Available online at www.sciencedirect.com
SCIENCE DIRECT®
Advances in Water Resources 28 (2005) 393–403
Advances in Water Resources
www.elsevier.com/locate/advwatres

Interface dynamics in randomly heterogeneous porous media

Yu.N. Lazarev [a], P.V. Petrov [a], Daniel M. Tartakovsky [b,*]

[a] Mathematical Division, Institute of Technical Physics, P.O. Box 245, Snezhinsk 456770, Russia
[b] Theoretical Division, Los Alamos National Laboratory, Group T-7, MS B284, Los Alamos, NM 87545, USA

Received 28 May 2004; received in revised form 18 October 2004; accepted 5 November 2004

Abstract

We consider the dynamics of a fluid interface in heterogeneous porous media, whose hydraulic properties are uncertain. Modeling hydraulic conductivity as a random field of given statistics allows us to predict the interface dynamics and to estimate the corresponding predictive uncertainty by means of statistical moments. The novelty of our approach to obtaining the interface statistics consists of dynamically mapping the Cartesian coordinate system onto a coordinate system associated with the moving front. This transforms a difficult problem of deriving closure relationships for highly nonlinear stochastic flows with free surfaces into a relatively simple problem of deriving stochastic closures for linear flows in domains with fixed boundaries. We derive a set of deterministic equations for the statistical moments of the interfacial dynamics, which hold in one and two spatial dimensions, and analyze their solutions for one-dimensional flow.

Keywords: Free surface; Conductivity tensor; Random fluctuations; Stochastic; Moment equations

1. Introduction

Free surface (interface, moving front) problems arise in a variety of applications, such as wetting and drying of porous media, pumping in unconfined aquifers, secondary oil recovery, DNAPL migration and remediation, seawater intrusion, etc. Traditional deterministic modeling of these and other similar phenomena assumes that the subsurface environment is homogeneous and/or that the relevant system parameters, such as hydraulic conductivity and dispersivity, are known with certainty in all of their relevant details. However, in most applications, interfaces propagate in heterogeneous environments, whose system parameters can only be sampled at selected locations in space and/or time. The need to assign parameter values to the points where measurements are not available, combined with measurement errors, introduces parameter uncertainty. This, in turn, leads to uncertainty in predictions of the interface dynamics.

Uncertainty in hydraulic conductivity $K(\mathbf{x})$ and other system parameters is conveniently quantified by treating them as random fields, whose sample statistics are inferred from data [1–5]. This renders the corresponding flow and transport equations stochastic. Solutions of these equations (hydraulic head, the velocity and position of a free surface, etc.) are given in terms of probability density functions or, equivalently, ensemble moments. Usually, the first moment (ensemble mean) provides the estimate or prediction of the system behavior, and the second moment (variance or standard deviation) quantifies the predictive uncertainty.

While flow and transport in randomly heterogeneous porous media with fixed boundaries have been studied extensively [1–5], stochastic analysis of the interfacial

* Corresponding author. Tel.: +1 505 667 0968; fax: +1 505 665 5757.
E-mail addresses: yulaz@snezhinsk.ru (Yu.N. Lazarev), pvpetrov@snezhinsk.ru (P.V. Petrov), dmt@lanl.gov (D.M. Tartakovsky).

0309-1708/$ - see front matter © 2004 Elsevier Ltd. All rights reserved.
doi:10.1016/j.advwatres.2004.11.003

dynamics in random media is still in its infancy. A reason for the relative lack of progress in analyzing this important problem is its high degree of nonlinearity. Since the randomness of hydraulic conductivity of a porous medium causes the free surface dynamics to be stochastic, ensemble averaging of the flow equations involves calculating ensemble means of such quantities as integrals of random functions over random domains and random functionals. One approach to dealing with this problem is to employ simplifying physical assumptions—such as the Dupuit approximation to model seawater intrusion in costal aquifers [6] and flow towards wells in unconfined aquifers [7] or a uniform flow approximation to describe free-surface flows [8]—which effectively eliminate moving boundaries (interfaces). A numerical Monte Carlo study of water tables in a heterogeneous dam was reported in [9].

The first attempt to rigorously analyze the interface dynamics in randomly heterogeneous porous media dealt with the gravity-free propagation of wetting fronts [10]. It relied on the expansions of integrals over the random domains into a Taylor series around the corresponding ensemble mean geometries. To make the analysis and numerical implementation of this procedure tractable, the authors found it necessary to linearize the problem by retaining only the leading terms in such expansions. This approach was used to describe the dynamics of phreatic surfaces [11], DNAPL fingers [12], and immiscible fluids [13] in heterogeneous porous media. However, the linearization procedure lying at the heart of these solutions is less than optimal, in that the subsequent perturbation expansions do not contain all the relevant terms [10].

The main goal of this study is to introduce an approach that does not require a linearization of the kind proposed in [10]. We formulate governing equations for the interface dynamics in random porous media in Section 2. The key part of our approach, a stochastic mapping of the random, time-varying flow domain onto a fixed domain, is presented in Section 3. Section 4 provides the corresponding mappings for the flow equations. This enables us to use standard perturbation techniques to derive, in Sections 5 and 6, closure approximations for the stochastic flow equations in two dimensions. Section 7 contains a brief outline of a numerical algorithm for solving the resulting deterministic moment equations. In Section 8, we analyze the accuracy of our approximations in a one-dimensional setting, by comparing the analytical solutions of moment equations with their exact counterparts.

2. Problem formulation

Consider the motion of a fluid–fluid interface in a randomly heterogeneous porous medium Ω_T that is bounded by the surface Γ_T. Following [10], we set gravity, capillary length, and the viscosity of one fluid to zero. In the inviscid fluid (air), the pressure is constant and may be set to zero. The viscous, incompressible fluid (water) occupies the flow domain Ω ($\Omega \in \Omega_T$), which is bounded either entirely by a free surface γ or by a combination of γ and some segments of Γ_T (Fig. 1). Such flow is described by a combination of Darcy's law and mass conservation,

$$\mathbf{q}(\mathbf{r},t) = -K(\mathbf{r})\nabla h(\mathbf{r},t), \quad \nabla \cdot \mathbf{q} = f(\mathbf{r},t), \quad \mathbf{r} \in \Omega(t), \tag{1}$$

subject to the boundary conditions

$$h(\mathbf{r},t) = H(\mathbf{r},t), \quad \mathbf{r} \in \Gamma_D, \tag{2a}$$

$$\mathbf{n}(\mathbf{r}) \cdot \mathbf{q}(\mathbf{r},t) = S(\mathbf{r},t), \quad \mathbf{r} \in \Gamma_N, \tag{2b}$$

$$h(\mathbf{r},t) = 0, \quad \mathbf{r} \in \gamma(t) \tag{2c}$$

where $\mathbf{q}$ is the Darcy flux, K is the hydraulic conductivity of a porous medium, h is the hydraulic head, f is the source function, and $\mathbf{n}$ is unit normal to the surface $\Gamma = \Gamma_D \cup \Gamma_N \cup \gamma$ consisting of Dirichlet segments Γ_D, Neumann segments Γ_N, and a moving front γ. The functions H and S are the prescribed hydraulic head and flux on the Dirichlet and Neumann boundary segments, respectively. The dynamics of the free surface $\gamma(t)$ is described by

$$\frac{d\mathbf{R}}{dt} = \frac{V_n(\mathbf{R},t)\mathbf{n}}{n_e} = \frac{\mathbf{V}(\mathbf{R},t)}{n_e}, \quad \mathbf{R} \in \gamma(t), \tag{2d}$$

where n_e is porosity, $\mathbf{V}$ is the Darcian velocity of the moving front γ, and mass conservation requires that V_n, the normal velocity of the front, satisfies $V_n(\mathbf{R},t) = \mathbf{q}(\mathbf{R},t) \cdot \mathbf{n}(\mathbf{R},t)$. Eqs. (1)–(2) constitute the widely used Green and Ampt [14] model for the propagation of wetting fronts in porous media.

Uncertainty in the hydraulic conductivity of a porous medium is captured by representing $K = K(\mathbf{r})$ as a ran-

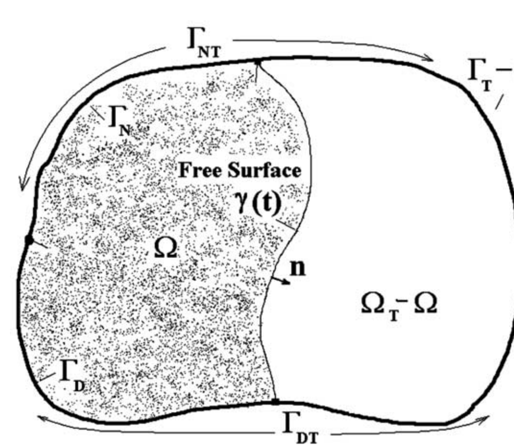

Fig. 1. A schematic representation of the dynamics of free surfaces in porous media.

dom field with given mean $\overline{K}$, variance σ_K^2, and a two-point correlation function $\rho_K(\mathbf{r}_1, \mathbf{r}_2)$. Other possible sources of randomness, which we do not consider here, are the driving forces f, H, and S, and porosity n_e. (Since the random effects of initial conditions and driving forces are additive, they can be easily incorporated into the present analysis following the procedure outlined in [15]. It is common (e.g., [5] and references therein) to treat porosity as a deterministic function rather than as a random field. One can extend our analysis to incorporate the randomness of porosity by treating its variance as an additional perturbation parameter, e.g., [16].) Our goal is to develop a set of deterministic equations for the mean and variance of the system states. The former estimates the interfacial dynamics, while the latter quantifies the uncertainty associated with such an estimate.

3. Stochastic mapping of the flow domain

Consider a curvilinear coordinate system (ξ, η), which is tied to the moving interface $\gamma(t)$. An advantage of using such a coordinate system is that the random, time-varying flow domain Ω in the (x, y) Cartesian coordinate system becomes a fixed regular-shaped domain (e.g., a square or a rectangle) W in the (ξ, η) coordinate system (see Fig. 2).

Following [17,18], we define a stochastic mapping $\Omega \rightarrow W$ $(0 \leqslant \xi \leqslant 1, 0 \leqslant \eta \leqslant 1)$ as a solution of the Laplace equations

$$\frac{\partial^2 x}{\partial \xi^2} + \frac{\partial^2 x}{\partial \eta^2} = 0, \quad \frac{\partial^2 y}{\partial \xi^2} + \frac{\partial^2 y}{\partial \eta^2} = 0, \tag{3}$$

subject to the boundary conditions

$$x(1, \eta) = x_\gamma(\eta), \quad y(1, \eta) = y_\gamma(\eta) \tag{4a}$$

$$x(0, \eta) = x_{\Gamma_D}(\eta), \quad y(0, \eta) = y_{\Gamma_D}(\eta) \tag{4b}$$

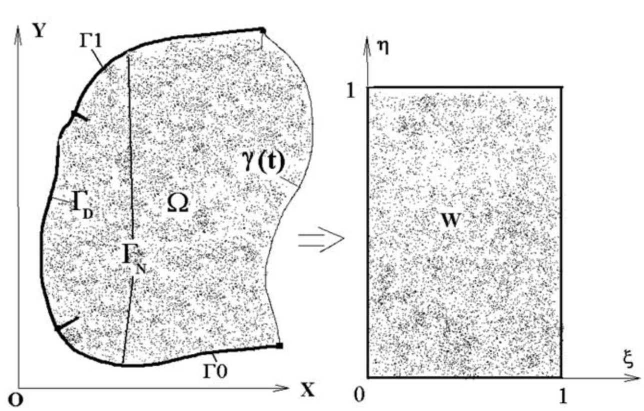

Fig. 2. A mapping of the flow domain.

and

$$x(\xi, 0) = x_{\Gamma_0}(\xi), \quad y(\xi, 0) = y_{\Gamma_0}(\xi) \tag{4c}$$

$$x(\xi, 1) = x_{\Gamma_1}(\xi), \quad y(\xi, 1) = y_{\Gamma_1}(\xi), \tag{4d}$$

where $x_{\Gamma_D}(\eta)$, $y_{\Gamma_D}(\eta)$, $x_{\Gamma_0}(\xi)$, $y_{\Gamma_0}(\xi)$, $x_{\Gamma_1}(\xi)$, and $y_{\Gamma_1}(\xi)$ are the known functions that describe the boundaries Γ_D and $\Gamma_N = \Gamma_0 \cup \Gamma_1$, respectively.

For the mapping (3) and (4) to exist, it is necessary that the boundary of the flow domain be piecewise smooth [10]. This condition holds for most physical applications, such as (unstable) front propagation in porous media. Moreover, as will become clear below, it is sufficient for (3) and (4) to exist in a weak sense, which further smooths the boundary through its ensemble averaging.

We use Reynolds decomposition $A = \overline{A} + \widetilde{A}$ to represent a random field A as the sum of its mean $\overline{A}$ and a zero-mean random fluctuation $\widetilde{A}$. (In the following, we use $\overline{A}$ and $\langle A \rangle$ interchangeably to indicate the ensemble mean of A.) Then stochastic averaging of (3) and (4) yields the ensemble mean component of the stochastic mapping as a solution of

$$\frac{\partial^2 \bar{x}}{\partial \xi^2} + \frac{\partial^2 \bar{x}}{\partial \eta^2} = 0 \tag{5}$$

subject to

$$\bar{x}(1, \eta) = \bar{x}_\gamma(\eta), \quad \bar{x}(\xi, 0) = x_{\Gamma_0}(\xi), \tag{6a}$$

$$\bar{x}(0, \eta) = x_{\Gamma_D}(\eta), \quad \bar{x}(\xi, 1) = x_{\Gamma_1}(\xi). \tag{6b}$$

Here $\bar{x}_\gamma(0) = x_{\Gamma_0}(1)$ and $\bar{x}_\gamma(1) = x_{\Gamma_1}(1)$.

Let us introduce the Green's function $L(\xi, \eta | \xi_1, \eta_1)$ as a solution of the Poisson equation,

$$\frac{\partial^2 L}{\partial \xi_1^2} + \frac{\partial^2 L}{\partial \eta_1^2} = -\delta(\xi_1 - \xi)\delta(\eta_1 - \eta), \tag{7}$$

subject to the homogeneous boundary conditions,

$$\begin{aligned} L(\xi, \eta \mid \xi_1 = 0, \eta_1) &= L(\xi, \eta \mid \xi_1 = 1, \eta_1) \\ &= L(\xi, \eta \mid \xi_1, \eta_1 = 0) = L(\xi, \eta \mid \xi_1, \eta_1 = 1) = 0. \end{aligned} \tag{8}$$

Then (5) and (6) can be recast as

$$\begin{aligned} \bar{x}(\xi, \eta) = &- \int_0^1 \left[\bar{x}_\gamma(\eta_1) \frac{\partial L}{\partial \xi_1}_{|_{\xi_1 = 1}} - x_{\Gamma_D}(\eta_1) \frac{\partial L}{\partial \xi_1}_{|_{\xi_1 = 0}} \right] d\eta_1 \\ &- \int_0^1 \left[x_{\Gamma_1}(\xi_1) \frac{\partial L}{\partial \eta_1}_{|_{\eta_1 = 1}} - x_{\Gamma_0}(\xi_1) \frac{\partial L}{\partial \eta_1}_{|_{\eta_1 = 0}} \right] d\xi_1. \end{aligned} \tag{9}$$

An expression for $\bar{y}$ is obtained in a similar fashion.

To obtain an equation for the random fluctuations $\tilde{x}$, we subtract (5) and (6) from (3) and (4), which gives

$$\frac{\partial^2 \tilde{x}}{\partial \xi^2} + \frac{\partial^2 \tilde{x}}{\partial \eta^2} = 0 \tag{10}$$

subject to

$$\tilde{x}(1,\eta) = \tilde{x}_\gamma(\eta), \quad \tilde{x}(\xi,0) = \tilde{x}_{\Gamma_0}(\xi), \tag{11a}$$

$$\tilde{x}(0,\eta) = 0, \quad \tilde{x}(\xi,1) = \tilde{x}_{\Gamma_1}(\xi). \tag{11b}$$

To find the boundary functions $\tilde{x}_{\Gamma_0}(\xi)$ and $\tilde{x}_{\Gamma_1}(\xi)$, we note that both x and $\bar{x}$ belong to Γ_0 and Γ_1, and that the following equalities hold,

$$\tilde{x}_{\Gamma_0}(1) = \tilde{x}_\gamma(0), \quad \tilde{x}_{\Gamma_0}(0) = 0,$$
$$\tilde{x}_{\Gamma_1}(1) = \tilde{x}_\gamma(1), \quad \tilde{x}_{\Gamma_1}(0) = 0. \tag{12}$$

Let $\theta = (1+\tilde{\theta})\xi$, where $\langle\tilde{\theta}\rangle = 0$, be a random variable describing the random variation of the coordinate x along boundaries Γ_0 and Γ_1. Expanding $x_{\Gamma_0}(\theta)$ and $x_{\Gamma_1}(\theta)$ in a Taylor series, and retaining the leading terms in these expansions, yields

$$x_{\Gamma_0}(\theta) \approx x_{\Gamma_0}(\bar{\theta}) + \frac{\partial x_{\Gamma_0}}{\partial\bar{\theta}}\xi\tilde{\theta}, \quad x_{\Gamma_1}(\theta) \approx x_{\Gamma_1}(\bar{\theta}) + \frac{\partial x_{\Gamma_1}}{\partial\bar{\theta}}\xi\tilde{\theta}, \tag{13}$$

and

$$\tilde{x}_{\Gamma_0} = \frac{\partial x_{\Gamma_0}}{\partial\bar{\theta}}\xi\tilde{\theta}, \quad \tilde{x}_{\Gamma_1} = \frac{\partial x_{\Gamma_1}}{\partial\bar{\theta}}\xi\tilde{\theta}. \tag{14}$$

Combining (12) and (14) gives

$$\tilde{x}_{\Gamma_0}(\xi) = \tilde{x}_\gamma(0)\xi\frac{\mathrm{d}x_{\Gamma_0}}{\mathrm{d}\xi}\left(\frac{\mathrm{d}x_{\Gamma_0}}{\mathrm{d}\xi}\right)^{-1}_{\xi=1},$$
$$\tilde{x}_{\Gamma_1}(\xi) = \tilde{x}_\gamma(1)\xi\frac{\mathrm{d}x_{\Gamma_1}}{\mathrm{d}\xi}\left(\frac{\mathrm{d}x_{\Gamma_1}}{\mathrm{d}\xi}\right)^{-1}_{\xi=1}. \tag{15}$$

In terms of the Green's function (7) and (8), the solution of (10) and (11) can be written as

$$\tilde{x}(\xi,\eta) = \int_0^1 \tilde{x}_{\Gamma_0}(\xi_1)\frac{\partial L}{\partial\eta_1}\Big|_{\eta_1=0}\mathrm{d}\xi_1 - \int_0^1 \tilde{x}_{\Gamma_1}(\xi_1)\frac{\partial L}{\partial\eta_1}\Big|_{\eta_1=1}\mathrm{d}\xi_1 - \int_0^1 \tilde{x}_\gamma(\eta_1)\frac{\partial L}{\partial\xi_1}\Big|_{\xi_1=1}\mathrm{d}\eta_1. \tag{16}$$

An expression for $\tilde{y}$ is obtained in a similar fashion.

Eq. (16) and the corresponding equation for $\tilde{y}$ define the linear integral operators $\widehat{X}$ and $\widehat{Y}$ that relate the mapping fluctuations inside the flow domain, $\tilde{x}(\xi,\eta)$ and $\tilde{y}(\xi,\eta)$, to their counterparts on the moving interface, $\tilde{x}_\gamma$ and $\tilde{y}_\gamma$, i.e.,

$$\tilde{x}(\xi,\eta) = \widehat{X}\cdot\tilde{x}_\gamma, \quad \tilde{y}(\xi,\eta) = \widehat{Y}\cdot\tilde{y}_\gamma. \tag{17}$$

4. Transformed flow equations

Let the subscripts ξ and η denote the partial derivatives with respect to ξ and η, respectively, and

$$J = \frac{\partial(x,y)}{\partial(\xi,\eta)} = x_\xi y_\eta - x_\eta y_\xi \tag{18}$$

denote the mapping Jacobian. Then

$$\frac{\partial}{\partial x} = \frac{y_\eta}{J}\frac{\partial}{\partial\xi} - \frac{y_\xi}{J}\frac{\partial}{\partial\eta}, \quad \frac{\partial}{\partial y} = -\frac{x_\eta}{J}\frac{\partial}{\partial\xi} + \frac{x_\xi}{J}\frac{\partial}{\partial\eta} \tag{19}$$

and (1) becomes

$$\frac{\partial y_\eta q_1}{\partial\xi} - \frac{\partial y_\xi q_1}{\partial\eta} - \frac{\partial x_\eta q_2}{\partial\xi} + \frac{\partial x_\xi q_2}{\partial\eta} = Jf[x(\xi,\eta),y(\xi,\eta)]. \tag{20}$$

The Darcy flux components q_1 and q_2 are given by

$$q_1 = -K[x(\xi,\eta),y(\xi,\eta)]\left(\frac{y_\eta}{J}\frac{\partial h}{\partial\xi} - \frac{y_\xi}{J}\frac{\partial h}{\partial\eta}\right), \tag{21a}$$

$$q_2 = -K[x(\xi,\eta),y(\xi,\eta)]\left(-\frac{x_\eta}{J}\frac{\partial h}{\partial\xi} + \frac{x_\xi}{J}\frac{\partial h}{\partial\eta}\right). \tag{21b}$$

Substituting (21) into (20) and denoting $F = Jf$ yields

$$-\frac{\partial}{\partial\xi}K^{11}\frac{\partial h}{\partial\xi} - \frac{\partial}{\partial\eta}K^{22}\frac{\partial h}{\partial\xi} + \frac{\partial}{\partial\xi}K^{12}\frac{\partial h}{\partial\eta} + \frac{\partial}{\partial\eta}K^{21}\frac{\partial h}{\partial\xi} = F, \tag{22}$$

where the components of the hydraulic conductivity tensor are given by

$$K^{11} = K\frac{x_\eta^2 + y_\eta^2}{J}, \quad K^{22} = K\frac{x_\xi^2 + y_\xi^2}{J},$$
$$K^{12} = K^{21} = K\frac{x_\xi x_\eta + y_\xi y_\eta}{J}. \tag{23}$$

Expressions (23) can be rewritten as

$$K^{\alpha\beta} = \left(\mathfrak{R}^{-1^{\mathrm{T}}}\mathfrak{R}^{-1}\right)^{\alpha\beta}, \quad \alpha,\beta = 1,2,$$
$$\mathfrak{R} = \frac{1}{\sqrt{KJ}}\begin{Vmatrix} x_\xi & y_\xi \\ x_\eta & y_\eta \end{Vmatrix}. \tag{24}$$

Since in general the mapping $\Omega \to W$ is not orthogonal, $K^{12} \neq K^{21} \neq 0$.

While hydraulic conductivity in the fixed coordinate system (x,y) was taken to be a scalar, hydraulic conductivity in the moving coordinate system (ξ,η) becomes a second rank tensor. Of course, the flow equation (22) remains valid even if hydraulic conductivity in the (x,y) coordinate system were a tensor.

Since the transformed flow equations involve first derivatives x_ξ, x_η, y_ξ, and y_η, the boundary Γ (or, more precisely, its ensemble mean) must be at least once differentiable. This explains the existence condition for the mapping $\Omega \to W$ in Section 3.

Boundary conditions for the flow equation (22) are derived by recasting (2) in the moving coordinate system. For the Dirichlet boundary segments this gives

$$h(\xi=0,\eta) = H\left[x_{\Gamma_\mathrm{D}}(\eta), y_{\Gamma_\mathrm{D}}(\eta)\right], \quad h(\xi=1,\eta) = 0. \tag{25a}$$

Likewise, the conditions on the Neumann boundaries transform into

$$-q_2(\eta=0) = K^{22}\left[x_{\Gamma_0}(\xi), y_{\Gamma_0}(\xi)\right]\frac{\partial h}{\partial \eta} - K^{21}[x_{\Gamma_0}(\xi), y_{\Gamma_0}(\xi)]\frac{\partial h}{\partial \xi} = \sqrt{x_\xi^2 + y_\xi^2}S[x_{\Gamma_0}(\xi), y_{\Gamma_0}(\xi)] \tag{25b}$$

and

$$-q_2(\eta=1) = K^{22}\left[x_{\Gamma_1}(\xi), y_{\Gamma_1}(\xi)\right]\frac{\partial h}{\partial \eta} - K^{21}[x_{\Gamma_1}(\xi), y_{\Gamma_1}(\xi)]\frac{\partial h}{\partial \xi} = -\sqrt{x_\xi^2 + y_\xi^2}S[x_{\Gamma_1}(\xi), y_{\Gamma_1}(\xi)]. \tag{25c}$$

The equations for the interface dynamics become (Appendix A)

$$\frac{\partial x_\gamma}{\partial t} = \chi^x \frac{\partial h}{\partial \xi}, \quad \frac{\partial y_\gamma}{\partial t} = \chi^y \frac{\partial h}{\partial \xi}, \tag{26a}$$

where

$$\chi^x = -\frac{K}{n_e J}\frac{\partial y_\gamma}{\partial \eta}, \quad \chi^y = \frac{K}{n_e J}\frac{\partial x_\gamma}{\partial \eta}. \tag{26b}$$

Introducing a new notation for the coordinates $\xi^1 = \xi$ and $\xi^2 = \eta$, and using the Einstein summation convention and tensorial notation allows us to recast (20) and (21) in a compact form

$$\frac{\partial q^\alpha}{\partial \xi^\alpha} = F, \quad q^\alpha = -K^{\alpha\beta}\frac{\partial h}{\partial \xi^\beta} \quad \alpha, \beta = 1, 2. \tag{27}$$

Finally, introducing a hydraulic resistivity tensor

$$Z^{\alpha\beta} = \left(K^{-1}\right)^{\alpha\beta} = \left(\Re\Re^{\mathrm{T}}\right)^{\alpha\beta} \tag{28}$$

transforms the flow Eq. (27) into

$$\frac{\partial q^\alpha}{\partial \xi^\alpha} = F, \quad \frac{\partial h}{\partial \xi^\alpha} = -Z^{\alpha\beta}q^\beta, \quad \left(\xi^1, \xi^2\right) \in W. \tag{29}$$

This is the form we use below to derive moment equations for hydraulic head and the interface dynamics.

5. Statistical moments of head

Stochastic averaging of the flow equation (29), defined on the fixed domain W and subject to the Dirichlet and Neumann boundary conditions (25), has received considerable attention [1–5,19]. Most of these studies have assumed that hydraulic conductivity (resistivity) is a scalar, while in (29) it is a tensor.

To simplify presentation, we set the source function and boundary fluxes to zero, i.e., $f = 0$ and $S = 0$. (One can easily incorporate nonzero deterministic f and S into the following analysis.) Taking the ensemble average of (29) and (25) yields equations for the mean hydraulic head

$$\frac{\partial \bar{q}^\alpha}{\partial \xi^\alpha} = 0, \quad -\frac{\partial \bar{h}}{\partial \xi^\alpha} = \overline{Z}^{\alpha\beta}\bar{q}^\beta + \left\langle \widetilde{Z}^{\alpha\beta}\tilde{q}^\beta \right\rangle \tag{30}$$

subject to the boundary conditions

$$\bar{h}\left(\xi^1 = 0, \xi^2\right) = H\left(\xi^2, t\right), \quad \bar{h}\left(\xi^1 = 1, \xi^2\right) = 0, \tag{31a}$$

$$\bar{q}^2\left(\xi^1, \xi^2 = 0\right) = 0, \quad \bar{q}^2\left(\xi^1, \xi^2 = 1\right) = 0. \tag{31b}$$

We use a perturbation expansion in the powers of the conductivity fluctuations to approximate the second moment $\langle \widetilde{Z}^{\alpha\beta}\tilde{q}^\beta\rangle$ in (30). The second-order (in the standard deviation of conductivity) approximation of $\langle \widetilde{Z}^{\alpha\beta}\tilde{q}^\beta\rangle$ gives rise to the nonlocal mean flow equation (Appendix B),

$$-\frac{\partial \bar{h}}{\partial \xi^\alpha} = \left[\overline{Z}^{\alpha\beta} - \left\langle \widetilde{Z}^{\alpha\alpha_1}\left(\overline{Z}^{-1}\right)^{\alpha_1\beta_1}\widetilde{Z}^{\beta_1\beta}\right\rangle\right]\bar{q}^\beta(\boldsymbol{\xi}) + \int_0^1\int_0^1 \left\langle \widetilde{Z}^{\alpha\alpha_1}T^{\alpha_1\beta_1}\widetilde{Z}_1^{\beta_1\beta}\right\rangle \bar{q}^\beta(\boldsymbol{\xi}_1)\mathrm{d}\boldsymbol{\xi}_1, \tag{32}$$

where $\mathbf{Z} = \mathbf{Z}(\boldsymbol{\xi})$, $\mathbf{Z}_1 = \mathbf{Z}(\boldsymbol{\xi}_1)$, and, as before, the summation over the repeated indexes is implied. The tensor $\mathbf{T}$ in (32) is defined by

$$T^{\alpha_1\beta_1} = \left(\overline{Z}^{-1}\right)^{\alpha_1\alpha_2}\frac{\partial^2 E(\boldsymbol{\xi} \mid \boldsymbol{\xi}_1)}{\partial \xi^{\alpha_2}\partial \boldsymbol{\xi}_1^{\beta_2}}, \left(\overline{Z}_1^{-1}\right)^{\beta_2\beta_1}, \tag{33}$$

where $E(\boldsymbol{\xi}|\boldsymbol{\xi}_1)$ is the Green's function defined as a solution of

$$\frac{\partial}{\xi_2^\alpha}\left[\left(\overline{Z}^{-1}\right)^{\alpha\beta}\frac{\partial E}{\partial \xi_2^\beta}\right] = -\delta\left(\xi_2^1 - \xi_1^1\right)\delta\left(\xi_2^2 - \xi_1^2\right) \tag{34}$$

subject to the boundary conditions

$$E\left(\boldsymbol{\xi}_1 \mid \xi_2^1 = 0, \xi_2^2\right) = 0, \quad E\left(\boldsymbol{\xi}_1 \mid \xi_2^1 = 1, \xi_2^2\right) = 0, \tag{35a}$$

$$\left(\overline{Z}^{-1}\right)^{2\alpha}\frac{\partial G}{\partial \xi_2^\alpha}\bigg|_{\xi_2^2=0} = 0, \quad \left(\overline{Z}^{-1}\right)^{2\alpha}\frac{\partial G}{\partial \xi_2^\alpha}\bigg|_{\xi_2^2=1} = 0. \tag{35b}$$

To obtain the second-order approximations of the correlation matrices of $\mathbf{Z}$ in (32), we linearize the random fluctuations $\widetilde{Z}^{\alpha\beta}$ about the corresponding means,

$$\widetilde{Z}^{\alpha\beta}\left(\tilde{x}, \tilde{y}, \widetilde{K}; \boldsymbol{\xi}\right) \approx Z_x^{\alpha\beta}\tilde{x}(\boldsymbol{\xi}) + Z_y^{\alpha\beta}\tilde{y}(\boldsymbol{\xi}) + Z_K^{\alpha\beta}\widetilde{K}[\bar{x}(\boldsymbol{\xi}), \bar{y}(\boldsymbol{\xi})], \tag{36}$$

where $Z_x^{\alpha\beta}$, $Z_y^{\alpha\beta}$, and $Z_K^{\alpha\beta}$ are the linear deterministic operators defined by (C.1)–(C.3) in Appendix C. Hence, the correlation matrices in (32) can be expressed, up to second order, in terms of the cross-correlations between $\tilde{x}$, $\tilde{y}$, and $\widetilde{K}$. These, in turn, are related to the statistics of the interface fluctuations $\tilde{x}_\gamma$ and $\tilde{y}_\gamma$ by (17).

For completeness, we outline a procedure for calculating the head covariance in Appendix B.

6. Statistical moments of the interface dynamics

The ensemble averaging of (26) yields

$$\frac{\partial \bar{x}_\gamma}{\partial t} = \bar{\chi}^x \frac{\partial \bar{h}}{\partial \xi^1} + \left\langle \tilde{\chi}^x \frac{\partial \tilde{h}}{\partial \xi^1} \right\rangle. \tag{37}$$

To derive an expression for the mixed moment in (37), we note that the second-order approximation of $\tilde{\chi}^x$ is derived from a Taylor expansion as

$$\tilde{\chi}^x\left(\tilde{x}_\gamma, \tilde{y}_\gamma, \widetilde{K}\right) \approx \chi^x_k \widetilde{K} + \chi^x_x \tilde{x}_\gamma + \chi^x_y \tilde{y}_\gamma, \tag{38}$$

where the deterministic expansion coefficients χ^x_k, χ^x_x and χ^x_y are given by (C.4)–(C.6) in Appendix C. Subtracting (37) from (26), and retaining the second-order terms gives

$$\frac{\partial \tilde{x}_\gamma}{\partial t} = \bar{\chi}^x \frac{\partial \tilde{h}}{\partial \xi^1} + \tilde{\chi}^x \frac{\partial \bar{h}}{\partial \xi^1}. \tag{39}$$

Substituting (38) and a similar expansion for the hydraulic head fluctuations $\tilde{h}$ into (39) leads to

$$\frac{\partial \tilde{x}_\gamma(\xi^2_1)}{\partial t} = X_k(\xi^2_1, \boldsymbol{v})\widetilde{K}(\boldsymbol{v}) + X_x(\xi^2_1, \xi^2_3)\tilde{x}_\gamma(\xi^2_3) + X_y(\xi^2_1, \xi^2_3)\tilde{y}_\gamma(\xi^2_3), \tag{40}$$

where the deterministic coefficients X_k, X_x, and X_y are given by (C.7) in Appendix C. Similarly, an equation for $\tilde{y}_\gamma$ is

$$\frac{\partial \tilde{y}_\gamma(\xi^2_1)}{\partial t} = Y_k(\xi^2_1, \boldsymbol{v})\widetilde{K}(\boldsymbol{v}) + Y_x(\xi^2_1, \xi^2_3)\tilde{x}_\gamma(\xi^2_3) + Y_y(\xi^2_1, \xi^2_3)\tilde{y}_\gamma(\xi^2_3). \tag{41}$$

Equations for covariances $C^\gamma_{xx}(\xi^2_1, \xi^2_2) = \langle \tilde{x}_\gamma(\xi^2_1)\tilde{x}_\gamma(\xi^2_2)\rangle$ and $C^\gamma_{yy}(\xi^2_1, \xi^2_2) = \langle \tilde{y}_\gamma(\xi^2_1)\tilde{y}_\gamma(\xi^2_2)\rangle$, and cross-covariance $C^\gamma_{xy}(\xi^2_1, \xi^2_2) = \langle \tilde{x}_\gamma(\xi^2_1)\tilde{y}_\gamma(\xi^2_2)\rangle$ are derived from (40) and (41) by noting that

$$\frac{\partial C^\gamma_{xx}(\xi^2_1, \xi^2_2)}{\partial t} = \left\langle \frac{\partial \tilde{x}_\gamma(\xi^2_1)}{\partial t}\tilde{x}_\gamma(\xi^2_2) \right\rangle + \left\langle \frac{\partial \tilde{x}_\gamma(\xi^2_2)}{\partial t}\tilde{x}_\gamma(\xi^2_1) \right\rangle \tag{42a}$$

and

$$\frac{\partial C^\gamma_{xy}(\xi^2_1, \xi^2_2)}{\partial t} = \left\langle \frac{\partial \tilde{x}_\gamma(\xi^2_1)}{\partial t}\tilde{y}_\gamma(\xi^2_2) \right\rangle + \left\langle \frac{\partial \tilde{y}_\gamma(\xi^2_2)}{\partial t}\tilde{x}_\gamma(\xi^2_1) \right\rangle. \tag{42b}$$

This gives

$$\begin{aligned}\frac{\partial C^\gamma_{xx}(\xi^2_1, \xi^2_2)}{\partial t} = {} & X_k(\xi^2_1, \boldsymbol{v})C^\gamma_{Kx}(\boldsymbol{v}, \xi^2_2) \\ & + X_x(\xi^2_1, \xi^2_3)C^\gamma_{xx}(\xi^2_2, \xi^2_3) \\ & + X_y(\xi^2_1, \xi^2_3)C^\gamma_{yy}(\xi^2_2, \xi^2_3) \\ & + X_k(\xi^2_2, \boldsymbol{v})C^\gamma_{Kx}(\boldsymbol{v}, \xi^2_1) \\ & + X_x(\xi^2_2, \xi^2_3)C^\gamma_{xx}(\xi^2_1, \xi^2_3) \\ & + X_y(\xi^2_2, \xi^2_3)C^\gamma_{yy}(\xi^2_1, \xi^2_3),\end{aligned} \tag{43}$$

$$\begin{aligned}\frac{\partial C^\gamma_{xy}(\xi^2_1, \xi^2_2)}{\partial t} = {} & X_k(\xi^2_1, \boldsymbol{v})C^\gamma_{Ky}(\boldsymbol{v}, \xi^2_2) \\ & + X_x(\xi^2_1, \xi^2_3)C^\gamma_{xy}(\xi^2_3, \xi^2_2) \\ & + X_y(\xi^2_1, \xi^2_3)C^\gamma_{yy}(\xi^2_2, \xi^2_3) \\ & + X_k(\xi^2_2, \boldsymbol{v})C^\gamma_{Kx}(\boldsymbol{v}, \xi^2_1) \\ & + X_x(\xi^2_2, \xi^2_3)C^\gamma_{xx}(\xi^2_1, \xi^2_3) \\ & + X_y(\xi^2_2, \xi^2_3)C^\gamma_{xy}(\xi^2_1, \xi^2_3),\end{aligned} \tag{44}$$

and an equation for $C^\gamma_{yy}(\xi^2_1, \xi^2_2)$ which is analogous to (43).

To derive approximate solutions for cross-covariances $C^\gamma_{Kx}(\boldsymbol{v}, \xi^2) = \langle \widetilde{K}(\boldsymbol{v})\tilde{x}_\gamma(\xi^2)\rangle$ and $C^\gamma_{Ky}(\boldsymbol{v}, \xi^2) = \langle \widetilde{K}(\boldsymbol{v})\tilde{y}_\gamma(\xi^2)\rangle$, we note that their second-order approximations involve only the leading term in an expansion of conductivity fluctuations, $\widetilde{K} \approx \widetilde{K}(\bar{x}, \bar{y})$. (The dependence of $\widetilde{K}$ on $\tilde{x}$ and $\tilde{y}$ enters the third- and higher-order terms.) Then

$$\frac{\partial \widetilde{K}}{\partial t} = \widehat{C}\widetilde{K}, \quad \widehat{C} = \frac{\partial \bar{x}}{\partial t}\frac{\partial}{\partial \bar{x}} + \frac{\partial \bar{y}}{\partial t}\frac{\partial}{\partial \bar{y}}. \tag{45}$$

Combining (45) with (9) yields

$$\widehat{C} = \mathbf{U}\frac{\partial}{\partial \boldsymbol{\xi}} \tag{46a}$$

where $\mathbf{U} = (U_1, U_2)^{\mathrm{T}}$ is given by

$$U_1 = \frac{1}{\Delta}\left(\bar{y}_{\xi^2}\frac{\partial \bar{x}}{\partial t} - \bar{x}_{\xi^2}\frac{\partial \bar{y}}{\partial t}\right), \quad U_2 = \frac{1}{\Delta}\left(-\bar{y}_{\xi^1}\frac{\partial \bar{x}}{\partial t} + \bar{x}_{\xi^2}\frac{\partial \bar{y}}{\partial t}\right), \tag{46b}$$

$$\Delta = \bar{x}_{\xi^1}\bar{y}_{\xi^2} - \bar{x}_{\xi^2}\bar{y}_{\xi^1}, \tag{46c}$$

and

$$\frac{\partial}{\partial t}\begin{pmatrix}\bar{x}(\boldsymbol{\xi}, t) \\ \bar{y}(\boldsymbol{\xi}, t)\end{pmatrix} = -\int_0^1 \frac{\partial L(\boldsymbol{\xi} \mid \xi^1_1 = 1, \xi^2_1)}{\partial \xi^1_1}\frac{\partial}{\partial t}\begin{pmatrix}\bar{x}_\gamma(\xi^2_1, t) \\ \bar{y}_\gamma(\xi^2_1, t)\end{pmatrix}\mathrm{d}\xi^2_1. \tag{46d}$$

Multiplying (40) with $\widetilde{K}$, taking the ensemble mean in a manner similar to (42), and accounting for (45) and (46) leads to

$$\begin{aligned}\frac{\partial C^\gamma_{Kx}(\boldsymbol{v}, \xi^2)}{\partial t} = {} & \widehat{C}(\boldsymbol{v}, \boldsymbol{v}_1)C^\gamma_{Kx}(\boldsymbol{v}_1, \xi^2) \\ & + X_k(\xi^2, \boldsymbol{v}_1)\rho_K(\boldsymbol{v}, \boldsymbol{v}_1) \\ & + X_x(\xi^2, \xi^2_1)C^\gamma_{Kx}(\boldsymbol{v}, \xi^2_1) \\ & + X_y(\xi^2, \xi^2_1)C^\gamma_{Ky}(\boldsymbol{v}, \xi^2_1).\end{aligned} \tag{47}$$

An analogous procedure applied to (41) leads to an equation for $C^\gamma_{Ky}(\boldsymbol{v}, \xi^2)$.

Eqs. (43), (44) and (47) are subject to the homogeneous initial conditions. A conductivity correlation function in the moving coordinate system $\rho_K(\boldsymbol{v}, \boldsymbol{v}_1)$ at time t is computed, to second order in conductivity fluctuations, at the mean coordinates.

7. Numerical implementation

We present a detailed description of our numerical algorithm and its implementation in a companion paper. A brief outline is as follows.

- Given the mean location of the interface at time t, solve (3) and (4) to construct the dynamic mapping $\Omega \to W$.
- Compute the correlation matrices $\mathbf{Z}$, $\mathbf{Z}_1$, and $\mathbf{T}$ in the nonlocal mean flow equation (32).
- Solve the mean flow equation (32) and equations for the second moments (Appendix B) to obtain the mean hydraulic head $\bar{h}$ and the hydraulic head variance σ_h^2.
- Calculate the mean velocity of the interface from (37) and compute the mean position of the interface at time $t + \Delta t$.
- Solve Eqs. (43), (44) and (47) to obtain cross-covariances C_{xx}^{γ}, C_{yy}^{γ}, C_{xy}^{γ}, C_{Kx}^{γ}, and C_{Ky}^{γ} at time $t + \Delta t$.
- Repeat calculations.

8. A computational example

While in general our moment equations have to be solved numerically, some flow scenarios are amenable to analytical treatment. Consider the one-dimensional front propagation in a randomly heterogeneous porous medium of log-normal hydraulic conductivity $K = \ln Y$ with geometric mean $K_g = \exp(\overline{Y})$, variance σ_Y^2, correlation function ρ_Y, and correlation length λ. The front is driven by hydraulic head $h(0) = H_0$ imposed at the boundary $x = 0$.

We recast the problem in a dimensionless form by introducing

$$x_d = \frac{x}{\lambda}, \quad t_d = 2\frac{tK_g H_0}{n_e \lambda^2}, \quad K_d = \frac{K}{K_g}, \quad h_d = \frac{h}{H_0}. \tag{48}$$

In the following, we drop the subscript d.

8.1. Mapping

Solving the one-dimensional version of (3) and (4) yields a mapping

$$x = x_\gamma \xi, \tag{49a}$$

whose Jacobian is

$$J = \frac{\partial x}{\partial \xi} = x_\gamma. \tag{49b}$$

8.2. Transformed flow equations

The mapping (49) transforms flow equations into the one-dimensional version of (29),

$$\frac{\partial q}{\partial \xi} = 0, \quad \frac{\partial h}{\partial \xi} = -Zq, \quad h(0) = 1, \quad h(1) = 0. \tag{50a}$$

Hydraulic resistivity $Z \equiv Z^{11}$ is obtained from (24) and (28) as

$$Z = x_\gamma K^{-1}. \tag{50b}$$

8.3. Statistical moments of head

The one-dimensional version of (30) and (31) gives

$$\frac{\partial \bar{q}}{\partial \xi} = 0, \quad \frac{\partial \bar{h}}{\partial \xi} = -\bar{Z}\bar{q} - \left\langle \widetilde{Z}\tilde{q} \right\rangle, \quad \bar{h}(0) = 1, \quad \bar{h}(1) = 0. \tag{51}$$

To close (51), i.e., to compute the mixed moment $\langle \widetilde{Z}\tilde{q} \rangle$, we seek the first-order (in σ_Y^2) approximation of the mean hydraulic head, $\bar{h} = \bar{h}^{(0)} + \bar{h}^{(1)} + O(\sigma_Y^4)$.

Consider the normalized dimensionless hydraulic resistivity,

$$z = Z/\bar{x}_\gamma. \tag{52}$$

Since

$$\overline{K} = K_g(1 + \sigma_Y^2/2) + O(\sigma_Y^4)$$

and

$$\langle \widetilde{K}^2 \rangle = \sigma_Y^2 + O(\sigma_Y^4),$$

it follows from (50b) and (52) that

$$\bar{z} = 1 + \frac{\sigma_Y^2}{2} - \Phi - \xi\frac{\partial \Phi}{\partial \xi}, \quad \tilde{z} = \frac{\tilde{x}_\gamma}{\bar{x}_\gamma} - \widetilde{K}, \quad \Phi = \frac{\left\langle \widetilde{K}\tilde{x}_\gamma \right\rangle}{\bar{x}_\gamma}, \tag{53}$$

where $\widetilde{K} = \widetilde{K}[\bar{x}(\xi)]$.

The one-dimensional Green's function in (34) and (35) is given by

$$E(\xi \mid \xi_1) = (\xi_1 - \xi)\theta(\xi - \xi_1) + (1 - \xi_1)\xi, \tag{54}$$

where $\theta(\xi)$ is the Heaviside function denned as $\theta = 1$ for $\xi \geqslant 0$ and $\theta = 0$ otherwise. Substituting (54) into the one-dimensional versions of (32) and (33), and introducing $Q = q\bar{x}_\gamma$, yields a solution for the mean hydraulic head,

$$-\frac{\partial \bar{h}}{\partial \xi} = \overline{Q}\left[\bar{z}(\xi) - \int_0^1 C_z(\xi, \nu)\,d\nu\right], \quad \frac{\partial \overline{Q}}{\partial \xi} = 0. \tag{55}$$

The normalized mean flux $\overline{Q}$ is obtained by integrating the first equation in (55), while taking into account the boundary conditions (50),

$$\overline{Q} = \left[\int_0^1 \bar{z}(\nu)\,d\nu - \int_0^1 \int_0^1 C_z(\mu, \nu)\,d\mu\,d\nu\right]^{-1}. \tag{56}$$

It follows from (53) that the covariance function $C_z(\mu,\nu)=\langle\tilde{z}(\mu)\tilde{z}(\nu)\rangle$ in (55) and (56) is given by

$$C_z(\mu,\nu)=\rho_Y[\bar{x}_\gamma(\mu-\nu)]-\Phi(\mu)-\Phi(\nu)+r_\gamma, \tag{57}$$

where $r_\gamma=\sigma_\gamma^2/\bar{x}_\gamma^2$ and $\sigma_\gamma^2=\langle\tilde{x}_\gamma^2\rangle$.

Substituting (54) into the one-dimensional versions of (B.3) and (B.4) yields an expression for the random fluctuations of hydraulic head,

$$\tilde{h}(\xi)=\overline{Q}\left[\xi\int_0^1\tilde{z}(\nu)\,d\nu-\int_0^\xi\tilde{z}(\nu)\,d\nu\right],\quad \widetilde{Q}=-\overline{Q}\int_0^1\tilde{z}(\nu)\,d\nu \tag{58}$$

Hence, the variances of hydraulic head and flux are given by

$$\frac{\sigma_h^2}{\overline{Q}^2}=\xi^2\int_0^1\int_0^1 C_z(\mu,\nu)\,d\mu\,d\nu-2\xi\int_0^1\int_0^\xi C_z(\mu,\nu)\,d\mu\,d\nu+\int_0^\xi\int_0^\xi C_z(\mu,\nu)\,d\mu\,d\nu, \tag{59}$$

and

$$\sigma_Q^2=\overline{Q}^2\int_0^1\int_0^1 C_z(\mu,\nu)\,d\mu\,d\nu, \tag{60}$$

respectively.

8.4. Statistical moments of the interface dynamics

The equations of motion of the interface (37) and (39) can now be written as

$$\frac{\partial\bar{x}_\gamma}{\partial t}=\frac{\overline{Q}(\xi=1)}{2\bar{x}_\gamma},\quad \frac{\partial\tilde{x}_\gamma}{\partial t}=\frac{\widetilde{Q}(\xi=1)}{2\bar{x}_\gamma}. \tag{61}$$

Recalling the definition of $\tilde{z}$ in (53), it follows from (61) that

$$\frac{\partial}{\partial t}\left(\frac{\tilde{x}_\gamma}{\bar{x}_\gamma}\right)=-\frac{\overline{Q}}{2\bar{x}_\gamma^2}\left[\int_0^1\tilde{z}(\nu)d\nu+\frac{\tilde{x}_\gamma}{\bar{x}_\gamma}\right]=\frac{\overline{Q}}{2\bar{x}_\gamma^2}\left[\int_0^1\widetilde{K}[\bar{x}(\nu)]\,d\nu-2\frac{\tilde{x}_\gamma}{\bar{x}_\gamma}\right]. \tag{62}$$

The one-dimensional version of (45) and (46) gives an equation for the conductivity fluctuations,

$$\frac{\partial\widetilde{K}}{\partial t}=\frac{\xi}{\bar{x}_\gamma}\frac{\partial\bar{x}_\gamma}{\partial t}\frac{\partial\widetilde{K}}{\partial\xi}=\frac{\overline{Q}\xi}{2\bar{x}_\gamma^2}\frac{\partial\widetilde{K}}{\partial\xi}. \tag{63}$$

Combining (62) with (63) leads to equations for the covariances r_γ and Φ,

$$\frac{\partial r_\gamma}{\partial t}=\frac{\overline{Q}}{\bar{x}_\gamma^2}\left[\int_0^1\Phi(\nu)\,d\nu-2r_\gamma\right], \tag{64}$$

and

$$\frac{\partial\Phi}{\partial t}-\frac{\overline{Q}\xi}{2\bar{x}_\gamma^2}\frac{\partial\Phi}{\partial\xi}=\frac{\overline{Q}}{2\bar{x}_\gamma^2}\left[\int_0^1\rho_Y[\bar{x}(\xi),\bar{x}(\nu)]\,d\nu-2\Phi(\xi)\right], \tag{65}$$

respectively. Integrating (64) and (65) subject to homogeneous initial conditions gives

$$r_\gamma=\int_0^1\int_0^1(1-\xi)(1-\eta)\rho_Y[\bar{x}_\gamma(\xi-\eta)]\,d\xi\,d\eta \tag{66}$$

and

$$\Phi(\xi)=\int_0^1(1-\eta)\rho_Y[\bar{x}_\gamma(\xi-\eta)]\,d\eta. \tag{67}$$

Eqs. (55)–(57), (59)–(61), (66) and (67) form a closed set of deterministic equations for the statistics of the interface dynamics and related state variables.

8.5. Comparison with exact solutions

The direct integration of flow equations (50) leads to

$$h=1-Q^{-1}\int_0^\xi z(\nu)\,d\nu,\quad Q^{-1}=\int_0^1 z(\nu)\,d\nu. \tag{68}$$

The statistics of the interface dynamics can be computed from (68) exactly provided a porous medium is perfectly correlated ($\lambda\to\infty$), i.e., hydraulic conductivity is a random constant [10]. Indeed, for perfectly correlated media (68) gives

$$h=1-\frac{x}{x_\gamma},\quad q=\frac{K}{x_\gamma},\quad x_\gamma^2=Kt, \tag{69}$$

which gives exact analytical expressions for the mean and variance of the interface position [10],

$$[\bar{x}_\gamma]_{\text{exact}}=e^{\sigma_Y^2/8}\sqrt{t},\quad [\sigma_\gamma^2]_{\text{exact}}=\left(e^{\sigma_Y^2/2}-e^{\sigma_Y^2/4}\right)t. \tag{70}$$

Thus the mean position of the interface scales as $\sqrt{t}$, while its variance increases linearly with t. Additionally, the normalized cross-covariance $\Phi=\langle\widetilde{K}\tilde{x}_\gamma\rangle/\bar{x}_\gamma$ has the form

$$[\Phi]_{\text{exact}}=e^{9\sigma_Y^2/8}-e^{5\sigma_Y^2/8} \tag{71}$$

and is time invariant.

Next we compare the first-order perturbation solutions derived in the previous section with their exact counterparts. Since for perfectly correlated media $C_Y=\sigma_Y^2$, (66) and (67) yield

$$r_\gamma=\frac{\sigma_Y^2}{4},\quad \Phi=\frac{\sigma_Y^2}{2}. \tag{72}$$

Then it follows from (53) that $\bar{z}=1$ and $\sigma_z^2\equiv\rho_Y-2\Phi+r_\gamma=\sigma_Y^2/4$, so that (56) gives

$$\overline{Q}=\left(1-\frac{\sigma_Y^2}{4}\right)^{-1}. \tag{73}$$

Substituting (73) into (61) leads to perturbation approximations for the mean and variance of the interface position,

$$\bar{x}_\gamma = \sqrt{\overline{Q}t} = \sqrt{\frac{t}{1-\sigma_Y^2/4}} = \left(1+\frac{\sigma_Y^2}{8}+\mathrm{O}(\sigma_Y^4)\right)\sqrt{t} \quad (74a)$$

and

$$\sigma_\gamma^2 \equiv \bar{x}_\gamma^2 r_\gamma = \frac{\sigma_Y^2}{4}\left(1+\frac{\sigma_Y^2}{8}\right)^2 t = \left(\frac{\sigma_Y^2}{4}+\mathrm{O}(\sigma_Y^4)\right)t. \quad (74b)$$

The comparison of (70) and (74) reveals that our perturbation solutions (i) give the correct time evolution of the interface statistics, and (ii) are indeed the first-order (in the log conductivity variance σ_Y^2) approximations of their exact counterparts. This is not the case with the linearized solutions, which can be found in Section 4.2 of [10].

Another advantage of the proposed approach is that it involves relative fluctuations of the dependent and independent random fields (e.g., $\tilde{x}_\gamma/\bar{x}_\gamma$ and $\widetilde{Q}/\overline{Q}$), rather than their absolute counterparts (e.g., $\tilde{x}_\gamma$ and $\widetilde{Q}$). The former can be small even when the latter are large, which is important for the accuracy of perturbation solutions. In particular, it follows from (74b) and (72) that the coefficient of variation of the interface position $\rho_\gamma \equiv \sigma_\gamma/\bar{x}_\gamma = \sigma_Y/2$ is less than 1 even for highly heterogeneous media with $\sigma_Y^2 < 4$, while the corresponding variance σ_γ^2 increases with time and, hence, can be arbitrary large.

9. Summary and conclusions

We considered interface dynamics in heterogeneous porous media whose hydraulic parameters are uncertain. To predict the evolution of a fluid–fluid interface and to quantify the uncertainty associated with such a prediction, we treated the hydraulic conductivity (permeability) of a porous medium as random and the corresponding governing equations as stochastic. The previous attempts to address this problem involve mathematical objects—such as integrals of random functions over random domains and random functionals—that are not readily amenable to standard perturbation techniques. To overcome this difficulty, we introduced a dynamic stochastic mapping of the domain with moving boundaries onto a fixed domain. This allowed us to use the well-understood ensemble averaging approaches to derive deterministic differential equations for the statistical moments of hydraulic head, Darcian flux, and interface dynamics.

We used perturbation expansions in a small parameter σ_Y^2, the variance of log hydraulic conductivity, to derive closure approximations for these moment equations. This formally limits the applicability of our approach to mildly heterogeneous porous media ($\sigma_Y^2 < 1$). However, the comparison of analytical solutions of the one-dimensional moment equations with their exact counterparts demonstrates that the perturbation approximations remain accurate for σ_Y^2 as large as 2.

Our study leads to the following major conclusions.

- The proposed approach yields a self-consistent first-order (in the variance of log hydraulic conductivity σ_Y^2) approximation of the statistics of the interface dynamics. This is in contrast with the existing linearized perturbation solutions, which omit some of the relevant terms in the corresponding expansions.
- For one-dimensional free-surface flow, the mean position of the interface $\bar{x}_\gamma$ scales as $\sqrt{t}$, while its variance σ_γ^2 increases linearly with time t.
- The corresponding coefficient of variation $\rho_\gamma \equiv \sigma_\gamma/\bar{x}_\gamma$, a key measure of predictive uncertainty, is time invariant and remains relatively small ($\rho_\gamma < 1$) even for highly heterogeneous media with the variance of log hydraulic conductivity $\sigma_Y^2 < 4$.

Acknowledgments

This work was performed under the auspices of the U.S. Department of Energy (DOE) through the Initiatives for Proliferation Prevention Program (IPP), the DOE/BES Program in the Applied Mathematical Sciences, Contract KC-07-01-01, and the Los Alamos National Laboratory LDRD Program.

Appendix A. Equations for the interface dynamics

The stochastic mapping $\Omega \to W$ transforms the dynamics conditions on the interface (2d) into

$$\mathbf{n}_\gamma \cdot \mathbf{q} = V_n \quad (A.1)$$

and

$$\frac{\partial x_\gamma}{\partial t} = \frac{V_x(x_\gamma, y_\gamma)}{n_e(x_\gamma, y_\gamma)}, \quad \frac{\partial y_\gamma}{\partial t} = \frac{V_y(x_\gamma, y_\gamma)}{n_e(x_\gamma, y_\gamma)}. \quad (A.2)$$

Here $x_\gamma = x_\gamma(\eta, t)$, $y_\gamma = y_\gamma(\eta, t)$, and the normal to the free surface $\mathbf{n}_\gamma$ is given by

$$\mathbf{n}_\gamma = \frac{\nabla\gamma}{|\nabla\gamma|} = \frac{(\partial y_\gamma/\partial\eta)\mathbf{e}_x - (\partial x_\gamma/\partial\eta)\mathbf{e}_y}{\sqrt{(\partial x_\gamma/\partial\eta)^2 + (\partial y_\gamma/\partial\eta)^2}}, \quad (A.3)$$

where $\mathbf{e}_x$ and $\mathbf{e}_y$ denote the unit vectors in the Cartesian (x, y) coordinate system.

Substituting (A.3) and the Darcy flux (21) evaluated at the interface into (A.1) yields

$$V_n = -\frac{K}{J\sqrt{(\partial x_\gamma/\partial\eta)^2 + (\partial y_\gamma/\partial\eta)^2}} \times \left\{ \left[\left(\frac{\partial x_\gamma}{\partial\eta}\right)^2 + \left(\frac{\partial y_\gamma}{\partial\eta}\right)^2 \right] \frac{\partial h}{\partial\xi} - \left(\frac{\partial x_\gamma}{\partial\xi}\frac{\partial x_\gamma}{\partial\eta} + \frac{\partial y_\gamma}{\partial\xi}\frac{\partial y_\gamma}{\partial\eta} \right) \frac{\partial h}{\partial\eta} \right\}. \tag{A.4}$$

Since the interface is an equipotential, i.e., a surface of the constant hydraulic head, the tangential derivative of the hydraulic head $\partial h/\partial\eta \equiv 0$. Hence, it follows from (A.3) and (A.4) that the components of the interface velocity vector $\mathbf{V} = V_n\mathbf{n}_\gamma$ are given by

$$V_x = -\frac{K}{J}\frac{\partial y_\gamma}{\partial\eta}\frac{\partial h}{\partial\xi}, \quad V_y = \frac{K}{J}\frac{\partial x_\gamma}{\partial\eta}\frac{\partial h}{\partial\xi}. \tag{A.5}$$

Substituting (A.5) into (A.2) gives (26).

Appendix B. Mixed moments

To derive the second-order approximation of $\langle \widetilde{Z}^{\alpha\beta}\widetilde{q}^\beta \rangle$ in (30), we consider an equation for the hydraulic head and flux fluctuations, which is obtained by subtracting (30) and (31) from (29) and (25) and retaining the terms up to $\widetilde{Z}^2$-order,

$$\frac{\partial\widetilde{q}^\alpha}{\partial\xi^\alpha} = 0, \quad -\frac{\partial\widetilde{h}}{\partial\xi^\alpha} = \overline{Z}^{\alpha\beta}\widetilde{q}^\beta + \widetilde{Z}^{\alpha\beta}\overline{q}^\beta \tag{B.1}$$

subject to the boundary conditions

$$\tilde{h}(\xi^1 = 0, \xi^2) = 0, \quad \tilde{h}(\xi^1 = 1, \xi^2) = 0, \tag{B.2a}$$

$$\tilde{q}^2(\xi^1, \xi^2 = 0) = 0, \quad \tilde{q}^2(\xi^1, \xi^2 = 1) = 0. \tag{B.2b}$$

In terms of $E(\boldsymbol{\xi}_1|\boldsymbol{\xi}_2)$, the Green's function defined by (34) and (35), the solution of (B.1) and (B.2) is

$$\tilde{h}(\boldsymbol{\xi}) = -\int_0^1\int_0^1 \frac{\partial E(\boldsymbol{\xi}\mid\boldsymbol{\xi}_1)}{\partial\xi_1^\alpha}\left(\overline{Z}^{-1}\right)^{\alpha\alpha_1}\widetilde{Z}^{\alpha_1\beta}\overline{q}^\beta\,d\boldsymbol{\xi}_1. \tag{B.3}$$

It follows from (B.1) and (B.3) that

$$\tilde{q}^\alpha(\boldsymbol{\xi}) = -\left(\overline{Z}^{-1}\right)^{\alpha\alpha_1}\widetilde{Z}^{\alpha_1\beta}\overline{q}^\beta(\boldsymbol{\xi}) + \left(\overline{Z}^{-1}\right)^{\alpha\alpha_1} \times \int_0^1\int_0^1 \frac{\partial^2 E(\boldsymbol{\xi}\mid\boldsymbol{\xi}_1)}{\partial\xi^{\alpha_1}\partial\xi_1^{\alpha_2}}\left(\overline{Z}^{-1}\right)^{\alpha_2\beta_2}\widetilde{Z}^{\beta_2\beta}\overline{q}^\beta\,d\boldsymbol{\xi}_1. \tag{B.4}$$

Substituting (B.4) into (30) gives the nonlocal mean flow Eq. (32).

(Co)variances of hydraulic head and Darcy's flux are obtained by squaring (B.3) and (B.4) and taking the ensemble mean.

Appendix C. Differential operators and expansion coefficients

Linear deterministic operators $Z_x^{\alpha\beta}$, $Z_y^{\alpha\beta}$, and $Z_K^{\alpha\beta}$ in (36) are given by

$$Z_x^{\alpha\beta} = \frac{1}{J_0\overline{K}}\begin{Vmatrix} \bar{x}_{\xi^1}\frac{\partial}{\partial\xi^1} + \bar{y}_{\xi^1}\frac{\partial}{\partial\xi^2} & 0 \\ \bar{x}_{\xi^2}\frac{\partial}{\partial\xi^1} + \bar{y}_{\xi^2}\frac{\partial}{\partial\xi^2} & 0 \end{Vmatrix} - \frac{1}{J_0}\begin{Vmatrix} \bar{x}_{\xi^1}^2 + \bar{y}_{\xi^1}^2 & \bar{x}_{\xi^1}\bar{x}_{\xi^2} + \bar{y}_{\xi^1}\bar{y}_{\xi^2} \\ \bar{x}_{\xi^1}\bar{x}_{\xi^2} + \bar{y}_{\xi^1}\bar{y}_{\xi^2} & \bar{x}_{\xi^2}^2 + \bar{y}_{\xi^2}^2 \end{Vmatrix} \times \left(\bar{y}_{\xi^2}\frac{\partial}{\partial\xi^1} - \bar{y}_{\xi^1}\frac{\partial}{\partial\xi^2}\right), \tag{C.1}$$

$$Z_y^{\alpha\beta} = \frac{1}{J_0\overline{K}}\begin{Vmatrix} 0 & \bar{x}_{\xi^1}\frac{\partial}{\partial\xi^1} + \bar{y}_{\xi^1}\frac{\partial}{\partial\xi^2} \\ 0 & \bar{x}_{\xi^2}\frac{\partial}{\partial\xi^1} + \bar{y}_{\xi^2}\frac{\partial}{\partial\xi^2} \end{Vmatrix} - \frac{1}{J_0}\begin{Vmatrix} \bar{x}_{\xi^1}^2 + \bar{y}_{\xi^1}^2 & \bar{x}_{\xi^1}\bar{x}_{\xi^2} + \bar{y}_{\xi^1}\bar{y}_{\xi^2} \\ \bar{x}_{\xi^1}\bar{x}_{\xi^2} + \bar{y}_{\xi^1}\bar{y}_{\xi^2} & \bar{x}_{\xi^2}^2 + \bar{y}_{\xi^2}^2 \end{Vmatrix} \times \left(\bar{x}_{\xi^1}\frac{\partial}{\partial\xi^2} - \bar{x}_{\xi^2}\frac{\partial}{\partial\xi^1}\right), \tag{C.2}$$

and

$$Z_K^{\alpha\beta} = -\frac{1}{\overline{\overline{K}}}\begin{Vmatrix} \bar{x}_{\xi^1}^2 + \bar{y}_{\xi^1}^2 & \bar{x}_{\xi^1}\bar{x}_{\xi^2} + \bar{y}_{\xi^1}\bar{y}_{\xi^2} \\ \bar{x}_{\xi^1}\bar{x}_{\xi^2} + \bar{y}_{\xi^1}\bar{y}_{\xi^2} & \bar{x}_{\xi^2}^2 + \bar{y}_{\xi^2}^2 \end{Vmatrix}, \tag{C.3}$$

where $J_0 = \bar{x}_{\xi^1}\bar{y}_{\xi^2} - \bar{x}_{\xi^2}\bar{y}_{\xi^1}$.

Expansion coefficients χ_k^x, χ_x^x, and χ_y^x in (38) are given by

$$\chi_x^x = \frac{\overline{K}\bar{y}_{\gamma\xi^2}}{n_e\left(\bar{x}_{\gamma\xi^1}\bar{y}_{\gamma\xi^2} - \bar{x}_{\gamma\xi^2}\bar{y}_{\gamma\xi^1}\right)^2}\left(\bar{y}_{\gamma\xi^1}\frac{\partial}{\partial\xi^2} - \bar{y}_{\gamma\xi^2}\frac{\partial}{\partial\xi^1}\right), \tag{C.4}$$

$$\chi_y^x = \frac{\overline{K}\bar{y}_{\gamma\xi^2}}{n_e\left(\bar{x}_{\gamma\xi^1}\bar{y}_{\gamma\xi^2} - \bar{x}_{\gamma\xi^2}\bar{y}_{\gamma\xi^1}\right)^2} \times \left(\frac{\bar{x}_{\gamma\xi^1}\bar{y}_{\gamma\xi^2} - \bar{x}_{\gamma\xi^2}\bar{y}_{\gamma\xi^1}}{\bar{y}_{\gamma\xi^2}}\frac{\partial}{\partial\xi^2} - \bar{x}_{\gamma\xi^1}\frac{\partial}{\partial\xi^2} + \bar{x}_{\gamma\xi^2}\frac{\partial}{\partial\xi^1}\right), \tag{C.5}$$

and

$$\chi_K^x = \frac{\bar{y}_{\gamma\xi^2}}{n_e\left(\bar{x}_{\gamma\xi^1}\bar{y}_{\gamma\xi^2} - \bar{x}_{\gamma\xi^2}\bar{y}_{\gamma\xi^1}\right)}. \tag{C.6}$$

Coefficients X_k, X_x, and X_y in (40) are given by

$$X_\delta = \chi_\delta^x\frac{\partial\bar{h}}{\partial\xi^1} - \bar{\chi}^x\int_0^1\int_0^1 \frac{\partial^2 E(\boldsymbol{\xi}\mid\boldsymbol{\xi}_1)}{\partial\xi^1\partial\xi_1^\alpha}\left(\overline{Z}^{-1}\right)^{\alpha\alpha_1}Z_\delta^{\alpha_1\beta}\bar{q}_\beta d\boldsymbol{\xi}_1, \quad \delta = k, x, y. \tag{C.7}$$

References

[1] Dagan G. Flow and transport in porous formations. New York: Springer-Verlag; 1989.

[2] Gelhar LW. Stochastic subsurface hydrology. New Jersey: Prentice Hall; 1993.

[3] Cushman JH. The physics of fluids in hierarchical porous media: Angstroms to miles. New York: Kluwer Academic Pub.; 1997.

[4] Dagan G, Neuman SP, editors. Subsurface flow and transport: a stochastic approach. New York: Cambridge; 1997.

[5] Rubin Y. Applied stochastic hydrogeology. New York: Oxford University Press; 2003.

[6] Dagan G, Zeitoun DG. Seawater–freshwater interface in a stratified aquifer of random permeability distribution. J Contam Hydrol 1998;29(3):185–203.

[7] Dagan G, Zeitoun DG. Free-surface flow toward a well and interface upconing in stratified aquifers of random conductivity. Water Resour Res 1998;34(11):3191–6.

[8] Amir O, Dagan G. Uniform steady free-surface flow in heterogeneous porous formations. J Fluid Mech 2002;454:327–43.

[9] Fenton GA, Griffiths DV. Statistics of free surface flow through stochastic earth dam. J Geotech Eng—ASCE 1996; 122(6):427–36.

[10] Tartakovsky DM, Winter CL. Dynamics of free surfaces in random porous media. SIAM J Appl Math 2001;61(6): 1857–76.

[11] Tartakovsky DM. Stochastic analysis of heterogeneous phreatic aquifers. Water Resour Res 1999;35(12):3941–6.

[12] Tartakovsky AM, Neuman SP, Tartakovsky DM. Mean and variance of DNAPL finger development in a saturated, randomly heterogeneous porous medium. Dev Water Sci 2002;47:1307–14.

[13] Tartakovsky AM, Neuman SP, Lenhard RJ. Immiscible front evolution in randomly heterogeneous porous media. Phys Fluids 2003;15(11):3331–41.

[14] Green WH, Ampt GA. Studies in soil physics. I. The flow of air and water through soil. J Agric Sci 1911;4:1–24.

[15] Tartakovsky DM, Neuman SP. Extension of "Transient flow in bounded randomly heterogeneous domains. 1. Exact conditional moment equations and recursive approximations". Water Resour Res 1999;35(6):1921–5.

[16] Hassan AE. Water flow and solute mass flux in heterogeneous porous formations with spatially random porosity. J Hydrol 2001;242(1–2):1–25.

[17] Goloviznin VM, Simacheva OG. On one method of constructing computational grids in domains with curved boundaries. J Comp Math Math Phys 1983;5:1245–9 (in Russian).

[18] Thompson J, Warsi Z, Mastin C. Numerical grid generation. Elsevier Science Publishing Co., Inc.; 1985.

[19] Tartakovsky DM, Neuman SP. Transient flow in bounded randomly heterogeneous domains. 1. Exact conditional moment equations and recursive approximations. Water Resour Res 1998; 34(1):1–12.