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Prediction of solute dispersion in heterogeneous porous media: effects of ergodicity and hydraulic conductivity discretisation

J.A. Tompkins[a,]*, K.C. Gan[a], H.S. Wheater[a], F. Hirano[b]

[a]*Department of Civil Engineering, Imperial College, London SW7 2BU, UK*

[b]*Underground Engineering Department, Shimizu Institute of Technology, 4-17, Etchujima, 3-chome, Tokyo, Japan*

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Abstract

The performance of a stochastic numerical modelling procedure to simulate dispersion of a conservative solute in two-dimensional heterogeneous hydraulic conductivity fields is investigated in a series of numerical experiments, the results of which are compared with theoretical predictions. Random hydraulic conductivity fields are generated with a prescribed statistical structure, a finite difference model is used to obtain the flow field and particle tracking reproduces the dispersive properties.

For comparison between stochastic numerical methods and stochastic theories for solute transport, fulfilment of the ergodic requirement is necessary, consequently aspects of simulated solute plume behaviour are investigated with respect to ergodicity. Application of numerical stochastic methods is hampered by the large associated computational burden, which is affected by a range of factors, not least the level of discretisation of the hydraulic conductivity field. The experiments detailed here investigate the effects of hydraulic conductivity discretisation and the effects of initial solute source area for a range of log–permeability variances. An increasing deviation from Dagan's linear theory is observed for increasing coarseness of discretisation. A tendency to ergodic conditions is found for a smaller initial source area than previously reported.

* Corresponding author.

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1. Introduction

The transport of solutes in groundwater systems is a complex process, and models have an important role to play, not only in predicting the fate of contaminants, but also in the interpretation of data and in system characterisation.

An underlying problem in all field-scale model applications is that of system and parameter uncertainty. This applies to the geo-hydrological characterisation of a groundwater system, representation of boundary conditions, etc. but is a particular problem for the spatial characterisation of aquifer properties. Data collection costs are high and aquifer properties are subject to a high degree of spatial variability. It follows that appropriate modelling approaches must recognise the issue of uncertainty and allow for its representation.

A second problem is a fundamental difficulty of appropriate representation of transport processes. The classical approach to modelling contaminant transport is based on the Bear–Bachmat advection–dispersion formulation (Bear, 1979), in which solute advection at the mean flow velocity is modified by spreading due to processes of local irregular advection and molecular diffusion, conventionally represented as a Fickian process and characterised by dispersivity (a tensor of second order with three principal directions). Several difficulties arise, often there are insufficient data to characterise the dispersivity tensor in anything other than a highly simplified form, and more fundamentally, there are problems concerning the Fickian representation. In practice, application of classical theory results in an apparent scale-dependence of dispersivity (Anderson, 1979; Gelhar, 1986).

One response to the problem of uncertainty has been an increased interest in stochastic methods, which provide a formal framework for the treatment of uncertainty. Such methods can be combined with alternative approaches to the representation of dispersion which accommodate scale-dependence via a non-parametric framework.

In this paper analytical and numerical stochastic approaches to ground-water modelling are briefly introduced. Two key issues concerning numerical model application and validation are discretisation scale and the fulfilment of the ergodic requirement. Criteria for these are evaluated through a series of synthetic numerical experiments.

2. Stochastic approaches to groundwater flow

It has been argued that the spatial variability of aquifer properties is such that their unique, deterministic, description is not feasible (Rubin, 1990), and this is formally recognised in the stochastic approach, in which aquifer properties are regarded as random variables with known distributions. It thus follows that the outputs from a stochastic model are probabilistic, characterised, for example, by the statistical moments or the full probability density function (p.d.f) of the variables of interest. Commonly such methods are based on modelling hydraulic conductivity as a spatial random function, for which the lognormal distribution is generally accepted. This leads to the formulation of the velocity field as a spatial random function.

Stochastic models may be classified as analytical or numerical. (A recent review of the former is given in Gelhar (1993).) Analytical solutions are generally based on linearisation of the governing, stochastic equations using spectral, perturbation or hybrid spectral-perturbation methods. In spectral methods (Bakr et al., 1978; Gutjahr et al., 1978; Gelhar et al., 1979; Gutjahr and Gelhar, 1981; Gelhar, 1986; inter alia) parameters are described in terms of their mean and a fluctuation about the mean; this produces deterministic equations for the means and equations for the fluctuations which can be solved using inverse Fourier transforms. The perturbation approach (Tang and Pinder, 1979; Winter et al., 1984; Neuman et al., 1987; inter alia) uses a Taylor series expansion of the flow-transport equations followed by the elimination of all non-linear terms in the perturbation. Gelhar and Axness (1983) developed a hybrid spectral-perturbation approach.

A general theoretical approach to transport in heterogeneous formations was presented by Dagan (1982, 1984, 1987) based on a perturbation analysis. For the transport of passive solutes under steady uniform average flow conditions over an infinite domain in which hydraulic conductivity is represented as a stationary, log–normally distributed function of small variance (shown by Freeze (1975) and Hoeksema and Kitanidis (1985) to be upheld in field studies), the statistical moments of velocity and concentration were derived in terms of the statistical structure of the spatial conductivity heterogeneity. Thus, the time-dependent development of dispersivity was modelled and was found to be consistent with the asymptotic results of Gelhar and Axness (1983).

Analytical solutions have provided important theoretical insights into the dispersion process, and provide tractable methods for estimation of the moments of the output distributions under idealised conditions. Application to field situations has been limited, although detailed experiments at the Borden site and Cape Cod aquifer have provided data for testing, with encouraging results (Freyberg, 1986; Mackay et al., 1986; Barry et al., 1988; Garabedian et al., 1991).

However, analytical solutions have been developed for a restricted set of conditions, e.g. an infinite domain, steady, uniform flow, and spatially stationary and homogeneous properties (typically log–normally distributed hydraulic conductivity of low variance). For more general applications, numerical stochastic methods are required. In principle, these allow for simulation of complex systems, subject to a variety of boundary conditions, sources and sinks, unsteady flow and non-stationary material properties. Commonly, Monte Carlo simulations are used to generate alternative, equally likely, realisations of the system. The ensemble of realisations is then used to define the statistics of the required outputs.

An increase in computational capability has led to a propagation of these stochastic numerical approaches to the representation of transport processes in groundwater systems (for example, Van Rooy, 1987; Varljen and Shafer, 1991; Tompson and Gelhar, 1990; Valocchi, 1990; Bellin et al., 1991). The objectives of these approaches include the validation of the existing analytical dispersion models, the definition of well capture zones and the delineation of potential or existing contaminant plumes.

These methodologies are based on the hypothesis that the use of finely discretised random fields to represent the heterogeneity of hydraulic conductivity will, in conjunction with particle tracking, account for hydrodynamic solute dispersion. Dispersion is most often represented by the variance of particle spatial positions relative to a plume centroid.

These numerical methods are invaluable in that they augment the findings of the analytical methods and extend the range of prediction and solute modelling beyond the limitations imposed by the assumptions of the theoretical approaches. There are, however, several conceptual and practical points which have to be resolved before numerical stochastic models can be usefully applied to problems in the field. Primarily there needs to be a link between numerical methods and analytical stochastic theories, and in this respect the fulfilment of the ergodic requirement is important and needs to be investigated. Also, in practice, there is a need to balance computational efficiency with solution accuracy and in this respect the key issues relate to the dimensionality of the solution, the discretisation of the hydraulic conductivity field and the number of realisations used.

This paper contains details of a series of stochastic numerical experiments which utilise a non-parametric approach to the representation of the dispersion of an inert solute in heterogeneous porous media. The nub of the numerical stochastic methodology adopted is the assumption that the mechanical component of the dispersion process can be represented solely by small-scale velocity fluctuations and that these fluctuations can be attributed to local variations in hydraulic conductivity. Therefore, it is evident from the underlying hypothesis of the modelling approach that the discretisation of the hydraulic conductivity field plays an important role in the simulation of dispersion.

Ergodicity is a mathematical concept which, in the case of spatial fields, implies that the properties of a realisation of a random function are representative of the ensemble properties of the underlying function. This effectively requires that there is sufficient sampling to ensure a correct representation of the underlying distribution. The validity of stochastic theories concerning solute dispersion depends on the fulfilment of this hypothesis.

For numerical approaches, the ergodic requirement has a bearing on the size of the domain to be modelled to facilitate valid comparison with theoretical results, while the conductivity scale determines its fineness of discretisation. Both aspects must be selected as a compromise between computational burden and solution accuracy, however, there are few guidelines at present in the literature. Unless the effects on results are known and quantified, practical application of the stochastic methodology will be hampered.

3. The role of ergodicity in dispersion

As mentioned above, the analytical approaches of Dagan (1982, 1984, 1987), Gelhar and Axness (1983) and Neuman et al. (1987) are all underlain by the assumption of ergodicity. A detailed statement of ergodicity can be found in most references on probability or stochastic processes (e.g. Blum, 1982; Rosenblatt, 1985; Cressie, 1991), and a consideration of the various formulations of the ergodic theory is given in Adler (1981).

It is currently accepted (Dagan, 1989; Cressie, 1991; Gelhar, 1993) that in spatial applications the ergodic hypothesis holds for a spatial random field if the spatial covariance tends to zero over the spatial extent of the field; this will apply if the length scale of the field under consideration is much larger than the length scale of the field correlation. In terms of a stochastic representation of flow through porous media the fulfilment of the ergodic hypothesis can thus be taken to imply that each realisation of the random hydraulic conductivity field is fully representative of the ensemble of possible realisations. For solute transport, ergodicity of the concentration field associated with the underlying spatially random hydraulic conductivity field requires that the plume centroid moves at the mean field velocity (U) and that the effective longitudinal dispersion coefficient D_L (and hence the rate of change of the spatial second moments) tends to a fixed value. However, if the ergodic requirement is not fulfilled, the attributes of plume movement will deviate from theoretical predictions.

In general, if the spatial extent of a pulse of solute introduced into a heterogeneous velocity field is small compared with the hydraulic conductivity correlation scale it is subergodic, in which case estimates of its centre of mass and spatial variance relative to the plume centroid will differ from its ensemble counterparts and the ensemble longitudinal dispersion will be less than the asymptotic value predicted by Dagan (1982, 1984, 1987) or Gelhar and Axness (1983). The statistical moments of the plume will change as it moves through the heterogeneous velocity field, and its shape will vary erratically with time. As the plume continues to move, it will expand and become much larger than the hydraulic conductivity correlation scale. It is only beyond this point that moment measurements from individual simulations exhibit ensemble characteristics. This plume behaviour must be considered when comparing individual plume moments with the stochastic theoretical results. It is only meaningful to compare the moments of plumes generated under differing flow conditions when the ergodic requirement has been met. Thus, the range of validity of the hypothesis and its consequent effects on dispersion are of great importance in the numerical simulation of solute transport (Gelhar, 1993). An example of plume evolution from non-ergodic to ergodic conditions can be seen in Tompson and Gelhar (1990).

A useful measure of the fulfilment of the ergodicity requirement is the comparison of the longitudinal plume variance with respect to the centroid trajectory (S_{11}) and the longitudinal plume variance with respect to the expected flow trajectory (X_{11}). The former refers to the observed spread about the plume centroid for an individual realisation, the latter to the spread about the expected ensemble centroid.

These two terms (S_{11} and X_{11}) are related through the following equation (Kitanidis, 1988; Dagan, 1989, 1990).

$$X_{11}(t) + S_{11}(0) = S_{11}(t) + R_{11}(t) \qquad (1)$$

where $X_{11}(t)$ is the ensemble longitudinal variance with respect to the expected plume centroid, $S_{11}(0)$ is the initial particle variance with respect to the source centroid for a given realisation, $S_{11}(t)$ is the particle variance at time t with respect to the plume centroid for a given realisation, and $R_{11}(t)$ is the variance of the plume centroid with respect to the expected plume centroid.

As R_{11} reduces, individual realisations become representative of the ensemble characteristics and there is a tendency toward ergodicity, because then the actual plume centroid approximates the expected.

In practical terms for solute transport, ergodicity may be said to be achieved if one of the following criteria is fulfilled:

(1) $\mathrm{d}R_{11}/\mathrm{d}t \rightarrow 0$, which implies that the centroid moves at the average field velocity (G. Dagan, personal communication, 1992);

(2) a match is obtained between the ensemble mean $\langle S_{11} \rangle$ and S_{11} for a single realisation (Gelhar, 1993);

(3) a match is demonstrated between S_{11} for a single realisation and an analytically generated variance value (this is using the assumption that since the analytical approaches are underlain by the ergodic hypothesis, their results will be implicitly ergodic).

There are several approaches which tackle the problem of the ergodic requirement. For example, Salandin and Rinaldo (1990) achieve ensemble statistics by releasing one particle for each random realisation of the hydraulic conductivity field, thus generating only uncorrelated paths. This implies that the plume resulting from the combined extent of the individual statistically-independent particle positions will cover several integral scales, therefore for a large number of realisations the resulting spatial moments from such single particle simulations will fulfil the ergodic assumption, and Salandin and Rinaldo (1990) have shown the results to be compatible with the analytical results of Dagan (1982, 1984, 1987). The spatial second moments in this case are calculated as the spatial moments of all particles taken about the mean centroid position (the variance here is equivalent to X_{11} in Eq. (1)). Alternatively Tompson and Gelhar (1990) used one single realisation of a large field and assumed that at large times the cloud would encounter sufficient hydraulic conductivity variations to ensure ergodicity and thus tend to the asymptotic macrodispersion value. However, Salandin and Rinaldo (1990) express doubts as to whether the field used is sufficiently large to ensure full sampling.

It can be seen from the various alternative numerical approaches that the ergodic requirement is fulfilled by ensuring that particles traverse a sufficiently large portion of the hydraulic conductivity domain, and that this ensures that the resulting plume statistics are representative of those for the ensemble. This can be done by using a large number of realisations, by increasing the travel time or distance, or by increasing the initial spatial extent of the plume source. Dagan (1991) investigated the effects of ergodicity on the behaviour of spatial moments. He showed that the controlling factor for the fulfilment of the ergodicity requirement in solute transport is the ratio of l_2, the transverse dimension of the solute input area, to λ_Y, the log-conductivity correlation scale, the longitudinal dimension l_1 having no effect since in a steady flow field the streamlines will be aligned through the input area and thus the cloud particle paths are correlated.

Dagan (1991) found analytically that if the ratio of l_2 to λ_Y is not larger than a given threshold value, the ensemble spatial moments are smaller than those obtained at the ergodic limit and are controlled by the value of l_2 irrespective of the relative value of λ_Y or the number of realisations. For increasing values of l_2 the ensemble spatial moments will tend to their ergodic limit and then be controlled by the value of λ_Y. This means that for a cloud with an initial source area to integral scale ratio less than the required value, the solute body will disperse modestly around its centroid. However, the centroid itself is subjected to a random motion of increasing uncertainty.

Numerical approaches are invaluable in the development of stochastic methodologies for groundwater flow, however a heavy computational burden may be imposed by the large field size or high number of realisations required to fulfil the ergodic assumption, depending in part on solute source characteristics. Therefore, it is important to investigate the physical requirements for fulfilment of the hypothesis in order to provide guidelines for numerical simulations.

4. Discretisation of hydraulic conductivity

The issue of discretisation is extremely important for the application of numerical stochastic methods, both when considering theoretical comparisons and plume identification. The level of discretisation determines the plume variance and the magnitude of numerical effects influencing particle tracking. The discretisation of hydraulic conductivity is often arbitrarily chosen to match the solution grid, and it is generally perceived (e.g. Davis, 1986) that the smaller the hydraulic conductivity discretisation the better will be the subsequent reproduction of dispersion. However, owing to the computational expense invoked by the use of fine mesh grids to represent hydraulic conductivity fields a guide to the relationship between an increase in the level of spatial discretisation of hydraulic conductivity and the corresponding increase in the accuracy of the description of dispersion, would be useful. Although this has been considered analytically by Ababou et al. (1989), few detailed quantitative investigations of this hypothesis have been made.

The salient issue is the number of hydraulic conductivity points per integral scale that are required to reproduce correctly the spatial second moments. Since dispersion is affected by the discretisation of both the hydraulic conductivity grid and the flow solution grid, it is necessary to separate these two components to assess the contribution from the hydraulic conductivity discretisation.

5. Experimental aims

The objectives of the experiments detailed herein are threefold: to provide a comparison with analytical solutions; to assess the effect on this relationship of the initial solute source dimensions, and hence fulfilment of the ergodic requirement; and to investigate the level of discretisation of the hydraulic conductivity field. The first comparison will also serve to verify the methodology, anchoring it to a theoretical base.

The experiments enable an investigation of the relative behaviour of the plume spatial second moments X_{11} and S_{11} for a range of initial source dimensions. Checks on ergodicity are made through the observation of the behaviour of $\mathrm{d}R_{11}/\mathrm{d}t$, a comparison of individual and ensemble longitudinal variances ($\langle S_{11}\rangle$ and S_{11}), and through a comparison of theoretical and numerical results. The theoretical model used for prediction of X_{11} is that of Dagan (1982, 1984, 1987); despite the approximations and simplifications used in the derivation of this approach it is generally believed that it provides an accurate model of longitudinal dispersion and it has been successfully fitted to the Borden aquifer plume (Freyberg, 1986; Barry et al., 1988). Since Dagan's model is implicitly ergodic we believe that a comparison of its predicted theoretical variances and numerical results in an appropriate indicator for ergodicity, although not a rigorous evaluation.

The experiments also examine the role of hydraulic conductivity discretisation in the description of dispersion and indicate appropriate values for the practical application of stochastic dispersion models. The spatial discretisation of the finite difference model grid was kept constant to eliminate variability of boundary and numerical effects, thus the combined effects of permeability and solution grid discretisation have not been considered.

6. Experimental procedure

The experiments consider the movement of a conservative tracer convected under steady-state conditions by a random velocity field arising from a heterogeneous hydraulic conductivity field. Both the velocity and log–hydraulic conductivity fields were treated as stationary spatial random functions. The field generation and flow and transport simulation were couched within a stochastic framework. Essentially the experimental procedure has no reliance on dispersion parameters and uses the stochastic simulation of hydraulic conductivity and the subsequent advective movement of particles over the resulting flow field to replicate dispersive processes.

The turning bands method, developed by Matheron (1973), was used to generate random, stationary, isotropic, log–normally distributed two-dimensional hydraulic conductivity fields with prescribed mean, variance, and covariance function. The spectral method of Mantoglou and Wilson (1982) was used for line generation and 50 evenly distributed lines were used. The number of spectral harmonics (150) and the width of the bands (one-half the discretisation spacing) were selected as a compromise between computing speed and accuracy. Generated hydraulic conductivity field statistics were reproduced to the same level of accuracy as that encountered in similar work in the literature.

A regularly spaced block-centred finite difference grid was used. Measuring 500×500 blocks, the node separation was 1 m, resulting in a modelled area of $500\,\mathrm{m} \times 500\,\mathrm{m}$. The nominal aquifer depth was 10 m. The flow situation was confined between two fixed head and two no-flow boundaries. A single porosity value of 0.3 was used for the whole domain. The head gradient across the field was 0.5 m. Hydraulic conductivity was generated over the domain as a spatial random variable with an exponential structure for which the natural log–mean conductivity value was 1.0 and the log–standard deviation ranged from 0.2 to 1.0. The resulting random field had a correlation length (λ_Y) of 5 m. The resulting average field velocity was 9×10^{-3} m day^{-1}.

The hydraulic conductivity field was simulated at several different levels of discretisation. The finite difference grid node spacing was kept constant and different sized blocks of hydraulic conductivity, centred upon the discrete point values and generated via turning bands, were superimposed upon this grid. Thus, the experiment was primarily influenced by the discretisation of hydraulic conductivity rather than numerical effects of the solution grid discretisation. The levels of discretisation used were 1 m ($0.2\,\lambda_Y$), 2 m ($0.4\,\lambda_Y$) and 5 m (λ_Y). Fifty simulations were carried out at each level of discretisation. For a source size of at least ten correlation lengths this was observed to be adequate.

Over the discretised domain, the hydraulic heads were solved for prescribed boundary conditions using the preconditioned conjugate gradient option of the USGS finite difference model MODFLOW (McDonald and Harbaugh, 1988).

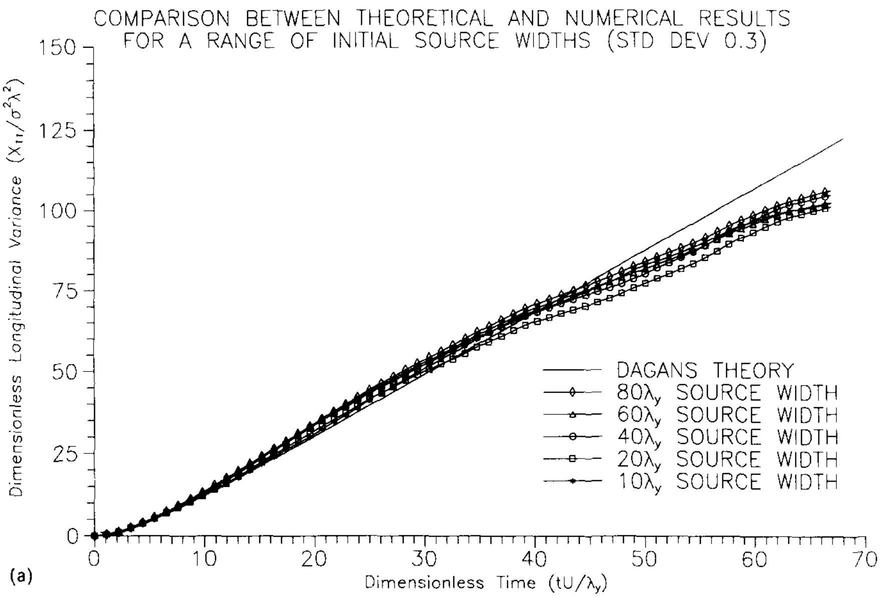
The computed heads were differentiated to derive the velocity through each cell face which served as the input to the particle tracking software, MODPATH (US Geological Survey, 1989). This uses the semianalytical method of Pollock (1988) for the computation of particle pathlines. Velocities were interpolated linearly within a cell from the face velocities, and an analytical expression describing the flow path within a cell. Small-scale diffusion and microdispersion within the grid cell were ignored.

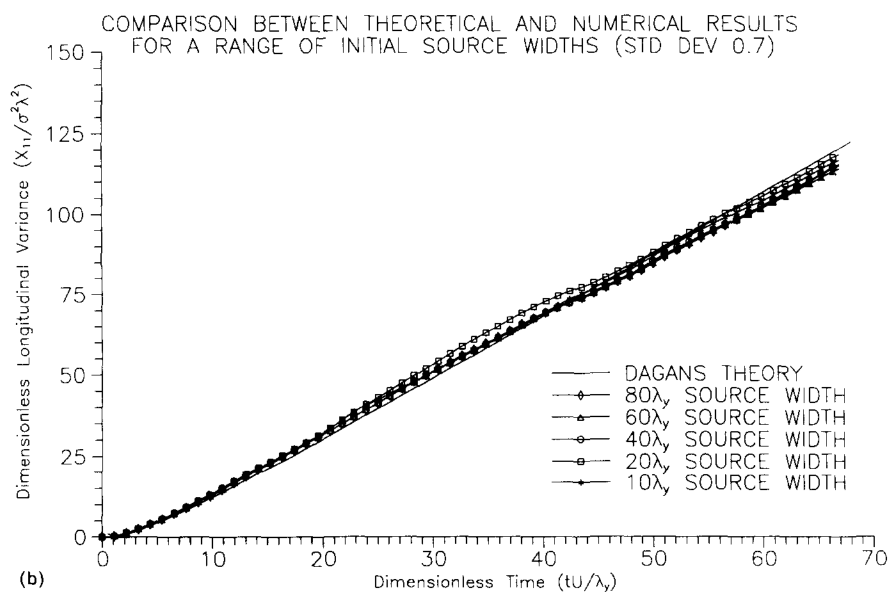
As noted above, an important aspect of the approach is that the resulting solute dispersion is represented as entirely resulting from advective processes caused by small-scale velocity variations, with no additional dispersion terms being used.

The solute source was represented by rectangular blocks of particles of variable size, with the longer axis oriented perpendicular to the direction of flow. The number of particles used in the representation of the source can also have an effect on dispersion, however this is only significant for small particle numbers (tens of particles). Here 1200 particles were used for each source size, evenly distributed within the source area, and it was found that an increase in this number had little effect on the dispersion characteristics. Five different source areas were considered. For each the longitudinal dimension (l_1) was 1 m and the transverse dimensions (l_2) were 50 m, 100 m, 200 m, 300 m and 400 m, respectively. Thus, these represent areas ranging from $0.2\,\lambda_Y \times 80\,\lambda_Y$ to $0.2\,\lambda_Y \times 10\,\lambda_Y$.

Bellin et al. (1991) estimated that velocity fields are affected by the boundary conditions for a region of up to $3\,\lambda_Y$ (for medium-scale log–variances). Hence, to avoid boundary effects the source area was located 15 m from the edge of the domain, equivalent to three correlation lengths. It can therefore be assumed that the Dagan (1984, 1987) assumption of an infinite field holds for these simulations.

The variance of each of the resulting plumes was calculated as it traversed a randomly generated hydraulic conductivity domain. The process is set in a stochastic framework and the individual variances were combined and averaged over each set of 50 realisations. Both the individual particle variance from the actual plume centroid


COMPARISON BETWEEN THEORETICAL AND NUMERICAL RESULTS
FOR A RANGE OF INITIAL SOURCE WIDTHS (STD DEV 0.3)
Dimensionless Longitudinal Variance ($X_{11}/\sigma^2\lambda^2$)
150
125
100
75
50
25
0
0
10
20
30
40
50
60
70
Dimensionless Time (tU/λ_y)
DAGANS THEORY
80λ_y SOURCE WIDTH
60λ_y SOURCE WIDTH
40λ_y SOURCE WIDTH
20λ_y SOURCE WIDTH
10λ_y SOURCE WIDTH
(a)


COMPARISON BETWEEN THEORETICAL AND NUMERICAL RESULTS
FOR A RANGE OF INITIAL SOURCE WIDTHS (STD DEV 0.7)
Dimensionless Longitudinal Variance ($X_{11}/\sigma^2\lambda^2$)
150
125
100
75
50
25
0
0
10
20
30
40
50
60
70
Dimensionless Time (tU/λ_y)
DAGANS THEORY
80λ_y SOURCE WIDTH
60λ_y SOURCE WIDTH
40λ_y SOURCE WIDTH
20λ_y SOURCE WIDTH
10λ_y SOURCE WIDTH
(b)

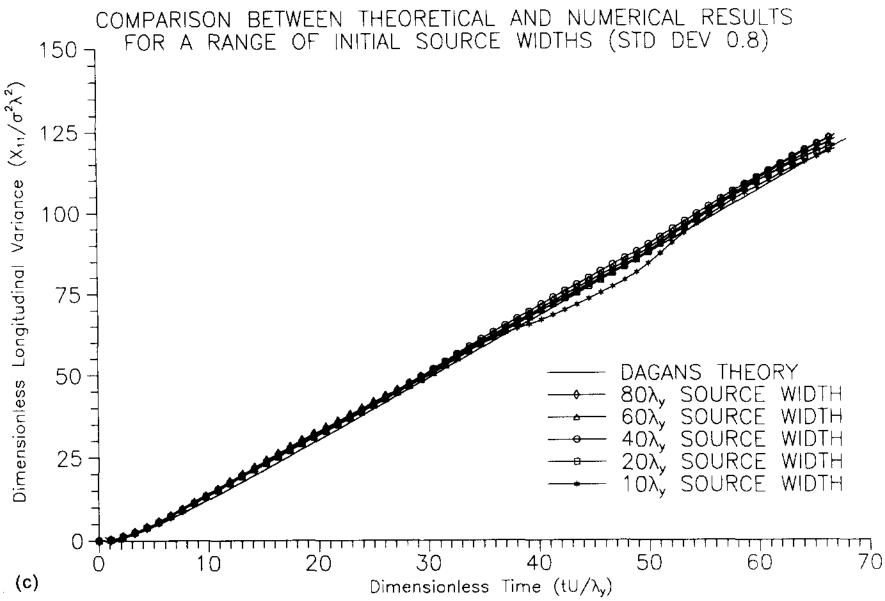


Fig. 1. Graph of dimensionless longitudinal variance ($X_{11}/\sigma^2\lambda_Y^2$) vs. dimensionless time (tU/λ_Y), for a hydraulic conductivity log standard deviation of 0.3 (a), 0.7 (b), 0.8 (c), and a range of initial source widths.

S_{11} and the variance of the plume centroid with respect to the expected centroid R_{11} were recorded, then using the initial variance $S_{11}(0)$, the longitudinal variance with respect to the expected centroid X_{11} could be computed via Eq. (1).

7. Results

Figures 1–5 show a comparison of theoretical and numerical results for source widths ranging from 80 λ_Y to 10 λ_Y and a range of variances (σ_Y^2) of the hydraulic conductivity field. Results are presented for dimensionless longitudinal variance relative to the expected advective centroidal position ($X_{11}/\sigma_Y^2\lambda_Y^2$), dimensionless longitudinal variance relative to the plume centroidal position ($S_{11}/\sigma_Y^2\lambda_Y^2$) and dimensionless centroidal variance relative to the expected centroid ($R_{11}/\sigma_Y^2\lambda_Y^2$), as a function of dimensionless time (tU/λ_Y). Figures 1–3 and Fig. 5 show the averaged results of 50 simulations, any increase in the number of realisations having very little effect on the results, which can therefore be regarded as ensemble values. The results shown in Fig. 4 pertain to a single realisation.

Figures 1(a), (b) and (c) show a good match between the experimental variance and Dagan's linear theory for all source sizes considered, for log–standard deviations of the hydraulic conductivity field of 0.3, 0.7 and 0.8. Similar results were obtained for the full range of log–standard deviations considered (i.e. 0.2–1.0). More importantly, there is a consistency between the source area results. This is in agreement with theory and implies that the variance in the mean plume trajectory accounts for the difference between X_{11} and S_{11}. Figures 2(a), (b) and (c) show the values of S_{11} for the full range of source sizes. It can be seen that the deviation from the expected theoretical variance increases as the source size decreases. However, the major point to notice here is that the change in S_{11} is greatest between 10 λ_Y and 20 λ_Y; the values from 20 λ_Y to 80 λ_Y, although deviating slightly from the theory, are very similar. Figure 3 augments the above results, showing only small-scale fluctuations of R_{11} for source widths ranging from 80 λ_Y to 20 λ_Y, indicating $dR_{11}/dt \approx 0$, but in comparison, the 10 λ_Y source width gives rise to an increasing value of R_{11} with time.

When we consider the results of an individual realisation simulation for the same variances as the ensemble values (Fig. 4), deviations from the theoretically derived variance and the numerical results shown in Fig. 1(a) are observed. However, the major features are reproduced and again the results for the 10 λ_Y manifest the greatest deviation from the theoretical variance.

The results of varying the hydraulic conductivity discretisation are shown in Figs. 5(a), (b) and (c). Results are shown for the 80 λ_Y source width, however the results are replicated for all source sizes. The results are for log–standard deviations of the hydraulic conductivity field of 0.3, 0.7 and 0.8, respectively. It can be seen that there is a good match between the longitudinal variances for 1 m (0.2 λ_Y) discretisation and Dagan's theoretical longitudinal variance ($X_{11}/\sigma_Y^2\lambda_Y^2$). The 2 m (0.4 λ_Y) discretisation also provides a reasonable match to the theory, having the same trend and behaviour as the 1 m results. However, as the discretisation becomes coarser, the solution is less stable and can be observed to converge at an overestimated longitudinal variance, the gradient of the line representing the 5 m (λ_Y) discretisation

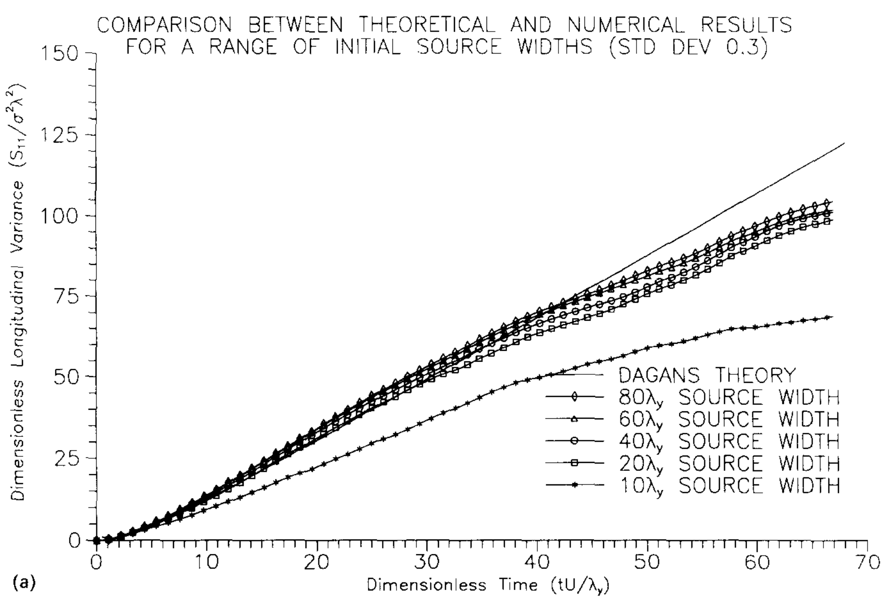
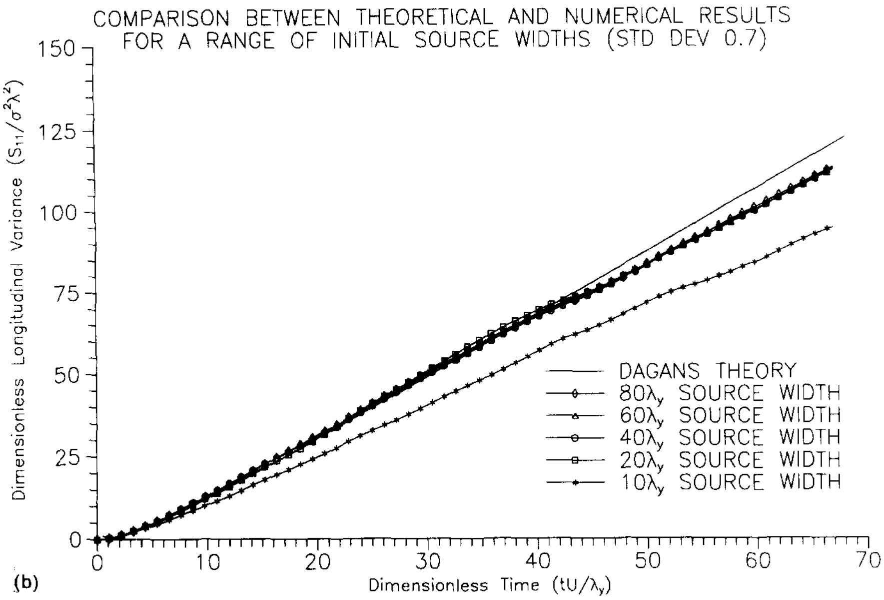


Fig. 2. Graph of dimensionless longitudinal variance ($S_{11}/\sigma^2\lambda_Y^2$) vs. dimensionless time (tU/λ_Y), for a hydraulic conductivity log standard deviation of 0.3 (a), 0.7 (b), 0.8 (c), and a range of initial source widths.


COMPARISON BETWEEN THEORETICAL AND NUMERICAL RESULTS
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Dimensionless Longitudinal Variance ($S_{11}/\sigma^2\lambda^2$)
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DAGANS THEORY
80λ_y SOURCE WIDTH
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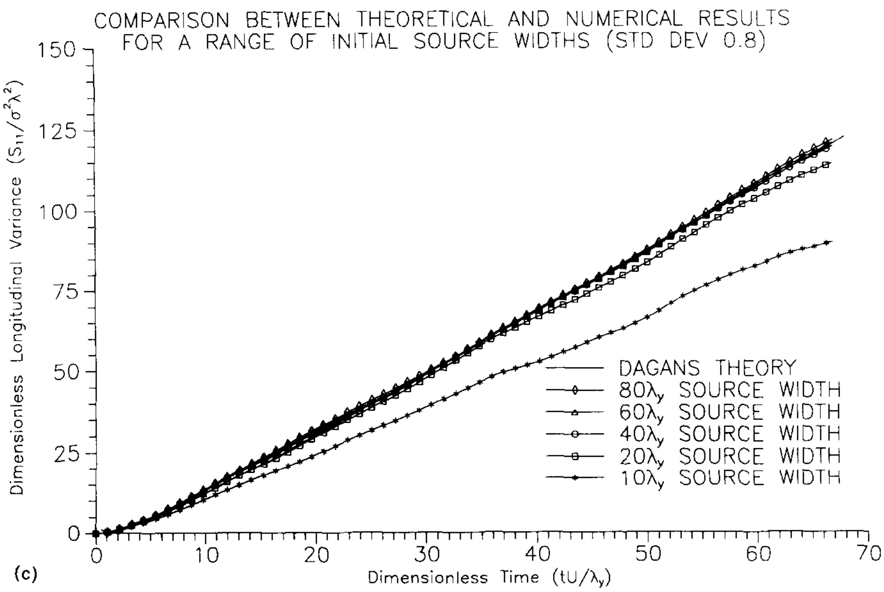
20λ_y SOURCE WIDTH
10λ_y SOURCE WIDTH
0
10
20
30
40
50
60
70
Dimensionless Time (tU/λ_y)

(b)


COMPARISON BETWEEN THEORETICAL AND NUMERICAL RESULTS
FOR A RANGE OF INITIAL SOURCE WIDTHS (STD DEV 0.8)
Dimensionless Longitudinal Variance ($S_{11}/\sigma^2\lambda^2$)
150
125
100
75
50
25
0
DAGANS THEORY
80λ_y SOURCE WIDTH
60λ_y SOURCE WIDTH
40λ_y SOURCE WIDTH
20λ_y SOURCE WIDTH
10λ_y SOURCE WIDTH
0
10
20
30
40
50
60
70
Dimensionless Time (tU/λ_y)

(c)

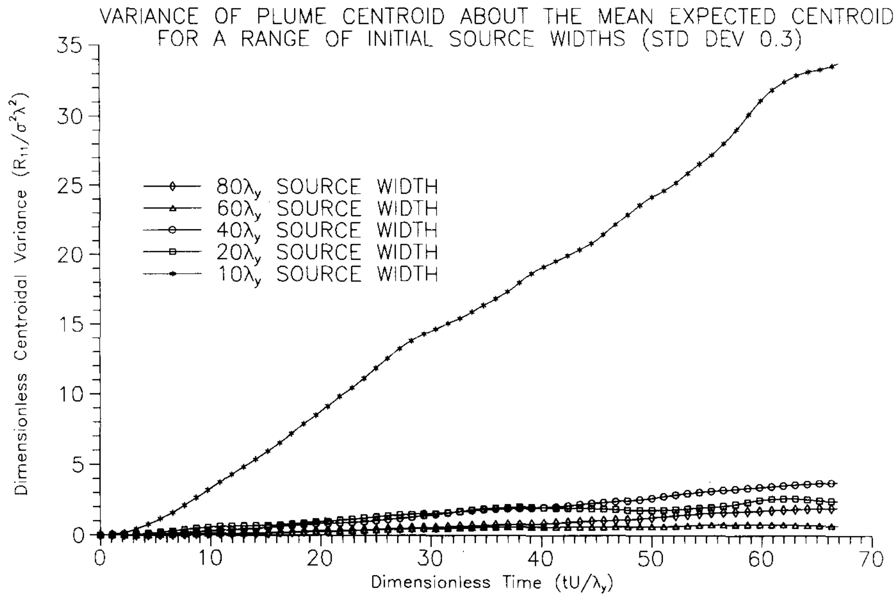


Fig. 3. Graph of dimensionless centroidal variance ($R_{11}/\sigma^2\lambda_Y^2$) vs. dimensionless time (tU/λ_Y), for a hydraulic conductivity log standard deviation of 0.3 and a range of initial source widths.

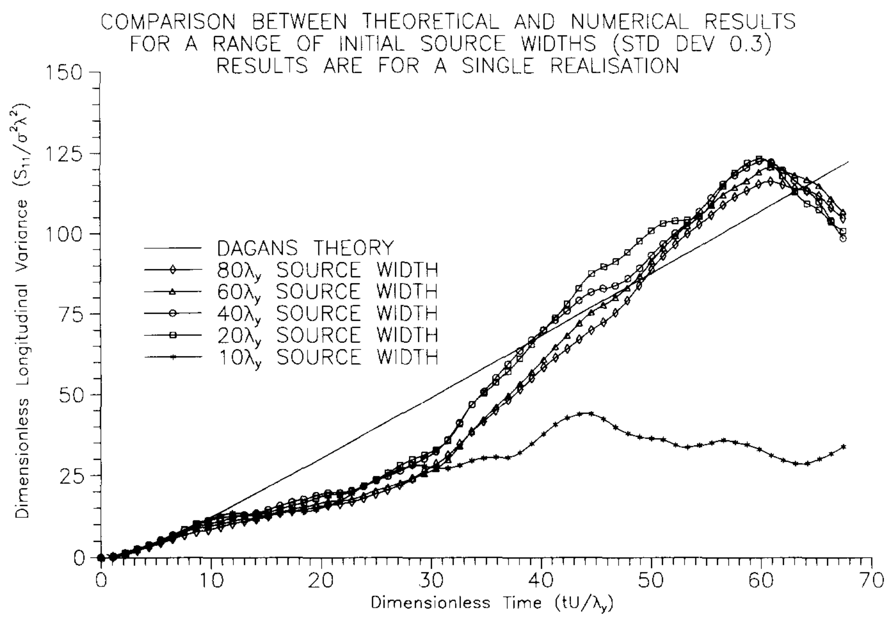


Fig. 4. Graph of dimensionless longitudinal variance ($S_{11}/\sigma^2\lambda_Y^2$) vs. dimensionless time (tU/λ_Y), for a single realisation of a hydraulic conductivity field with log standard deviation of 0.3 and a range of initial source widths.

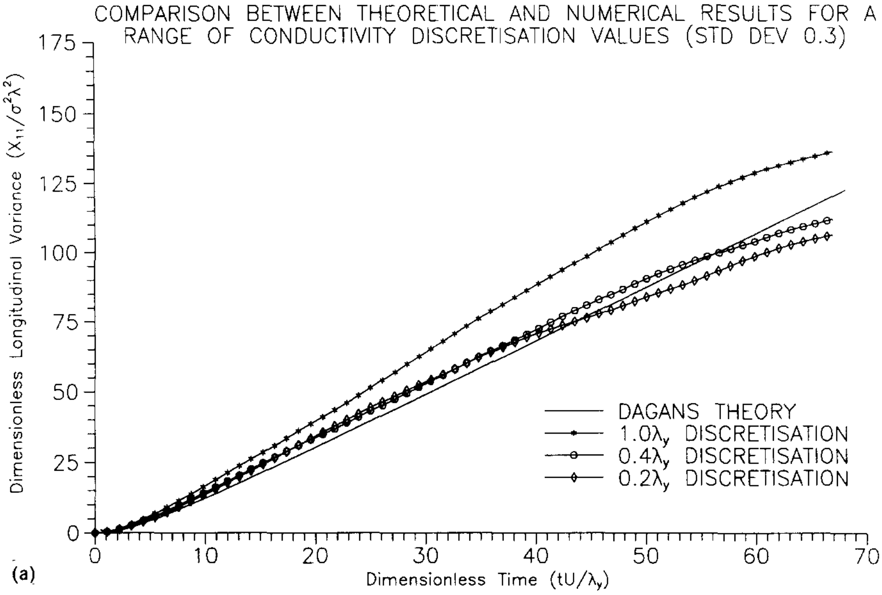
differing markedly from that of the theory. In general, it can be seen that the fit deteriorates as the level of discretisation decreases and that this deterioration is augmented by an increase in the variance of field heterogeneity.

8. Discussion and conclusions

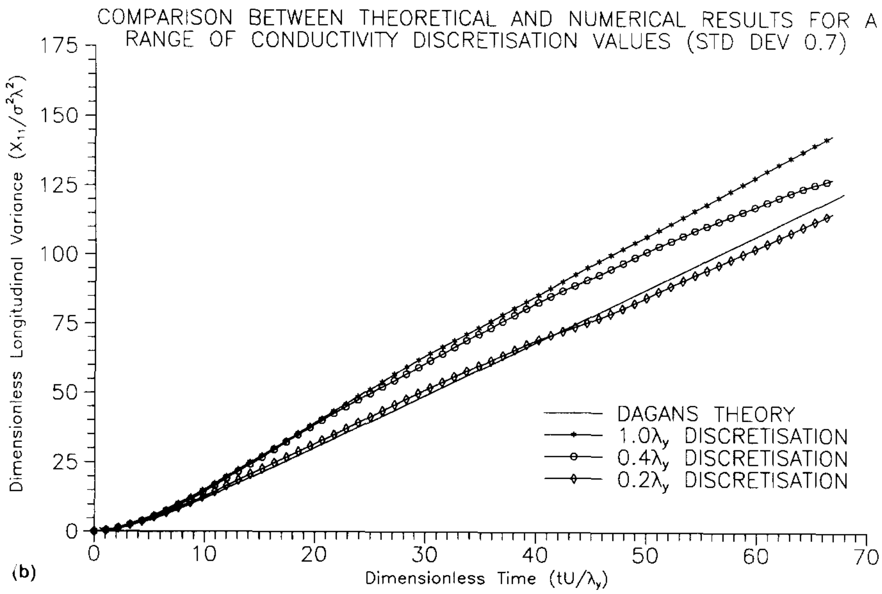
The results demonstrate a match between the numerical method and the main accepted analytical results, and this can be taken as a validation of the use of a numerical stochastic methodology in which transport processes are represented purely by small-scale advection, with no recourse to additional dispersion terms. They also show that in the subergodic range, plume variance manifests itself as both S_{11} and R_{11}, with their sum X_{11} remaining constant for various initial source widths l_2. Thus, X_{11} can be considered as appropriate for the comparison of plume statistics in the subergodic range. A tendency to ergodicity was found for a source dimension l_2 of only 20 λ_Y which is less than predicted in Dagan (1991) and Valocchi (1990) but is in keeping with the comments in Cvetkovic et al. (1992).

Dagan (1991) derived an analytical expression for D_L and investigated its dependence on l_2/λ_Y and the point at which it tended to its ergodic limit. With reference to the work of Valocchi (1990), an l_2 value of 10^2 times the correlation length was postulated as the value required to ensure ergodicity. The results in Fig. 4 pertaining to a single realisation are similar to those of Valocchi (1990) and show that even for a source size of 80 λ_Y there is failure to match the ensemble variance. Dagan (1991) also comments on the behaviour of D_L with increasing source size, showing that the approach to the ergodic limit increases rapidly with increasing l_2 and this is replicated in our ensemble results. However, although the value of 10^2 may be appropriate for an exact fulfilment of the ergodic requirement, the results have shown that for l_2/λ_Y ratios greater than 20 the difference between theoretical and numerical variances is relatively small and that $\mathrm{d}R_{11}/\mathrm{d}t \approx 0$. Cvetkovic et al. (1992) derived expressions of the covariance of mass flux and the cumulative mass flux as functions of l_2/λ_Y and also showed (for both two- and three-dimensional conditions) that for an l_2/λ_Y of 20, near-ergodic conditions were achieved. It therefore appears that an l_2 of 20 λ_Y is sufficient to provide near-ergodic conditions. It may be possible (G. Dagan, personal communication, 1993) that the use of $\langle S_{11}\rangle$ rather than effective dispersion coefficients $1/2\,\langle \mathrm{d}S_{11}/\mathrm{d}t\rangle$ accounts for this earlier stabilisation, and this is currently under investigation.

Ababou et al. (1989) suggested that discretisation effects may be avoided when the number of points per integral scale is greater than $1+\sigma_Y^2$. Bellin et al. (1991) obtained similar results, observing higher longitudinal variance for coarser grid discretisations, and a convergence of solutions for values of discretisation below $1+\sigma_Y^2$. These findings are echoed in the results obtained here. For discretisations below this value the longitudinal variances tend to those of Dagan's theory, above this value the results are unstable and converge to incorrect asymptotic values. However, it was observed that although this criterion gives a good indication of the level at which deviation from the theory occurs, it is not a threshold value and degradation in


COMPARISON BETWEEN THEORETICAL AND NUMERICAL RESULTS FOR A RANGE OF CONDUCTIVITY DISCRETISATION VALUES (STD DEV 0.3)
Dimensionless Longitudinal Variance $(X_{11}/\sigma^2\lambda^2)$
Dimensionless Time (tU/λ_y)
DAGANS THEORY
$1.0\lambda_y$ DISCRETISATION
$0.4\lambda_y$ DISCRETISATION
$0.2\lambda_y$ DISCRETISATION
0
25
50
75
100
125
150
175
0
10
20
30
40
50
60
70

(a)


COMPARISON BETWEEN THEORETICAL AND NUMERICAL RESULTS FOR A RANGE OF CONDUCTIVITY DISCRETISATION VALUES (STD DEV 0.7)
Dimensionless Longitudinal Variance $(X_{11}/\sigma^2\lambda^2)$
Dimensionless Time (tU/λ_y)
DAGANS THEORY
$1.0\lambda_y$ DISCRETISATION
$0.4\lambda_y$ DISCRETISATION
$0.2\lambda_y$ DISCRETISATION
0
25
50
75
100
125
150
175
0
10
20
30
40
50
60
70

(b)

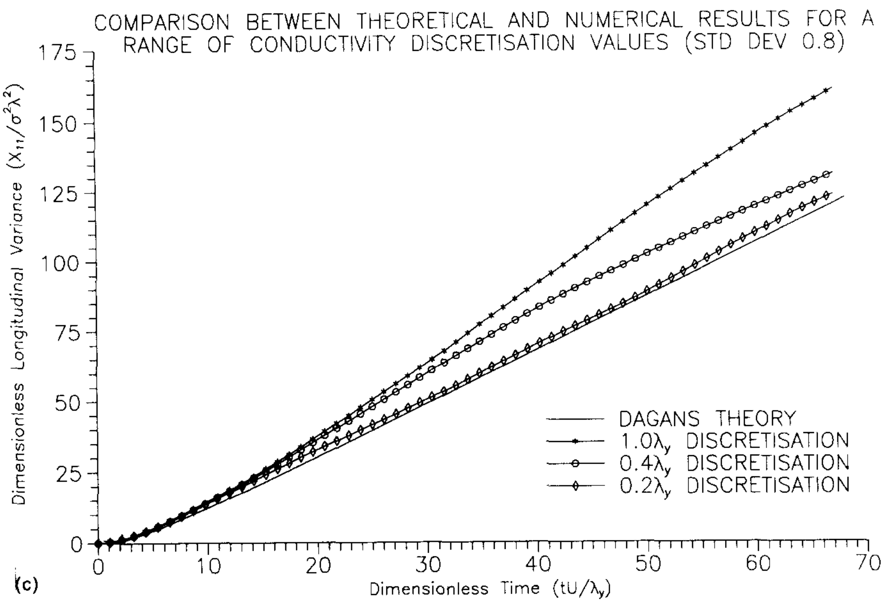


Fig. 5. Graph of dimensionless longitudinal variance ($X_{11}/\sigma^2\lambda_Y^2$) vs. dimensionless time (tU/λ_Y), for a hydraulic conductivity log standard deviation of 0.3 (a), 0.7 (b), 0.8 (c), and a range of conductivity discretisation values.

performance is gradual, with all changes in discretisation affecting the resulting longitudinal variances.

The increased longitudinal variances for the coarser grids may be due to the poor description of the correlation structure causing abrupt changes in conductivity between adjacent cells. Also, the representation of the variogram of the spatial hydraulic conductivity field, specified a priori, may break down as the conductivity integral scale is exceeded by the discretisation, although the field will still yield the correct statistics. This may be the reason for the marked deviation from theory for the discretisations greater than the integral scale.

Therefore the main specific conclusions are:

(1) that the ratio of source size to characteristic length scale of conductivity correlation is evidently an important factor in dispersion;

(2) that a source dimension l_2 of 20 λ_Y may be adequate to ensure near-ergodic conditions;

(3) that the use of a grid resolution greater than $1 + \sigma_Y^2$ is computationally wasteful in terms of increasing the accuracy of dispersion.

More generally, the results validate the stochastic numerical procedure, but for a relatively simple case. More complex applications which better represent natural systems are required. Furthermore, investigations are needed of the extent to which incorporation of increasing levels of data availability, through the use of conditioning and screening algorithms, affects the computational efficiency of the Monte Carlo-based scheme.

9. Acknowledgements

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