbf{y}, \mathbf{x}, t) \\ & \nabla_y^T \langle h^{(1)}(\mathbf{y}, s)\rangle_c + \nabla_x u_c^{(3)}(\mathbf{y}, \mathbf{x}, t)\nabla_y^T \langle h^{(0)}(\mathbf{y}, s)\rangle_c] \\ & + \frac{1}{K_G(\mathbf{x})}\nabla_y^T \mathbf{p}_c^{(3)}(\mathbf{x}, \mathbf{y}, t, s) + \frac{1}{K_G(\mathbf{y})}\nabla_x \mathbf{p}_c^{(3)T}(\mathbf{y}, \mathbf{x}, s, t) \\ & + \frac{1}{K_G(\mathbf{x})K_G(\mathbf{y})}[\boldsymbol{\beta}_c^{(3)}(\mathbf{y}, \mathbf{x}, t)\nabla_y^T \langle h^{(0)}(\mathbf{y}, s)\rangle_c \\ & + \nabla_x \langle h^{(0)}(\mathbf{x}, t)\rangle_c \boldsymbol{\beta}_c^{(3)T}(\mathbf{x}, \mathbf{y}, s)]\end{aligned} \tag{D18}$$

where it is understood that $\nabla_y^T \mathbf{p}_c(\mathbf{x}, \mathbf{y}, t, s) = \langle K'(\mathbf{x})\nabla_x h'(\mathbf{x}, t)\nabla_y^T h'(\mathbf{y}, s)\rangle_c$ is a dyadic, the same being true in

$$
\begin{aligned}
\frac{C_{qc}^{(4)}(\mathbf{x}, \mathbf{y}, t, s)}{K_G(\mathbf{x})K_G(\mathbf{y})} &= -\frac{\mathbf{r}_c^{(2)}(\mathbf{x}, t)\mathbf{r}_c^{(2)T}(\mathbf{y}, s)}{K_G(\mathbf{x})K_G(\mathbf{y})} + \nabla_x\nabla_y^T C_{hc}^{(4)}(\mathbf{x}, \mathbf{y}, t, s) \\
&+ \frac{\sigma_Y^2(\mathbf{x}) + \sigma_Y^2(\mathbf{y})}{2}\nabla_x\nabla_y^T C_{hc}^{(2)}(\mathbf{x}, \mathbf{y}, t, s) \\
&+ \nabla_x\langle h^{(0)}(\mathbf{x}, t)\rangle_c \nabla_y^T\langle h^{(0)}(\mathbf{y}, s)\rangle_c \\
&\left[\frac{\langle Y'(\mathbf{x})Y'^3(\mathbf{y})\rangle_c + \langle Y'^3(\mathbf{x})Y'(\mathbf{y})\rangle_c}{6}\right. \\
&\left. + \frac{\langle Y'^2(\mathbf{x})Y'^2(\mathbf{y})\rangle_c - \sigma_Y^2(\mathbf{x})\sigma_Y^2(\mathbf{y})}{4}\right] + [\nabla_x\langle h^{(1)}(\mathbf{x}, t)\rangle_c \\
&\nabla_y^T\langle h^{(0)}(\mathbf{y}, s)\rangle_c + \nabla_x\langle h^{(0)}(\mathbf{x}, t)\rangle_c\nabla_y^T\langle h^{(1)}(\mathbf{y}, s)\rangle_c] \\
&\frac{\langle Y'(\mathbf{x})Y'^2(\mathbf{y})\rangle_c + \langle Y'^2(\mathbf{x})Y'(\mathbf{y})\rangle_c}{2} + [\nabla_x\langle h^{(2)}(\mathbf{x}, t)\rangle_c \\
&\nabla_y^T\langle h^{(0)}(\mathbf{y}, s)\rangle_c + \nabla_x\langle h^{(0)}(\mathbf{x}, t)\rangle_c\nabla_y^T\langle h^{(2)}(\mathbf{y}, s)\rangle_c \\
&+ \nabla_x\langle h^{(1)}(\mathbf{x}, t)\rangle_c\nabla_y^T\langle h^{(1)}(\mathbf{y}, s)\rangle_c]\langle Y'(\mathbf{x})Y'(\mathbf{y})\rangle_c \qquad \text{(D19)} \\
&+ \frac{1}{K_G(\mathbf{x})}[\nabla_x\langle h^{(2)}(\mathbf{x}, t)\rangle_c\nabla_y^T u_c^{(2)}(\mathbf{x}, \mathbf{y}, s) + \nabla_x\langle h^{(1)}(\mathbf{x}, t)\rangle_c \\
&\nabla_y^T u_c^{(3)}(\mathbf{x}, \mathbf{y}, s) + \nabla_x\langle h^{(0)}(\mathbf{x}, t)\rangle_c\nabla_y^T u_c^{(4)}(\mathbf{x}, \mathbf{y}, s)] \\
&+ \frac{1}{K_G(\mathbf{y})}[\nabla_x u_c^{(2)}(\mathbf{y}, \mathbf{x}, t)\nabla_y^T\langle h^{(2)}(\mathbf{y}, s)\rangle_c \\
&+ \nabla_x u_c^{(3)}(\mathbf{y}, \mathbf{x}, t)\nabla_y^T\langle h^{(1)}(\mathbf{y}, s)\rangle_c + \nabla_x u_c^{(4)}(\mathbf{y}, \mathbf{x}, t) \\
&\nabla_y^T\langle h^{(0)}(\mathbf{y}, s)\rangle_c] + \frac{1}{K_G(\mathbf{x})}\nabla_y^T\mathbf{p}_c^{(4)}(\mathbf{x}, \mathbf{y}, t, s) + \frac{1}{K_G(\mathbf{y})} \\
&\nabla_x\mathbf{p}_c^{(4)T}(\mathbf{y}, \mathbf{x}, s, t) + \frac{1}{K_G(\mathbf{x})K_G(\mathbf{y})}[\boldsymbol{\beta}_c^{(4)}(\mathbf{y}, \mathbf{x}, t) \\
&\nabla_y^T h^{(0)}(\mathbf{y}, s) + \boldsymbol{\beta}_c^{(3)}(\mathbf{y}, \mathbf{x}, t)\nabla_y^T\langle h^{(1)}(\mathbf{y}, s)\rangle_c \\
&+ \nabla_x h^{(0)}(\mathbf{x}, t)\boldsymbol{\beta}_c^{(4)T}(\mathbf{x}, \mathbf{y}, s) + \nabla_x\langle h^{(1)}(\mathbf{x}, t)\rangle_c\boldsymbol{\beta}_c^{(3)T}(\mathbf{x}, \mathbf{y}, s) \\
&+ \boldsymbol{\alpha}_c^{(4)}(\mathbf{x}, \mathbf{y}, t, s)].
\end{aligned}
$$

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S. P. Neuman, Department of Hydrology and Water Resources, The University of Arizona, Building 11, P.O. Box 210011, Tucson, AZ 85721-0011.

D. M. Tartakovsky, Geoanalysis Group, Earth and Environmental Sciences Division, Los Alamos National Laboratory, Los Alamos, NM 87545.

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