EIS000029

"Donald L. Baker" <don.baker@aquarien.com> on 09/02/99 06:28:55 PM

Please respond to don.baker@aquarien.com

To: EISR/YM/RWDOE

cc:

Subject: Comment on the draft EIS

RECEIVED

SEP 0 2 1999

Please be informed that I wish this e-mail and attachment to be entered into the public record of comment on the Draft Environmental Impact Statement, DOE/EIS-0350D.

1 How can you draft an impact statement when you haven't accounted for all the modeling errors?

This is the summary for the attached file, ympquea2.pdf.

Some Questions for the Modelers of Unsaturated Flow and Transport for the Yucca Mountain Project, Hanford Tank Initiative, Nevada Test Site and other DOE Programs.

Submitted by
Donald L. Baker, Ph.D. Soil Physics
Aquarius Engineering
2000 West Maine Street
Fayetteville, AR 72701
www.aquarien.com

Summary

1 continued

Recent work (publications and draft papers on www.aquarien.com) in numerical methods for modeling the vertical unsaturated flow of water in porous media has uncovered previously unrecognized errors in standard methods. These errors may affect the validity and reliability of models that attempt to predict the flow of water and the transport of hazardous and nuclear waste on the scale of tens to thousands of years. The following questions and three-point grid test demonstrate how the common arithmetic mean of intergrid unsaturated hydraulic conductivity violates Darcy's law for vertical unsaturated flow in all but a few trivial conditions, and can even violate the mathematical minimum-maximum principle for elliptic boundary value problems (steady-state flow problems). By contrast, a Darcian intergrid conductivity mean for the exponential pressure-conductivity relation solves such problems perfectly. The numerical examples in the appendix compare parallel models of a relaxing wet pulse in a long, vertical fracture, using the exponential pressure-conductivity relation. One model uses the arithmetic mean, and the other the analytic Darcian mean, with exactly the same adaptive time steps for both. The arithmetic mean model exhibits a dry spike that grows with the logarithm of time, and oscillations similar to numerical dispersion, both associated with space steps where the arithmetic mean can violate the min-max principle. By contrast, the Darcian mean model is smooth and well-behaved.

Sincerely,
Don Baker
mailto://don.baker@aquarien.com

EIS000029

- ympquea2.pdf

2

~~Supplemental Material~~

EIS000029

Some Questions for the Modelers of Unsaturated Flow and Transport for the Yucca Mountain Project, Hanford Tank Initiative, Nevada Test Site and other DOE Programs.

Submitted by
Donald L. Baker, Ph.D. Soil Physics
Aquarius Engineering
2000 West Maine Street
Fayetteville, AR 72701
www.aquarien.com

Summary

Recent work (publications and draft papers on www.aquarien.com) in numerical methods for modeling the vertical unsaturated flow of water in porous media has uncovered previously unrecognized errors in standard methods. These errors may affect the validity and reliability of models that attempt to predict the flow of water and the transport of hazardous and nuclear waste on the scale of tens to thousands of years. The following questions and three-point grid test demonstrate how the common arithmetic mean of intergrid unsaturated hydraulic conductivity violates Darcy's law for vertical unsaturated flow in all but a few trivial conditions, and can even violate the mathematical minimum-maximum principle for elliptic boundary value problems (steady-state flow problems). By contrast, a Darcian intergrid conductivity mean for the exponential pressure-conductivity relation solves such problems perfectly. The numerical examples in the appendix compare parallel models of a relaxing wet pulse in a long, vertical fracture, using the exponential pressure-conductivity relation. One model uses the arithmetic mean, and the other the analytic Darcian mean, with exactly the same adaptive time steps for both. The arithmetic mean model exhibits a dry spike that grows with the logarithm of time, and oscillations similar to numerical dispersion, both associated with space steps where the arithmetic mean can violate the min-max principle. By contrast, the Darcian mean model is smooth and well-behaved.

X 3

Some Questions on Model Validity

Would you agree that it is necessary for a modeler of unsaturated flow to be cognizant of all the sources and relative magnitudes of error in his or her numerical calculations? Would you agree that this allows a modeler to construct a variable or adaptive grid so as to produce the least error? If not, make an irrefutable scientific argument for the contrary view.

Would you agree that any method of calculating steady-state unsaturated flow would be both physically and mathematically invalid if it violated either the minimum-maximum principle for elliptic boundary value problems (D.W. Zachmann & P. DuChateau, 1986, Schaum's Outline Series, Theory and Problems of Partial Differential Equations, pp 19-21) or Darcy's law? If not, can you give a scientific justification for your answer that is beyond all refutation?

Would you contend that any such method that commits either of these violations in a model of steady-state flow is then valid to use in a model of transient flow? If so, can you give a scientific justification for your answer that is beyond all refutation?

Would you agree that any method that commits one or both of these violations would be inappropriate to use in models designed to predict and assure the safety of a nuclear waste site over the scale of thousands of years? If not, can you give a scientific justification for your answer that is beyond refutation?

Can you demonstrate that all the methods that you use for calculating unsaturated flow in your models do not violate either the min-max principle or Darcy's law in any case or regime in which your models are used? If not, can you give a scientific justification that is beyond all refutation for why your models should be considered to be valid and reliable?

Do you recognize equation [1] as Darcy's law in the finite form and [2] as Darcy's law in the continuum form?

[1] $\bar{q} = -Ks \cdot Kv \cdot \frac{\Delta H}{\Delta x} = -Ks \cdot Kv \cdot \frac{\Delta x - \Delta \psi}{\Delta x}$, where q-bar (m/s) is the mean mass flow across the vertical distance, Δx (m), Ks (m/s) is saturated hydraulic conductivity, Kv is the mean relative hydraulic conductivity across vertical Δx, and ΔH (m) is the total hydraulic head difference across Δx, where $H = x-\psi$, x (m) is the vertical position or head and ψ (m) is the matric suction (or negative pressure) head.

[2] $q = -K(\psi) \cdot \frac{\partial H}{\partial x} = -K(\psi) \cdot \frac{\partial x - \partial \psi}{\partial x}$

Consider the three-point system of steady-state, constant, vertical, unsaturated flow in a homogeneous porous medium in Figure 1, with fixed boundary conditions $\psi2(x2)$ and $\psi0(x0)$, where $x0 = 0$, $x1 = \Delta x$ and $x2 = 2 \cdot \Delta x$ in the vertical. Let Km be the estimate of unsaturated hydraulic relative conductivity mean between x0 and x2, and kml and kmu be the estimates by the same method between x0 and x1, and x1 and x2, respectively. Let H0, H1 and H2 be the total heads at x0, x1 and x2, such that $H0 = -\psi0$, $H1 = \Delta x-\psi1$ and $H2 = 2 \cdot \Delta x-\psi2$. Would you agree that equation [3] is an accurate and valid application of Darcy's law in [1] in this case?

~~2~~
4

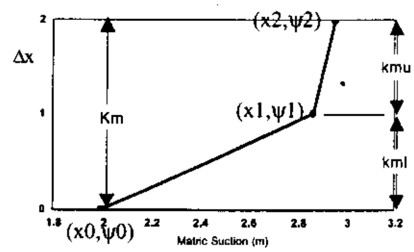

Figure 1: Three-Point System of Steady-State Flow

$$[3]\ \frac{-q \cdot \Delta x}{Ks} = Km \cdot (H2 - H0)/2 = kml \cdot (H1 - H0) = kmu \cdot (H2 - H1)$$

If one solves the two right-hand-sides of [3] against Km·(H2-H0) for H1, sets them equal and divides out common terms of (H2-H0), the result is then equation [4]. Would you agree that in order to satisfy Darcy's law and calculate the same constant flow on both the Δx and 2·Δx scales, that any method to estimate the intergrid conductivity means, Km, kml and kmu, would also have to satisfy equation [4]? And would you agree that if it failed to satisfy equation [4] that this would raise a legitimate question as to its validity in a model of unsaturated flow? If not, please demonstrate mathematically why not.

$$[4]\ Km = \frac{2 \cdot kml \cdot kmu}{kml + kmu}$$

Suppose that the method in question is the arithmetic mean, such that Km = (kr0+kr2)/2, kml = (kr0+kr1)/2 and kmu = (kr1+kr2)/2, where kr0 = kr(ψ0), kr1 = kr(ψ1), kr2 = kr(ψ2) and kr(ψ) is the unsaturated relative conductivity relation for the porous medium in Figure 1. Substitute the arithmetic means for kml and kmu into equation [3] and cancel common terms, like 2. Would you agree that equation [5] is a valid result and the only unknown in the equation is ψ1, which can be solved be iteration or Newton's method? Equations [4] and [5] are both derived from equation [3]. Would you agree that the value of kr1 = kr(ψ1) resulting from [5] determines the values of kml and kmu, and that substituting them back into equation [4] is a reasonable way to check the mathematical and physical validity of the arithmetic mean, or any other method of estimation?

$$[5]\ (kr(\psi 1) + kr2) \cdot (H2 - \Delta x + \psi 1) - (kr0 + kr(\psi 1)) \cdot (\Delta x - \psi 1 - H0) = 0$$

Consider a porous medium where the unsaturated conductivity relation is determined by equation [6], with η = 8.1 and ψd = 0.08 m. Given the expected values published in Schenker, et al. (1995, Stochastic hydrogeological unites and hydrogeological properties development for total-system performance assessments, Sandia Report SAND94-0244*UC-814 under DOE contract DE-AC04-94AL85000), is this a reasonable possible expression for the relative conductivity of a fracture in Topopah Spring welded volcanic tuff, if one uses a Mualem or Burdine transformation to derive kr(ψ) from the pressure-saturation parameters given in Schenker, et al? If not, can you specify a more correct set of η and ψd parameters to use in this example?

~~3~~
5

$$[6]\quad kr(\psi) = \begin{cases} 1 & ,\psi \le \psi d \\ (\psi d / \psi)^{\eta} & ,\psi > \psi d \end{cases}$$

, where ψd = "displacement pressure" head (m) and η is a fitting parameter.

Please verify that Table 1 is the set of solutions to equation [5], given equation [6], with ψd = 0.08 and η as given in column 2. Is it not apparent from this table that for η = 8.1 the arithmetic mean produces a value of $\psi 1$ that violates the min-max principle for any Δx greater than about 0.50366 m? It is possible to show that the arithmetic mean satisfies both equations [4] and [5] in the trivial case of pure gravity flow, where $\psi 0 = \psi 1 = \psi 2$. But is it not apparent from Table 1 that the arithmetic mean fails satisfy Darcy's law in steady state flow for $\psi 0 \neq \psi 2$ and Δx > 0.50366 m? Is it not also apparent that the arithmetic mean likely violates the min-max principle for η = 2.1 and 4 and for Δx > 0.80422 and 0.56667 m, respectively? If you do not agree, can you demonstrate the opposite mathematically?

Table 1: Solutions to Figure 1 with the Arithmetic Mean

The variables η, Δx, $\psi 0$, $\psi 1$ and $\psi 2$ are as described above. The variable, $\psi 1$, is determined by the solution to equation [5], kr1=kr(y1) = $(0.08/\psi 1)^{\eta}$, kml = (kr0+kr1)/2, kmu = (kr1+kr2)/2, Km = (kr0+kr2)/2 and the mean of means is 2·kml·kmu/(kml+kmu), the right-hand-side of equation [4]. The $\psi 1$ column tests conformity to the min-max principle, that $\psi 1$ is included in the range [$\psi 0$,$\psi 2$]. Rows 8 and 9 show violation of the min-max principle. Rows 1,2 and 7 show the boundary of violation for the min-max principle. The last two columns on the right test the balance of equation [4] for the arithmetic mean, which fails in every row.

	η	Δx (m)	$\psi 0$ (m)	y1 (m)	y2 (m)	kr1	kml	kmu	Km	mean of means rhs of [4]
1	2.1	0.80422	0.5	1	1	.004972	.013142	.004972	.013142	.007214
2	4.0	0.56667	0.5	1	1	4.1e-5	.000348	4.1e-5	.000348	7.33e-5
3	8.1	0.001	0.5	0.58860	1	9.54e-8	2.26e-7	4.83e-8	1.79e-7	7.97e-8
4	8.1	0.01	0.5	0.59200	1	9.11e-8	2.24e-7	4.62e-8	1.79e-7	7.66e-8
5	8.1	0.1	0.5	0.63450	1	5.11e-8	2.05e-7	2.66e-7	1.79e-7	4.71e-8
6	8.1	0.5	0.5	0.99634	1	1.34e-9	1.79e-7	1.32e-9	1.79e-7	2.63e-9
7	8.1	0.50366	0.5	1	1	1.3e-9	1.79e-7	1.3e-9	1.79e-7	2.59e-9
8	8.1	1	0.5	1.494	1	5.0e-11	1.79e-7	6.8e-10	1.79e-7	1.35e-9
9	8.1	2	0.5	2.4873	1	8.1e-13	1.79e-7	6.5e-10	1.79e-7	1.3e-9

Consider again equations [4] and [5], which derive from Darcy's law for steady-state flow that is constant in space in equation [3]. Is it not apparent from these equations that a method of estimating an intergrid hydraulic conductivity mean that upholds Darcy's law must contain an accounting for the model vertical space step term, Δx?

It may be possible that the non-Darcian flow errors generated by the arithmetic mean are small enough to make it of practical use in some modeling regimes. Can you provide a mathematical

4
6

justification for when this would be the case? Can your justification account for both the pressure-conductivity relation, kr(ψ), and the model vertical space step size, Δx?

If you are using some other method of estimating the intergrid hydraulic conductivity mean in your models, can you perform this analysis and demonstrate that any other method you use does not produce similar violations of Darcy's law and the min-max principle?

If not, would you agree that a method that did account for both kr(ψ) and Δx, and did not violate either Darcy's law or the min-max principle would be more appropriate for use in both models of steady-state and transient flow?

Do you again recognize equation [2] as the continuum form of Darcy's law? Consider that if kr is a function of ψ and ψ is a function of x, then kr is also a function of x. Do you recognize equation [7] as the expression of flow that is constant in space, and equation [8] ([7] applied to [2]) as the expression of steady-state flow that is constant in space and time, as long as the boundary conditions are constant in time? If the conductivity relation and its inverse are as described in [9], please verify that [9] and the spatial distribution of kr(x) in [10] satisfy [8].

[7] $$-\frac{\partial(q / Ks)}{\partial x} = 0$$

[8] $$\frac{\partial}{\partial x}\left[kr(\psi(x)) \cdot \frac{\partial}{\partial x}\left(x - \psi(x)\right)\right] = \frac{\partial kr(x)}{\partial x} \cdot \left[1 - \frac{\partial y(x)}{\partial x}\right] - kr(x) \cdot \frac{\partial^2 \psi}{\partial x^2} = 0$$, where the boundary conditions are (x1=0,ψ1) lower and (x2=Δx,ψ2) upper and constant in time, which may also be expressed as (0,kr1=kr(ψ1)) and (Δx,kr2=kr(ψ2)).

[9] $kr(x) = \exp(\eta \cdot (\psi d - \psi(x)))$, $\psi(x) = \psi d - \ln(kr(x)) / \eta$

[10] $kr(x) = a \cdot \exp(-\eta \cdot x) + b$, $a = \dfrac{kr1 - kr2}{1 - \exp(-\eta \cdot \Delta x)}$, $b = \dfrac{kr2 - kr1 \cdot \exp(-\eta \cdot \Delta x)}{1 - \exp(-\eta \cdot \Delta x)}$

Equation [11] is [1] rewritten. Equation [12] is the integration of [2], allowing that kr(ψ(x)) can also be expressed as kr(x). Do you recognize [13] and its implication as a legitimate definition of mean flow in a problem [8] where the flow is constant in time and space, and the resulting value of Kv as the legitimate definition of a mean intergrid hydraulic conductivity in that problem? Please verify that substituting [9] and [10] into the definition of Kv in [13] produces the expression in [14].

[11] $-\bar{q} \cdot \Delta x / Ks = Kv \cdot (\Delta x - \Delta\psi)$

[12] $$-\frac{1}{Ks}\int q\,dx = \int kr(x)\,dx - \int kr(\psi)\,d\psi$$

[13] $$\bar{q} = \frac{1}{\Delta x}\int q\,dx \Rightarrow Kv = \frac{\int kr(x)\,dx - \int kr(\psi)\,d\psi}{\Delta x - \Delta\psi}$$

[14] $$Kv = \frac{u \cdot \left(kr2 - kr1 \cdot e^{-u}\right)}{\left(1 - e^{-u}\right) \cdot \left(u - \ln(kr1 / kr2)\right)}$$, $u = \eta \cdot \Delta x$

Since Kv is derived from the analytic solution to the steady-state problem in equation [8], it is called a Darcian mean. Do you see that this approach depends intimately on the pressure-

~~5~~
7

conductivity relation, kr(ψ), in [9]? Please verify that as kr1 goes to kr2, Kv goes to Kv = kr1 = kr2, that as Δx goes to zero, Kv goes to (kr1-kr2)/ln(kr1/kr2) and that as Δx goes to +infinity, Kv goes to kr2. Note that the first limit perfectly predicts that when ψ0 = ψ2 in the case of pure gravity flow, that ψ0 = ψ1 = ψ2.

Let Kv be expressed as a function Kv(kr1,kr2,Δx). Referring to the problem in Figure 1 and equations [3] and [4], let Km = Kv(kr0,kr2,2·Δx), kml = Kv(kr0,kr1,Δx) and kmu = Kv(kr1,kr2,Δx). The result, using the exponential conductivity relation in [9] is shown in Table 2. {Note: The exponential conductivity relation in [9] is used here instead of the Brooks-Corey relation in [6] because there is as yet no explicit analytic solution for Kv with [6]. But the results of using the arithmetic mean with an exponential kr(ψ) are much the same character as in Table 1.} In every row of Table 2, the min-max principle is preserved and equation [4] is balanced. Is it not apparent that the Darcian mean represents not just the estimate of the mean necessary to solve the problem in Figure 1, given the conductivity relation in [9], but the true mean that perfectly satisfies Darcy's law in this case?

Table 2: Solutions to Figure 1 with a Darcian Mean

The variables η, Δx, ψ0, ψ1 and ψ2 are as described above. The variable, ψ1, is determined by the solution to equation [5], kr1=kr(y1) = exp(η·(ψd-ψ1)), kml = Kv(kr0,kr1,Δx), kmu = Kv(kr1,kr2,Δx), Km = Kv(kr0,kr2,2·Δx) and the mean of means is 2·kml·kmu/(kml+kmu), the right-hand-side of equation [4]. The ψ1 column tests conformity to the min-max principle, that ψ1 is included in the range [ψ0,ψ2]. The last two columns on the right test the balance of equation [4]. In each case, the min-max principle and Darcy's law are perfectly preserved.

	η	**Δx (m)**	**ψ0 (m)**	**y1 (m)**	**y2 (m)**	**kr1**	**kml**	**kmu**	**Km**	**mean of means rhs of [4]**
1	2.1	0.80422	0.5	0.87887	1	0.1868	0.2259	0.1594	0.1964	0.1964
2	4.0	0.56667	0.5	0.88249	1	0.0404	0.0722	0.0296	0.0420	0.0420
3	8.1	0.001	0.5	0.58392	1	0.0169	0.0242	0.0048	0.0080	0.0080
4	8.1	0.01	0.5	0.58836	1	0.0163	0.0237	0.0046	0.0077	0.0077
5	8.1	0.1	0.5	0.64069	1	0.0107	0.0184	0.0029	0.0050	0.0050
6	8.1	0.5	0.5	0.91656	1	0.0011	0.0034	6.8e-4	0.0011	0.0011
7	8.1	0.50366	0.5	0.91831	1	0.0011	0.0034	6.8e-4	0.0011	0.0011
8	8.1	1	0.5	0.99790	1	5.9e-4	0.0012	5.8e-4	7.7e-4	7.7e-4
9	8.1	2	0.5	0.999··	1	5.8e-4	7.7e-4	5.8e-4	6.6e-4	6.6e-4

If you do not agree, please offer the proof, consisting of a set of conditions and numerical values for which Kv either violates the min-max principle or Darcy's law using [3] and [4]. Please explain under what valid scientific principle the YMP modelers at the DOE Lawrence Berkeley National Laboratory may claim that this approach to calculating intergrid hydraulic conductivity means is not physically based and cannot be valid in the gravity flow case where ψ0 = ψ1 = ψ2. Please extend that argument to explain why one cannot take any other conductivity relation, such as [6], solve the elliptic boundary value problem [8] numerically, and thus obtain kr(x) and a valid numerical value for Kv. Is it not apparent that this approach for develops Darcian means for steady-state flow? If you disagree, can you demonstrate that it will produce a worse answers in numerical transient flow models than commonly-used means, such as the arithmetic mean, that do not account for kr(ψ) or Δx, and occasionally violate the min-max principle?

In the finite method expression [15] of Richards' equation for unsaturated flow in a homogeneous medium, modelers sometimes make separate calculations for the intergrid hydraulic conductivity means for gravity (advective), Kx, and capillary (diffusive) flow, Kψ. This may be justified by using [13], as in [16], redefining the integrals as the respective mean conductivities, Kx and Kψ, over Δx and Δψ [17]. But notice that in general it is difficult, if not impossible, to know the spatial distribution, kr(x), between grid points in a transient flow problem. It is common to calculate the integral that defines Kψ, but to substitute a much simpler mean, such as the arithmetic mean, for Kx. Notice the effect that such a substitution in [16] has on the mathematically equivalent [15], since Kv can now be defined as in [18]. Near hydrostatic conditions, Δx goes to Δψ, and Kv in [18] suffers from division by zero, producing a singularity with limits at ±infinity, if Kx and Kψ are not perfectly related through the derivations of Darcian means presented here. Can you certify that you do not use any such method in your models? If you do, can you provide mathematical proof that the errors generated by the singularity are not significant in every case?

[15] $\theta_i^{j+1} = \theta_i^j + r \cdot \left[Kv_{i+1/2} \cdot \left(H_{i+1} - H_i \right) - Kv_{i-1/2} \cdot \left(H_i - H_{i-1} \right) \right],\ r = Ks \cdot \Delta t / \Delta x^2$

[16]

$$\theta_i^{j+1} = \theta_i^j + r \cdot \left[\left.\frac{Kx\Delta x - K\psi\Delta\psi}{\Delta x - \Delta\psi}\right|_{i+1/2} \left.(\Delta x - \Delta\psi)\right|_{i+1/2} - \left.\frac{Kx\Delta x - K\psi\Delta\psi}{\Delta x - \Delta\psi}\right|_{i-1/2} \left.(\Delta x - \Delta\psi)\right|_{i-1/2} \right]$$

$$= \theta_i^j + \frac{\Delta t \cdot Ks}{\Delta x}\left(Kx_{i+1/2} - Kx_{i-1/2}\right) - r \cdot \left[K\psi_{i+1/2} \cdot \left(\psi_{i+1} - \psi_i\right) - K\psi_{i-1/2} \cdot \left(\psi_i - \psi_{i-1}\right) \right]$$

[17] $Kx = \frac{1}{\Delta x} \cdot \int kr(x)\,dx\ ,\ K\psi = \frac{1}{\Delta\psi} \cdot \int kr(\psi)\,d\psi$

[18] $Kv = \frac{Kx \cdot \Delta x - K\psi \cdot \Delta\psi}{\Delta x - \Delta\psi}$

What is the difference between determining that an error is tolerable and denying that it even exists? Is it logical and legitimate to say that a "carefully designed grid system" eliminates an error that one claims does not exist? Is it possible that carefully accounting for all the errors is a prerequisite for designing a grid system? And finally, if one scientist has a calculator, and another can show that for even one case the calculator gives back 2.5 for 1+1, which scientist has the responsibility to demonstrate the practical usefulness and validity of the calculator in all cases?

Appendix: Numerical Examples - Parallel Models of a Relaxing Wet Pulse Using the Arithmetic and Darcian Means (excerpts from a paper in progress)

Now consider a numerical experiment for a long, vertical, homogeneous fracture described by pressure-conductivity relation [9] and the pressure-saturation relation [19], using parameters, Ks = 0.00474 m/s, η = 6.4 (1/m), ψd = 0.08 m, θs = 1, θr = 0.0395 and β = 0.64 (1/m). These conductivity parameters very crudely model an average fracture in Topopah Spring welded volcanic tuff (Schenker, et al., 1995), with the saturation parameters chosen simply and arbitrarly to keep count of mass balance. A fracture of depth, xl = 512 m, is modeled with a finite difference form of the Richards' unsaturated flow equation [15], using the modified Picard method (Celia, et al., 1990) with an adaptive time step (Baker, et al., 1998). In this case, just to make x equal to depth, x will be positive downwards. The upper boundary will be a matric suction (2.95823 m) such that kr = 10^{-8}. The lower boundary is no-flow and set up such that the depth, xl, is constant no matter how many grid points, 0 to np, in the model.

[19] $\frac{\theta-\theta_r}{\theta_s-\theta_r}=\begin{cases}1 & ,\psi\le\psi_d\\ \exp(\beta\cdot(\psi_d-\psi)) & ,\psi>\psi_d\end{cases}$, where θ = volumetric water content (m^3/m^3, effectively dimensionless) θr = residual water content, θs = saturated water content, and β and ψd are fitting parameters

The initial condition of all the grid points in the model will be a matric suction such that kr = 10^{-8}, except for the points from 0.35*xl to 0.45*xl, which shall be set to a positive pressure head of 1 m (ψ = -1 m). The number of points, np, in model will be an even multiple of 10, such as, 40, 60, 100, 140, 200, 280, 400, giving space steps of Δx = 12.8, 8.533, 5.12, 3.657, 2.56 1.829 and 1.28 m for xl = 512 m. {Note: The same errors occur in smaller reaches, but the large-scale plots make the dispersive nature of some oscillations more apparent.}

Because the mass inflow and outflow at the boundaries of this experiment will be orders of magnitude smaller than the mass flow in the interior, the relative global mass balance, as defined by Celia, et al., will not be used. Instead, each time step will be calculated to converge to an error, rmb, in the equivalent depth of water of 10^{-10} m. The error, rmb = sumth - flx, where sumth = $\frac{\Delta x}{2}\cdot\sum_{i=1}^{np}\left(\theta_{i-1}^{j+1}-\theta_{i-1}^{j}+\theta_i^{j+1}-\theta_i^{j}\right)$ is the trapezoidal integral of the mass change in the model during one time step, and flx = $-Km_{1/2}$*(H1-H0)*Δt/Δx is the mass flow into the upper boundary of the model in one time step. $Km_{1/2}$ is the intergrid hydraulic conductivity mean between the x0 = 0 upper boundary and the first grid point at x1 = Δx.

In this case, two models will be run in parallel for comparison. One uses the arithmetic mean, Ka, for the intergrid conductivity mean. The other uses the Darcian mean in [14], Kv. The model using the Darcian mean will be set to adjust the time steps so that it converges to rmb < 10^{-10} m in 40 iterations or less. The model using the arithmetic mean will use exactly the same time steps, but will be allowed to converge in 80 iterations or less. If the either model does not converge in the alloted number of iterations, then the time step is reset and reduced, and both models are rerun for that time step. If the Darcian mean model converges in less than 40 iterations, the time step is increased slightly. The maximum time step is limited to $5(10^5)$ s. In this way, any difference between the two models involving time step as well as space step discretization error is removed. Both are equally affected.

Figure 2a shows the results for the arithmetic mean model for np = 40, Δx = 12.8 m, at t = 0, 10, $0.512(10^6)$, $1.024(10^6)$, $2.048(10^6)$ and $4.096(10^6)$ s. Figure 2b shows the results in the same run for the Darcian mean model. Note the different vertical scales, necessary due to radically different responses. This is the model of an initial-condition pressure pulse that should be both relaxing and drifting downwards in the fracture. In the first ten seconds, the arithmetic mean model produces excess negative matric suction (positive pressure) heads that are non-physical.

The Darcian mean model, by contrast, relaxes completely to the just under saturation near a matric suction of 0.08 m, with no apparent change in pulse shape.

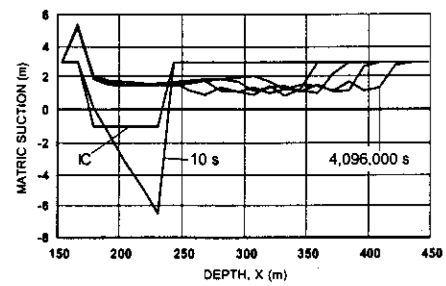

Figure 2a: Arithmetic Mean Model
Initial pulse of y = -1 m between 0.35xl and 0.45xl, relaxing and translating with time, for np = 40 at t = 0, 10, $0.512(10^6)$, $1.024(10^6)$, $2.048(10^6)$ and $4.096(10^6)$ s, in the example fracture

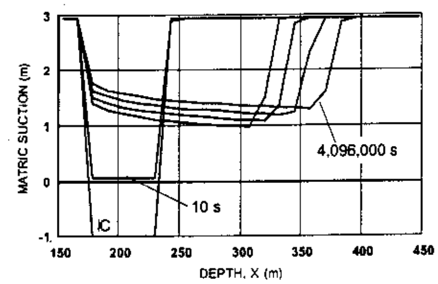

Figure 2b: Darcian Mean Model
for np = 40 running in parallel with the same time steps in the same fracture and the same output times.

As the models progress, the arithmetic mean model develops a persistent non-physical spike in matric suction at the top edge of the pulse (left on graph). This is a direct result of violation of the min-max principle, as demonstrated in the three-point grid test in the questions above. The arithmetic mean model also develops severe oscillations in the peak of the pulse, producing many non-physical peaks that are consistent with the concept of mass clumping due to a differential error in hydraulic conductivity between wet-over-dry and dry-over-wet conditions. By contrast, the Darcian mean model is very smooth and well-behaved.

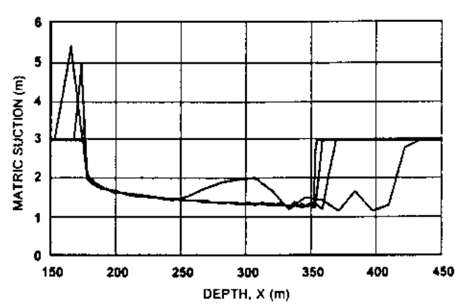

Figure 3a: Arithmetic Mean Model
Convergence to the fine-grid solution, for np = 40, 100, 200 and 400, or Δx = 12.8, 5.12, 2.56 and 1.28 m.

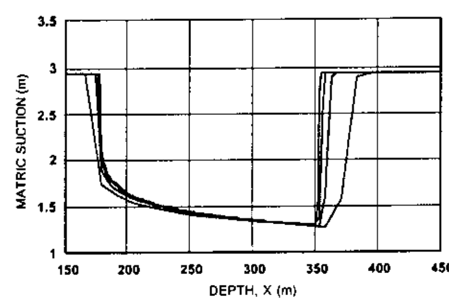

Figure 3b: Darcian Mean Model
Convergence to the fine-grid solution, for np = 40, 100, 200 and 400, or Δx = 12.8, 5.12, 2.56 and 1.28 m. Parallel time step run with Arithmetic mean model.

9

Figures 3a and b show the convergence of the arithmetic mean and Darcian mean models for np = 40, 100, 200 and 400, or Δx = 12.8, 5.12, 2.56 and 1.28 m, at t = 4.096(10^6)s. As step size goes down, the trailing edge suction spike and the leading edge oscillations in the arithmetic mean model decrease. Both models converge to the same fine-grid solution, but the Darcian mean model shows superior error and stability characteristics.

Non-Darcian flow errors are not apparent in this example for vertical space step sizes below where the arithmetic mean actually violates the min-max principle. But in another example (Baker, 1999b), of infiltration into a fracture to less then 1 cm, with space steps from 1.5 mm to 21 μm, and an adaptive grid set to maintain a constant ratio between adjacent grid conductivities, using the arithmetic mean produced errors in the wetting front position of up to 18.75%, compared to 0.36% for an approximate Darcian mean. It may be that non-Darcian flow errors are tolerable in many cases, but this cannot be certified unless they are actually accounted.

The oscillations in the leading edge of the pulse in the arithmetic mean model are reminiscent of numerical dispersion in hyperbolic systems. But classical numerical dispersion is created by the differing speeds of propagation of different frequency components of the pulse. Here the differing speeds of propagation are generated directly by errors in the intergrid conductivity mean, and depend as well on the slope of the pulse. This kind of oscillation has been seen previously in fracture flow infiltration using a van-Genuchten-style conductivity relation in Baker, et al. (1999a).

Figure 4 shows how the matric suction spike evolves as a function of time and model vertical space step size, Δx. The trend, out to 83,886,100 s in model time, is for the non-physical spike to increase logarithmically in time, once it starts to develop. The plot for np = 40, Δx = 12.8 m, is atypical, possibly because of increasing space step discretization error. Note that the plots for 1.829 and 2.56 m start to decrease before rising above the initial conditions behind the pulse. The reasons for delayed onset and the apparent logarithmic increase of the dry spike are not fully understood at this time.

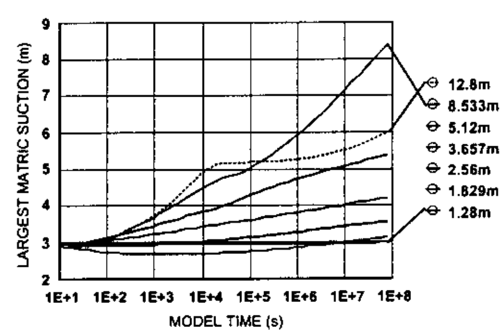

Figure 4: Trailing Edge Matric Suction Spike
for arithmetic mean model for np = 40, 60, 100, 140, 200, 280 and 400, Δx = 12.8 to 1.28m; The grid point with the largest spike value at t = 8.39(10^8) s is tracked from t = 10 to 8.39(10^8) s.

Although it does not show well, note that even for np = 400, Δx = 1.28 m, the grid point at the trailing edge of the initial pulse rises from the initial condition of 2.95823 m to 2.99623 m at the end of the run. There is no physical reason for it to do so; the gravity flow into the fracture is the same as in the fracture to the top edge of the relaxing pulse. If the pulse were diffusing upwards, the trend would be in the opposite direction. If the pulse had reached the no-flow lower boundary and the fracture were filling with water, due to the upper boundary inflow of $4.74(10^{-10})$ m/s, the trend would be in the opposite direction. The model end time is about 2.63 years, and the non-physical spike for the $\Delta x = 1.28$ m case is just beginning to show. This does not bode well for models that use the arithmetic mean, or any other significantly non-Darcian mean in violation of the min-max principle, to predict flow over scales of thousands of years.

References

Baker, D.L., M.E. Arnold and H.D. Scott, 1998. Some comparisons of new time steps for mass-conservative infiltration models, not yet published, draft available at: http://www.aquarien.com.

Baker, D.L., M.E. Arnold and H.D. Scott. 1999a. Some analytical and approximate Darcian means, GROUND WATER, v.37, no.4, pp. 532-538.

Baker, D.L. 1999b. Some methods to examine the validity of Darcian means, submitted to Journal of Hydrology, 1999, draft available at http://www.aquarien.com.

Celia, M.A., E.T. Bouloutas and R.L. Zarba. 1990. A general mass-conservative numerical solution for the unsaturated flow equation. Water Resources Research 26 (7), 1483-1496.

DuChateau, P. and D.W. Zachmann. 1986. Schaum's Outline of Theory and Problems of Partial Differential Equations. McGraw-Hill, New York, 241p, ISBN 0-07-017897-6.

Schenker, A.R., D.C. Guerin, T.H. Robey, C.A. Rautman and R.W. Bernard. 1995. Stochastic hydrogeological units and hydrogeologic properties development for total-system performance assessments, Sandia Report SAND94-0244 * UC-814, Prepared by Sandia National Laboratories, Albuquerque NM 87185 and Livermore CA 84550 for the United States Department of Energy under Contract DE-AC04-94AL85000, 87p + appendices.

H
13