## Review of Comments by Dr. D.L. Baker Regarding Calculation of Darcian Interblock Conductivity Means in Vertical Unsaturated Water Flow

by

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### Introduction

The purpose of this review is to consider comments made to U.S. Nuclear Regulatory Commission (NRC) staff by Dr. Donald Baker, of Aquarius Engineering, concerning the approach used by the U.S. Department of Energy (DOE) for calculating inter-grid-block hydraulic conductivity in the unsaturated flow model used for performance evaluations of the proposed nuclear waste repository at Yucca Mountain. A brief background of Dr. Baker's concern is first given, followed by a discussion of interblock relative conductivity calculation methods, conclusions and recommendations.

### Background

Most of the following background discussion is based on information provided on CD-ROM by Dr. Baker;[1] much of the same information contained on the CD-ROM is currently available on the Aquarius Engineering Internet site.[2]

In 1997, Dr. Baker was awarded a DOE Phase I Small Business Innovation Research contract, DE–FG02–97ER82329. With this funding, Dr. Baker developed a mathematical and modeling framework for calculating interblock hydraulic conductivity means for vertical unsaturated water flow. In his report to DOE, Baker (1998) described an approach for calculating what he referred to as Darcian mean flows between grid cells. Baker (1998) also concluded that "common standard methods of calculating vertical, unsaturated, single-phase flow between model grid cells can produce predicted flow in error up to six orders of magnitude, in the wrong directions, or with effectively misplaced hydrostatic conditions." Such a conclusion calls into question the appropriateness of the DOE unsaturated flow model for Yucca Mountain, which uses the "common standard" upwind weighting method for calculation of interblock hydraulic conductivity.

Dr. Baker's concerns were related to DOE and reviewed by Liu and Bodvarsson (1999), who concluded the following:

1. "There is no physical reasoning to support that Dr. Baker's Darcian mean approach is more rigorous than any of the commonly used schemes in general cases."

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[1]D. Baker. Letter to U.S. Nuclear Regulatory Commission, dated September 23, 1998, with an attached CD-ROM entitled "Capabilities in Developing Leading Edge Numerical Modeling."

[2]Internet site http://www.aquarien.com accessed December 19, 2002.

2. "It is misleading to only compare Darcian mean approaches with hydraulic conductivities at grid cell interfaces, in two-node systems with fixed capillary pressures at the nodes, in order to evaluate prediction errors for water flow."

3. "Significant differences between Darcian means and hydraulic conductivities calculated from commonly used schemes occur only when the capillary pressures (or relative hydraulic conductivities) at two nodes are very different (e.g., many orders of magnitude). This extreme condition is unlikely to occur in simulations with carefully designed grid systems."

In an April 15, 1999, letter[3] to NRC, Dr. Baker responded to Liu and Bodvarsson (1999), and persisted in his claim that his work "makes a lot of the models used to characterize Yucca Mountain and other nuclear waste suspect." In that same letter, Dr. Baker inquired whether NRC would be willing to support an unsolicited proposal to continue his work on the Darcian mean approach, or to provide a statement that the work needs to be done that could be included in a proposal to the National Science Foundation. While NRC offered no support, staff did take note of Dr. Baker's concerns.

In June 1999, Dr. Baker submitted written comments to public meetings of the Advisory Committee on Nuclear Waste, and the Nuclear Waste Technical Review Board. These written comments basically provided a summary of the Darcian mean approach and rebutted the review by Liu and Bodvarsson (1999).

In a May 2002 email message,[4] Dr. Baker advised NRC staff that 585 PowerPoint tutorial slides on the Darcian mean approach were available on the Aquarius Engineering Internet site (www.aquarien.com), and that these slides answered criticisms of his previous work by Liu and Bodvarsson (1999). Dr. Baker further indicated his belief that the "modeling gurus for Yucca Mountain" had unfairly criticized his work with "bad math and science," and he requested that his concern be included as a comment in an NRC public meeting.

To address Dr. Baker's concerns, a review of his Darcian mean approach is provided in the following sections, and an evaluation is made to assess whether his conclusions indicate potential problems with the modeling approach used by DOE for the Yucca Mountain site. Although all of the aforementioned references were reviewed, particular attention was paid to an article by Baker, et al. (1999) that was published in the journal *Ground Water*, which is the most recent peer-reviewed and published version of his work on Darcian means.

**Calculation of Interblock Relative Conductivity in Unsaturated Zone Numerical Flow Models**

At issue is the calculation of interblock relative conductivity in finite-difference models of infiltration. Infiltration is typically described by Richards equation, but the calculation of interblock conductivity is a generic step in obtaining numerical solutions to partial differential

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[3]D. Baker. Letter to D. Brooks, U.S. Nuclear Regulatory Commission, April 15, 1999.

[4]D. Baker. Email message to N. Coleman, U.S. Nuclear Regulatory Commission, May 15, 2002.

equation that describe the evolution of a conserved quantity (mass, energy, etc.). In one-dimension, Richards equation is written

$$\frac{\partial \theta}{\partial t} = -\frac{\partial q}{\partial z}$$

$$q = -K_s k_r \frac{\partial}{\partial z}[z + h]$$

where $t$ is time, $z$ is vertical elevation, $\theta$ is the volumetric water content, $K_s$ the saturated conductivity, $k_r$ the relative conductivity, and $h$ is pressure head. Constitutive relationships are used to relate $h$ and $\theta$, and to define $k_r$ as a function of the dependent variable ($\theta$ or $h$). In a finite-difference approximation to Richards equation, the flux across the interface between two model nodes is calculated from Darcy's law as

$$q_{12} = \overline{K}[z_2 - z_1 + h_2 - h_1]$$

where the subscripts 1 and 2 denotes properties at center of model cells 1 and 2, and the symbol $\overline{K}$ is the interblock (total) conductivity, which must be related to quantities that are defined at cell centers. Specifically, the interblock conductivity needs to be related to the block saturated conductivities defined at blocks 1 and 2 ($K_{s1}$ and $K_{s2}$, respectively), which are properties of the medium, and to the relative conductivities defined at block centers ($k_{r1}$ and $k_{r2}$), which depend on the medium and the local saturation conditions. There are many ways to combine $K_{s1}$ and $K_{s2}$ and $k_{r1}$ and $k_{r2}$ to obtain $\overline{K}$ (e.g. Aziz and Settari, 1979). These are often referred to as conductivity weighting schemes.

It is useful and customary to write the $\overline{K}$ as a product $\overline{K} = \overline{K}_S\ \overline{k}_r$, where $\overline{K}_S$ is the interblock saturated conductivity, and $\overline{k}_r$ is the interblock relative conductivity. Baker restricts his attention to the situation where $K_S$ is constant and only deals with the calculation of the interblock relative conductivity $\overline{k}_r$. The following focuses on the calculation of the interblock relative conductivity.

The DOE unsaturated zone models use different weighting schemes for $\overline{K}_S$ and $\overline{k}_r$. Specifically, $\overline{K}_S$ is defined by harmonic averaging cell values for $K_{s1}$ and $K_{s2}$, whereas $\overline{k}_r$ is defined by upwind weighting using the following criteria:

$$\overline{k}_r = k_{r1} \quad \text{if flow is from node 1 to node 2}$$
$$\overline{k}_r = k_{r2} \quad \text{if flow is from node 2 to node 1}$$

This approach is standard in applications such as petroleum reservoir simulation (Aziz and Settari, 1979) and in geothermal modeling (Pruess, 1991), as well as in hydrologic modeling. The upwind weighting method is also used in DOE thermal hydrological and thermal hydrological chemical modeling. Independent computer codes, such as MULTIFLO (Lichtner, 1996; Painter, et al., 2001), developed for NRC also employ the upwind weighting scheme.

Building on earlier work of Warrick (1991), Baker (1998) developed weighting schemes for interblock relative conductivity. The first, the so-called Darcian mean, requires solution to a partial differential equation at each time step, a procedure that is feasible for research purposes but which may be impractical to implement in a production model because of large computational requirements. When $k_r$ is of the exponential form, the Darcian mean has an analytical solution, which is more practical to implement. For more realistic versions of $k_r$, no explicit analytical result is known. However, Baker (1998, 1999) developed an approximate version appropriate when $k_r$ follows the Brooks-Corey model. He called this the piecewise Brooks-Corey Darcian. The resulting weighting scheme is a highly non-linear combination of the $k_{r1}$ and $k_{r2}$ variables, but tends to weight the upwind value heavily, similar to the first-order upwind weighting. The method does perform well in numerical tests.

To test the accuracy of conventional weighting schemes, Baker (1999) fixes relative conductivity at two nodes and shows that approximating the interblock conductivity with the arithmetic mean results in large errors when there is large contrast between $k_{r1}$ and $k_{r2}$. This comparison can be highly misleading, however, for the following three reasons. First, it is not very informative to fix relative conductivity and solve for flux without also imposing mass conservation. In practice, the interblock conductivity models are integrated into finite difference solutions to mass conservation equations, and a more useful comparison is to actually solve Richards equation with different assumptions about the interblock conductivities. Second, the arithmetic (and presumably other) approximations to the interblock relative conductivities are poor approximations only when there is large contrast in relative conductivity between nodes. In systems with homogeneous rock properties, the focus of Baker's work, arbitrarily large changes in relative conductivity between successive grid nodes can always be eliminated by grid refinement; indeed, a properly implemented finite difference grid would not contain such large contrasts in saturation and thus $k_r$. The Darcian mean concept applies to homogeneous systems, and is thus not an option for systems with heterogeneous rock properties, which may support large changes in $k_r$. Finally, the comparison of methods made by Baker focuses on the arithmetic mean values of $k_r$ and does not consider the upwind weighting method, the standard approach for these types of problems and the method used primarily by DOE in their unsaturated zone modeling efforts.

Baker also solves Richards equation using the arithmetic mean and the Brooks-Corey Darcian mean to approximate interblock conductivities, and compares the results. The arithmetic mean correctly reproduces the analytical result when the grid is fine, but causes non-physical oscillations when the grid spacing is greater than a critical size. Such oscillations are well-known numerical artifacts of applying central difference schemes on coarse grids, and are the primary motivation for the broad adoption of upwind weighting schemes. The Brooks-Corey Darcian result does not suffer these oscillations, but does cause broadening of the sharp wetting front for coarse grids, similar to the first-order upwind scheme. No comparisons with the upwind scheme were shown by Baker, et al. (1999), but they do note that the upwind scheme performed similarly to the Brooks-Corey Darcian, producing an error about twice that of the Brooks-Corey Darcian. Given the fact that the Brooks-Corey Darcian requires considerably more floating point operations at each time step due to its non-linear nature, a factor-of-two reduction in error is not significant.

The Brooks-Corey Darcian applied to a vertical infiltration problem is a special case of a higher-order upwind scheme. More conventional higher-order methods (e.g., Leonard, 1979, 1984) have been widely used to solve similar types of conservation equations, and are able to track sharp fronts with high accuracy. However, we are not aware of efforts to use these to solve Richards equation.

**Discussion**

The approaches proposed by Baker appear to be physically and mathematically correct for one-dimensional, single-phase infiltration in single-continuum homogeneous media. However, the method does not appear to offer a significant improvement over the methods used by DOE for unsaturated zone flow modeling for the following reasons:

1. Upwind weighting, the primary method used by DOE, appears to be adequate provided the computational grid is properly refined. Calculations by Baker, et al. (1999) confirm this for vertical infiltration problems, as does general experience within the computational science community on similar types of flux conservation equations.

2. The unsaturated flow fields used to calculate radionuclide transport in DOE performance assessments are steady-state. Steady-state simulations are less susceptible to numerical artifacts as compared with transient simulations, the focus of Baker's work.

3. For the same grid size, the Brooks-Corey Darcian method offers only a modest reduction in error over the first-order upwind method. Given the additional computational burden imposed by the use of the non-linear Brooks-Corey Darcian method, it is not clear that the method offers any improvement in computational efficiency when compared on the basis of floating point operations.

4. The methods based on Darcian mean are not developed for dual-continuum systems, for systems with higher dimensionality, or for systems with heterogeneity in the saturated hydraulic conductivity.

**Conclusions and Recommendation**

There is no evidence to suggest that the conductivity weighting methods used by DOE are producing inaccurate results. The methods are consistent with standard practice in the computational science community and should produce physically correct results provided that care is taken in designing computational grids.

The methods proposed by Baker are not sufficiently developed for use in a heterogeneous dual-permeability, multi-dimensional model. Moreover, they do not appear to offer any significant improvement in computational efficiency compared to standard first-order upwind weighting.

Staff recommend no further action.

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