# Scale-dependent Dispersivity: a Velocity Fluctuation Model

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**Abstract:** In the previous paper, it was shown that the cumulative effect of multiple one-dimensional velocity fluctuations can explain qualitative features of the observed scale dependent dispersivity in natural aquifers, but not the magnitude of the effect. It is plausible that in real systems the enhancement of dispersion caused by a single fluctuation may be larger than that derived for the 1-dimensional stepped fluctuation, because for example there are additional enhancement mechanisms in 2- and 3-dimensional systems. However this paper shows that to achieve the observed magnitude, it is not enough to increase the size of enhancement factor but in addition the rate at which the effect of a single fluctuation changes with fluctuation length and with position along the fluctuation sequence need to be modified. Several variations are explored. Simple assumptions are shown to lead to dispersivity formulas in terms of purely algebraic power laws, while more elaborate assumptions yield expressions that are still analytic but contain non-elementary functions. In either case it is possible to find the required variation of the dispersivity over 3 or more orders of magnitude and with curve shapes that are consistent with historical observations Moreover, this is achieved with plausible parameter values, leading for example to the conjecture that in the observed systems the porous medium could not have been homogeneous on a scale of more than centimeters. The model presented is schematic in the sense that it contains some detail assumptions not derived from first principles, but is believed to capture the essentials of the mechanism that causes scale dependent dispersivity. It sets some boundaries for viable detail models, but within those boundaries the final predictions are not very sensitive to the detail assumptions. A key merit of the treatment is that it identifies crucial variables that need to be measured or controlled in experimental studies.

*Keywords: scale-dependent; dispersivity; solute transport; porous medium.*

## 1. INTRODUCTION

Since the publication of collected experimental measurements of the dispersion of solutes in aquifers by Lallemand and Peaudecerf (1978), Gelhar (1986) and others, it has been known that the longitudinal dispersivity of natural porous media varies over several orders of magnitude with the scale of the experiment. While this dependence is roughly linear over a moderate range, it becomes non-linear for the complete range of 5 orders of magnitude covered by available data. It was shown in a previous paper by Verwoerd and Kulasiri (2003) that several features of the observed changes in dispersivity are explained by a model that incorporates the effects of a variable drift velocity, such as may be expected in a non-homogeneous medium, on solute dispersion. To facilitate calculation in detail, this model only considered 1-dimensional flow and modeled fluctuations in drift velocity as discrete steps. Perhaps not surprising for such an idealized model, the final results were not able to explain the magnitude of the observed effect although qualitative as well as some quantitative features, such as that the dispersivity increase is far slower than linear at large scales, did emerge without any need for specific parameter fitting.

This paper presents an extension of that model, which endeavors to keep those successful features and the overall structure of the model, while identifying plausible modifications of details that do produce quantitative agreement with the observed magnitude of dispersivity changes.

## 2. MODEL FORMULATION

As a starting point, the essentials of the 1D-step model for fluctuations defined on a regular spatial grid with a spacing $L$ can be summarised as follows:

- A single macroscopic velocity fluctuation enhances dispersion above the diffusive value for an average flow velocity, by a factor approximated by

$$f_m = 1 + \frac{3Q\lambda}{1 + 3m\lambda} \qquad (1)$$

We refer to $f_m$ as the "enhancement factor" and the additive second term in this equation as the "enhancement".

- The fluctuation length $3\,L$ is represented in this equation by a scaled spacing parameter $\lambda = L/\Lambda$. Here $\Lambda$ is an inherent length scale defined in terms of the average drift velocity $V$, initial plume variance $S^2$ and stochastic amplitude $\gamma$:

$$\Lambda \equiv \frac{V\,S^2}{\gamma^2} \approx 2\,S^2\,\frac{P}{p} \qquad (2)$$

  where $P$ is the Peclet number of the flow and $p$ the pore diameter of the medium.

- As a plume traverses the medium, it encounters fluctuations in a sequence indicated by the index $m$ featuring in equation 1.

- The cumulative effect of the fluctuation sequence up to $m = M$, is obtained by multiplying the $f_m$. Expressing M in terms of a scaled traversal length $\Gamma = x/\Lambda$ the combined enhancement factor $F(\Gamma)$ is

$$F(\Gamma) = \prod_{m=1}^{\Gamma/3\lambda} f_m \qquad (3)$$

- $F(\Gamma)$ behaves differently above and below a transition point at $\Gamma = 1$, as a result of the different nature of the dependence of $f_m$ on $m$, above and below $m = 1/3\lambda$.

- Above 1, the behavior of $F$ is essentially as $\Gamma^{Q}$. Here the amplitude of the fluctuations determines Q, and the value of 0.32 that fits experiments is similar although somewhat larger than those estimated from the 1D-step model.

- Below 1, $F$ grows exponentially with $\Gamma$, and this behavior is compatible with the observations.

- However, it only reaches a value proportional to $e^Q$ when $\Gamma = 1$. This is far smaller than the $F$ value of the order of 1000 at the transition point suggested by the observations [Gelhar 1986].

Consideration of these items shows that it is the last point that causes the failure of the model to achieve quantitative agreement. Because of the product form of $F$, values above $\Gamma = 1$ would automatically be raised to the required level if those below are adjusted to yield a realistic value at the transition point.

This leads us to the proposition that experimental evidence requires us to increase the values of the single fluctuation enhancement $f_m$ and/or their rate of decline with $m$, in the range of $m$ values below $1/3\lambda$.

Within the confines of the 1D-step model a plausible reason why equation (1) might underestimate $f_m$ is the neglect of non-Gaussian distortion of the plume by each step. The assumption of abrupt steps in the 1D-step model may also contribute to this because it has been shown [Verwoerd and Kulasiri, 2002] that e.g. linearly slanted steps have associated exponential effects on dispersion. Finally it has been established that in higher dimensional systems transverse variations in flow velocity, such as the stratified flow investigated by Gelhar et al (1979), can also enhance longitudinal dispersion.

We leave the investigation of mechanisms responsible for a larger enhancement factor for later study and here focus on discovering how equation (1) needs to be modified in order to reflect the observed dispersivity behavior. For easy comparison we rewrite equation (1) to incorporate a modifying factor $W(\lambda,m)$ in the form

$$f_m = 1 + \frac{3Q\lambda}{1+3\lambda m} W(\lambda,m) \qquad (4)$$

To retain the 1D-step model for large traversal lengths where it works satisfactorily, we require that $W(\lambda,m) = 1$ at or above $m = 1/3\lambda$ but assume that it is $>1$ below the transition.

Taking the existence of a transition as an experimental fact, and observing that $m$ is a discrete variable, we conclude that a separation into two regions can only happen if $3\lambda << 1$. Other than that, $\lambda$ is left free, but the simplifying assumption made in the 1D-step model that there is a single dominating fluctuation length is kept. Then $\lambda$ remains constant while calculating $F$, and so the main question is how $f_m$ needs to depend on $m$ in order to produce a value $F(1) \approx 1000$.

## 3. TRIAL MODIFYING FUNCTIONS

In choosing functional forms for $W(\lambda,m)$ to investigate, it is desirable to keep the resulting form of $f_m$ simple enough that expressions for $F(\Gamma)$ remains tractable, preferably splitting into factors that dominate above and below the transition, as was the case in the 1D-step model. It is helpful in this regard to separate the question of an assumed $m$-dependence into two parts: take the value of $W(\lambda,m)$ at $m = 0$ as an unknown fixed value $w >> 1$, determined later, and try various expressions that allow $W$ to decay from this value to 1 at the transition point in a plausible way.

For the first trial, we note that equation (1) was arrived at in the 1D-step model as a simplifying expression that produced the correct dominating terms in series expansions about the points $\lambda = 0$, $m = 1/2\lambda$ and $m = \infty$. It was a remarkable feature in the underlying theory that all three of these coefficients were proportional to the same number $Q$. An obvious generalization would be to assume that the appropriate $Q$ values can be different; in particular, that the $Q$ value for the $m = 0$ limit is much larger than for the $m = \infty$ limit. To fully determine the expression for $W$ it is also necessary to choose an interpolating $Q$ value at the transition point, $Q_t$. It turns out that the expression for F becomes intractable unless the very specific choice

$$\frac{5}{Q_t} = \frac{3}{Q_\infty} + \frac{2}{Q_0} \qquad (5)$$

is made, and this leads to

$$W_1(\lambda, m) = \frac{(1+3\lambda m)\,w}{1+3\lambda m w} \qquad (6)$$

where, in effect, $Q_0 = w\,Q_\infty$. However, when the calculation of $F$ is done with this trial function, it is found that the value of $F(1)$ is practically independent of $w$ and the required value cannot be achieved for any choice of $w$. The hyperbolic decay of $f_m$ values with $m$ that is implicit in equation (6) is simply too fast to allow a sufficient accumulation of the enhancement effects to explain the observed dispersivity growth.

This raises the question whether it is at all possible to achieve large values of $F(1)$ by boosting the lower range $f_m$ by a plausible amount. To facilitate answering this question, the product in equation (3) can be split for $\Gamma > 1$ into the product of the low range part $m \le 1/3\lambda$ and the high range part $m > 1/3\lambda$. In the high range part we use equation (1) for $f_m$, in effect taking W = 1 in that range. Then, we might make the extreme assumption that in the low range $f_m$ is a constant; if it is not possible to achieve the required enhancement from this, it would indeed be necessary to conclude that models of the kind that we are investigating are incompatible with observations. The corresponding expression for $W$ is the second trial expression:

$$W_2(\lambda, m) = w(1+3\lambda m) \qquad (7)$$

In this case, it is easily seen that $F(1) = (1+3\lambda Q w)^{1/3\lambda}$ which behaves like $F(1) = e^{Q w}$ for small $\lambda$, and with plausible choices of Q = 0.32, $\lambda = 0.001$ and $w = 25$ a value of more than 1000 is obtained.

This shows that it is feasible to obtain the required overall enhancement by several orders of magnitude without an excessive value of $w$. However, the assumption implicit in equation (7) that each subsequent single fluctuation, up to the transition point, produces the same enhancement, does not appear very plausible. Neither does the discontinuous drop at the transition point that this implies.

The next trial function eliminates these objections by assuming a linear decrease of $f_m$ that joins continuously to the high range values at $m = 1/3$:

$$W_3(\lambda, m) = (1+3\lambda m)(w + \tfrac{3}{2}\lambda m - 3w\lambda m) \qquad (8)$$

and taking $W = 1$ for $m \ge 1/3\lambda$ as before. It is found that once more $F$ can be calculated analytically, although a complicated expression is obtained, but the main result is that once more $F(1) \approx 1000$ can be obtained for a reasonable, if somewhat larger, $w$ value than that used in trial 2.

In trials 2 and 3 the essential mechanism to achieve a large enhancement was to replace the hyperbolic decrease of $f_m$, by a constant and a linear decrease respectively. The final set of trial functions aim to revert closer to the original form by retaining the hyperbolic term, but considering it to be the first term in a series expansion about the transition point and so taking $W$ to be of the form:

$$W(\lambda, m) = w + g\,\frac{3\lambda m}{1+3\lambda m} \qquad (9)$$

where $g$ is a coefficient still to be chosen. This expression stays approximately constant at the value $w$ for small $m$, becomes linear near the transition point and saturates to $(w+g)$ at large $m$.

For trial 4, we make the simplest possible choice of taking $g = 0$. This gives a behavior of $f_m$ intermediate between those of trials 2 and 3 and as could be expected, once more $F(1) \approx 1000$ is obtained for a $w$ value intermediate between those of trials 2 and 3.

Trial 5 is constructed by choosing the value $g = 2(1-w)$, which ensures continuity at the transition point. The resulting decline of $f_m$ is sharper than in trial 3. The drawback of the more complicated form of $W$ in this trial is that it is no more possible to reduce the resulting $F$ to analytical form in terms of simple functions; instead an expression in terms of Pochhammer functions of an irrational and possibly complex argument is obtained. The result of numerical evaluation confirms that also in this case the required enhancement is obtained.

Trials 2-5 all rely on splitting the range of the $m$-product in equation (3) so that tractable

expressions for the low *m* factor could be obtained while maintaining the high *m* factor, as it already reflects the observed behavior. As trial 5 already leads to abandonment of the tractability aim, there is no point in enforcing the range splitting either. So finally, trial 6 reverts to a single product expression over the whole range, and makes the choice $g = (1-w)$ to ensure that $W = 1$ holds when $m \gg 1/3\lambda$. Once again, numeric evaluation is necessary, but the required enhancement values are attained and moreover the kink in the *W*-curves of trials 2-5 is completely eliminated to give the most plausible behavior of all the trials considered.

In the work so far, *w* has been taken as a constant, because any $\lambda$-dependence that it has, is not relevant for calculations based on a fixed $\lambda$ value. On the other hand, $\lambda$ itself is unknown except that it has to be $\ll 1$. So knowledge of how *w* depends on $\lambda$ may be used to estimate $\lambda$, once a suitable *w* value has been found e.g. by fitting $F(\Gamma)$ curves to experimental observations.

In the 1D-step model, as approximated by equation (1), the enhancement produced by a fluctuation is just proportional to its scaled length $\lambda$. It is plausible that the enhancement should vanish as $\lambda \to 0$, but at the other extreme where $\lambda \to \infty$, such behavior is not plausible. Indeed, it has been shown [Verwoerd and Kulasiri, 2001] that the effects of a single step decays away from the step on a length scale related to the extension of the contaminant plume, so the effects of a stepped fluctuation must also become negligible if the fluctuation length is much larger than the plume extension. Indeed, the unlimited increase of the enhancement with $\lambda$ is just an artifact of approximating $f_m$ in the 1D-step model by the dominating term at $\lambda = 0$; the full expression deviates from linearity as shown in figure 1.

A simple assumption that vanishes at $\lambda \to 0$ while avoiding unrealistic growth at large $\lambda$ values, is a fractional power law:

$$w(\lambda) = (3\lambda)^{n-1} \qquad (10)$$

Also shown in figure 1, is a comparison of this formula for $n = 1/3$ with the actual curve obtained from the 1D-step model; it represents a fairly uniform increase of the enhancement beyond the 1D-step model values.
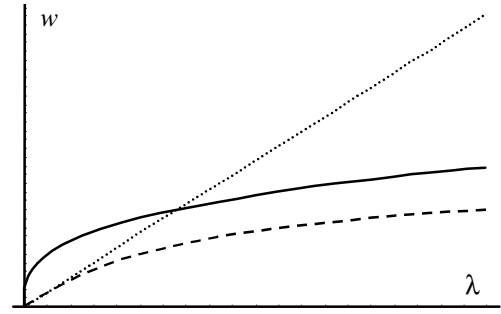


**Figure 1.** Eq (10) (solid line) compared to the $\lambda$-dependence of the 1D-step model (dashed) and its linear approximation (dotted).

In addition, it is compatible with the *w*-values of the order of 25 to 50 at $\lambda = 0.001$ that were obtained from the trial functions above. Similar agreements can be obtained with other *n* values but only within fairly narrow limits of the order of $0.2 < n < 0.6$, depending on what is considered a reasonable range for $\lambda$.

## 4. COMPARING TRIAL FUNCTIONS

The trial functions proposed above represent quite a large range of modification of the 1D-step model enhancement as function of *m*, as demonstrated by figure 2. For comparison, the same value $w = 25$ was used for all curves:
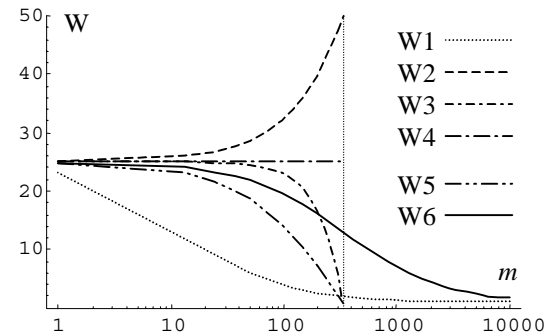


**Figure 2.** Trial modifying functions as functions of fluctuation count *m*.

Figure 3 shows the dispersivity curves calculated from the split range trial functions *W2* to *W5*, via the cumulative enhancement factor *F*, and compares these to experimental values.

Parameters were chosen by the following procedure. Inspection of the measured values suggests that the transition between low and high range behaviors takes place at approximately 30 meters, so this was chosen as the length scale $\Lambda$. To obtain a smooth buildup of the dispersivity to the observed large value at the transition point without an excessive enhancement by a single fluctuation, a large number of factors are needed in the product appearing in equation (3) which means that $\lambda$ must be quite small. We chose $\lambda =$

0.001, but this value can be adjusted by an order of magnitude either way without affecting the results significantly. The combination of the chosen $\Lambda$ and $\lambda$ values imply that the physical length of the dominating fluctuation is about 9 cm, which also appears very reasonable from a physical point of view. The value of $Q$ is simply the slope of the high range dispersivity on a logarithmic plot, and from the data a value of $Q = 0.32$ has been chosen.
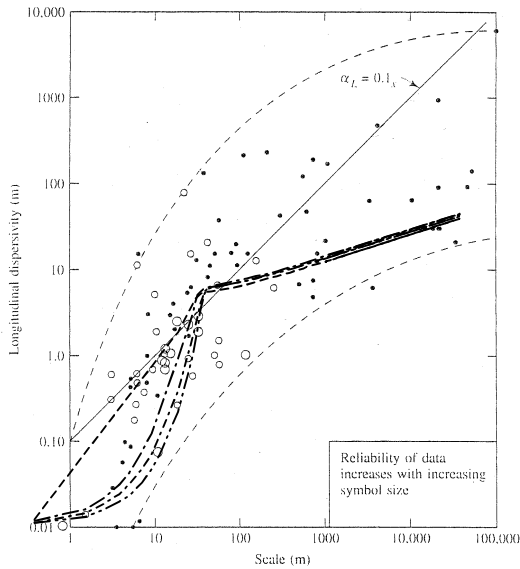


**Figure 3.** Dispersivity calculated from split range trial functions W2 to W5, compared to experimental values [Fetter (1999)and Gelhar(1986)]. Plot styles as for figure 2.

This leaves only the single parameter $w$ to be used for fitting the calculated dispersion curves to the data. The values obtained by manual adjustment are $w = 20, 38, 29, 64$ for trials 2, 3, 4 and 5 respectively, and these yield the curves shown in figure 3, all of which are in reasonable agreement with the measurements.

A striking feature of the plots is that despite wide variations in the underlying trial functions, the dispersivity curves are very similar. This observation applies even more strongly if the implausible trial 2 is excluded. That gives some retrospective justification for the rather ad hoc way in which the trial functions were constructed.

A similar comparison is done next for the continuous range trial function *W6*. In this case, the transition takes place more gradually and this is accommodated by a slight downwards adjustment of the assumed scale length $\Lambda$ to a value of 10 m. A consistent physical fluctuation length is maintained by correspondingly increasing $\lambda$ to 0.0035. Manual fitting then leads to $w = 24$, and the resulting dispersivity curve is shown in figure 4.
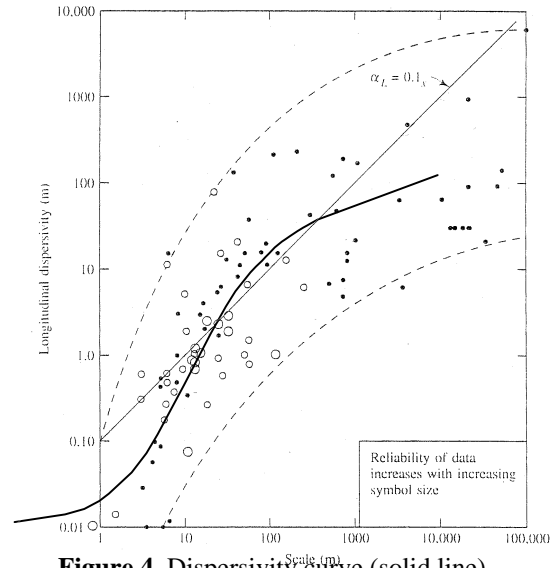


**Figure 4.** Dispersivity curve (solid line) calculated from continuous range trial function W6 compared to experimental values.

It is seen that an even better fit to the observations is obtained, suggesting that the rather sharp transitions in figure 3 was an artifact of the range splitting simplification used for the initial trials.

In none of the results presented was an optimized fit of parameters attempted, as this would not be justified in view of the large variations in the measured data collected from many experiments. Instead, the point made is that with only a few parameters, of which only one is freely fitted while the rest are determined by their physical interpretation and qualitative features of the data, an excellent representation is obtained of the rather complicated observed dispersivity behavior encompassing about 4 orders of magnitude in size and 5 in spatial range.

As further confirmation of the plausibility of the model, figure 5 shows the actual single fluctuation enhancement values represented by the parameters that fit the data.

For the 1D-step model, the enhancement by the first fluctuation would be 0.1%; but in order to fit observations, this is increased to 2 % for trial 6 and somewhat higher values for the split range models. While the increase relative to the 1D-step model is substantial, the effect of any single fluctuation remains only a small perturbation of the background diffusive plume growth. There is obviously a reciprocal relationship between this behavior and the value of $\lambda$. For example, at the extreme of choosing $3\lambda = 1$, only a single fluctuation would fit into the interval covered by the length scale. Hence not only would there be a single discontinuous jump in the dispersivity, but the enhancement would have to be the absurd

value of 1000. This argument shows that whatever one considers to be a plausible maximum for the single fluctuation enhancement, places an upper limit to the value that can be chosen for $\lambda$. The values presented above shows that it is possible to reconcile the enhancement value and the fluctuation length in a plausible way.
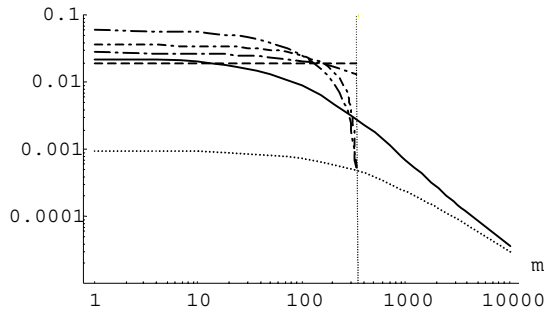


**Figure 5.** Enhancement by fluctuation number *m*. Dotted line is the 1D-step model, other curves as in figure 2.

Yet another plausibility test of the model is to compare the value of the length scale $\Lambda$ as inferred from the data with the expression in terms of flow parameters that is given by equation (2). As a ballpark figure we take the pore diameter as p = $10^{-4}$ m and the initial Gaussian plume variance as given by $S = 10^{-2}$ m. Then the $\Lambda$ values of 10 or 30 m as used above implies a longitudinal Peclet number in the range 5 to 15, which appears quite reasonable. Most likely the actual values of *P*, *p* and *S* in the various experiments from which data were collected for figures 3 and 4 were all different, which may account for some of the variability in the measured values.

Trial function *W2* may be considered an upper limit on plausible *W*-functions as it does not allow for any decrease in the enhancement as the plume is dispersed, while a lower limit must be somewhere between *W1* (which attenuates too fast to fit the data) and *W5* that does fit. These limits give some guidance on viable assumptions.

## 5. CONCLUSIONS

The model presented here succeeds very well in explaining the rather dramatic changes of observed dispersivity over several orders of magnitude as a function of the length scale of the experiment.

The final results are expressed in terms of a set of four parameters, but it is emphasized that the model is not just a curve fitting exercise. Each of the parameters has a particular physical interpretation, and the values obtained have been shown to be physically meaningful in terms of this context. Moreover, the structure of the model has a solid grounding on a detailed first principles calculation of the interaction between dispersion and drift velocity variations in a 1-dimensional flow. In fact, only one aspect of the 1D model needed to be modified: the enhancement of dispersion by a single fluctuation needs to be boosted by a considerable amount to reflect the observed dispersivity rise. We expressed that boost by a modifying function *W*, and showed that a considerable range of postulated *W* functions give similar levels of agreement of calculated dispersivity curves with measured values.

The main outstanding issue to be addressed in future elaborations of the model is to identify mechanisms for the required boost and hence to derive W in a systematic and detailed way. Some refinements of the 1D model are still possible, but it seems likely that the major source of the boost will be from additional mechanisms for interaction between dispersion and velocity fluctuations coming into play in 2- and 3-dimensional systems.

## 6. REFERENCES

Fetter, C.W, Contaminant Hydrogeology, 2$^{nd}$ ed. Prentice-Hall, London, 1999.

Gelhar, L.W. , A.L. Gutjahr and R.L. Naff, Stochastic analysis of macrodispersion in a stratified aquifer, *Water Resources Research,* 15(6), 1387-1397, 1979

Gelhar, L.W., *Water Resources Research,* 22(9), 135S-145S, 1986.

Lallemand-Barres, P and P. Peaudecerf, *Bulletin*, Bureau de Recherches Géologiques et Miniéres, Sec ¾, 277-284 , 1978.

Verwoerd, W.S. and D. Kulasiri, Solute Dispersion in Porous Flow with a Constant Velocity Gradient, *ASM 2002 conference proceedings*, Crete, Greece, 501-505, 2002

Verwoerd, W.S. and D. Kulasiri, The effects of variable flow velocity on contaminant dispersion in porous flow, *MODSIM 2001 conference proceedings Vol. 1*, Canberra, Australia, 401-406, 2001

Verwoerd, W.S. and D. Kulasiri, Solute Dispersion by 1D Stepped Velocity Fluctuations, *MODSIM 2003 conference proceedings, Townsville, Australia,* 2003.