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A Note on the Recent Natural Gradient Tracer Test at the Borden Site

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The variance in particle position, a measure of dispersion, is reviewed in the context of certain models of flow in random porous media. Asymptotic results for a highly stratified medium and an isotropic medium are particularly highlighted. Results of the natural gradient tracer test at the Borden site are reviewed in light of these models. This review suggests that the moments obtained for the conservative tracers at the Borden site could as well be explained by a model that more explicitly represents the three-dimensional nature of the flow field.

INTRODUCTION

In this note we wish to discuss certain aspects of a natural gradient tracer test recently performed at the Borden site, Ontario, Canada. The results of the test, as well as the reduced data, have been reported on in a series of articles by *Mackay et al.* [1986], *Freyberg* [1986], *Roberts et al.* [1986], and *Sudicky* [1986]. In this test, two conservative (as well as other) tracers were injected into a rather uniform sand aquifer over a 1.6-m depth in a simulated pulse consisting of 12 m^3 of solution. The resulting tracer cloud was then allowed to drift with the natural gradient while being observed through multilevel samplers, consisting of collection tubes set to various depths, which were arranged in a regular grid along the flow path. Concentrations, measured from samples taken from these tubes, were depth integrated and this reduced data set was used to estimate horizontal moments of the tracer cloud. Our note concerns the time modeling of the second moment, or variance, of this cloud. Particulars concerning the test are to be found in the aforementioned reports.

The objective of the large-scale field tests is, in no small part, to test recently advanced theories of dispersion in heterogeneous porous media. These theories in general require a knowledge of two medium parameters: the variance in the logarithm of hydraulic conductivity and the correlation length scale of this quantity. The investigators at the Borden site, in a laudable effort culminating from intensive sampling of the medium, provide us with estimators of these parameters. The concentration variance model used by these investigators for a conservative tracer, however, does not admit three-dimensional flow [see *Freyberg*, 1986, equation (12); *Sudicky*, 1986, equation (14)]. We propose a model that does admit three-dimensional flow and that also allows for a highly stratified medium.

In order to make our note more lucid, we first derive certain theoretical results concerning the time behavior of the second moment of a tagged particulate of water moving through a medium in which the hydraulic conductivity is spatially variable but statistically homogeneous. Many of these results have been reported on previously by *Dagan* [1984]; we expand slightly on his earlier results and particularize them to discussing the natural gradient tracer test. Subsequently, we discuss the estimated second moments from the Borden tracer test and their relation to these theoretical models.

THEORETICAL CONSIDERATIONS

The vectoral position $\boldsymbol{\chi}(t)$ of a fluid particulate moving through a three-dimensional medium is accurately described by the model

$$\boldsymbol{\chi}(t) = \int_0^t \mathbf{U}(\boldsymbol{\chi}(t))\, dt + \boldsymbol{\chi}(0) \tag{1}$$

where $\mathbf{U}(\mathbf{x})$, $\mathbf{x} = (x_1, x_2, x_3)$ is the Eulerian velocity field [*Phythian*, 1975]. Since this form is rather intractable, a first-order approximation of the particle path is commonly used in the integrand of (1); that is, $\mathbf{X}(t) \approx \bar{\mathbf{U}}t$, where $\bar{\mathbf{U}} = E(\mathbf{U})$ is assumed constant. Thus (1) becomes

$$\boldsymbol{\chi}(t) = \int_0^t \mathbf{U}(\bar{\mathbf{U}}t)\, dt \tag{2}$$

where we have neglected $\boldsymbol{\chi}(0)$ without loss of generality. In addition, if a coordinate axis is chosen such that $\bar{\mathbf{U}} = (\bar{U}_1, 0, 0)$, then (2) can be written

$$\boldsymbol{\chi}(t) = (1/\bar{U}_1) \int_0^{\bar{U}_1 t} \mathbf{U}(z, 0, 0)\, dz \tag{3}$$

We will then be concerned principally with the component of $\boldsymbol{\chi}(t)$ that lies in the $E(\mathbf{U})$ direction, which is $\chi_1(t)$ in the case of (3). The variance of this component, where $\mathbf{U}(\mathbf{x})$ is a second-order stationary random field, is

$$\mathrm{Var}\,[\chi_1] = (2/\bar{U}_1{}^2) \int_0^{\bar{U}_1 t} (\bar{U}_1 t - s_1)\, \mathrm{Cov}_{u_1}(s_1, 0, 0)\, ds_1 \tag{4}$$

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where Cov_{u_1} (s) is the covariance function of the $u_1 = U_1 - \bar{U}_1$ component of the velocity field (see, for example, *Taylor* [1921]). Equation (4) is unchanged in form for the case of two-dimensional flow: the velocity covariance function need only represent a two-dimensional process, while $\bar{U}_1$ should be the appropriate mean velocity for this case.

With this initial information, it is well to consider first an overly simple model. Assume that flow is present in a perfectly stratified aquifer and that the mean flow is parallel to stratification. Then (3), where $\chi = (\chi_1, 0, 0)$, is exact and the mean and variance in particle position are

$$E(\chi_1) = \bar{U}_1 t = \bar{K}Jt/n \qquad (5a)$$

$$\mathrm{Var}\,[\chi_1] = t^2\,\mathrm{Var}\,[U_1] = \sigma_K{}^2 J^2 t^2/n^2 \qquad (5b)$$

respectively, where J is the gradient of the flow system, $\bar{K}$ and $\sigma_K{}^2$ are the mean and variance of the hydraulic conductivity fields, and n is the mean porosity. The result follows because K, in case (5), is a function of x_3 only. In reality, (5b) represents the early time behavior of almost all three-dimensional transport problems because most media exhibit some degree of stratification.

Dagan [1987] has proposed a significant variant of the perfectly stratified model. He considers a model in which the hydraulic conductivity within each layer is variable but assumes that no single layer can communicate with its neighbors. The interlayer variability is taken to be two dimensional, parallel to bedding. That is, hydraulic conductivity is a random function of space only in the plane perpendicular to the direction of stratification. In this case, the ensemble mean particle position becomes

$$E(\chi_1) = U_g t = K_g Jt/n \qquad (6)$$

where U_g and K_g are the geometric means of velocity and hydraulic conductivity, respectively, and J now represents the mean gradient. Taking $\bar{U}_1 = U_g$ in (4), then, the variance in particle position becomes

$$\mathrm{Var}\,[\chi_1] = \sigma_Y{}^2\lambda^2 A_g(\tau) \qquad (6')$$

where $\sigma_Y{}^2$ is the variance in the logarithm of the hydraulic conductivity, $Y = \ln K$, λ is the horizontal length scale of the medium approximately equivalent to the horizontal dimension of a heterogeneity, and $\tau = U_g t/\lambda$. The dimensionless variance $A_g(\tau)$ is dependent upon the particular covariance function chosen to represent the correlation structure of the two-dimensional hydraulic conductivity field. In the case where an isotropic negative exponential is used to represent this behavior, *Dagan* [1984, 1987] found that

$$A_g(\tau) = \beta\{2\tau + 3[1/2 - C + (e^{-\tau}(\tau+1) - 1)/\tau^2 - E_1(\tau) - \ln\tau]\} \qquad (7)$$

where C is Euler's number and $E_1(\tau)$ is a first-order exponential integral. The constant β results from deriving the two-dimensional hydraulic conductivity field necessary to (4) by averaging a three-dimensional process over one vertical length scale. The intent of β is to compensate for the use of a two-dimensional correlation function when the hydraulic conductivity field is technically a three-dimensional process. Again, for the specific covariance function selected by *Dagan* [1987], $\beta = 0.74$. With these inputs, (6') will have early and late time behavior

$$\mathrm{Var}\,[\chi_1] \sim 3/8\beta\sigma_Y{}^2 U_g{}^2 t^2 \qquad t \to 0 \qquad (8a)$$

$$\mathrm{Var}\,[\chi_1] \sim 2\beta\sigma_Y{}^2\lambda U_g t \qquad t \to \infty \qquad (8b)$$

respectively. Note that the intent of (6) is to approximate dispersion in three-dimensional media that is so highly stratified that the intralayer correlation in flow is insignificant.

In order to contrast the above two-dimensional approximator with an actual three-dimensional case, we derive the variance in particle position for two cases where flow is three dimensional. We assume that the logarithm of hydraulic conductivity, $Y = \ln K$, has a negative exponential correlation structure such that its spectrum can be expressed as

$$S_Y(\mathbf{k}) = \frac{\sigma_Y{}^2\lambda^2\lambda_3}{\pi^2}(1 + \lambda^2(k_1{}^2 + k_2{}^2) + \lambda_3{}^2 k_3{}^2)^{-2} \qquad (9)$$

where k_i is the wave number in the i direction and λ or λ_3 are the corresponding length scales. Then, from *Gelhar and Axness* [1983, equation (61)] the spectrum of the velocity field in the $\bar{U}_1$ direction can be expressed as

$$S_{u_1}(\mathbf{k}) = (K_g J/n)^2((k_2{}^2 + k_3{}^2)/k^2)^2 S_Y(\mathbf{k}) \qquad (10)$$

where $k^2 = \mathbf{k}\cdot\mathbf{k}$, and it has been assumed that x_1 is parallel to k_1, such that stratification, if present, is parallel to the mean flow direction. Noting that $U_g = K_g J/n$, then the covariance function of the u_1 process becomes

$$\mathrm{Cov}_{u_1}(\mathbf{s}) = U_g{}^2 \int e^{i\mathbf{k}\cdot\mathbf{s}}((k_2{}^2 + k_3{}^2)/k^2)^2 S_Y(\mathbf{k})\,d\mathbf{k} \qquad (11)$$

which, upon substitution into (4) gives the result that

$$\mathrm{Var}\,[\chi_1] = \frac{2}{\gamma^2}\int (1 - e^{ik_1\bar{U}_1 t})/(k_1{}^2)((k_2{}^2 + k_3{}^2)/k^2)^2 S_Y(\mathbf{k})\,d\mathbf{k} \qquad (12)$$

where $\gamma = \bar{U}_1/U_g$. Letting $\mathbf{z} = (\lambda k_1, \lambda k_2, \lambda_3 k_3)$ then (12) takes the form

$$\mathrm{Var}\,[\chi_1] = \lambda^2\sigma_Y{}^2 A(\tau)/\gamma^2 \qquad (13a)$$

where

$$A(\tau) = \frac{2}{\pi^2}\int \frac{1 - \mathrm{Cos}\,(z_1\tau)}{z_1{}^2}\left(\frac{z_2{}^2 + \mu^2 z_3{}^2}{z_1{}^2 + z_2{}^2 + \mu^2 z_3{}^2}\right)^2 \frac{d\mathbf{z}}{(1 + z^2)^2} \qquad (13b)$$

and $\tau = \bar{U}_1 t/\lambda$, $\mu = \lambda/\lambda_3$. In general, (13b) is rather difficult to resolve. However, two asymptotes of interest can be obtained, one by assuming μ to be very large, i.e., the stratified case, and the other by letting $\mu = 1$, i.e., the isotropic case. We examine the stratified case first.

Allowing μ to be large in (13b) results in the approximation that $A(\tau) \to A_s(\tau)$, where

$$A_s(\tau) = \frac{2}{\pi^2}\int \frac{1 - \mathrm{Cos}\,(z_1\tau)}{z_1{}^2}\frac{d\mathbf{z}}{(1 + z^2)^2} = 2[\tau - 1 + e^{-\tau}] \qquad (14)$$

On the other hand, when $\mu = 1$ in (13b) then $A(\tau) \to A_i(\tau)$, where

$$A_i(\tau) = \frac{2}{\pi^2}\int \frac{1 - \mathrm{Cos}\,(z_1\tau)}{z_1{}^2}\left(\frac{z_2{}^2 + z_3{}^2}{z^2}\right)^2 \frac{d\mathbf{z}}{(1 + z^2)^2}$$

$$= A_s(\tau) + B(\tau) \qquad (15a)$$

$$B(\tau) = -2\left\{\frac{5}{3} + \left[\frac{8}{\tau^3} - \frac{4}{\tau} - \left(\frac{8}{\tau^3} + \frac{8}{\tau^2} - 1\right)e^{-\tau}\right]\right\} \qquad (15b)$$

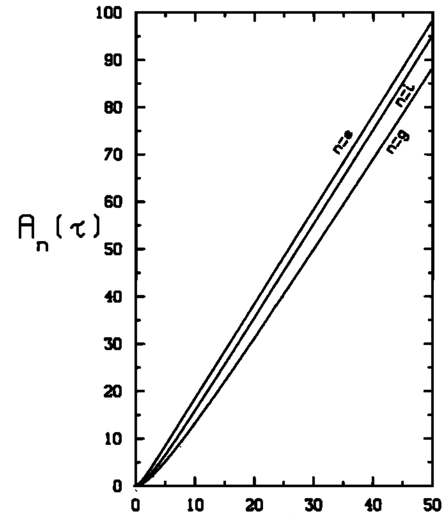

Fig. 1. Dimensionless variance in particle position: $A_g(\tau)$, equation (7); $A_s(\tau)$, equation (14); and $A_i(\tau)$, equation (15).

It can be verified that this solution is identical to that of *Dagan* [1984]. The mean velocity $\bar{U}_1$ for the stratified case should approach the arithmetic mean; i.e.,

$$\bar{U}_1 = K_g \exp(\sigma_Y^2/2)J/n \tag{16}$$

while that for the isotropic case is

$$\bar{U}_1 = K_g \exp(\sigma_Y^2/6)J/n \tag{16'}$$

[*Gelhar and Axness*, 1983, equation (60)]. Thus one would expect the mean velocity to be somewhat greater than the geometric mean for these three-dimensional models. We note that the early and late time variance asymptotes for the stratified model are

$$\mathrm{Var}[\chi_1] = \sigma_Y^2 U_g^2 t^2 \qquad t \to 0 \tag{17a}$$

$$\mathrm{Var}[\chi_1] = 2\sigma_Y^2 \lambda \bar{U}_1 t/\gamma^2 \qquad t \to \infty \tag{17b}$$

while for the isotropic model these asymptotes are

$$\mathrm{Var}[\chi_1] = \tfrac{8}{15}\sigma_Y^2 U_g^2 t^2 \qquad t \to 0 \tag{18a}$$

$$\mathrm{Var}[\chi_1] = 2\sigma_Y^2 \lambda \bar{U}_1 t/\gamma^2 \qquad t \to \infty \tag{18b}$$

[*Dagan*, 1984]. Result (17*b*) is equivalent to (65*a*) of *Gelhar and Axness* [1983], while result (18*b*) is equivalent to their (33); these results are equal when mean flow is parallel to stratification as in the case of (17*b*). It is important to note that all three models (equations (8*a*), (17*a*), and (18*a*)) indicate an early time behavior proportional to t^2. However, the stratified case (17*a*) will respond the most rapidly, while the two-dimensional approximator (8*a*) will respond least rapidly. Note that when K is lognormally distributed, (17*a*) is a first-order approximation of (5*b*). The large time behavior of the two-dimensional approximator (8*b*) differs from these by a factor of $\beta\gamma$. Dimensionless curves for the three cases are presented in Figure 1; note that τ is a different dimensionless parameter in the case of the two-dimensional approximator (7) as compared to the three-dimensional case (13).

It should be noted that all these results assume a certain ergodicity in order that the ensemble averages reported above can be applied to a real-world situation. In the case of the stratified models (5) and (6), the ergodic state can be achieved by averaging over many layers in the vertical direction, considering that flow, in these cases, is parallel to stratification. In the case of (13) it is less obvious that an ergodic state can be achieved by this means, especially if $\mu = 1$ and λ is large relative to the injection zone. However, in the situation at hand, λ_3 is small relative to the zone of injection so that although the spatial concentration information is correlated, it should yield averages which approximate the ensemble moments. Indeed, the smoothing seen in the depth-averaged concentrations, versus the three-dimensional data set [*Mackay et al.*, 1986], is indicative that ergodicity is a functional hypothesis in this case.

INTERPRETATION

Freyberg [1986] and *Sudicky* [1986] collected and presented a considerable amount of information concerning the variability of the medium and flow field. From these data, the following parameter values are indicated:

$$\sigma_Y^2 = 0.29$$

$$\bar{U}_1 = 0.091 \text{ m/day}$$

$$\gamma = 1.16$$

$$\lambda = 2.8 \text{ m}$$

$$U_g = K_g J/n = 0.078 \text{ m/day}$$

Note that as discussed by *Sudicky* [1986], $\bar{U}_1$ calculated from (16*a*) using the above values of σ_Y^2 and U_g is very close to the field value reported above. If these values are incorporated into (7), (14), and (15), then curves *g*, *s*, and *i*, respectively, of Figure 2 result. If, in addition, the moment data from *Freyberg* [1986, Table 3] are plotted on the same graph, then it would appear that the two-dimensional approximator (7) fits the field data most closely; indeed, the fit is remarkable. (We have used all field moment values, even though there is some question as to the validity of the oldest bromide moment; see *Freyberg* [1986].) Differences between this fit and that of Sudicky are primarily the result of using a geometric mean velocity in (7).

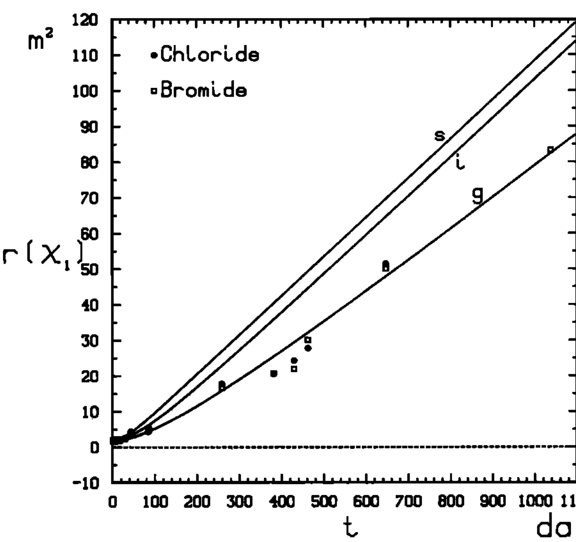

Fig. 2. Variance curves as calibrated with field data from Borden site. Point variance estimates from tracer results at Borden site [*Freyberg*, 1986].

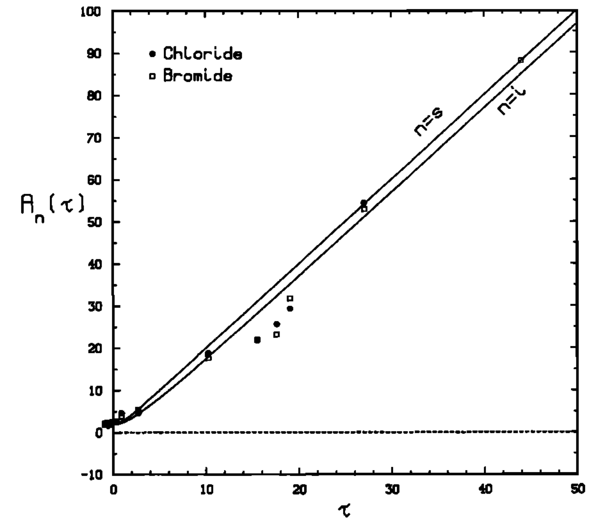

Fig. 3. Best fit of point variance estimates to three-dimensional flow models: $\lambda = 2.1$ m.

The best fit derived from Figure 2 is all the more remarkable considering the physical basis of the underlying model (7). No vertical flow component is permitted with this model, yet there is an abundance of data to indicate that a vertical component should be present. *Sudicky* [1986] reports a horizontal to vertical anisotropy in hydraulic conductivity of 1.3, which is exceedingly small (see, for example, *Weeks* [1969]). The plume, as an apparent result of a density contrast [*Sudicky*, 1986, p. 2702], sank readily in the initial part of the test, indicating that layers do communicate. Indeed, the plots by Sudicky [1986, Figures 6 and 7] of the hydraulic conductivity field indicate a less than perfect stratification. Finally, the good fit of the field data to (16) indicates that while the medium is stratified, flow is three dimensional. However, theoretically all second-moment data for a three-dimensional flow field should fall between curves *s* and *i* on Figure 2, disallowing for noise. The depth-integrated data from *Freyberg* [1986] clearly do not fall in this range, when the field data are taken at face value.

Examination of Figure 2 indicates that the good fit associated with the two-dimensional approximator is largely the result of two effects. The ultimate slope of the approximator is significantly less than that of the three-dimensional models, and the early time behavior is more subdued. Given the good relationship between field measurement of $\bar{U}_1$ and K_g and $\sigma_Y{}^2$, the estimated values of these parameters appear very reliable. We consider it more likely that the field estimate of λ could be in error; indeed, a maximum likelihood approach as suggested by *Vecchia* [1988] should yield superior estimates of this parameter. Alternate λ values could decrease the ultimate slope of the three-dimensional models, as suggested by (17*b*) and (18*b*). The subdued nature of the initial moment data, as presented by *Freyberg* [1986] in Table 3, could be related to problems associated with simulating, in the field, a hypothetical pulse injection of tracer.

As originally injected, the tracer preferentially displaced the ambient fluid in the vicinity of the well bores where the medium was more permeable. With regard to the depth-integrated concentration data, this displacement caused the tracer to immediately appear "dispersed" in the medium. However, this dispersal is contrary to what one would expect from a nonintrusive pulse of tracer in a natural gradient test. That is, the tracer, in this real-world test, was actually pushed upgradient by the forced injection of the tracer solution. That part of the tracer in the more permeable part of the medium would be more easily flushed by the natural flow, causing the upgradient part of the cloud to be reunited with the main body of the cloud. During this period, little apparent additional dispersion would occur.

In addition to the above possibility, it is probable that a density contrast between the injected tracer and the ambient water caused the centroid of the tracer cloud to move downward, perpendicular to the direction of stratification. This downward movement occurred at a velocity equivalent to 40% of the mean horizontal velocity in days 1 through 9, 15% in days 11 through 29, and at a rate of about 10% or less thereafter (as calculated from *Freyberg* [1986, Table 3]). This additional component of velocity perpendicular to stratification has the effect of reducing dispersion in the direction of stratification [*Matheron and deMarsily*, 1980]. However, since stratification is approximately horizontal, second-moment estimates derived from depth-integrated concentration measurements should reflect this component of dispersion. Thus one would expect that particularly during the initial period of the tracer test, moment estimates would be smaller because of this additional velocity component. Whatever the reason, we note that the variance in the tracer cloud is little changed over the first 29 days of the test [*Freyberg*, 1986, Table 3].

Given these two lines of reasoning, then, we consider it appropriate to investigate the sorts of length scales and, if necessary, time compensation needed in order to make the moment data fit the three-dimensional models. This was accomplished by first multiplying the variance estimates from Table 3 of *Freyberg* [1986] by $\gamma^2/\lambda^2\sigma_Y{}^2$ and their corresponding times by $\bar{U}_1/\lambda$, causing both qualities to take on a nondimensional character appropriate for plotting on Figure 1. Actually, the nondimensionalized data were plotted separately but on graphs with the same scaling as Figure 1, and λ was allowed to take on different values from plot to plot ($\sigma_Y{}^2$ and γ were held constant at their field values). Attempts were then made to fit the various plots to the large time part of the curves representing the three-dimensional process in Figure 1 (curves *s* and *i*), regardless of the placement of the early time data. In this manner, we were able to find two values of λ that in our consideration, give an adequate fit to the three-dimensional models. These fits are shown in Figures 3 and 4 for values of λ equal to 2.1 and 2.0 m, respectively. For a λ of 2.1 m a time compensation in the initial part of the data approximately equal to one dimensionless time unit τ (or a t of 23 days) was required to allow an adequate fit to the late time slope, while no time compensation was required for a λ of 2.0 m. Although, given the noise in the data, both models are probably equally realizable, we prefer Figure 3 as being sightly more aesthetic. Note that as a curve-fitting procedure, neither figure offers any advantage over the fit in Figure 2; indeed, if anything they may be somewhat inferior.

Conclusion and Discussion

In our view, the results of the previous section place the investigator in a bit of a quandary. On the one hand, the original Borden site studies, with model (7) as a basis for fitting field moments, allows only for two-dimensional flow.

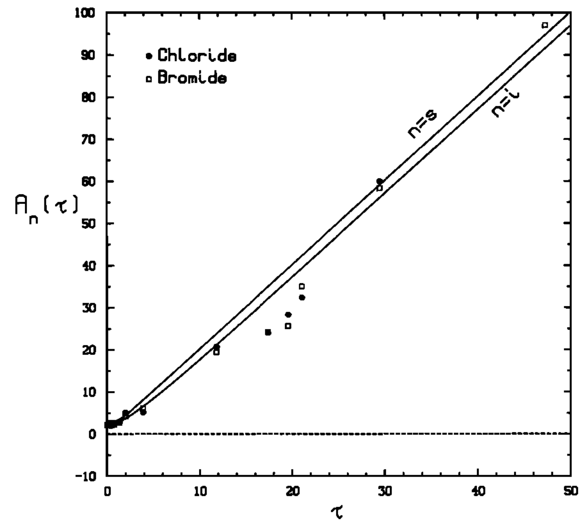

Fig. 4. Best fit of point variance estimates to three-dimensional flow models: $\lambda = 2.0$ m.

On the other hand, model (13*b*), which allows for three-dimensional flow, does not supply a superior fit to the concentration moments, especially when the original field statistics for media and velocity properties are considered. Thus the investigator has a choice of selecting what is probably an inferior model with an apparent superior fit, or what is probably a superior model with an apparent inferior fit. We have demonstrated that a relatively small change (25%) in one of the parameters (λ) will cause (13*b*) to have an adequate fit. In addition, we have discussed possible early time inconsistencies in modeling a field pulse input, which could cause discrepancies in fitting a theoretical model to field moments. Finally, we have presented evidence that points to a three-dimensional flow field. Thus while we cannot conclude that (13*b*) is superior to (7), we certainly do not feel that the fit demonstrated in Figure 2 makes (7) superior to (13*b*). We suggest that (13*b*) should have been the superior model and puzzle over its lack of fit to the field moments.

This note does point up the need for enhanced methods of determining the statistical properties of the medium. To even the casual observer, the work necessary to produce the variogram estimates provided by *Sudicky* [1986] must have been tremendous. Yet, we are neglecting data that reflect the variability in hydraulic conductivity because we lack adequate procedures to turn this information into statistical estimates of medium properties. These data are the variations in concentration and hydraulic head that are available from the multilevel collection tubes at these sites. Inverse procedures, along the lines of *Hoeksema and Kitanidis* [1985], are needed to turn these variations into independent estimates of medium properties. The production of these procedures will not be an easy task because of the time-dependent nature of this data, which results in an immense quantity of temporal and spatial information. This is not to detract from the work of the investigators at the Borden site; we firmly believe that this kind of experimentation is necessary if the hydrologist is ever to understand dispersion in porous media.

It is interesting to note that if one were to derive a longitudinal dispersivity α_L for the stratified model (14), then it would appear [*Fisher*, 1966]

$$\alpha_L = \sigma_Y{}^2 \lambda \gamma^{-2}(1 - e^{-\tau})$$

where $\tau = t\bar{U}_1/\lambda$. This form has been proposed, on an ad hoc basis, by *Pickens and Grisak* [1981, equation (11)] as a means for modeling scale-dependent dispersion. Indeed, given the little difference between forms (14) and (15), and the fact that most sedimentary aquifers are to some degree stratified, this form may find considerable application in this area.

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