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Stochastic averaging of nonlinear flows in heterogeneous porous media

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We consider flow in partially saturated heterogeneous porous media with uncertain hydraulic parameters. By treating the saturated conductivity of the medium as a random field, we derive a set of deterministic equations for the statistics (ensemble mean and variance) of fluid pressure. This is done for three constitutive models that describe the nonlinear dependence of relative conductivity on pressure. We use the Kirchhoff transform to map Richards equation into a linear PDE and explore alternative closures for the resulting moment equations. Regardless of the type of nonlinearity, closure by perturbation is more accurate than closure based on the non-perturbative Gaussian mapping. We also demonstrate that predictability of unsaturated flow in heterogeneous porous media is enhanced by choosing either the Brooks–Corey or van Genuchten constitutive model over the Gardner model.

1. Introduction

Modelling fluid flow and transport in natural porous media, such as soils, aquifers, oil and gas reservoirs, is complicated by the high degree of heterogeneity combined with insufficient data characterizing the relevant medium properties. These properties and parameters can be conveniently described by random fields, whose statistics are usually inferred from experimental data. This renders the corresponding flow and transport equations stochastic (Dagan 1989; Gelhar 1993; Cushman 1997; Dagan & Neuman 1997). While significant progress has been made in analysing linear phenomena in random porous media, such as flow in fully saturated media (Batchelor 1974; Rubinstein 1986; Rubinstein & Torquato 1989; Indelman 1996) and transport of conservative solutes (Winter, Newman & Neuman 1984; Koch & Brady 1987; Dagan 1991; Rubin *et al.* 1999; Indelman & Dagan 1999), there are considerably fewer rigorous studies of nonlinear random phenomena.

Multiphase flows, in general, and unsaturated flow, in particular, are typical examples of such nonlinear phenomena. Consider Richards equation,

$$\frac{\partial \theta}{\partial t} = -\nabla \cdot \boldsymbol{q} + f, \qquad \boldsymbol{q} = -K(\boldsymbol{x}, \psi)\nabla(\psi + x_3), \tag{1.1}$$

which is commonly used to describe unsaturated flow (flow in partially saturated porous media). Here $\theta(\psi)$ is the normalized saturation of a medium, $\boldsymbol{q}$ is the macroscopic (Darcian) flux of a fluid, ψ is the fluid pressure, and f represents a source term. The vertical coordinate x_3 accounts for gravitational force. At full saturation, the medium conductivity $K \equiv K_s$ is a property of the porous medium only. For partially saturated media, it also depends on the fluid pressure, so that $K(\psi) = K_s K_r(\psi)$ where the relative conductivity $K_r(\psi) \leqslant 1$.

We concetrate on quantifying uncertainty that is caused by saturated conductivity K_s, since its random effects are multiplicative. Driving forces (the source term f and boundary conditions) often serve as additional sources of randomness, but their effects are additive and thus are easier to analyse. For flow in porous media, the uncertainty in K_s and the multiplicative noise it induces are ubiquitous. This is in contrast to statistical hydrodynamic models that typically arise from the Landau and Lifshitz theory of hydrodynamic fluctuations (Landau & Lifshitz 1959), which adds a random component to the otherwise deterministic fluxes. Such models roughly correspond to (1.1) wherein K_s is deterministic so that f is the only source of randomness. Except for simple flow scenarios amenable to analytical treatment, a standard approach is to use the linearization $K_r(\psi) \approx \kappa = constant$ (e.g. Garcia *et al.* 1987).

Similarly, most moment analyses of unsaturated flow (Yeh, Gelhar & Gutjahr 1985; Mantoglou & Gelhar 1987; Russo 1995; Zhang, Walstrom & Winter 1998) use Taylor expansion of the relative conductivity $K_r(\psi)$ around a mean pressure $\langle\psi\rangle$ to linearize Richards equation (1.1) by setting $\langle K_r(\psi)\rangle \approx K_r(\langle\psi\rangle)$. For these approaches to be workable, it is necessary that the corresponding infinite Taylor series can be accurately approximated by a finite number of terms (often just by the leading term). This requires, in turn, that pressure variance σ_ψ^2, or more precisely the coefficient of variation $\sigma_\psi/\langle\psi\rangle$ be small. Clearly, this condition cannot be verified *a priori*, since it involves the unknown pressure statistics. Moreover, the random pressure field is expected to be statistically non-homogeneous leading to non-uniform accuracy throughout the flow domain. The Kirchhoff mapping (Tartakovsky, Neuman & Lu 1999) and a Gaussian approximation (Amir & Neuman 2001) have been successfully used to derive differential equations for statistical moments of ψ (and flux $\boldsymbol{q}$) without linearization.

Excepting Zhang *et al.* (1998), existing ensemble moment analyses of Richards equation employ the Gardner model of relative conductivity, $K_r(\psi) = \exp(-\alpha\psi)$, where α is the inverse of capillary length. While convenient mathematically, the Gardner model often fits experimental data poorly and hence is rarely used in practical applications. The main goal of this study is to investigate the effects of using more realistic models of relative conductivity, such as the Brooks–Corey and van Genuchten models, on the quality of prediction of unsaturated flow in randomly heterogeneous porous media. Unlike Zhang *et al.* (1998), we do so without linearizing $K_r(\psi)$, which allows us to isolate the nonlinearity effects.

We start by formulating a set of stochastic partial differential equations (PDEs) that describe flow in unsaturated randomly heterogeneous porous media in § 2. In §§ 3–5 we employ the Kirchhoff mapping to derive, without linearizing the constitutive law $K_r(\psi)$, a set of deterministic PDEs for the ensemble mean and variance of pressure head. The accuracy of the closure approximations, which are required to derive these equations, is analysed in § 6 by comparing, for two-dimensional flow, the solutions of our moment equations with Monte Carlo simulations. A specific focus of this analysis is the influence of nonlinearities (i.e. of the constitutive model) on our ability to quantify uncertainty in the fluid behaviour in heterogeneous porous media.

2. Problem formulation

In a steady-state regime and in the absence of gravity, Richards equation reads

$$\nabla \cdot [K(\boldsymbol{x}, \psi)\nabla\psi] + f = 0. \tag{2.1}$$

The stochastic flow equation (2.1) is subject to the boundary conditions,

$$\psi(\boldsymbol{x}) = \Psi(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Gamma_D, \tag{2.2a}$$

$$K(\boldsymbol{x}, \psi)\nabla\psi \cdot \boldsymbol{n}(\boldsymbol{x}) = Q(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Gamma_N, \tag{2.2b}$$

where $\Psi(\boldsymbol{x})$ is a randomly prescribed pressure head on Dirichlet boundary segments Γ_D, $Q(\boldsymbol{x})$ is a randomly prescribed flux across Neumann boundary segments Γ_N, $\boldsymbol{n} = (n_1, n_2, n_3)^T$ is a unit outward normal to the boundary $\Gamma = \Gamma_D \cup \Gamma_N$ of the flow domain Ω. Though it is not strictly necessary, we assume for simplicity that the source and boundary functions $f(\boldsymbol{x})$, $\Psi(\boldsymbol{x})$ and $Q(\boldsymbol{x})$ are prescribed in a statistically independent manner.

While neglecting gravity limits the applicability of the model (1.1), it allows us to conduct a rigorous analysis of the effects of nonlinearity in $K_r(\psi)$ on the statistical moments of pressure ψ. Despite its theoretical and practical importance, this subject has not been previously addressed. In particular, the following questions remain unanswered. How does a choice of the constitutive model $K_r(\psi)$ influence our ability to estimate (predict) fluid flow behaviour in heterogeneous porous media with uncertain hydraulic parameters? What is its impact on uncertainty estimates?

Among physical phenomena described by (2.1) are unsaturated flow in horizontal fractures, vertical infiltration into soils whose saturated zone is thick and is not influenced by the water table (Gelhar 1993, p. 183) and moisture redistribution in heavy soils with high pressure gradients (Childs & Collis-George 1950). It is also used to infer soil–water diffusivity from laboratory experiments (Bruce & Klute 1956). Equally important are other applications, such as real gas flow (Tartakovsky & Guadagnini 2001) and nonlinear heat (Carslaw & Jaeger 1959) and electrical (Jang, Barber & Hu 1998) conductance.

To complete the description of unsaturated flow given by (2.1), it is necessary to specify the functional dependence $K_r(\psi)$. We will consider three commonly used models: the Gardner model,

$$K_r(\psi) = \mathrm{e}^{-\alpha\psi}, \tag{2.3}$$

the Brooks–Corey model,

$$K_r(\psi) = \left|\frac{\psi}{\psi_c}\right|^{-\omega} \quad \text{for} \quad \psi \geqslant \psi_c, \qquad K_r(\psi) = 1 \quad \text{for} \quad \psi < \psi_c, \tag{2.4}$$

and the van Genuchten model,

$$K_r(\psi) = (1 + |\beta\psi|^n)^{-5m/2}[(1 + |\beta\psi|^n)^m - |\beta\psi|^{n-1}]^2, \qquad m = 1 - \frac{1}{n}. \tag{2.5}$$

(As defined above, the pressure ψ is non-negative throughout the flow domain and is often referred to as suction.) A particular constitutive model is usually selected based on experimental data. While most analytical studies of unsaturated flow in porous media use the Gardner model because of its simplicity, the Brooks–Corey and van Genuchten models usually fit data better. Hence, they are most often used in practical applications.

All or none of the fitting parameters α, ψ_c, ω, β and n can be considered random, depending on field-based information. However, unlike the parameter α in the Gardner model, whose statistical properties have been classified for a wide variety of soil types, little is known about the statistics of the fitting parameters which appear in the Brooks–Corey and van Genuchten models. Hence, we assume these parameters to be deterministic, so that K_s and f are the only sources of randomness. Treating the fitting parameters as correlated random variables is relatively straightforward, but cumbersome (Lu *et al.* 2002).

To make a meaningful comparison between the pressure statistics computed with alternative models (2.3), (2.4) or (2.5) we use the equivalence criteria established in Morel-Seytoux *et al.* (1996). It requires the preservation of the maximum value of the effective capillary drive, also referred to as a macroscopic capillary length,

$$H_c = \int_0^\infty K_r(s)\,\mathrm{d}s, \tag{2.6}$$

and relates the fitting parameters between models. Effective capillary drive is directly related to the Kirchhoff transform used in our subsequent analysis.

Randomness of (or, equivalently, uncertainty in) the medium's conductivity K_s and driving forces f, Ψ and Q render the pressure dynamics random (uncertain). The optimal unbiased estimate of pressure head ψ in the L^2 norm is provided by the ensemble mean $\langle\psi\rangle$, while the uncertainty associated with such an estimate is quantified by pressure variance σ_ψ^2. Our main goal is to derive and analyse deterministic equations for these two quantities, thus eliminating the need for computationally expensive Monte Carlo simulations.

3. Stochastic averaging

For any $K_r(\psi)$, the Kirchhoff mapping,

$$\Phi[\psi(\boldsymbol{x})] = \int_\psi^\infty K_r(s)\,\mathrm{d}s, \tag{3.1}$$

transforms (2.1) into a linear stochastic PDE,

$$\nabla\cdot[K_s(\boldsymbol{x})\nabla\Phi(\boldsymbol{x})] + f = 0. \tag{3.2}$$

Transformation of the boundary conditions (2.2) yields

$$\Phi(\boldsymbol{x}) = H(\boldsymbol{x}), \qquad \boldsymbol{x}\in\Gamma_D, \tag{3.3a}$$

$$K_s(\boldsymbol{x})\nabla\Phi(\boldsymbol{x})\cdot\boldsymbol{n}(\boldsymbol{x}) = Q(\boldsymbol{x}), \qquad \boldsymbol{x}\in\Gamma_N, \tag{3.3b}$$

where H is the Kirchhoff transform of Ψ. We use Reynolds decomposition $\mathscr{A} = \langle\mathscr{A}\rangle + \mathscr{A}'$ to represent a random field $\mathscr{A}$ as the sum of its mean, $\langle\mathscr{A}\rangle$, and a zero-mean random fluctuation, $\mathscr{A}'$. Then stochastic averaging of the transformed flow equation yields

$$\nabla\cdot[\langle K_s\rangle\nabla\langle\Phi\rangle] + \nabla\cdot\boldsymbol{r} + \langle f\rangle = 0. \tag{3.4}$$

We obtain a closure approximation for the cross-product term $\boldsymbol{r}(\boldsymbol{x}) \equiv \langle K_s'\nabla\Phi'\rangle$ through the perturbation expansion in σ_Y^2, the variance of the log conductivity $Y = \ln K_s$. Despite some earlier reservations (e.g. Frisch 1968), applying this approach to linear stochastic PDEs like (3.2), proved to be remarkably robust even for relatively high values of σ_Y^2 (Guadagnini & Neuman 1999*b*). (Note that if K_s were deterministic, i.e. if the randomness were due to the additive noise f only, the Kirchhoff mapping (3.1) would yield the exact averaged equation for Φ. This relatively simple setting corresponds, for example, to flow of water in natural environments, where the major source of uncertainty is recharge or evapotranspiration.)

Consider an asymptotic series $\langle\Phi\rangle = \langle\Phi^{(0)}\rangle + \langle\Phi^{(1)}\rangle + O(\sigma_Y^4)$. Let $K_g \equiv \exp(\langle Y\rangle)$ denote the geometric mean of K_s and $G(\boldsymbol{y},\boldsymbol{x})$ denote the zeroth-order mean Green's function defined by $\nabla\cdot[K_g\nabla G] + \delta(\boldsymbol{x}-\boldsymbol{y}) = 0$ subject to the appropriate homogeneous boundary conditions. Since $\langle K_s\rangle = K_g(1+\sigma_Y^2/2+\cdots)$, the first two terms in this expansion ($i = 1, 2$) satisfy

$$\nabla \cdot \left[K_g \nabla \left\langle \Phi^{(i)} \right\rangle\right] + \mathscr{F}_i = 0, \tag{3.5}$$

where the source terms are $\mathscr{F}_0 \equiv \langle f \rangle$ and $\mathscr{F}_1 \equiv \nabla \cdot [K_g(\sigma_Y^2/2)\nabla\langle \Phi^{(0)}\rangle + \boldsymbol{r}^{(1)}]$. The first-order approximation of the mixed moment $\boldsymbol{r}$ is given by (Guadagnini & Neuman 1999*a*)

$$\boldsymbol{r}^{(1)} = \int_{\Omega} K_g C_Y \nabla_{\boldsymbol{y}} \nabla_{\boldsymbol{x}}^T G \nabla_{\boldsymbol{y}} \left\langle \Phi^{(0)} \right\rangle \mathrm{d}\boldsymbol{y}, \tag{3.6}$$

where $C_Y(\boldsymbol{y}, \boldsymbol{x}) = \langle Y'(\boldsymbol{y}) Y'(\boldsymbol{x})\rangle$ is the two-point covariance function of Y. Equation (3.5) is subject to the boundary conditions

$$\left\langle \Phi^{(i)} \right\rangle = \mathscr{H}_i, \qquad \boldsymbol{x} \in \Gamma_D, \tag{3.7a}$$

$$K_g \nabla \left\langle \Phi^{(i)} \right\rangle \cdot \boldsymbol{n} = \mathscr{Q}_i, \qquad \boldsymbol{x} \in \Gamma_N, \tag{3.7b}$$

where the boundary terms are $\mathscr{H}_0 \equiv \langle H \rangle$, $\mathscr{H}_1 \equiv 0$, $\mathscr{Q}_0 \equiv \langle Q \rangle$, and $\mathscr{Q}_1 \equiv -\boldsymbol{n} \cdot [K_g(\sigma_Y^2/2) \nabla\langle \Phi^{(0)}\rangle + \boldsymbol{r}^{(1)}]$.

Two important points regarding this approach deserve to be mentioned. First, it allows for statistically heterogeneous (non-stationary) random fields K_s. Secondly, unlike closures based on the direct interaction approximation or the Corsin conjecture (Kraichnan 1987; Neuman & Orr 1993), the recursive approximation does not result in a non-local, integro-differential equation. Hence, there is no need for localization of (3.6).

4. Uncertainty quantification

We use σ_Φ^2, the variance of the Kirchhoff variable Φ, to quantify the uncertainty associated with our estimate $\langle \Phi \rangle$. A set of deterministic partial differential equations for the first-order approximations of the covariance $C_\Phi(\boldsymbol{x}, \boldsymbol{y}) \equiv \langle \Phi'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle$ and the cross-covariance $C_{K\Phi}(\boldsymbol{x}, \boldsymbol{y}) \equiv \langle K_s'(\boldsymbol{x})\Phi'(\boldsymbol{y})\rangle$ are obtained from (3.2)–(3.3) as (Guadagnini & Neuman 1999*a*)

$$\nabla_{\boldsymbol{x}} \cdot \left[K_g \nabla_{\boldsymbol{x}} C_\Phi^{(1)}(\boldsymbol{x}, \boldsymbol{y}) + C_{K\Phi}^{(1)}(\boldsymbol{x}, \boldsymbol{y}) \nabla_{\boldsymbol{x}} \left\langle \Phi^{(0)}(\boldsymbol{x}) \right\rangle\right] = 0, \tag{4.1}$$

subject to the boundary conditions

$$C_\Phi^{(1)}(\boldsymbol{x}, \boldsymbol{y}) = 0, \qquad \boldsymbol{x} \in \Gamma_D, \tag{4.2a}$$

$$\boldsymbol{n}(\boldsymbol{x}) \cdot \left[K_g \nabla_{\boldsymbol{x}} C_\Phi^{(1)}(\boldsymbol{x}, \boldsymbol{y}) + C_{K\Phi}^{(1)}(\boldsymbol{x}, \boldsymbol{y}) \nabla_{\boldsymbol{x}} \left\langle \Phi^{(0)}(\boldsymbol{x}) \right\rangle\right] = 0, \qquad \boldsymbol{x} \in \Gamma_N, \tag{4.2b}$$

and

$$C_{K\Phi}^{(1)}(\boldsymbol{x}, \boldsymbol{y}) = -K_g \int_{\Omega} K_g C_Y(\xi, \boldsymbol{x}) \nabla_\xi G(\xi, \boldsymbol{y}) \cdot \nabla_\xi \left\langle \Phi^{(0)}(\xi) \right\rangle \mathrm{d}\boldsymbol{\xi}. \tag{4.3}$$

The Kirchhoff transform variance $\sigma_\Phi^2(\boldsymbol{x})$ is calculated by taking the limit of $C_\Phi(\boldsymbol{x}, \boldsymbol{y})$ as $\boldsymbol{y} \to \boldsymbol{x}$ once (4.1)–(4.3) have been solved. Note that these equations are valid for a deterministic source function f. The extension to random f is straightforward (Tartakovsky & Neuman 1999).

5. Statistical moments of pressure

The statistics of the Kirchhoff transform, Φ, derived in the previous section are independent of the constitutive law, $K_r(\psi)$. Since the Darcian velocity (mass flux) $\boldsymbol{q}$ is readily expressed in terms of the Kirchhoff transform as $\boldsymbol{q} = -K_s \nabla \Phi$, estimating its averaged behaviour and quantifying the corresponding uncertainty does not require further approximations. This is of particular importance for transport phenomena in porous media, since the Darcian velocity $\boldsymbol{q}$ and its statistics serve as input parameters in the advection or advection–dispersion equations (Dagan 1991; Indelman & Dagan 1999).

At the same time, the pressure distribution estimates do depend on the constitutive law, $K_r(\psi)$. We explore two alternative strategies to obtain the statistics of pressure ψ. The first relies on perturbation expansions of the inverse Kirchhoff mapping. The second is based on the assumption that the Kirchhoff variable Φ is Gaussian. Both approaches are compared with Monte Carlo simulations, which are treated as exact.

5.1. *Perturbation solution*

5.1.1. *Gardner model*

For the Gardner model of relative conductivity (2.3), the first-order approximations of the pressure estimate, $\langle \psi_{GR} \rangle$, and the pressure variance, $\sigma^2_{\psi_{GR}}$, are given by equations (45)–(47) of Tartakovsky *et al.* (1999).

5.1.2. *Brooks–Corey model*

Evaluating the Kirchhoff transform (3.1) of the Brooks–Corey model (2.4) and its inverse yields

$$\psi_{BC} = \begin{cases} \dfrac{\omega\psi_c}{\omega-1} - \Phi, & \dfrac{\psi_c}{\omega-1} \leqslant \Phi \leqslant \dfrac{\omega\psi_c}{\omega-1} \equiv H_c, \\ \psi_c\left(\dfrac{\omega-1}{\psi_c}\Phi\right)^{1/(1-\omega)}, & 0 \leqslant \Phi < \dfrac{\psi_c}{\omega-1}. \end{cases} \tag{5.1}$$

Then mean pressure is approximated by $\langle \psi_{BC}^{[1]} \rangle = \langle \psi_{BC}^{(0)} \rangle + \langle \psi_{BC}^{(1)} \rangle$, where

$$\langle \psi_{BC}^{(0)} \rangle = \begin{cases} \dfrac{\omega\psi_c}{\omega-1} - \langle \Phi^{(0)} \rangle, & \dfrac{\psi_c}{\omega-1} \leqslant \langle \Phi^{(0)} \rangle \leqslant H_c, \\ \psi_c\left(\dfrac{\omega-1}{\psi_c}\langle \Phi^{(0)} \rangle\right)^{1/(1-\omega)}, & 0 \leqslant \langle \Phi^{(0)} \rangle < \dfrac{\psi_c}{\omega-1}, \end{cases} \tag{5.2}$$

and

$$\langle \psi_{BC}^{(1)} \rangle = \begin{cases} -\langle \Phi^{(1)} \rangle, & \dfrac{\psi_c}{\omega-1} \leqslant \langle \Phi^{[1]} \rangle \leqslant H_c, \\ \left(\dfrac{\langle \Phi^{(1)} \rangle}{\langle \Phi^{(0)} \rangle} + \dfrac{\omega}{1-\omega}\dfrac{\left[\sigma^2_\Phi\right]^{(1)}}{2\langle \Phi^{(0)} \rangle^2}\right)\dfrac{\langle \psi_{BC}^{(0)} \rangle}{1-\omega}, & 0 \leqslant \langle \Phi^{[1]} \rangle < \dfrac{\psi_c}{\omega-1}. \end{cases} \tag{5.3}$$

The pressure variance is given to the first order by

$$\left[\sigma^2_{\psi_{BC}}\right]^{(1)} = \begin{cases} \left[\sigma^2_\Phi\right]^{(1)}, & \dfrac{\psi_c}{\omega-1} \leqslant \langle \Phi^{[1]} \rangle \leqslant H_c, \\ \dfrac{1}{(1-\omega)^2}\left(\dfrac{\langle \psi_{BC}^{(0)} \rangle}{\langle \Phi^{(0)} \rangle}\right)^2 \left[\sigma^2_\Phi\right]^{(1)}, & 0 \leqslant \langle \Phi^{[1]} \rangle < \dfrac{\psi_c}{\omega-1}. \end{cases} \tag{5.4}$$

5.1.3. *Van Genuchten model*

Owing to the complexity of the van Genuchten model (2.5), its Kirchhoff transform (3.1) cannot be evaluated analytically. To derive the inverse mapping we expand (3.1) in a Taylor series about $\langle \psi \rangle$,

$$\Phi(\psi) = \int_{\langle \psi \rangle}^{\infty} K_r(s)\,\mathrm{d}s + \psi' K_r(\langle \psi \rangle) + \frac{\psi'^2}{2}\frac{\mathrm{d}K_r}{\mathrm{d}s}\bigg|_{s=\langle \psi \rangle} + \cdots. \tag{5.5}$$

Expanding the ensemble mean of (5.5) in a Taylor series about the zeroth-order approximation, $\langle \psi^{(0)} \rangle$, gives the implicit perturbation solutions

$$\left\langle \Phi^{(0)} \right\rangle = \int_{\langle \psi_{vG}^{(0)} \rangle}^{\infty} K_r(s)\, \mathrm{d}s, \tag{5.6}$$

and

$$\left\langle \Phi^{(1)} \right\rangle = K_r\left(\left\langle \psi_{vG}^{(0)} \right\rangle\right)\left\langle \psi_{vG}^{(1)} \right\rangle + \frac{\left[\sigma_{\psi_{vG}}^2\right]^{(1)}}{2} \frac{\mathrm{d}K_r}{\mathrm{d}s}\bigg|_{s=\langle \psi_{vG}^{(0)} \rangle}. \tag{5.7}$$

In a similar fashion, the first-order approximation of the pressure head variance, $\sigma_{\psi_{vG}}^2$, is obtained from (5.5) as

$$\left[\sigma_{\Phi}^2\right]^{(1)} = \left[\sigma_{\psi_{vG}}^2\right]^{(1)} K_r^2\left(\left\langle \psi_{vG}^{(0)} \right\rangle\right). \tag{5.8}$$

The perturbative nature of our solutions formally limits their applicability to small pressure variances, i.e. to a flow scenario with $\sigma_{\psi}^2 \ll 1$. However, numerical simulations reported in the following sections demonstrate that both pressure estimates and the uncertainty measures remain accurate for rather large values of σ_{ψ}^2. This remarkable accuracy might be due to the smoothing nature of the Laplacian in the linear flow equation (see, for example, the discussion of figure 6 in Glimm *et al.* 1992).

5.2. *Gaussian approximation*

The Gaussian approximation assumes that the Kirchhoff variable Φ is normal with mean $\langle \Phi(\boldsymbol{x}) \rangle$ and variance $\sigma_{\Phi}^2(\boldsymbol{x})$. Since Φ is defined on the interval $[0, H_c]$, its distribution is normalized with

$$A(\boldsymbol{x}) = \frac{1}{\sqrt{2\pi\sigma_{\Phi}^2}} \int_0^{H_c} \exp\left(-\frac{[\phi - \langle \Phi \rangle]^2}{2\sigma_{\Phi}^2}\right) \mathrm{d}\phi. \tag{5.9}$$

For the Gardner and Brooks–Corey models, explicit expressions relating ψ and Φ are available, e.g. (5.1), and calculating the moments of ψ requires a simple evaluation of numerical quadratures. For the van Genuchten model, the procedure to calculate the moments of ψ is similar, but uses an implicit dependence of ψ on Φ.

The accuracy and robustness of these approximations depend on the particular functional form of $K_r(\psi)$ in (2.3)–(2.5). We investigate this question in the following example by comparing our numerical solutions with Monte Carlo simulations. The latter are treated as exact.

6. Computational example

As an example, we consider two-dimensional flow in a heterogeneous medium whose saturated conductivity K_s is modelled as a statistically homogeneous, lognormal random field with an isotropic Gaussian covariance function,

$$C_Y(r) = \sigma_Y^2 \exp(-\pi r^2/4\lambda^2), \tag{6.1}$$

where $r = \|\boldsymbol{x} - \boldsymbol{y}\|$ is the separation distance and λ is the correlation length. In all simulations, we set $\lambda = 1$ and $\langle Y \rangle = 0$. The degree of heterogeneity varies from mild ($\sigma_Y^2 = 0.1$) to moderate ($\sigma_Y^2 = 1.0$) to relatively high ($\sigma_Y^2 = 2.0$).

Consider flow within a square domain, $\Omega = [L \times L]$, whose vertical boundaries ($x_1 = 0,\ L$) are impermeable and the lower boundary ($x_2 = 0$) is maintained dry ($\psi = \infty$). The upper boundary ($x_2 = B$) is subdivided into three equal segments. The Dirichlet condition $\psi = 0$ is prescribed on the central segment $L/3 \leqslant x_1 \leqslant 2L/3$, while the remaining two segments $0 \leqslant x_1 < L/3$ and $2L/3 < x_1 \leqslant L$ are impermeable.

Model parameters	α	ψ_c	ω	β	n
Gardner	0.01				
Brooks–Corey		77.27	4.40		
van Genuchten				7.46×10^{-3}	4.8

TABLE 1. The model parameters for the Gardner (2.3), Brooks–Corey (2.4), and van Genuchten (2.5) models. These parameters satisfy (2.6) with $H_c = 100$.

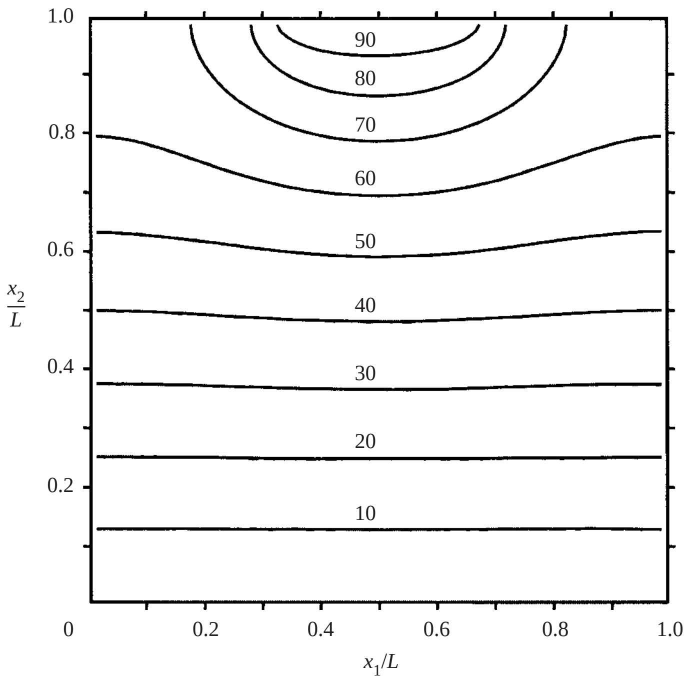

FIGURE 1. Mean Kirchhoff variable $\langle \Phi \rangle$ computed with MCS (solid line) and the perturbation closure of the moment equations (dash-dotted line) for $\sigma_Y^2 = 1$.

We prescribe an effective capillary drive of $H_c = 100$ on the Dirichlet segment of the upper boundary. Following Morel-Seytoux *et al.* (1996), (2.6) gives rise to the values of the fitting parameters in (2.3)–(2.5) that are summarized in table 1.

Moment equations (3.5)–(4.3) are solved by the non-local Galerkin finite elements algorithm (Guadagnini & Neuman 1999*a*) on the uniform grid consisting of 100×100 elements, whose size is $\Delta_{x_1} = \Delta_{x_2} = 0.25\lambda$. To gauge accuracy of the perturbation closure of the moment equations, we compare their solutions with those obtained from Monte Carlo simulations (MCS). The MCS consist of (i) generating multiple realizations of the saturated conductivity field $K_s(\boldsymbol{x})$, (ii) solving the (deterministic) flow equation for each realization, and (iii) obtaining the statistics of these solutions. Realizations of the random $K_s(\boldsymbol{x})$ fields were generated by means of the Gaussian sequential simulator SGSIM (Deutsch & Journel 1992). Depending on the value of σ_Y^2, between 2000 and 4000 realizations are required to obtain the prescribed ensemble statistics. Following standard practice, we treat the MCS results as exact.

Figures 1 and 2 compare the first-order approximations of the mean Kirchhoff transform, $\langle \Phi^{[1]} \rangle = \langle \Phi^{(0)} \rangle + \langle \Phi^{(1)} \rangle$, and its variance, $[\sigma_\Phi^2]^{[1]}$ with their MCS counterparts.

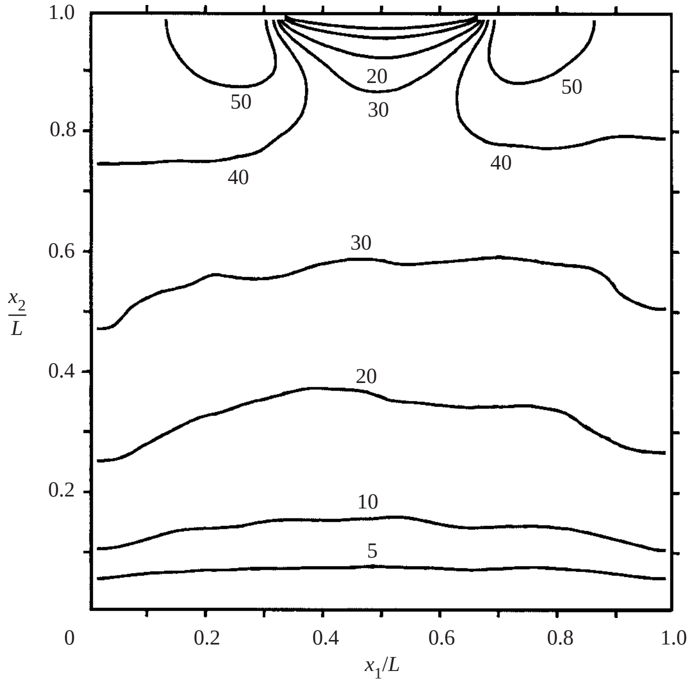

FIGURE 2. Variance of the Kirchhoff variable σ_Φ^2 computed with MCS (solid line) and the perturbation closure of the moment equations (dash-dotted line) for $\sigma_Y^2 = 1$.

In these and other figures we set $\sigma_Y^2 = 1$. While the perturbation solutions are formally valid for $\sigma_Y^2 \ll 1$, the agreement is excellent. The maximum discrepancies between the two methods are 0.05% for the mean and 2% for the variance.

The statistics of Φ and accuracy of their approximations remain the same regardless of the choice of the functional relationship $K_r(\psi)$. In contrast, the pressure statistics are highly sensitive to such a choice. Figure 3 shows the ensemble mean of the pressure, $\langle\psi\rangle$, computed via both the perturbation approximations (PA) of § 5.1 and the Gaussian approximation (GA) of § 5.2 for the Brooks–Corey model. Also added for comparison is $\langle\psi\rangle$ obtained via a simple mean field approximation (MF) that replaces the random conductivity field with its geometric mean. The latter coincides with the zeroth-order solution of the perturbation method. We can see that all approximations compare favourably with MCS and yield virtually indistinguishable solutions.

The accuracy of each approximation ($A = PA, GA$, or MF) is reported in terms of its relative error against the MCS results (MC),

$$\mathscr{E}_A = \frac{\langle\psi\rangle^A - \langle\psi\rangle^{MC}}{\langle\psi\rangle^{MC}} \times 100\%. \tag{6.2}$$

For $\sigma_Y^2 = 1$, the errors introduced by the perturbation approximation $\mathscr{E}_{PA}$ do not exceed 3% throughout the flow domain. Although not shown here, the perturbation closure remains remarkably accurate even for $\sigma_Y^2 = 2$. In this case, the maximum $\mathscr{E}_{PA}$ is about 10% in the vicinity of the lower boundary $x_2 = 0$ and remains below 5% elsewhere. The non-perturbative Gaussian approximation proves to be less accurate. We will explain this finding later in the paper. For $\sigma_Y^2 = 1$, the corresponding relative

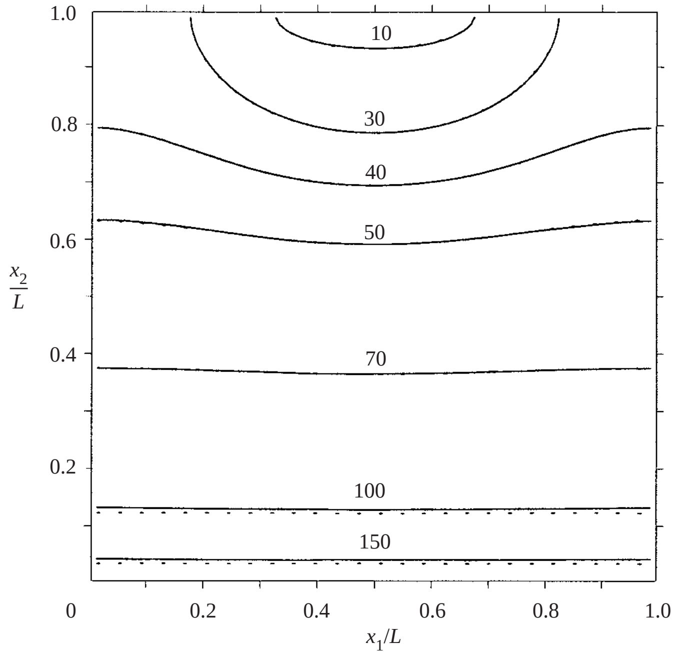

FIGURE 3. Mean pressure head $\langle\psi\rangle$ for the Brooks–Corey model computed with MCS (solid line), perturbation closure (dash-dotted line), Gaussian approximation (dashed line), and mean field approximation (dotted line).

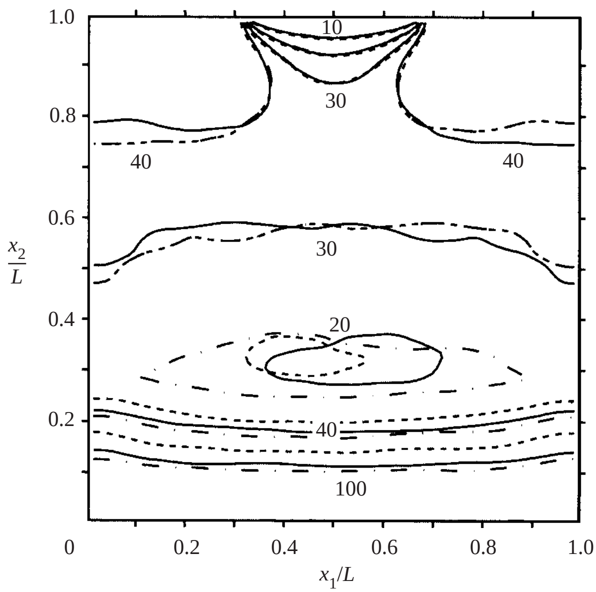

FIGURE 4. Pressure variance σ_ψ^2 for the Brooks–Corey model computed with MCS (solid line), the perturbation closure (dash-dotted line) and Gaussian approximation (dashed line).

error $\mathscr{E}_{GA}$ reaches the maximum value of 9% close to the upper boundary and does not exceed 4% elsewhere. For $\sigma_Y^2 = 2$, $\mathscr{E}_{GA}$ reaches a maximum value of 20% close to the upper boundary and does not exceed 7% elsewhere.

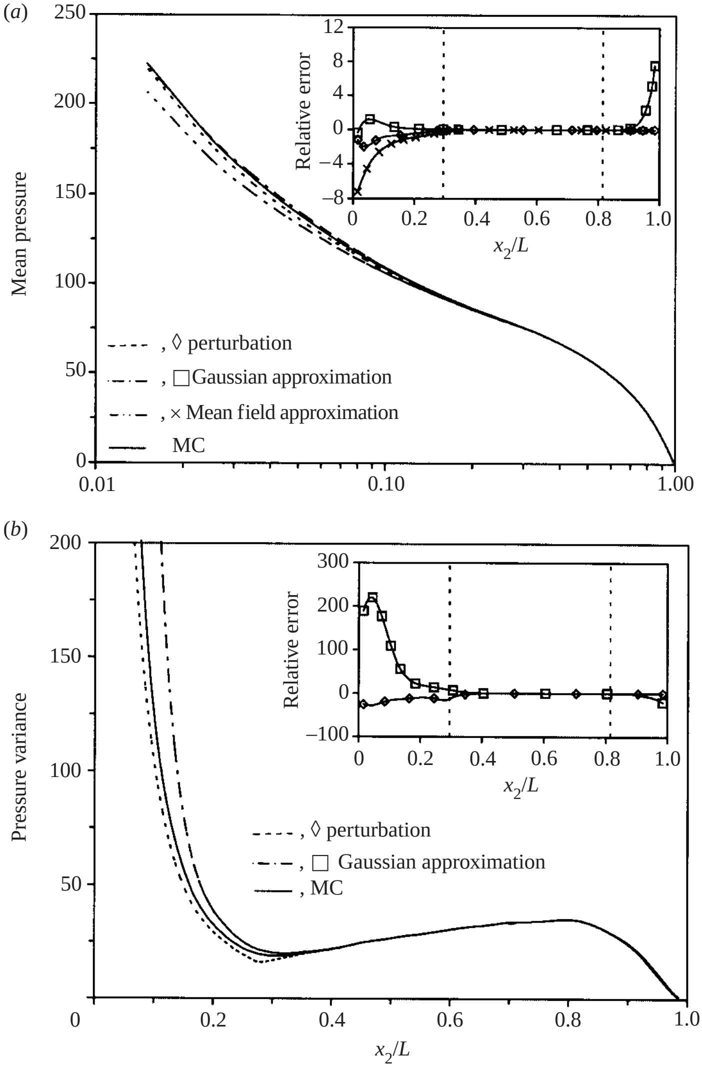

FIGURE 5. The Brooks–Corey model: vertical cross-section, $x_1 = 0.5L$, of (*a*) the mean pressure $\langle \psi_{BC} \rangle$ and (*b*) pressure variance $\sigma^2_{\psi_{BC}}$ computed with the perturbation closure (dashed line) and Gaussian approximation (dashed-dotted line).

Note that a much simpler mean-field approximation performs as well as the Gaussian one. Thus for $\sigma_Y^2 = 1$, the maximum global error of $\mathscr{E}_{MF} \approx 9\%$ is introduced by the mean field approximation and occurs close to the lower boundary. It does not exceed 5% elsewhere. This explains why rough estimates of pressure distributions, that treat the medium as homogeneous, often prove to be accurate. However, such analyses fail to quantify the predictive uncertainty. Moreover, the accuracy of the mean-field approximation deteriorates rapidly with increasing σ_Y^2.

Figure 4 provides a similar comparison for the pressure variance, σ_ψ^2. The accuracy of the perturbation closure is much superior to those obtained by the Gaussian approximation with the maximum errors $\mathscr{E}_{PA} \approx 35\%$ versus $\mathscr{E}_{GA} \approx 250\%$. Increasing σ_Y^2 to 2 does not alter this pattern significantly.

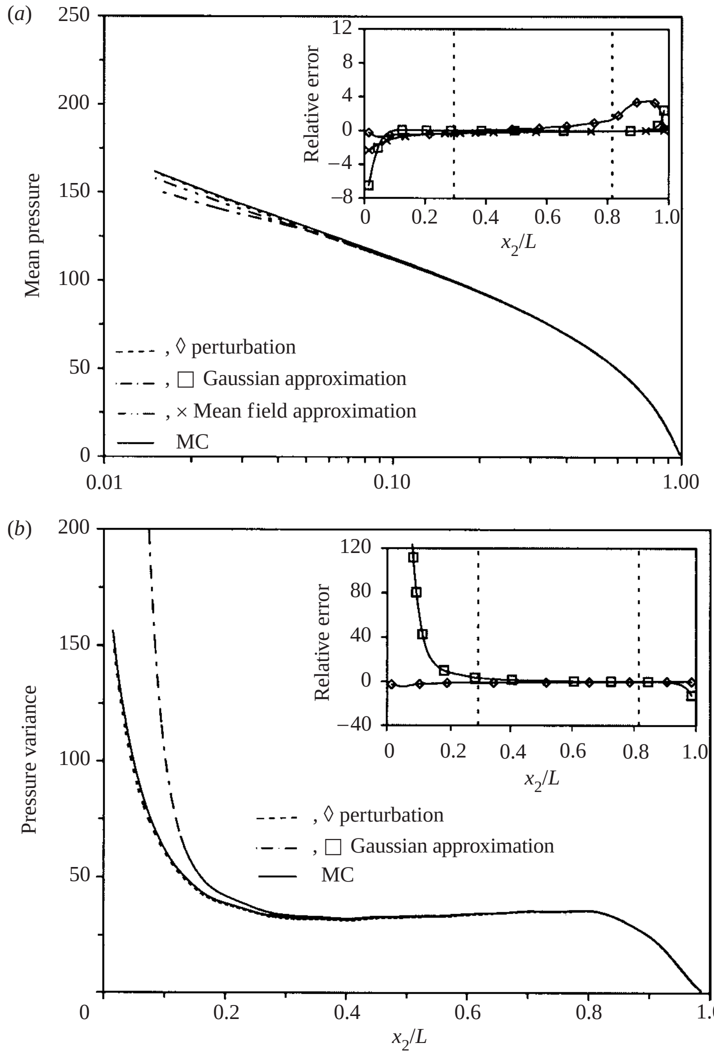

FIGURE 6. The van Genuchten model: vertical cross-section, $x_1 = 0.5L$, of (*a*) the mean pressure $\langle \psi_{vG} \rangle$ and (*b*) pressure variance $\sigma^2_{\psi_{vG}}$ computed with the perturbation closure (dashed line) and Gaussian approximation (dashed-dotted line).

Figures 5–7 demonstrate the fluid behaviour along the vertical cross-section $x_1 = 0.5$ for the Brooks–Corey, van Genuchten and Gardner models, respectively. The pressure estimates corresponding to the Brooks–Corey and van Genuchten models are very close, while the Gardner model gives rise to significantly higher mean pressure gradients. More important, the Brooks–Corey and van Genuchten constitutive laws result in mean pressure gradients that vary slowly in space over significant parts of the flow domain. As has been demonstrated in Tartakovsky *et al.* (1999), this is a necessary condition for the existence of effective relative permeability. The Gardner model results in more variable mean pressure gradients.

Another important feature revealed by figures 5–7 is that, regardless of the choice of the constitutive law, the pressure variance σ^2_ψ peaks in the vicinity of the lower boundary. This implies that dispersion of a conservative solute is largest when it is

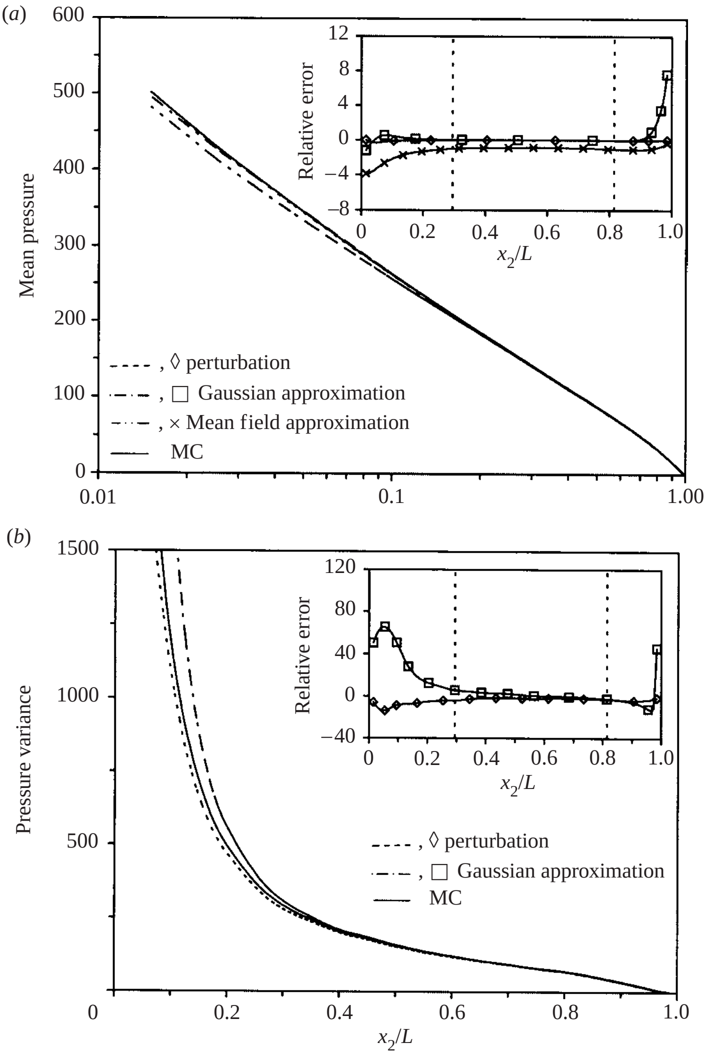

FIGURE 7. The Gardner model: vertical cross-section, $x_1 = 0.5L$, of (*a*) the mean pressure $\langle \psi_{GR} \rangle$ and (*b*) pressure variance $\sigma^2_{\psi_{GR}}$ computed with the perturbation closure (dashed line) and Gaussian approximation (dashed-dotted line).

released close to the dry condition. Uncertainty in the pressure estimates, as quantified by σ^2_ψ, is highest for the Gardner model. However, for all three constitutive laws the coefficient of variation, $\sigma_\psi / \langle \psi \rangle$, is less than one. For the Brooks–Corey and van Genuchten models, it varies between 0.01 and 0.02 and is an order of magnitude higher for the Gardner model. This indicates that predictability of flow in partially saturated porous media is enhanced by choosing either the Brooks–Corey or van Genuchten model.

Figures 5–7 also exhibit the relative errors in the pressure moments calculated with alternative approximations. The errors introduced by the Gaussian approximation increase with the proximity to the boundaries, while the perturbation closure remains accurate throughout the flow domain. To analyse in detail the breakdown of the non-perturbative Gaussian closure, we conduct a χ^2 test for Gaussianity on the

Kirchhoff variable distributions, $\Phi(\boldsymbol{x})$, obtained from the Monte Carlo simulations. Not surprisingly, $\Phi(\boldsymbol{x})$ passes the χ^2 test with a significance level of 1% away from the boundaries (the region between the two vertical dashed lines on figures 5–7) and fails the test otherwise. The Kirchhoff variable is highly non-Gaussian when the mean flow is strongly non-uniform ($x_2 \to 1$).

Overall, the perturbation closure performs remarkably well for all three constitutive models even for relatively large values of conductivity variance σ_Y^2. The simple mean field approximation leads to accurate estimates of the ensemble mean pressure head for the Brooks–Corey and van Genuchten models, and to less accurate estimates of mean pressure for the Gardner model (although the relative errors might be acceptable for practical estimation purposes). For all three constitutive models, the perturbation closure provides more accurate estimates of pressure variance than does the Gaussian approximation. The sole exception is the mean pressure estimate corresponding to the van Genuchten model, which is computed most accurately with the Gaussian approximation (figure 6). However, even in this case, the maximum relative error of 2% introduced by the perturbation approximation should be considered negligibly small.

7. Conclusions

We have analysed statistically flow in partially saturated heterogeneous porous media whose hydraulic parameters are uncertain. By treating saturated hydraulic conductivity as a random field, and the corresponding flow equations as stochastic, we have derived deterministic equations for the mean and variance of the pressure head. The former serves as the best estimate of pressure, while the latter quantifies uncertainty associated with such an estimate. We have used two alternative approximations to close these moment equations: closure by perturbation and Gaussian approximation. Monte Carlo simulations were used as a yardstick against which we compared the accuracy of each approximation. Our analysis leads to the following major conclusions.

(i) Kirchhoff mapping of the stochastic, nonlinear Richards equation and the subsequent closure by perturbation allow for accurate and robust approximations of the ensemble mean, $\langle \psi \rangle$, and variance, σ_ψ^2, of the pressure head. These approximations remain accurate for moderately large values of log-conductivity variance.

(ii) Accuracy and robustness of the closure approximations are influenced by the functional dependence of relative conductivity on pressure, $K_r(\psi)$. Regardless of the choice of $K_r(\psi)$, perturbation closure is more accurate than the Gaussian approximation. Gaussian approximation works well away from the flow domain boundaries and singularities, where flow is almost uniform in the mean.

(iii) The coefficient of variation, $\sigma_\psi / \langle \psi \rangle$, for the Gardner constitutive law is an order of magnitude higher than that for the Brooks–Corey and van Genuchten laws. This indicates that predictability of flow in partially saturated porous media is enhanced by choosing either the Brooks–Corey or van Genuchten models.

(iv) The pressure estimates corresponding to either Brooks–Corey and van Genuchten models are close and differ significantly from that corresponding to the Gardner model.

(v) Reliance on effective constitutive models is more accurate for the Brooks–Corey or van Genuchten constitutive laws than for the Gardner law. This is so, because the former two give rise to mean pressure gradients that vary slower in space than the mean pressure gradients arising from the latter.

Regardless of the constitutive law used and the closure approximation employed, the accuracy of pressure predictions and uncertainty estimates decreases in the vicinity of the flow domain boundaries. This study only begins to address this issue, while leaving a more complete analysis for future work.

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