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APPROXIMATING THE IMBIBITION AND ABSORPTION BEHAVIOR OF A DISTRIBUTION OF MATRIX BLOCKS BY AN EQUIVALENT SPHERICAL BLOCK

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ABSTRACT

A theoretical study is presented of the effect of matrix block shape and matrix block size distribution on liquid imbibition and solute absorption in a fractured rock mass. It is shown that the behavior of an individual irregularly-shaped matrix block can be modeled with reasonable accuracy by using the results for a spherical matrix block, if one uses an effective radius $\tilde{a} = 3V/A$, where V is the volume of the block and A is its surface area. In the early-time regime of matrix imbibition, it is shown that a collection of blocks of different sizes can be modeled by a single equivalent block, with an equivalent radius of $\langle a^{-1} \rangle^{-1}$, where the average is taken on a volumetrically-weighted basis. In an intermediate time regime, it is shown for the case where the radii are normally distributed that the equivalent radius is reasonably well approximated by the mean radius $\langle a \rangle$. In the long-time limit, where no equivalent radius can be rigorously defined, an asymptotic expression is derived for the cumulative diffusion as a function of the mean and the standard deviation of the radius distribution function.

INTRODUCTION

Yucca Mountain, Nevada, is the potential site of an underground high-level radioactive waste repository. The potential repository horizon is located above the water table, in a formation consisting of highly fractured volcanic tuff. Characterization of the hydrological behavior of the unsaturated zone at Yucca Mountain will require numerical simulation of transient infiltration processes in a fractured rock mass. Modeling of the performance of the repository after waste emplacement will require simulation of radionuclide transport in fractured rock. Both processes involve flow through a fracture network, with slow diffusion into matrix blocks. For quasi-steady-state processes that occur on a sufficiently slow time scale, it is often assumed that the fractured rock mass can be treated as an equivalent homogeneous porous medium.[1] For transient processes, such as infiltration of rainwater into the mountain, or the spread of radionuclides from a leaking waste canister, the "dual-porosity" nature of the medium must be accounted for. In a dual-porosity medium, the fractures provide most of the transmissivity of the rock mass, whereas most of the fluid storage takes place in the relatively impermeable matrix blocks.[2] An important parameter in a dual-porosity system is the characteristic length of the matrix blocks, which determines the time scale for which matrix effects are (or are not) important.[3,4] In this paper, we study two aspects of the effect of block geometry on matrix diffusion: finding the appropriate characteristic length for a matrix block, and finding an equivalent block size that can be used to represent a collection of matrix blocks of different sizes.

EQUIVALENT RADIUS OF A NON-SPHERICAL MATRIX BLOCK

The matrix blocks in the fractured units at Yucca Mountain are the regions of rock material that are formed by the sets of intersecting fractures. Since fractures are typically planar features, the matrix blocks will often be shaped like polyhedra. For example, parallel, orthogonal sets of fractures will give rise to matrix blocks that are parallelepipeds. The rate of imbibition of water into an unsaturated matrix block, or the rate of solute diffusion into a matrix block, will depend on both the size and shape of the block. Both processes are governed by diffusion-type equations, although for unsaturated rocks the "diffusion coefficient" is typically saturation-dependent, and not equal to a constant.[5-7] However, it is known that the imbibition of water into unsaturated matrix blocks behaves much like a constant-diffusivity process, with an "effective diffusivity" that depends on the initial saturation of the block, as well as on its hydrological properties. Hence, imbibition has often been modeled by a diffusion equation with a constant diffusivity.[8,9] Although this simplification is not strictly correct, it is a reasonable approximation. Using this approximation, the following equation will govern imbibition or drainage of water, or solute diffusion, into a matrix block:

$$\nabla^2 \theta(\mathbf{x}, t) = \frac{1}{D}\frac{\partial \theta}{\partial t}, \tag{1}$$

where $\mathbf{x}$ is the position vector of a generic point in the block, D is the diffusivity, and θ is the water content (or the solute concentration). The boundary and initial conditions are

$$\theta(\mathbf{x}, t=0) = \theta_i, \tag{2}$$

$$\theta(\mathbf{x} \in \Gamma, t>0) = 0, \tag{3}$$

where Γ denotes the outer boundary of the block. Note that if the diffusion process is mathematically linear, we can always redefine the dependent variable θ such that the boundary condition (3) is zero. Therefore, although the problem stated in eqs. (1-3) represents drainage of a block, it is mathematically equivalent to imbibition, and no distinction will be made in the remainder of the paper.

For processes that are governed by a linear diffusion equation, the diffusion rate is controlled by the diffusivity of the rock matrix, and by the geometric properties of the block. However, the specific geometric properties that control the diffusion rate at early times are not the same properties that control diffusion at late times. At early times, diffusion proceeds inward from the entire outer boundary of the block in a one-dimensional manner, without any regard for the local curvature of the surface. It is clear that this will be true at sufficiently small times;[10] furthermore, it can be demonstrated explicitly, for example, for a sphere, by comparing the small-time solution for diffusion into a sphere with the solution for diffusion into a half-space.[11] Hence, at small times the flux out of the block will be proportional to the outer surface area of the block, A, whereas the gross geometrical shape of the block will be irrelevant:[11]

$$q \approx \theta_i A \sqrt{D/\pi t}\,. \tag{4}$$

Eventually, when the diffusion process is complete, the total cumulative flux out of the block must be equal to the product of the block volume and the initial water content, i.e., $\theta_i V$. Hence, at small times, the *normalized* flux out of the block will be given by

$$q/V \approx (A/V)\sqrt{D/\pi t}\,. \tag{5}$$

The parameter $\tilde{a} = 3V/A$, which has dimensions of [length], can therefore be identified as a length scale for early-time diffusion; the factor 3 is included so that $\tilde{a}$ is equal to the radius when the block is spherical. Using $\tilde{a}$ as the length scale, the normalized flux can be expressed as

$$q/V \approx 3(D/\pi \tilde{a}^2 t)^{1/2}. \tag{6}$$

To study the imbibition rate at long times, and under quasi-steady-state conditions, we can formally analyze the solution to eqs. (1-3) in the time domain; an analogous analysis can also be carried out in the Laplace domain.[4,12] Using the method of separation of variables, we search for solutions to eq. (1) that have the form $\theta(\mathbf{x}, t) = F(\mathbf{x})G(t)$. The standard procedure[13] then leads to

$$\frac{\nabla^2 F(\mathbf{x})}{F(\mathbf{x})} = \frac{1}{D}\frac{G'(t)}{G(t)} = -\lambda, \tag{7}$$

where $'$ indicates differentiation with respect to time, and λ must be a constant that does not depend on $\mathbf{x}$ or t. The functions $F(\mathbf{x})$ therefore satisfy the equation

$$\nabla^2 F(\mathbf{x}) = -\lambda F(\mathbf{x}), \tag{8}$$

along with the boundary condition

$$F(\mathbf{x}) = 0 \quad \text{for all } \mathbf{x} \in \Gamma. \tag{9}$$

The allowable values of λ are therefore the eigenvalues of the Laplacian operator for the region occupied by the matrix block, with Dirichlet-type boundary conditions.

The eigenvalues can be found explicitly only for geometrically simple shapes, such as spheres, cylinders, cubes, etc. There will nevertheless always be an infinite set of eigenvalues λ_n, each corresponding to one or more eigenfunctions $F_n(\mathbf{x})$. For a finite-sized body, the eigenvalues will be discrete and positive, and can be labeled as $\lambda_1 < \lambda_2 < \cdots$. Although in certain cases an eigenvalue can have more than one independent eigenfunction associated with it, this possibility is of no importance for our purposes, so we ignore it. From eq. (7), we find that the time-dependent parts of the solutions are given by $G_n(t) = \exp(-\lambda_n D t)$. Hence, the general solution to eq. (1) can be written as

$$\theta(\mathbf{x}, t) = \sum_{n=1}^{\infty} C_n F_n(\mathbf{x}) e^{-\lambda_n D t}, \tag{10}$$

where the C_n are constants. The C_n are found from the initial conditions, although their precise values are not relevant to the present discussion.

The important implication of eq. (10) is that, for large times, the term involving λ_1 will dominate the series, since the other terms, corresponding to higher eigenvalues, will be exponentially smaller. The long-time behavior of the matrix block is therefore dominated by the *smallest* eigenvalue, $\lambda_1 \equiv \lambda_{min}$. These minimum eigenvalues can be found for various simple shapes from the solutions compiled in standard texts on heat conduction or diffusion.[11,14] For example, $\lambda_{min} = \pi^2/a^2$ for a sphere of radius a; $\lambda_{min} = \pi^2/L^2$ for a thin sheet of thickness L; $\lambda_{min} = 3\pi^2/L^2$ for a cubical block of length L; and $\lambda_{min} = z_1^2/a^2$ for a long cylinder of radius a, where $z_1 = 2.405$ is the first positive root of the Bessel function $J_o(z)$. For more general block shapes, the minimum eigenvalue λ_{min} cannot be found explicitly, and so it would be useful to be able to estimate λ_{min} by some approximate rule-of-thumb. We know that at small times, the characteristic length is given by $\tilde{a} = 3V/A$. It would be convenient to be able to use this same parameter to quantify the long-time behavior of the diffusion process. For a spherical block of radius a, $\lambda_{min} = \pi^2/a^2$, and $3V/A = a$, so λ_{min} can also be expressed as

$$\lambda_{min} = \frac{\pi^2}{(3V/A)^2} = \frac{\pi^2}{\tilde{a}^2}. \tag{11}$$

The question now arises as to what extent eq. (11) can be used as an approximation to λ_{min} for blocks of non-spherical shape. Although we cannot test this approximation for arbitrarily-shaped polyhedra, we can test it for blocks that are shaped like rectangular parallelepipeds, which will be the case if the fracture sets are orthogonal. For these shapes, the exact result is[14]

$$\lambda_{min}^{exact} = \pi^2 \left[\frac{1}{L_1^2} + \frac{1}{L_2^2} + \frac{1}{L_3^2} \right], \tag{12}$$

where L_1, L_2, and L_3 are the lengths of the three sides of the matrix block. The volume of the matrix block is $L_1L_2L_3$, and its outer surface area is $2(L_1L_2+L_2L_3+L_3L_1)$, so the approximation given by eq. (11) yields

$$\lambda_{min}^{apprx} = \frac{4\pi^2}{9} \left[\frac{1}{L_1} + \frac{1}{L_2} + \frac{1}{L_3} \right]^2. \tag{13}$$

The ratio of the approximate value of λ_{min} to the exact value is

$$\frac{\lambda_{min}^{apprx}}{\lambda_{min}^{exact}} = \frac{4(L_1L_2+L_2L_3+L_3L_1)^2}{9[(L_1L_2)^2+(L_2L_3)^2+(L_3L_1)^2]}. \tag{14}$$

The ratio in eq. (14) takes on maximum or minimum values when the ratios of the lengths take on their limiting values, i.e., $L_1 = L_2 \gg L_3$, etc. Table 1 summarizes these extreme cases, along with one arbitrarily chosen example. The table shows that the approximation (11) is reasonably accurate, in the sense that in no case does it grossly underpredict or overpredict the value of λ_{min}. In the worst case, which occurs for a long, prismatic block, the approximate method underpredicts λ_{min} by 55%. Since these cases cover a large range of aspect ratios of the matrix blocks, from sheets to cubes to long prisms, it seems reasonable to use expression (11) in the general case, when the fracture sets might not be orthogonal. In this regard, it is worth pointing out that the exact shapes of the matrix blocks at Yucca Mountain will probably never be known; at best, only rough knowledge of fracture spacings will be available. It is therefore sufficient to know that eq. (11) will always give the correct order-of-magnitude estimate for λ_{min}.

The above discussion shows that, to a reasonable approximation, diffusion into a matrix block can be quantified in terms of the characteristic length $\tilde{a} = 3V/A$, for both early and late times. Henceforth, we will use a to denote the "radius" of a matrix block, with the understanding that it actually represents $3V/A$.

Table 1. Relationship between matrix block geometry and λ_{min}. The matrix blocks are parallelepipeds with sides of length L_1, L_2, and L_3. The exact value of λ_{min} is given by eq. (10), and the approximate value is given by eq. (11).

Fracture spacing	Block shape	λ_{min}^{exact}	λ_{min}^{apprx}	$\lambda_{min}^{apprx}/\lambda_{min}^{exact}$
$L_1 = L_2 = L_3$	cube	$3\pi^2/L_3^2$	$4\pi^2/L_3^2$	4/3
$L_1 = L_2 \gg L_3$	thin sheet	π^2/L_3^2	$4\pi^2/9L_3^2$	4/9
$L_1 \gg L_2 = L_3$	long prism	$2\pi^2/L_3^2$	$16\pi^2/9L_3^2$	8/9
$L_1 = 2L_2 = 3L_3$	brick-like	$14\pi^2/9L_3^2$	$16\pi^2/9L_3^2$	8/7

EQUIVALENT RADIUS OF A DISTRIBUTION OF MATRIX BLOCKS

In a typical numerical simulation of flow and transport processes at Yucca Mountain, the computational gridblocks will be much larger than a typical matrix block. For example, in the three-dimensional site-scale model[15] that has been developed for the the unsaturated zone at Yucca Mountain, the computational gridblocks range in volume from 10^4 m^3 to 10^7 m^3, whereas the typical matrix block size will be orders of magnitude less.[16] Hence, each gridblock will contain a very large number of matrix blocks, whose radii will follow some distribution function. We now discuss the implications of having a distribution of radii, and examine to what extent, if any, these distributions can be replaced by some appropriate mean values. This analysis will be conducted for three cases: early time behavior using the exact solutions, early time behavior using the Warren-Root approximation, and late time behavior.

A. Early Times, Exact Model

Consider a computational gridblock that contains a certain number of discrete matrix blocks, each being characterized by a certain "radius" a. Let $\bar{\theta}(a,t)$ be the mean water content in a matrix block of radius a at time t, and let $\bar{\bar{\theta}}(t)$ be the mean water content of all the matrix blocks in that gridblock, each under the same initial and boundary conditions. We now show that for small times, diffusion into a collection of blocks can be modeled as diffusion into a single equivalent block, by use of the proper choice of the equivalent radius, a_{eq}. This case is actually of great practical interest, since it has been shown that tracer tests in fractured rock lasting as long as a few weeks can be successfully modeled using the "short time" assumption.[17]

At early times, which can be defined as the regime $Dt/a^2 < 0.01$, the mean water content in each block is given by[18]

$$\bar{\theta}(a,t) \approx \theta_i[1-(36Dt/\pi a^2)^{1/2}]; \tag{15}$$

this result can be found by integrating eq. (6), and applying initial condition (2). We now define two related distribution functions: $n(a)$, which quantifies the distribution of the number of matrix blocks having a given radius, and $v(a)$, which quantifies the distribution of the rock volume that is occupied by blocks having a given radius. Consider a computational gridblock having total volume V, or, more precisely, volume $(1-\phi_f)V$, where $\phi_f \ll 1$ is the fracture porosity. The number of matrix blocks in this gridblock whose radii lie between a_1 and a_2 will be given by

$$N(a_1<a<a_2) = \int_{a_1}^{a_2} n(a)da\,. \tag{16}$$

The total volume occupied by these matrix blocks is given by

$$V(a_1<a<a_2) = \int_{a_1}^{a_2} \frac{4\pi a^3}{3} n(a)da \equiv \int_{a_1}^{a_2} v(a)da\,, \tag{17}$$

where $v(a)=4\pi a^3 n(a)/3$. The normalization conditions for these two distributions are

$$\int_0^\infty v(a)da = \int_0^\infty \frac{4\pi a^3}{3} n(a)da = V\,. \tag{18}$$

The mean water content in the entire gridblock is then found by averaging $\bar{\theta}(a,t)$ over all matrix blocks:

$$\begin{aligned}\bar{\bar{\theta}}(t) &= \frac{1}{V}\int_0^\infty \bar{\theta}(a,t)v(a)da \\ &= \frac{1}{V}\int_0^\infty \theta_i\left[1-(36Dt/\pi a^2)^{1/2}\right]v(a)da \\ &= \theta_i\left[\frac{1}{V}\int_0^\infty v(a)da - (36Dt/\pi)^{1/2}\frac{1}{V}\int_0^\infty \frac{v(a)}{a}da\right] \\ &= \theta_i\left[1-\left[36Dt/\pi\langle a^{-1}\rangle_v^{-2}\right]^{1/2}\right].\end{aligned} \tag{19}$$

This expression has the same form as that for the single matrix block, eq. (15), so we see that the appropriate a_{eq} is $\langle a^{-1}\rangle_v^{-1}$, where the subscript v indicates that the average is taken with respect to the distribution function of the volume of the matrix blocks as a function of block radius. If we use the distribution function $n(a)$, on the other hand, eqs. (15,17) can be used to show that the equivalent radius is $\langle a^3\rangle_n/\langle a^2\rangle_n$. This expression for a_{eq} is identical to that which has been derived for the early-time behavior of a bed of spherical particles that had a surface-resistance term that was modeled using an analogy to convective heat transfer.[19] Han et al.[20] pointed out that this parameter represents (aside from a numerical constant) the ratio of mean block volume to mean surface area, and used it to correlate their experimental measurements of solute dispersion.

B. Early Times, Warren-Root Model

In many dual-porosity models for flow or diffusion in fractured rock masses, the Warren-Root approximation is used to model the flux between the fractures and the matrix blocks.[3] This model is based upon the assumption of quasi-steady-state behavior, and can be derived[18] from an analysis that utilizes the most-slowly-decaying mode in the Fourier series solution, as in eq.

(10). Hence this model is accurate in the late stages of matrix imbibition, but has been found to be very inaccurate at early times.[21] (Note that in studies of the *reservoir-scale* behavior of fractured rock masses, the terms "early time", "intermediate time", and "late time" are used with different meanings than in the present work). Nevertheless, because of the simplicity afforded by assuming that the flux is linearly proportional to the difference between the potential at the outer boundary of the matrix block (i.e., in the fractures), and the mean potential in the matrix block, $\bar{\psi}$, the Warren-Root approximation is widely–used.[9] It is therefore of interest to derive an expression for the equivalent radius of a collection of matrix blocks, at early times, using the Warren-Root model for the fracture/matrix interactions.

Strictly speaking, the driving force in the Warren-Root model is the potential difference between the matrix block and the adjacent fractures. Since we are assuming linear diffusion processes (in order to make the analysis tractable, and at the same time to focus on geometrical effects), there is no need here to make a distinction between saturation and potential. According to the Warren-Root model, then, the mean value of the water content in a matrix block of radius a, for the problem stated by eqs. (1-3), will at early times be given by[18]

$$\bar{\theta}(a,t) \approx \theta_i\left[1-(\pi^2 Dt/a^2)\right]. \tag{20}$$

Following the integration procedure that was shown in detail in the previous section utilizing the exact solution, we see that the early-time approximation to the mean water content in the entire gridblock will be given by

$$\bar{\bar{\theta}}(t) \approx \theta_i\left[1-(\pi^2 Dt/a_{eq}^2)\right], \tag{21}$$

where the equivalent radius is given by

$$a_{eq}^2 = \frac{1}{\langle a^{-2}\rangle_v} = \frac{\langle a^3\rangle_n}{\langle a\rangle_n}, \tag{22}$$

which is to say $a_{eq} = \langle a^{-2}\rangle_v^{-1/2}$. Rao et al. used this expression, without derivation, to rationalize their experimental results on solute transport in aggregated soils.[22] Except in the exceptional case where all matrix blocks have the same radius, the appropriate equivalent radius for the Warren-Root model in the early-time limit will therefore not be the same as that for the exact model.

C. Late Times, Exact or Warren-Root Model

The analyses given in the two previous sections show that, for early times, a collection of matrix blocks can rigorously be replaced by a single, equivalent matrix block of radius a_{eq}, where a_{eq} is defined in terms of certain moments of the block-size distribution function. We now examine whether or not an equivalent radius exists in the long-time, quasi-steady-state regime. Since the Warren-Root approximation is derived so that it gives the correct behavior in the long-time limit, we see immediately that the results in this regime will not depend on whether or not the exact solutions, or the Warren-Root approximation, is used. For completeness, we will base our analysis on the exact solution for diffusion into a sphere, which leads to the following expression[11] for the mean water content in a matrix block of radius a:

$$\frac{\bar{\theta}(a,t)}{\theta_i} = \frac{6}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}e^{-n^2\pi^2 Dt/a^2}. \tag{23}$$

The mean water content in the entire gridblock is then given by[23]

$$\frac{\bar{\bar{\theta}}(t)}{\theta_i} = \frac{6}{\pi^2 V}\sum_{n=1}^{\infty}\frac{1}{n^2}\int_0^{\infty} v(a)e^{-n^2\pi^2 Dt/a^2}da. \tag{24}$$

As the matrix block radius a appears in the denominator of the argument of the exponential terms, it is difficult[24] to extract any general results from eq. (24) that are independent of the distribution function $v(a)$. To proceed further to estimate the effect of having a distribution of radii, we must choose a specific form for the distribution function $v(a)$. Although a lognormal distribution is more commonly observed in geological studies,[25] in order to simplify the subsequent analysis we will follow Ruthven and Loughlin[23] and others in assuming that the radii of the blocks follow a Gaussian distribution of the form (Fig. 1)

$$v(a) = \frac{V}{\sqrt{2\pi}\sigma}e^{-\frac{(a-\mu)^2}{2\sigma^2}}, \tag{25}$$

where $\mu = \langle a\rangle_v$ is the mean radius, and σ is the standard deviation. Although this distribution has often been used to represent particle sizes, it is not strictly admissible, since it is not properly normalized if one imposes the additional constraint that a must be positive. However, as long as the "narrowness" parameter $s = \mu/\sigma$ is greater than about 3, the fraction of the distribution that has $a < 0$ will be negligible (<0.001; see Fig. 1), and eq. (25) can be used for $a > 0$ only. Moreover, we expect on physical grounds that the actual block size distributions will go to zero very rapidly as $a \to 0$, so that the cases that may occur in practice will have $s \geq 3$.

Use of the distribution (25) in eq. (24) leads to

$$\frac{\bar{\bar{\theta}}(t)}{\theta_i} = \frac{6}{\sqrt{2}\pi^{5/2}\sigma}\sum_{n=1}^{\infty}\frac{1}{n^2}\int_0^{\infty} e^{-(a-\mu)^2/2\sigma^2}e^{-n^2\pi^2 Dt/a^2}da. \tag{26}$$

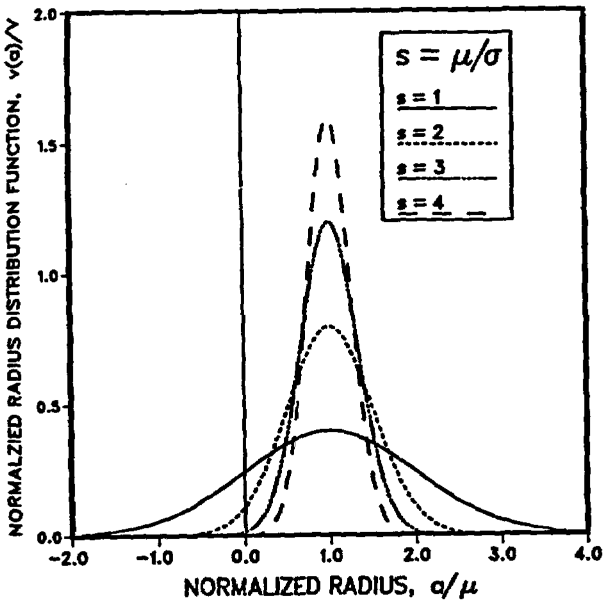

Fig. 1. Normal distribution of matrix block volume as a function of radius, as given by eq. (25), with mean μ and standard deviation σ. If $s=\mu/\sigma \geq 3$, the area under the curve that lies within the physically meaningless range $a<0$ is negligible, in which case eq. (25) is a permissable distribution function.

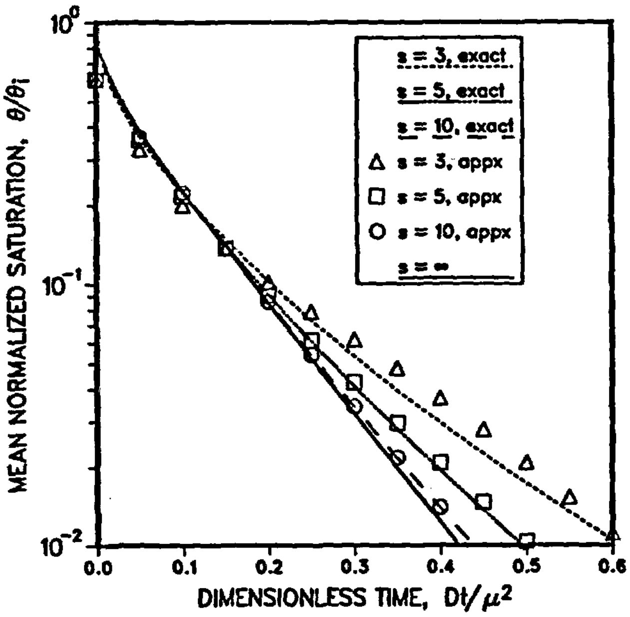

Fig. 2. Normalized mean saturation in a collection of matrix blocks, with boundary and initial conditions given by eqs. (2,3). The block radii follow a normal distribution, with mean radius μ, and standard deviation $\sigma=\mu/s$. Exact results are calculated from eq. (27), and approximate results are from eq. (32).

We now nondimensionalize the integrals appearing in eq. (26) by letting $z=a/\mu$ and $s=\mu/\sigma$, to arrive at

$$\frac{\bar{\theta}(t)}{\theta_i} = \frac{6s}{\sqrt{2}\pi^{5/2}}\sum_{n=1}^{\infty}\frac{1}{n^2}\int_0^{\infty} e^{-s^2(z-1)^2/2}e^{-n^2\pi^2 Dt/z^2\mu^2}dz\,. \quad (27)$$

At this point we restrict our attention to large values of t, in which case we retain only the first term in the summation:

$$\frac{\bar{\theta}(t)}{\theta_i} \approx \frac{6s}{\sqrt{2}\pi^{5/2}}\int_0^{\infty} e^{-s^2(z-1)^2/2}e^{-\pi^2 Dt/z^2\mu^2}dz\,. \quad (28)$$

The integral appearing in eq. (28) cannot be evaluated in closed form. But as we have already assumed that $s=\mu/\sigma>3$, we can use the fact that s is never small to develop an asymptotic expansion[26] for the integral as a function of the "large" parameter s^2. To accomplish this, we first note that as the term in the integrand that involves s^2 will be very localized in the vicinity of z=1, we can extend the lower limit of integration to $-\infty$. We then expand the other term in a power series in the variable $(z-1)$; a straightforward application of Taylor's formula yields

$$e^{-\tau/z^2} = e^{-\tau}\left[1+2\tau(z-1)+\tau(2\tau-3)(z-1)^2+\cdots\right], \quad (29)$$

where $\tau=\pi^2 Dt/\mu^2$. By letting $(z-1)=y$, eq. (28) can be written as

$$\frac{\bar{\theta}(t)}{\theta_i} \approx \frac{6se^{-\tau}}{\sqrt{2\pi}\,\pi^2}\int_{-\infty}^{\infty} e^{-\frac{s^2y^2}{2}}\left[1+2\tau y+\tau(2\tau-3)y^2+\cdots\right]dy. \quad (30)$$

We now make use of the known result[27]

$$\int_{-\infty}^{\infty} y^{2n}\exp(-s^2y^2/2)dy = \frac{1\times 3\times\cdots\times(2n-1)\sqrt{2\pi}}{s^{2n+1}}\,, \quad (31)$$

along with the observation that the terms involving odd powers of y will integrate out to zero. Hence, the mean water content will be given by

$$\frac{\bar{\theta}(t)}{\theta_i} \approx \frac{6e^{-\tau}}{\pi^2}\left[1+\frac{\tau(2\tau-3)}{s^2}\cdots\right], \quad (32)$$

where $\tau=\pi^2 Dt/\mu^2$. The leading term in eq. (32) agrees with the result that would be obtained in the $s \to \infty$ limit, which corresponds to an infinitely sharp distribution centered at $a = \mu$. The second term is a correction which reflects the existence of a finite value of the parameter $s = \mu/\sigma$. Note that eq. (32) is an asymptotic expansion in terms of the parameter s, and becomes more accurate as s increases, for any fixed t. It is not strictly meaningful to hold s fixed and let $t \to \infty$.

Fig. 2 shows a comparison between the approximate results found from the asymptotic expansion (32), and the exact results obtained from numerical evaluations of the *full* solution, which is given by eq. (27). The comparisons are shown for the cases $s = 3$, 5, and 10. The "long time" approximations become accurate when $Dt/\mu^2 > 0.1$; their accuracy is greater for larger values of s. The results for $s = 10$ are essentially the same as would be found for $s \to \infty$, in which case the curve approaches a straight line on the semi-log plot, as the curve drops off exponentially. Note, however, that the effect of having a finite variance in the distribution function causes the curves for $s < \infty$ to have a qualitatively different form for large times: the curves for finite s cannot be fit with an exponential function by *any* choice of an equivalent radius a_{eq}. On the other hand, it is worth noting that the divergence among the various curves does not become appreciable until a dimensionless time of about 0.2, at which time the diffusion process is about 90% complete. As $t \to 0$, the approximate curves extrapolate back to $6/\pi^2 = 0.608$ instead of 1.0, reflecting the neglect of the $n > 1$ terms in the summation. Note that the early-time regime, which was discussed in a previous section, corresponds to $Dt/\mu^2 < 0.01$, and so is not clearly discerned in Fig. 2. However, there is an intermediate time regime extending from about $0.01 < Dt/\mu^2 < 0.2$ for which the curves are very close together when μ is used as the length scale. Hence for most of the process, the (volumetric) mean radius, μ, provides an acceptable value for the equivalent radius a_{eq}.

SUMMARY

The effect of matrix block geometry on water imbibition and solute absorption, including the effect of block size distribution, has been studied from a theoretical point of view. In order to make the mathematics tractable, and to focus attention on the geometrical effects of matrix block size and shape, absorption and solute diffusion were both assumed to be governed by linear diffusion equations. First, it was shown that at early times, diffusion into a single block of volume V and surface area A is characterized by a length scale $\tilde{a} = 3V/A$. It was then shown that the long-time imbibition/drainage of polyhedral matrix blocks can be reasonably well approximated using this length scale, and the exact results for a spherical block.

Analyses were then conducted of the effect of having a distribution of matrix block sizes. It was shown that at early times, a collection of blocks can rigorously be replaced by an equivalent block whose radius is given by $\langle a^{-1} \rangle_v^{-1}$, where $\langle \rangle_v$ denotes an average taken on a volumetrically-weighted basis. If the Warren-Root approximation is used, however, it was found that $a_{eq} = \langle a^{-2} \rangle_v^{-1/2}$. Finally, an analysis was given for the long-time behavior of a collection of matrix blocks of different sizes, under the assumption that the block volume is normally distributed as a function of radius. An asymptotic expression was found for the diffusive behavior as a function of the parameter μ/σ, where μ is the mean and σ is the standard deviation of the distribution of block volume as a function of radius. Although it does not seem that such an aggregation of blocks can be rigorously replaced by any equivalent matrix block, it was found that through most of the diffusion process, the collection does behaves like a single matrix block having an equivalent radius $a_{eq} = \langle a \rangle_v$. It remains to be seen if the results are similar for the case of a log-normal distribution.

Based on numerical simulations of flow in fractured media, it has been concluded that once a collection of absorbing matrix blocks is coupled to the macroscopic flow field in the fracture network, the effects of any variance in the block size distribution are greatly mitigated.[28] Results for solute transport, on the other hand, seem to indicate that the variance in the block size distribution cannot be ignored when calculating breakthrough curves.[29] The theoretical results derived in this paper provide a basis for the investigation of the effect of block size and shape distribution on dual-porosity behavior. These results should therefore be useful in future systematic studies of the effect of block size distribution on transient infiltration and radionuclide transport at Yucca Mountain.

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