# A FINITE ELEMENT COLLOCATION METHOD FOR VARIABLY SATURATED FLOWS IN POROUS MEDIA

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# A Finite Element Collocation Method for Variably Saturated Flows in Porous Media

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One common formulation of Richard's equation for variably saturated flows in porous media treats pressure head as the principal unknown and moisture content as a constitutive variable. Numerical approximations to this "head-based" formulation often exhibit mass-balance errors arising from inaccuracies in the temporal discretization. This article presents a finite-element collocation scheme using a mass-conserving formulation. The article also proposes a computable index of global mass balance.

## I. INTRODUCTION

The ability to model water flows in variably saturated soils is importnt to several problems in water resources engineering, among them the prediction of water table contamination from sources at or near the earth's surface. The partial differential equations governing such flows are difficult to solve owing to their nonlinearity, and it is generally necessary to use numerical techniques such as finite differences or finite elements to produce approximate solutions. However, even with numerical schemes there remain difficulties, notably the conservation of mass. Discrete analogs to some formulations of variably saturated flow fail to produce approximate solutions that respect the global mass balance law, even though the original differential equation is derived from this law. We introduce an approach to this problem using finite element collocation. The key to the success of this approach is the choice of a formulation of the flow equation whose temporal discretization is a differential form of the global mass balance for each time interval. Thus the only mass-balance errors in the numerical solution are those arising from the use of a nonzero convergence criterion in the iterations used to advance between time levels. The use of finite element collocation to discretize the space derivatives guarantees approximations of high-order spatial accuracy while obviating the costs of integration and formal matrix assembly associated with other finite-element techniques.

## II. SETTING OF THE PROBLEM

The equation governing one-dimensional water flows in variably saturated soils has the form [1]

$$\frac{\partial}{\partial x}\left[K(h)\frac{\partial h}{\partial x} - K(h)\right] = C(h)\frac{\partial h}{\partial t}. \tag{1}$$

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Here $h$ stands for pressure head, measured in meters; $K$ represents the hydraulic conductivity of the soil, measured in meters/second; and $C$ is called the specific moisture capacity of the soil, measured in meters$^{-1}$. The specific moisture capacity $C$ accounts for the variation in the soil's dimensionless moisture content $\theta$ in response to changes in pressure head; specifically, $C = d\theta/dh$. In practice one uses experimental data to quantify the constitutive relationships $\theta(h)$ and $K(h)$.

Equation (1) casts the pressure head $h$ as the dependent variable, leaving $\theta$ and $K$ as nonlinear coefficients. As an alternative to this *h-based* formulation, we can pose the problem in terms of the moisture content $\theta$ as follows:

$$\frac{\partial}{\partial x}\left[D(\theta)\frac{\partial \theta}{\partial x} - K(\theta)\right] = \frac{\partial \theta}{\partial t}. \tag{2}$$

Here $K$ appears as a function of $\theta$, and $D = K\,dh/d\theta$ is the soil's hydraulic diffusivity, measured in meters$^2$/second. This is the *θ-based* formulation. Although Eq. (1) and (2) are equivalent by the chain rule, modelers prefer the h-based formulation in most practical problems, where spatial variations in soil properties and sharp gradients in $\theta$ can lead to poor behavior in the $\theta$-based formulation [2].

As a model problem we shall solve the initial-boundary value problem for variably saturated flow posed by Warrick et al. [3]. Let a soil column [0, 1.25] have an initial water saturation described by

$$\theta(x, 0) = \begin{cases} 0.15 + x/12, & 0 < x \le 0.6 \\ 0.2, & 0.6 < x < 1.25 \end{cases}, \tag{3a}$$

where $x$ stands for depth in meters from the surface. Assume that the pressure head at the surface is atmospheric, that is

$$h(0, t) = -0.14495\,, \tag{3b}$$

and that the pressure head gradient vanishes at the outflow,

$$\frac{\partial h}{\partial x}(1.25, t) = 0\,. \tag{3c}$$

For the constitutive relationships $K(h)$ and $C(h)$ we use the functions measured by Warrick et al. [3], which in SI units are

$$K(h) = \begin{cases} 1.157 \times 10^{-7}(19.34 \times 10^{5}|100h|^{-3.4095}), & h \le -0.29484 \\ 1.157 \times 10^{-7}(516.8|100h|^{-0.97814}), & h > -0.29484 \end{cases}$$

$$\theta(h) = \begin{cases} 0.6829 - 0.09524 \ln|100h|, & h \le -0.29484 \\ 0.4531 - 0.02732 \ln|100h|, & h > -0.29484 \end{cases}$$

Thus the prescribed atmospheric pressure head at $x = 0$ corresponds approximately to a moisture content $\theta(0, t) = 0.38$.

The numerical solution of this problem using finite elements is not entirely straightforward. The nonlinearities in the $h$-based flow equation can lead to poor global mass balance and thus to unacceptable numerical approximations.

Van Genuchten [4] demonstrates this difficulty quite clearly by comparing several Galerkin approximations to Eq. (1) with the auxiliary data (3). Figure 1 shows some of his results. Notice in particular that the wetting front in the solution using a Hermite cubic trial function with two-point Gauss quadrature on each element (marked "2GP, 3LP" in Fig. 1) lags the correct wetting front by a significant distance. This poor approximation apparently bodes ill for finite-element collocation on Hermite cubic spaces, since there is a direct algebraic correspondence between such collocation schemes and Galerkin's method on Hermite cubics with two-point quadrature [5]. We shall examine the difficulties with collocation in the next section.

Recognizing the importance of mass-balance errors, Milly [6] examines the effect of temporal discretization on the accuracy of the accumulation term $C\,\partial h/\partial t$ in Eq. (1). He proposes a global mass-balance criterion of the form

$$\frac{1}{\Delta t}\int_{\Omega}(\theta^{n+1}-\theta^{n})\,dx = \int_{\Omega}\left(K\frac{\partial h}{\partial x}-K\right)dx \tag{4}$$

where $\Omega = [0, 1.25]$ is the spatial domain of the flow, $\Delta t$ is the discrete time interval, and $n, n+1$ signify successive time levels. Milly attributes the mass balance errors plaguing various discrete analogs to failures to evaluate the coefficient $C(h)$ in a way that reflects the average behavior of the soil over each time interval. He advances an iterative scheme for approximating $C(h)$ that leads to arbitrarily good mass balance in the sense of Eq. (4), given a sufficient number of iterations.

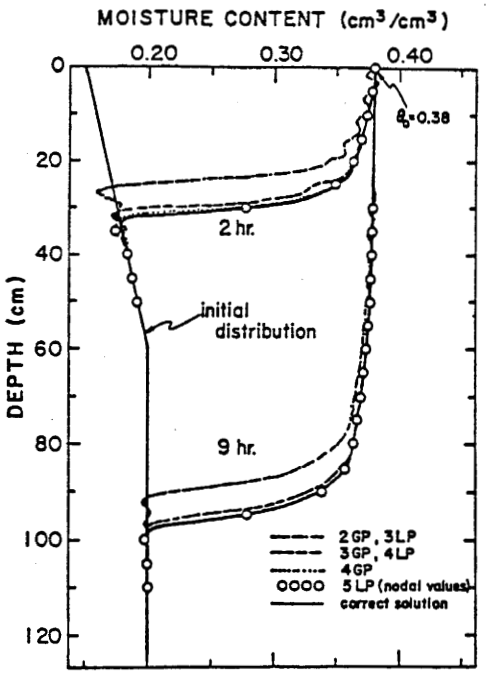


FIG. 1. Numerical moisture-content profiles computed from the $h$-based formulation using the Galerkin method on Hermite cubics with various quadrature schemes (from Reference [4]).

We propose a finite element collocation scheme for variably saturated flows that conserves mass by a somewhat simpler device. Before describing this scheme, however, let us examine in detail the difficulties that arise in the straightforward application of collocation approximation to Eq. (1).

## III. COLLOCATION USING THE *h*-BASED FORMULATION

To construct a collocation approximation to Eq. (1), we can follow an approach that is analogous to Van Genuchten's [4]. Let us begin by discretizing Eq. (1) in time using an implicit Euler difference scheme:

$$K^{n+1}\frac{\partial^2 h^{n+1}}{\partial x^2} + \frac{\partial K^{n+1}}{\partial x}\frac{\partial h^{n+1}}{\partial x} - \frac{\partial K^{n+1}}{\partial x} - C^{n+1}\frac{h^{n+1} - h^n}{\Delta t} = 0 \qquad (5)$$

Here, as in Eq. (4), the superscripts $n, n+1$ indicate successive time levels and $\Delta t$ is the time interval between them. This approximation imposes a truncation error that is $O(\Delta t)$.

Since the coefficients $K^{n+1}, C^{n+1}$ depend on the unknown $h^{n+1}$, it is necessary to use an iterative method to advance Eq. (5) from one time level to the next. We can effect a Newton-like iteration scheme as follows:

$$K^{n+1,m}\frac{\partial^2}{\partial x^2}(h^{n+1,m} + \delta h) + \frac{\partial K^{n+1,m}}{\partial x}\frac{\partial}{\partial x}(h^{n+1,m} + \delta h) - \frac{\partial K^{n+1,m}}{\partial x} - \frac{C^{n+1,m}}{\Delta t}(h^{n+1,m} + \delta h - h^n) = 0. \qquad (6)$$

In this scheme, the variable $h^{n+1,m}$ signifies the known approximation to the new pressure head $h^{n+1}$ at the $m$-th iterative level; $K^{n+1,m}$ and $C^{n+1,m}$ stand for $K(h^{n+1,m})$ and $C(h^{n+1,m})$, respectively, and the unknown $\delta h$ represents an increment that must be added to $h^{n+1,m}$ to produce an improved approximation $h^{n+1,m+1}$. At each time level the iterative scheme begins with the initial value $h^{n+1,0} = h^n$ and ends by assigning $h^{n+1} = h^{n+1,m+1}$ when either the increment $\delta h$ or the residual

$$K^{n+1,m+1}\frac{\partial^2 h^{n+1,m+1}}{\partial x^2} + \frac{\partial K^{n+1,m+1}}{\partial x}\frac{\partial h^{n+1,m+1}}{\partial x} - \frac{\partial K^{n+1,m+1}}{\partial x} - \frac{C^{n+1,m+1}}{\Delta t}(h^{n+1,m+1} - h^n) = R^{n+1,m+1}$$

is sufficiently small.

To construct a collocation analog of this discrete-time scheme, let us approximate the unknown $\delta h$ by a piecewise Hermite cubic finite element representation:

$$\delta\hat{h}(x) = \sum_{i=1}^{N}[\delta_i H_{0,i}(x) + \delta_i' H_{1,i}(x)]. \qquad (7)$$

In this equation $H_{0,i}(x)$ and $h_{1,i}(x)$ are elements of the Hermite cubic basis for $C^1$ polynomial interpolation on a partition of $\Omega$, and $\delta_i$ and $\delta_i'$ stand for the

values of $\delta\hat{h}$ and $\partial(\delta\hat{h})/\partial x$, respectively, at node $i$ of the partition [7]. Once we have solved for the coefficients $\{\delta_i, \delta_i'\}_{i=1}^N$ in Eq. (7), we can compute a new iterative approximation to the pressure head in the obvious way:

$$\hat{h}^{n+1,m+1}(x) = \sum_{i=1}^{N} [(h_i^{n+1,m} + \delta_i)H_{0,i}(x) + (h_i'^{n+1,m} + \delta_i')H_{1,i}(x)].$$

There are several ways to represent the coefficients $K$ and $C$. One approach that seems to produce well-behaved approximations is simply to interpolate between the nodal values $K(h_i)$ or $C(h_i)$. If we use linear interpolation, then the representations become

$$\hat{K}(x) = \sum_{i=1}^{N} K(h_i)L_i(x)$$

$$\frac{\partial \hat{K}}{\partial x}(x) = \sum_{i=1}^{N} K(h_i)\frac{dL_i}{dx}(x)$$

$$\hat{C}(x) = \sum_{i=1}^{N} C(h_i)L_i(x)$$

where $\{L_i\}_{i=1}^N$ is the Lagrange basis for $C^0$ linear interpolation on the partition of $\Omega$ [7].

If we substitute all of these finite element approximations into the discrete-time equation (6), there remains the task of solving for the $2N$ unknowns $\{\delta_i, \delta_i'\}_{i=1}^N$. Since the boundary conditions translate to $h_0 = h(0,t)$ and $h_N' = \partial h/\partial x(1.25, t)$, we know that $\delta_1 = \delta_N' = 0$. To solve for the remaining $2N - 2$ unknowns, we collocate the finite-element approximation to Eq. (6). That is, we force

$$\hat{K}^{n+1,m}(\bar{x}_k)\frac{\partial^2}{\partial x^2}[\hat{h}^{n+1,m}(\bar{x}_k) + \delta\hat{h}(\bar{x}_k)] + \frac{\partial \hat{K}^{n+1,m}}{\partial x}(\bar{x}_k)\frac{\partial}{\partial x}[\hat{h}^{n+1,m}(\bar{x}_k) + \delta\hat{h}(\bar{x}_k)]$$
$$- \frac{\partial \hat{K}^{n+1,m}}{\partial x}(\bar{x}_k) - \frac{\hat{C}^{n+1,m}(\bar{x}_k)}{\Delta t}[\hat{h}^{n+1,m}(\bar{x}_k) + \delta\hat{h}(\bar{x}_k) - \hat{h}^n(\bar{x}_k)] = 0$$

at $2N - 2$ values $\bar{x}_k \in \Omega$. Douglas and Dupont [5] show that, if the finite element partition of $\Omega$ is uniform, then the optimal collocation points are the Gauss points

$$\bar{x}_k = x_i + \left(\frac{1}{2} \pm \frac{1}{\sqrt{3}}\right)\Delta x, \qquad i = 1, \ldots, N-1$$

where $\Delta x$ is the mesh of the partition. This scheme produces approximate solutions with a spatial error that is $O(\Delta x^4)$.

Figure 2 shows the numerical pressure head profiles at two and nine hours using this scheme with $\Delta x = 0.05$, $\Delta t = 240$, and an iterative convergence criterion requiring that the maximum residual $\max\{R^{n+1,m+1}(\bar{x}_k)\}_{k=1}^{2N-2}$ be less than $5.0 \times 10^{-6}$/s. Figure 3 depicts the corresponding moisture content distributions at two and nine hours, computed from the constitutive relationship $\theta(h)$. Observe that the wetting front at two hours lies at approximately $x =$

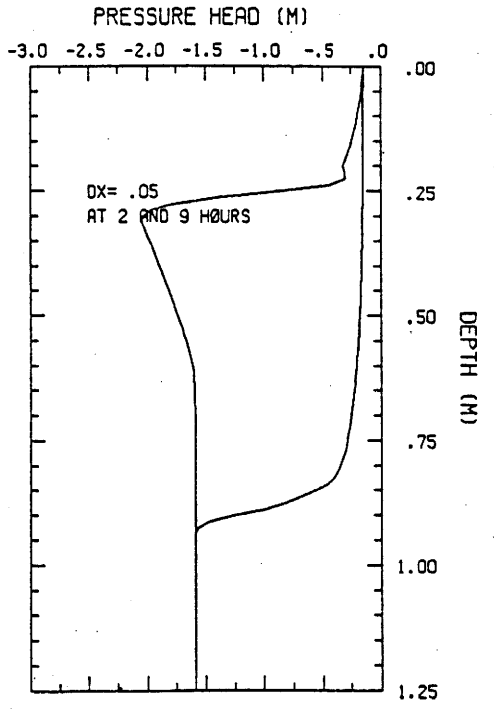


FIG. 2. Numerical pressure-head profiles computed from the $h$-based formulation using finite-element collocation.

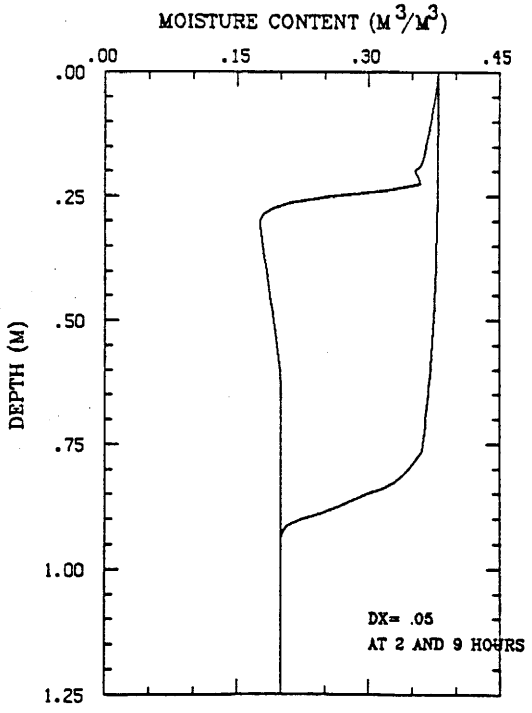


FIG. 3. Numerical moisture-content profiles computed from the $h$-based formulation using finite-element collocation.

0.24, which is very close to that in Van Genuchten's solution in Figure 1 using Hermite cubics with two-point Gauss quadrature on each element. Thus the collocation method outlined above exhibits mass-balance errors similar to those of the Galerkin method with two-point quadrature, as we expected on the strength of the theoretical correspondence between the two methods.

## IV. AN ALTERNATIVE COLLOCATION SCHEME

One can generate a mass-conserving collocation scheme by discretizing a differential equation derived directly from the global mass balance, Eq. (4), in the limit $\Delta t \to 0$. This yields a governing equation of the form

$$\frac{\partial}{\partial x}\left[K(h)\frac{\partial h}{\partial x} - K(h)\right] = \frac{\partial \theta}{\partial t}(h) \tag{8}$$

provided the integrands in the global equation are continuous. Since the left side of this equation is exactly the same as the left side of the $h$-based formulation (Eq. (1)), while the right side is simliar to that appearing in the $\theta$-based formulation (Eq. (2)), we might call Eq. (8) a *hybrid* formulation.

Let us discretize Eq. (8) in a fashion analogous to our treatment of Eq. (1). First, replace the time derivative by an implicit difference scheme having truncation error $O(\Delta t)$:

$$K^{n+1}\frac{\partial^2 h^{n+1}}{\partial x^2} + \frac{\partial K^{n+1}}{\partial x}\frac{\partial h^{n+1}}{\partial x} - \frac{\partial K^{n+1}}{\partial x} - \frac{\theta^{n+1} - \theta^n}{\Delta t} = 0.$$

Here $\theta^{n+1}, \theta^n$ stand for $\theta(h^{n+1}), \theta(h^n)$, respectively. Next, to accommodate the nonlinearities in $K$ and $\theta$, assume an iterative method of the form

$$K^{n+1,m}\frac{\partial^2}{\partial x^2}(h^{n+1,m} + \delta h) + \frac{\partial K^{n+1,m}}{\partial x}\frac{\partial}{\partial x}(h^{n+1,m} + \delta h) - \frac{\partial K^{n+1,m}}{\partial x} - \frac{1}{\Delta t}\left(\theta^{n+1,m} + \frac{d\theta^{n+1,m}}{dh}\,\delta h - \theta^n\right) = 0 \tag{9}$$

for updating the implicit coefficients from one time level to the next. Finally, project the unknowns $\delta h$ to Hermite cubic subspaces and the coefficients $K$ and $d\theta/dh = C$ to Lagrange linear subspaces as in Section III above.

There remains the question of a finite-element representation of $\theta$. We have found through numerical experiments that a Hermite cubic expansion of $\theta$ gives superior results. To effect such a representation, we use the chain rule to compute the nodal gradients in $\theta$:

$$\hat{\theta}(x) = \sum_{i=1}^{n}\left[\theta(h_i)H_{0,i}(x) + \frac{d\theta}{dh}(h_i)h_i' H_{1,i}(x)\right].$$

Then, using the finite element spatial discretizations together with the iterative time-stepping scheme in Eq. (9), we collocate at the $2N - 2$ Gauss points as before to advance the iterations from one time level to the next.

Figure 4 shows the pressure head profiles at two and nine hours using the new scheme with the same $\Delta x, \Delta t$, and convergence criteria as used in producing Figure 2. Figure 5 displays the corresponding profiles for moisture content. Notice that the wetting front at two hours in this plot falls at about $x = 0.30$, which agrees with the location of the wetting front that Van Genuchten identifies as the correct solution in Figure 1. Finite element collocation applied to the hybrid formulation in Eq. (8) apparently furnishes approximate solutions that more closely respect the balance of mass.

It is useful in checking a coded algorithm for this type of problem to have a computable technique for checking global mass balance. For the collocation method presented in this section we can readily derive such a technique. We wish to verify at any time level that Eq. (4) holds to a good approximation. It happens that each of the integrals in this equation can be rapidly computed using information that is already available from the collocation solution at each time step. Consider first the flux integral on the right side of Eq. (4). Since $\hat{h} \in C^1(\Omega)$ and $\hat{K} \in C^0(\Omega)$, the differential flux $(\hat{K}(\partial\hat{h}/\partial x) - \hat{K}) \in C^0(\Omega)$ and hence the fundamental theorem of calculus yields

$$\int_\Omega \frac{\partial}{\partial x}\left(\hat{K}\frac{\partial \hat{h}}{\partial x} - \hat{K}\right) dx = K(h_N)\,(h'_N - 1) - K(h_1)\,(h'_1 - 1)\,.$$

Now look at the accumulation integral on the left side of Eq. (4). This can be written as

$$\frac{1}{\Delta t}\int_\Omega (\hat{\theta}^{n+1} - \hat{\theta}^n)\, dx = \frac{1}{\Delta t}\sum_{i=1}^{N-1}\int_{x_i}^{x_{i+1}} (\hat{\theta}^{n+1} - \hat{\theta}^n)\, dx$$

But the integrand in each term in this decomposition is a cubic function of $x$, and so two-point Gauss quadrature suffices for the exact calculation of these integrals. Since the Gauss points are precisely the collocation points, the computation of the accumulation integral reduces to a sum of previously computed values:

$$\frac{1}{\Delta t}\int_\Omega (\hat{\theta}^{n+1} - \hat{\theta}^n)\, dx = \frac{\Delta x}{2\Delta t}\sum_{k=1}^{2N-2} (\hat{\theta}^{n+1} - \hat{\theta}^n)\Big|_{\bar{x}_k}$$

where each $\bar{x}_k$ is a collocation point.

Now we can define a mass balance index as the ratio of the accumulation integral to the flux integral:

$$I_{MB} = \frac{1}{K(h_n)\,(h'_n - 1) - K(h_1)\,(h'_1 - 1)}\,\frac{\Delta x}{2\,\Delta t}\sum_{k=1}^{2N-2} (\hat{\theta}^{n+1} - \hat{\theta}^n)\Big|_{\bar{x}_k}$$

For a perfectly conservative numerical scheme $I_{MB} = 1$. For real schemes, however, the necessity of stopping the time-stepping procedure after a finite number of iterations will generally prohibit an exact mass balance. Figure 6 exhibits ranges of values of $I_{MB}$ computed from the hybrid collocation scheme using several spatial meshes $\Delta x$. The plots show that the new formulation gives

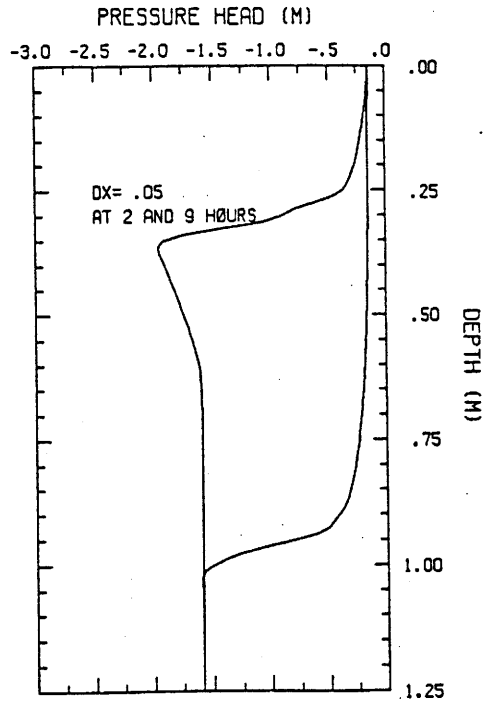


FIG. 4. Numerical pressure-head profiles computed from the hybrid formulation using finite-element collocation.

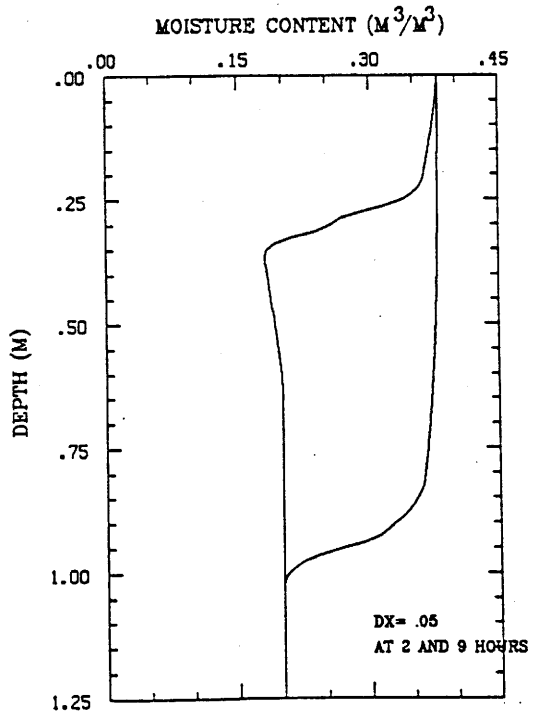


FIG. 5. Numerical moisture-content profiles computed from the hybrid formulation using finite-element collocation.

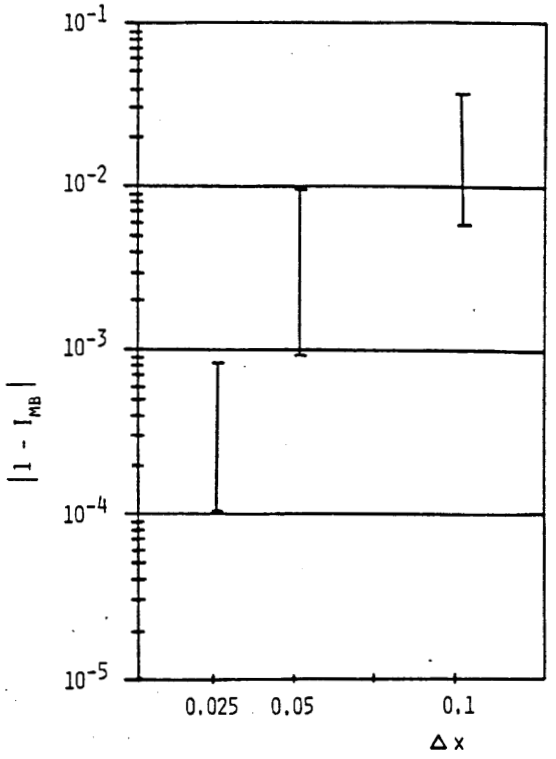


FIG. 6. Mass-balance error $|1 - I_{MB}|$ in the hybrid formulation using finite-element collocation with various spatial meshes.

reasonable global mass balances that improve upon refinement of the spatial partition. These results corroborate the good agreement between the profiles shown in Figure 5 and Van Genuchten's "correct solutions" plotted in Figure 1.

## V. CONCLUSIONS

The collocation scheme presented here gives numerical solutions to the variably saturated flow equation that enjoy high-order spatial accuracy and stand in quantifiable agreement with the principle of global mass balance. The choice of a hybrid formulation incorporating features of both the $h$-based and $\theta$-based flow equations proves instrumental in forcing mass conservation, since this formulation is directly descended from the global mass balance criterion. The direct projection of the accumulation term $\partial\theta/\partial t$ onto Hermite cubic interpolation polynomials avoids the delicate problem of choosing representative values for the time-varying coefficient that arises on applying the chain rule to this term. When one imposes an iterative time-stepping scheme upon this hybrid form in conjunction with finite element collocation, the individual collocation equations drive the mass-balance error at each collocation point toward zero as the iterations proceed.

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