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# The effects of non-linear bromide adsorption on apparent macrodispersivity

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# THE EFFECTS OF NON-LINEAR BROMIDE ADSORPTION ON APPARENT MACRODISPERSIVITY

by

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This thesis, submitted by Eron J. Dodak in partial fulfillment of the requirements for the Degree Master of Science from the University of North Dakota, has been read by the Faculty Advisory Committee under whom the work has been done and is hereby approved.

Scott F. Korom
(Chairman)

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Philip J. Gerla

This thesis meets the standards for appearance, conforms to the style and format requirements of the Graduate School of the University of North Dakota, and is hereby approved.

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Dean of the Graduate School

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| Department | Geology and Geological Engineering |
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To Robert and Darlene Dodak

# ABSTRACT

Macrodispersivity estimates are crucial in predicting the subsurface transport of contaminants. These predictions have become increasingly important as the number of contaminated sites continues to increase. In addition, the longevity of many contaminants can affect water quality over extended periods of time.

Anionic tracers such as bromide and chloride are commonly used as groundwater tracers in dispersivity experiments because they are inexpensive, easily detected, and are commonly believed to behave conservatively. It has been found, however, that anionic tracers do not always behave conservatively; sediments with a net positive surface charge can adsorb some of the tracer.

A weakly non-linear, experimentally derived Freundlich sorption isotherm was found to describe bromide adsorption in sediments from the Savannah River Site in South Carolina. The aim of this research was to quantify the effects of this sorption on apparent dispersivities relative to a conservative tracer. In addition, the effects on apparent dispersivities of injecting different amounts of tracer and omitting tracer concentrations below detection limits were evaluated.

Monte Carlo simulations were performed using SUTRA and WATSUTRA. The models were developed to simulate natural gradient tracer tests. Two types of hydraulic conductivity fields were generated using the Fast Fourier Transform method. One represented a weakly heterogeneous flow field, with physical parameters similar to the Borden aquifer in Ontario, Canada; the other represented a strongly heterogeneous flow

field with physical parameters similar to the Columbus aquifer in Mississippi. These hydraulic conductivity fields represent two extremes of aquifer conditions.

Forty simulations were performed in this study for eight cases. Five realizations were performed for each case; each realization was simulated for two years. Apparent dispersivities were calculated by the method of moments. Ensemble means were estimated by averaging the apparent longitudinal or horizontal transverse dispersivity values for the five realizations in each case. Null hypothesis testing was performed with a standard t-test to test the significance between the estimates for the ensemble means for various cases.

The following simplifying assumptions were used in this research:

1) Sorption according to the Freundlich isotherm was assumed to be a reversible equilibrium process. Thus, desorption followed the same isotherm as adsorption, only with decreasing concentrations, and both adsorption and desorption were rapid in comparison to advective flow.

2) The Freundlich isotherm was constant throughout the model domain.

3) The groundwater model employed was two-dimensional; vertical heterogeneity was not represented.

The results indicated the experimentally derived Freundlich isotherm, given the assumptions and limited number of realizations used in this study, did not significantly affect apparent plume dispersivity values. Thus, bromide was not found to be an unsuitable groundwater tracer. The quantity of tracer mass injected and omission of tracer concentrations below detection limits also did not have a significant effect on apparent dispersivity values. It was found that using tracer concentrations below detection level can adversely affect high-order spatial moments; this finding may, however, be unique to SUTRA and WATSUTRA or similar finite-element programs.

# INTRODUCTION

The quantification of macrodispersivity is important in assessing the spreading of a plume as it travels through an aquifer. Macrodispersivity affects the lateral, vertical, and longitudinal extent of a contaminant plume. The way in which a plume disperses as it moves though an aquifer will affect the type of remediation strategy best suited for a site. This has become increasingly important as the number of contaminated sites continues to increase. In addition, the longevity of many contaminants can affect groundwater quality over extended periods of time.

Over the past 40 years dispersivity research has moved from small-scale laboratory column tests, to larger-scale single-well tracer tests, and finally to large-scale natural gradient tracer tests. The advantage of the natural gradient tracer test is that it can be used to calculate longitudinal and transverse dispersivities on a field scale of hundreds of meters under natural groundwater flow conditions. Contaminant plumes found in nature are generally of this scale. The results of a natural gradient tracer test can be used as a predictive tool in subsurface transport and in transport model testing.

Conservative tracers are an important tool in natural gradient tests because they do not react with the solid or liquid phases in an aquifer; thus, the movement and spreading of the tracer is caused by groundwater flow. Anionic tracers such as bromide and chloride are commonly used as groundwater tracers because they are inexpensive, easily detected, and are commonly believed to behave conservatively. The conservative nature of anionic tracers is due to the net negative surface charge on many sediments, which repels anions and limits interaction between the anion and mineral surfaces.

There are two types of surface charges found on minerals, 1) constant surface charge minerals, which dominate in temperate climates, and 2) variable surface charge minerals, which dominate in tropical climates (Uehara and Gillman, 1981, p. 2-3). The charge on minerals with a constant surface charge is permanent. A perfectly formed crystal lattice will have no net surface charge because the atoms in the crystal are electrically balanced (Uehara and Gillman, 1981, p. 31). Some crystals do, however, possess defects within the crystal lattices. This is generally the result of isomorphic substitution, which is the substitution of an ion at a particular site in the crystal lattice with one of a different, generally lower, valence. The result is a charge imbalance in the crystal lattice that is permanent. This generally leads to a net negative surface charge, which is balanced by counterions in solution (Uehara and Gillman, 1981, p. 2). Anionic tracers such as bromide and chloride are generally conservative in sediments with constant charge minerals because the net negative surface charge of the sediments repels anionic tracers.

Some highly weathered sediments found in tropical climates, however, may have a net positive surface charge that may lead to adsorption of some of the anionic tracer. In such climates the constant surface charge minerals are generally severely altered or completely weathered out (Uehara and Gillman, 1981, p. 3). Sediments containing significant quantities of variably charged minerals such as Fe and Al oxides tend to adsorb anionic tracers (Uehara and Gillman, 1981, p. 43). The surface charge of the oxide is generated by potential-determining ions in solution, principally $H^+$ and $OH^-$. Thus, the pH governs the sign and magnitude of the charge. The pH where the net surface charge is zero is the zero point of charge (ZPC). This indicates that equal amounts of $H^+$ and $OH^-$ have been adsorbed onto the oxide's surface. The ZPC of Fe and Al oxides is generally within the range of pH 7-9, and depends on the composition and degree of crystallinity of the oxide (Uehara and Gillman, 1981, p. 46). At pH values below ZPC, more $H^+$ is adsorbed than $OH^-$; thus the mineral surface charge will be positive and an anionic tracer may be adsorbed onto the surface of the oxides to maintain charge neutrality. As a result, some of the tracer may be lost from solution.

Sediments with a net positive surface charge are present at the Savannah River Site (SRS) in South Carolina (Seaman et al., 1996). SRS is a 775 $km^2$ Department of Energy complex on the Atlantic Coastal Plain. Column studies were conducted on sediment samples from SRS (Korom, 1994, personal communication). The sediments are part of the Dry Branch Formation and consist primarily of medium- to fine-grained sands with less than one percent silt and clay. Undisturbed horizontal sediment cores were taken from an erosional cut approximately 60 feet deep (Korom, 1994, personal communication).

The column studies were performed with the samples by injecting known concentrations of tritium ($^3H$) and bromide ($Br^-$) through the column at an average rate of 0.103 m/day. The bromide had calcium as the carrier cation ($CaBr_2$). Tritium was used as the conservative tracer. The concentration of the influent was increased in order-of-magnitude increments and was then reduced sequentially to the initial low concentrations. Bromide concentrations of almost 4 orders of magnitude were tested. At each concentration, the amount of bromide adsorbed was calculated relative to tritium breakthrough curves (BTC), which were fitted using CXTFIT (Parker and van Genuchten, 1984). The difference between the tritium and bromide BTCs is related to the quantity of bromide adsorbed onto the sediment. The mass of bromide adsorbed per mass of sediment, $C_s$, was plotted against the mass of bromide per mass of water, C, on log-log axes. The resulting linear regression (95% confidence intervals on the regression) yielded the following equilibrium Freundlich isotherm:

$$C_s = 8.64 \times 10^{-5} (\rho C)^{(1/1.12)} \tag{1}$$

where ρ is the density of water ($M/L^3$). The sorption coefficient in the Freundlich isotherm, $8.64 \times 10^{-5}$, represents the y-intercept value of the line in the graph of log $C_s$ verses log C. The Freundlich exponent, $n = 1/1.12$, represents the slope of the line, and is defined for values $0 < n < 1$; a value of 1 indicates linear sorption. An implicit assumption of a Freundlich isotherm is that sorption equilibrium is rapid in comparison to advective groundwater flow (Fetter, 1993, p. 117).

The aim of this research was to quantify, using some simplifying assumptions, the effects of the non-linear sorption isotherm in Eq. (1) on apparent dispersivities relative to that of a conservative tracer. A numerical groundwater model was developed to quantify the effects because actual natural gradient tracer tests are costly to perform. This will provide guidelines on whether anionic tracers can be used in sediments onto which they are adsorbed following a similar sorption isotherm. This study also examined the effects of an order-of-magnitude difference in the amount of tracer mass used in the simulated natural gradient tests. In addition, the effects of omitting concentrations below a detection level, set at 0.1 part per million (ppm), were examined.

# BACKGROUND

The purpose of this section is to provide the reader with a general knowledge of solute transport and stochastic groundwater modeling. The basic concepts of solute transport will be discussed with an emphasis on dispersion, the focus of this study. Stochastic groundwater modeling, the approach to solute transport modeling used this study, will also be discussed.

## Solute Transport

Solute transport is the result of advection, mechanical dispersion, molecular diffusion, and chemical reactions. Advection is the movement of groundwater as a result of a hydraulic gradient. Mechanical dispersion is caused by variations in flow velocity at the pore and field scales. Molecular diffusion is the movement of a solute as a result of a concentration gradient. Mechanical dispersion requires advection; molecular diffusion does not. Mechanical dispersion and molecular diffusion are commonly combined into a quantity called hydrodynamic dispersion because they cannot be evaluated independently in flowing groundwater (Fetter, 1993, p. 51). Chemical reactions include sorption, transformation, and precipitation/dissolution. Adsorption of anionic tracers, the focus of this study, is commonly a result of ionic attractions between the tracer and aquifer sediments.

### Advection

Advection is described by Darcy's law, which states that the flow rate through a porous medium is proportional to the hydraulic gradient; the proportionality constant is hydraulic conductivity. The hydraulic conductivity is a measure of the permeability of sediments for a given fluid (generally water). Permeability is a measure of how readily fluids can move through a porous medium and is an intrinsic property of the porous medium. Darcy's law can be used to estimate groundwater velocity; the form used to calculate average linear velocity in the i direction is:

$$v_i = -(K/n)*(dh/dl) \tag{2}$$

where K is the hydraulic conductivity (L/T), n is effective porosity ($L^3/L^3$), and dh/dl is the hydraulic gradient (L/L).

### Hydrodynamic Dispersion

Hydrodynamic dispersion, as stated above, consists of two terms, mechanical dispersion and molecular diffusion. Mechanical dispersion is defined as dispersivity times average linear velocity. Dispersivity is a mixing length; it is an intrinsic property of the porous medium. It results from variations in flow velocity at the pore and field scales. If dispersion did not occur, there would be an abrupt interface between the solute and uncontaminated groundwater; the solute would move like a plug. The molecular diffusion component of hydrodynamic dispersion is a result of concentration gradients. Solutes in water spontaneously travel from areas of high concentration toward areas of low concentration. Molecular diffusion is a result of mixing caused by random molecular motions due to the thermal kinetic energy of the solute in solution (Domenico and Schwartz, 1990, p. 367).

The hydrodynamic dispersion coefficients in the longitudinal, $D_L$, and horizontal transverse, $D_T$, directions are:

$$D_L = \alpha_L v_i + D^* \tag{3}$$

$$D_T = \alpha_T v_i + D^* \tag{4}$$

where $\alpha_L$ is the longitudinal dispersivity (L), $\alpha_T$ is the transverse dispersivity (L), and D* is the effective molecular diffusion coefficient ($L^2/T$).

The longitudinal direction is parallel to the principal direction of flow; the horizontal transverse direction is in the horizontal plane perpendicular to the direction of flow. A third component, the vertical transverse direction, is commonly neglected because mixing in the vertical plane is very small in naturally stratified sediments (Gelhar et al., 1992).

In most groundwater systems the molecular diffusion term of hydrodynamic dispersion can be neglected because it is insignificant in comparison to mechanical dispersion. The only cases where diffusion would dominate are where concentration gradients are high and hydraulic gradients and/or hydraulic conductivities are low (Perkins et al., 1963).

Mechanical dispersion occurs at the pore and field scales. At the pore scale, mechanical dispersion is mainly due to heterogeneities in the sediment (Wang and Anderson, 1982, p. 175). The result of the heterogeneities (i.e. sediment grains) is varying pore size, flow path length, and velocity distributions in the pore (Fetter, 1993, p. 149). The pore size affects the velocity at which the water will travel; the smaller the pore, the more friction the water encounters with the grains and the slower it travels. Water flows along paths of varying lengths as it moves around individual sediment grains to go a given linear distance. The final cause of dispersion at the pore scale is the velocity distribution in the pore. Water travels fastest in the center of the pore throat and slower where it interacts with the grain surfaces. The factors listed above all cause the water to mix or disperse. Dispersivities at the pore scale are on the order of centimeters (Wang and Anderson, 1982, p. 175).

At the field scale dispersivity, also known as macrodispersivity, is the spreading of a plume at scales of tens to thousands of meters. It is caused by variations in aquifer parameters contained in Darcy's law (Eq. 2). Hydraulic conductivity is by far the most important of these parameters because it can vary several orders of magnitude in a distance of a few meters. Porosity and hydraulic gradient generally vary little in comparison. Thus, macrodispersivity is primarily the result of the variance in hydraulic conductivity of an aquifer. Dispersivities at the field scale are on the order of meters (Wang and Anderson, 1982, p. 175).

Groundwater flows preferentially along paths of the highest hydraulic conductivities. A low conductivity zone, such as a clay lens, will deflect groundwater around the zone. As a plume travels longer distances, more heterogeneities are encountered, and the macrodispersivity of the formation increases. This is known in the literature as the scale effect of dispersivity.

Neuman (1990) performed a fractal analysis on the scaling of longitudinal dispersivities. In the analysis, Neuman derived a semivariogram and fractal dimension that can be viewed as a universal scaling rule. This scaling rule essentially accounts for the self-similarity of natural log transformed hydraulic conductivity values from a wide range of geologic materials, flow conditions, and flow lengths. The universal scaling rule could therefore be used without describing any particular site, other than its length.

Gelhar et al. (1992) believe it is not appropriate to represent longitudinal dispersivity data by a single universal line. They argued the scale effect of dispersivity was less clear when the reliability of the data was considered. In the study they examined dispersivity calculations from 59 different field sites. The dispersivity values were rated by the type of test and method of data analysis. Highly reliable data were only available up to scales of about 300 m. They acknowledged a scale dependence of longitudinal dispersivity, but concluded that more reliable large-scale tests must be performed to determine the nature of the dependence.

Engesgaard et al. (1996) reported a field scale dispersion test on a scale of 1000 m. The researchers reported a longitudinal dispersivity value in the range of 1 to 10 m. The study results apparently do not support the hypothesis that longitudinal dispersivity increases indefinitely with scale.

### Methods of Calculating Dispersivity

There are principally three ways to estimate dispersivities at three different scales. At the pore scale, dispersivity can be estimated by performing laboratory column tests. This method only takes into account dispersion due to pore scale heterogeneities. At a scale of meters, single-well tracer tests can be performed which produce in situ dispersivity values representing the large-scale heterogeneities in the area affected by the test as well as those at the pore scale. At the scale of tens to thousands of meters (field scale), natural gradient tracer tests can be performed to produce in situ dispersivity estimates that take into account the large-scale heterogeneities over tens to thousands of meters as well as those at the pore scale. The natural gradient tracer test is the only method with which transverse dispersivities can be estimated and is the focus of this study.

The natural gradient tracer test involves a pulse injection of a tracer at a constant rate and concentration into an aquifer. Inherent in the test is the assumption that the injection rate is slow; the natural gradient must not be affected by the injection. Once the injection is complete, the tracer plume is allowed to move through the aquifer under natural gradient conditions. A three-dimensional array of sample wells is installed to measure the concentrations of the tracer plume through time. The result is a database of spatial and temporal concentration data providing "snapshots" of the plume through time.

Generally, the plume is monitored for a few years (Mackay et al., 1986; LeBlanc et al., 1991; Boggs et al., 1992).

Apparent macrodispersivities in the longitudinal and transverse directions are calculated from the concentration data by the method of moments. This involves summing the tracer concentrations and finding the variances about the center of mass of the plume. The average rate of change of the plume variance with respect to the center of mass is used to calculate apparent dispersivities (these calculations will be discussed in the Methods section).

## Stochastic Groundwater Modeling

There are two basic approaches to groundwater modeling, deterministic and stochastic. A deterministic model solves a partial differential equation (Eq. 5 below) for a given set of input values, aquifer parameters, and boundary conditions (Fetter, 1993, p. 77). The output variable, such as solute concentrations, have specific values at every point in the aquifer. An assumption in this approach is that the distribution of aquifer parameters is known. Thus, in deterministic modeling an "exact" output parameter is provided. The problem with such a model is the uncertainty in the characterization of the aquifer parameters. It is not possible to know the hydraulic conductivity of the aquifer sediments at every point in the system. Even if it were possible to test the hydraulic conductivity at every location in an aquifer, additional uncertainty results from experimental error.

A stochastic approach to groundwater modeling recognizes the statistical uncertainties involved in parameter estimation and provides a range of possible outcomes rather than an "exact" solution. This is important because knowledge of aquifer parameters will always be limited and therefore cannot provide an exact solution to the problem.

The type of stochastic groundwater modeling used in this study was a limited Monte Carlo analysis. Monte Carlo simulations are performed by generating random, but statistically equivalent, hydraulic conductivity fields over the entire model domain. The advection-dispersion equation is then solved using the generated aquifer parameters. The one-dimensional form of the advection-dispersion equation is (Fetter, 1993, p. 115):

$$\partial C/\partial t = D_L(\partial^2 C/\partial x^2) - v_i(\partial C/\partial x) - (\rho_d/n)(\partial C^*/\partial t) \qquad (5)$$

where $\rho_d$ is the bulk density of the aquifer ($M/L^3$), and $C^*$ is the amount of solute sorbed per unit weight of solid (M/M).

The advection-dispersion equation states that the rate of change in concentration with respect to time is equal to dispersion minus advection and sorption (this simplified form of the equation assumes there are no sources, sinks, or chemical reactions occurring other than sorption).

Hydraulic conductivity is one of the most important parameters in solute transport modeling because conductivities can vary several orders of magnitude for geologic materials. As such it is a parameter with great uncertainty. The hydraulic conductivity field is treated as a random variable with a given covariance structure. Each simulation conducted with a random hydraulic conductivity field constitutes a realization. The best estimate of the plume concentration solution is the ensemble mean. The ensemble mean is the mean of all possible random but equivalent populations (i.e. realizations) (Fetter, 1993, p. 81). A small number of realizations (e.g. five) is used to approximate the ensemble mean in a limited Monte Carlo analysis.

The covariance structure of the natural log transformed hydraulic conductivity (ln K) field consists of the mean, variance, and correlation lengths. The mean is the average of all ln K values. The variance is a measure of the spread of values about the mean ln K;

it is a measure of the heterogeneity in an aquifer. The correlation length is a measure of the distance that values are correlated from a given point in space. The correlation of two values decreases with increasing distance between them. There is a separate correlation length for every dimension used in the random field.

The correlation length can be thought of as a measure of the size of heterogeneities in an aquifer. The heterogeneities in a natural depositional system are the result of different local environments of deposition. In the horizontal plane they may represent deposits such as point bars and channel deposits in a meandering stream system. In the vertical plane the correlation length generally represents stratification.

Limited Monte Carlo simulations have been used to estimate the ensemble mean by using a small number of realizations. Burr et al. (1994) performed such a study with the geostatistical parameters of the Borden aquifer in Ontario, Canada. The ensemble mean in the study was estimated using only five realizations. The researchers performed an additional 20 realizations and found essentially identical results.

# PREVIOUS WORK

There are two main categories of previous work relevant to this study; field studies, which focus on natural gradient tracer tests, and numerical studies, which focus on stochastic groundwater modeling with sorbing solutes in heterogeneous aquifers. Both are reviewed below. In addition, a new groundwater modeling trend is discussed.

## Field Studies

### Natural Gradient Tracer Tests

Two natural gradient tracer tests are discussed in this section, the Borden and Columbus natural gradient tracer tests. These were chosen because they have well documented statistical parameters of hydraulic conductivity and they represent two extremes in aquifer parameters; the Borden site represents a weakly heterogeneous aquifer, the Columbus site represents a strongly heterogeneous aquifer.

#### Borden Site

A large-scale natural gradient tracer test was conducted in the unconfined sand aquifer underlying an inactive sand quarry at the Canadian Forces Base Borden in Ontario, Canada (Mackay et al., 1986). The purpose of this study was to produce a detailed and accurate data base describing the transport, transformation, and fate of conservative tracers (bromide and chloride) and halogenated organic contaminants in the saturated zone (Mackay et al., 1986). The data could then be used to evaluate dispersive transport models. This experiment was ideal for such evaluation because of the controlled initial conditions, long plume travel distance, and detailed three-dimensional resolution of concentration distributions and hydraulic conductivity fields. Detailed three-dimensional monitoring of solute concentrations through time provided "snapshots" of plume development, which could be used to calculate spatial moments to quantify the movement and spreading of the plumes through time.

The aquifer is composed of clean, well-sorted, fine- to medium-grained sand of glaciofluvial origin. Quartz, feldspar, and carbonates dominate the mineralogy of the sediments. The grains are subangular to well-rounded (Mackay et al., 1986).

The aquifer extends about 9 m below the horizontal quarry floor and is underlain by a thick silty clay deposit. The lower 2-3 m of the aquifer contains a landfill leachate plume. The water table depth is generally about 1.0 m below the quarry floor, but fluctuates seasonally. The average horizontal hydraulic gradient throughout the year in the study area is approximately 0.0043 (Sudicky, 1986). The aquifer is quite homogeneous compared to most aquifers. The bedding is approximately horizontal and parallel, but some cross and convolute bedding are also found. The main forms of spatial heterogeneity in the aquifer are thin lenses (0.02-0.1 m) of 2-5 m lateral extent composed of sediments of contrasting particle size distribution and hydraulic conductivity (Sudicky, 1986).

Sudicky (1986) examined the spatial structure of the hydraulic conductivity at the Borden site using 32 cores from two core transects. One transect was oriented in the direction of groundwater flow, the other was transverse to groundwater flow. Each core was approximately 2 m long and was obtained from depths of approximately 2.5 (top) to 4.5 m (bottom) below the quarry surface. The horizontal spacing of the cores was 1 m. Each core was divided into 0.05 m vertical intervals; each relatively homogeneous interval was dried and subjected to a permeameter test to determine its hydraulic conductivity. A total of 1279 hydraulic conductivity measurements were performed on the cores.

The geometric mean of the hydraulic conductivity measurements was found to be $9.75 \times 10^{-3}$ cm/s. Each hydraulic conductivity value was transformed into a natural log value (ln K); the geometric mean of ln K was -4.63. The variance of the mean ln K was found to be 0.29 with correlation lengths of 2.8 m in both horizontal directions and 0.12 m in the vertical direction (Sudicky, 1986). A reevaluation of the data by Woodbury and Sudicky (1991), which examined how assumptions and interpretations may affect the geostatistical parameters, yielded in the direction of flow, a variance of 0.24 and a correlation length of 5.1 m in the horizontal direction and 0.21 m in the vertical direction. The values in the direction transverse to flow were 0.37, 8.3 m, and 0.34 m, respectively.

The goal of the injection system was to create plumes of well defined geometry with a uniform distribution of solutes (Mackay et al., 1986). In addition, the injection was desired to be essentially instantaneous with little disturbance to the natural flow. A total of 12 $m^3$ of solution containing the nonreactive tracers and contaminants was injected into the aquifer over a 14.75-hour period. Nine wells were used to inject the solution.

A dense network of multilevel sampling wells was installed with horizontal spacing ranging from 1.0 to 4.0 m. Figure 1 shows the three-dimensional array of multilevel sampling wells. The vertical spacing of the sampling points ranged from 0.2 to 0.3 m. Samples were taken from the multilevel wells and analyzed for solute concentrations to provide "snapshots" in time of solute distributions. Over 11,000 samples were taken during 14 sampling sessions. The tracer test was monitored for 1038 days and the nonreactive plumes traveled more than 110 m.

Freyberg (1986) used the nonreactive tracer data (bromide and chloride) to calculate plume spatial moments, zeroth through second. The moments were used to calculate the total mass of solute, average plume velocity, and dispersivities. The moments were calculated in two dimensions; the vertical concentration values were

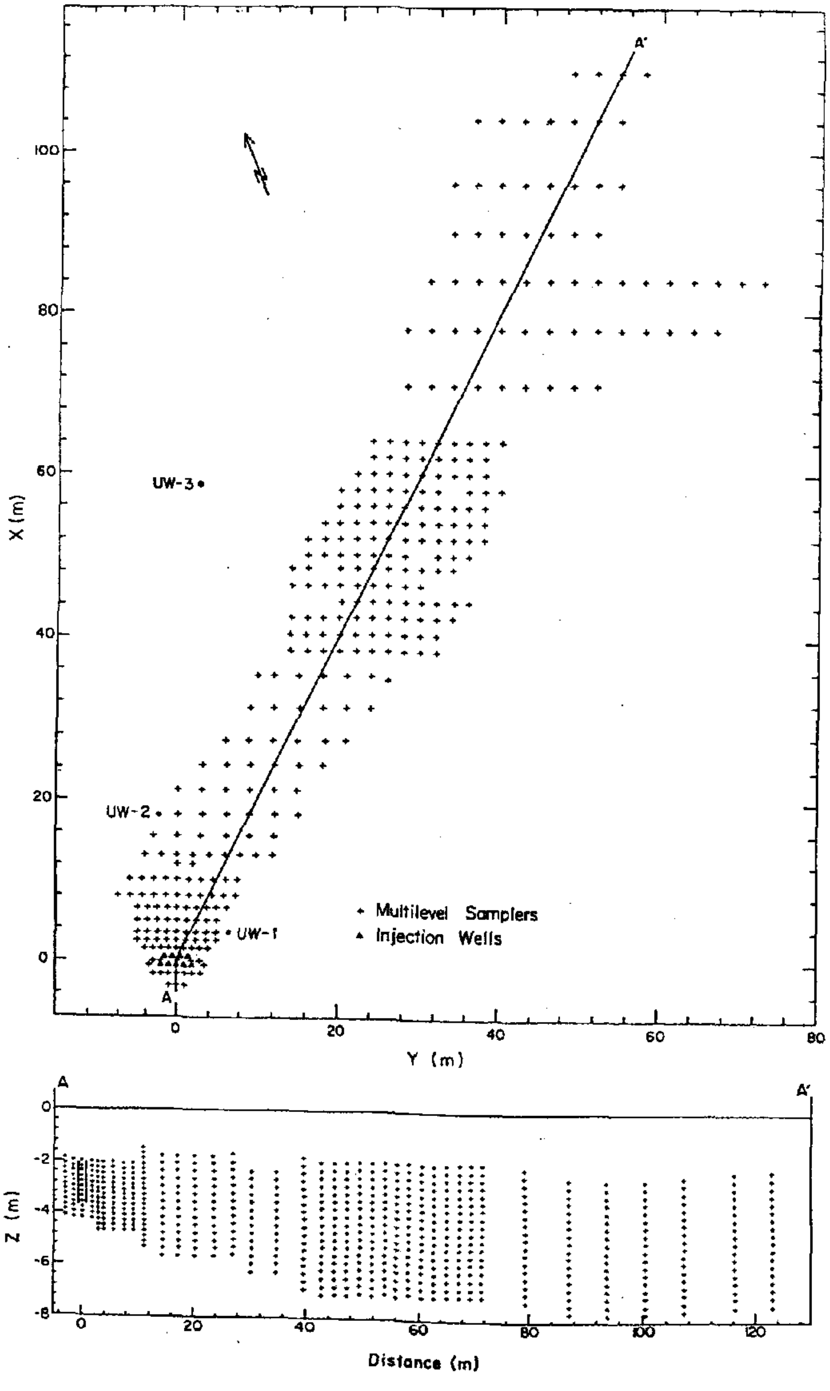


Figure 1. Three-dimensional array of multilevel sampling wells used to monitor the Borden natural gradient tracer test. Plus symbols represent multilevel sampling wells; triangles represent injection wells. Position labeled UW-3 is the location of the 32 cores used in calculating the geostatistical parameters of hydraulic conductivity. (Figure 5 of Mackay et al., 1986).

averaged. The average linear velocity of the plume was estimated at 0.091 m/day by examining the plume's center of mass as a function of time. The apparent dispersivities were calculated using the average plume velocity and the rate of change of plume variance with respect to time. The apparent longitudinal and horizontal transverse dispersivities were 0.36 m and 0.039 m, respectively.

### Columbus Site

A large-scale natural gradient tracer experiment was conducted in an unconfined aquifer at Columbus Air Force Base in northeastern Mississippi. The purpose of the experiment was to increase the existing information gathered from natural gradient tracer tests for a very heterogeneous aquifer (Boggs et al., 1992). The study would expand the spectrum of aquifer conditions for transport model testing. In addition, this study examined practical field methods for estimating the spatial variability of hydraulic conductivity. As with the Borden experiment, detailed three-dimensional monitoring of solute concentrations was performed to provide "snapshots" of plume development through time.

The aquifer is composed of poorly to well-sorted sandy gravel and gravelly sand with small amounts of silt and clay. The mineralogy of the sands and gravels consists of chert, feldspar and mica. The fine-grained materials (< 0.074 mm) consist of quartz, potassium feldspar, muscovite, and clay minerals. The clay minerals are predominantly kaolinites and illites with small amounts of montmorillonites and vermiculites (actually altered biotite). The sediments are commonly coated with iron oxides (Boggs et al., 1992).

The unconfined aquifer consists of an alluvial terrace deposit and averages approximately 11 m in thickness. An aquifer exposure adjacent to the site indicated the facies occur as irregular lenses and layers of up to 8 m wide and 1 m thick. The aquifer is underlain by an aquitard consisting of fine-grained marine sediments belonging to the

Eutaw Formation (Boggs et al., 1992). The hydraulic head field of the site exhibits complex temporal and spatial variability as a result of the heterogeneity of the aquifer and seasonal fluctuations of the water table. The average horizontal hydraulic gradient is approximately 0.003, and exhibits seasonal periodicity as a result of water table fluctuations. At many locations the vertical hydraulic gradient is greater than the horizontal gradient.

Rehfeldt et al. (1992) examined the spatial variability of hydraulic conductivity at the site. A total of 2187 hydraulic conductivity measurements were taken throughout the site. Many methods were employed in taking the conductivity measurements including the borehole flowmeter method, slug tests, and laboratory permeameter tests. Estimates of covariance parameters were found using indirect measures of hydraulic conductivity such as soil grain size distributions, surface geophysical surveys, and mapping of sediment facies in outcrop.

The values of hydraulic conductivity varied considerably throughout the site. Near the injection site the mean value of hydraulic conductivity was approximately $10^{-3}$ cm/s, while the mean value of the far downgradient region of the test site was 1-2 orders of magnitude larger (Boggs et al., 1992), for a mean range ln K of -6.9 to -2.3 (a single mean ln K value was not given for the site). The covariance parameters were estimated by two different methods. The first method assumed second-order stationarity of the hydraulic conductivity field. This method indicates the covariance between two points depends only on the distance between them and not on their spatial location; thus, the hydraulic conductivity field was assumed to be uniformly heterogeneous. In other words, it was assumed that there are no spatial trends in hydraulic conductivity values; features such as abandoned channel deposits were treated as large-scale heterogeneities. The values of ln K variance and correlation scales in the horizontal and vertical directions were found by this method to be 4.5, 12.8 m, and 1.6 m, respectively (Rehfeldt et al., 1992). The hydraulic conductivity field was found, however, to have a nonstationary character (i.e. spatial trends in hydraulic conductivity exist).

The second method used to calculate the covariance parameters assumed a nonstationary character and involved trend removal and the subsequent covariance analysis of the stationary residuals. Trend analysis is a mathematical method of separating a map into two components; that of a regional nature (trend), and local fluctuations (residuals) (Davis, 1986, p. 405). Thus, residuals are deviations from the general trend. The resulting values of variance and correlation scales in the horizontal and vertical directions using the trend removal method were found to be 2.7, 4.8 m, and 0.8 m, respectively (Rehfeldt et al., 1992).

A total of 10.07 $m^3$ of groundwater containing bromide and three organic tracers was pulse injected into the aquifer over a period of 48.5 hours. The slow injection rate was chosen to keep the disturbance of the natural flow system to a minimum. Five injection wells spaced 1 m apart in a linear array were used in the injection.

The monitoring system consisted of an array of 258 multilevel sampling wells (Boggs et al., 1992), having 6000 three-dimensional sampling points with which to monitor the plumes. The emphasis of the monitoring program, as with the Borden site, was to provide snapshots of plume development through time. Eight sampling sessions were performed during the experiment at intervals of five to 19 weeks. The experiment was monitored for 594 days.

Adams and Gelhar (1992) performed a spatial moment analysis on the bromide concentration data. An apparent longitudinal dispersivity value of 50-75 m was calculated from second-order spatial moments of the plume. The relationship between the second-order spatial moment and dispersivity assumes a uniform flow field with a Gaussian concentration distribution were present. The site, however, was shown to have a nonuniform flow field and non-Gaussian plume concentration distributions. The flow field was found to be accelerating in a downgradient direction; the groundwater velocity increased tenfold 100 m downgradient from the injection site. The researchers therefore performed a dispersivity calculation which assumed a nonuniform flow field. A longitudinal dispersivity value of 5-10 m was calculated using this approach, which is an order of magnitude larger than that of the weakly heterogeneous Borden site.

A decreasing mass balance for bromide throughout the experiment prompted studies to be performed to determine if bromide was being adsorbed onto the aquifer sediments (Boggs and Adams, 1992). As discussed earlier, researchers have shown that sediments containing significant quantities of variably charged minerals such as Fe and Al oxides may adsorb anionic tracers (Uehara and Gillman, 1981, p. 46). The pH governs the sign and magnitude of the oxide surface charge. The presence of iron oxides and kaolinite, in conjunction with the relatively low pH at the site (approximately 4.8), indicated that anion adsorption may be a factor (Boggs and Adams, 1992).

A column study was performed to estimate the effects of bromide adsorption relative to the conservative tracer, tritium. A linear sorption isotherm described the sorption that occurred in the column studies. The results of the bromide column studies indicated that approximately 20% of the bromide was being adsorbed. A retardation factor of 1.20 was estimated for bromide (Boggs and Adams, 1992). Boggs and Adams (1992) did not, however, test if the sorption was a function of concentration; one bromide concentration of 500 mg/l was used in the column studies.

Sorption was tested at the Columbus site because it can have profound effects on plume spreading. The effects of sorption were well illustrated in a natural gradient tracer test at Cape Cod, Massachusetts (LeBlanc et al., 1991). Figure 2 shows plume "snapshots" of bromide, lithium, and molybdate through time. It is clear from Figure 2 that the longitudinal spreading of the molybdate plume at 461 days was much larger than

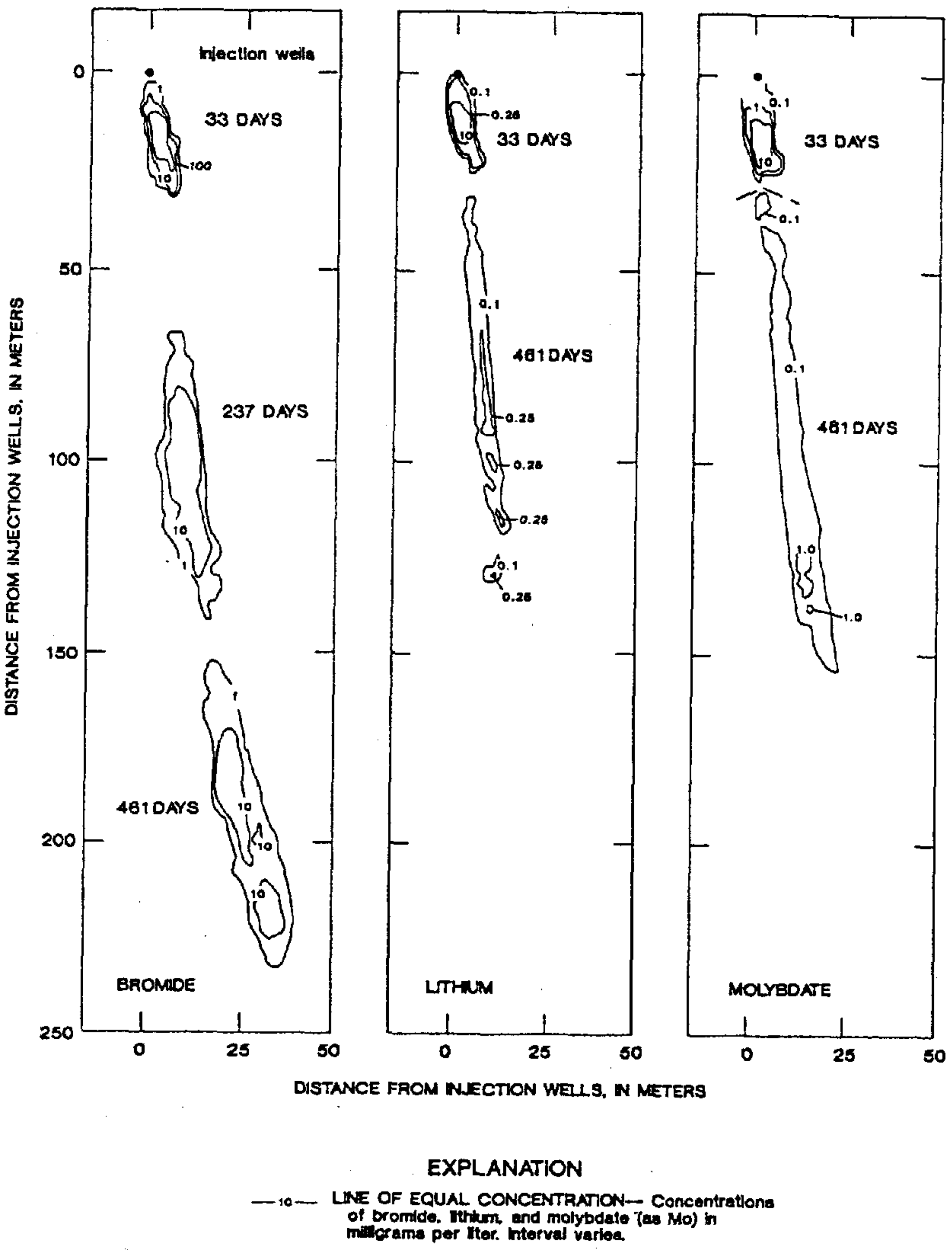


Figure 2. Plume "snapshots" of bromide, lithium, and molybdate at the Cape Cod natural gradient tracer test (Figure 10 of LeBlanc et al., 1991).

the conservative bromide plume. The enhanced longitudinal spreading was attributed to sorption (LeBlanc et al., 1991).

Natural gradient tracer tests are an important tool in examining the transport of solutes in a subsurface environment. They are, however, quite costly to perform. Many researchers are turning to numerical groundwater modeling to quantify solute transport because it is a cost-effective alternative to field natural gradient tracer tests.

## Numerical Studies

### The Effect of Sorption on Dispersion

Sorption of contaminants or tracers can profoundly affect plume spreading and dispersivities. Recently, researchers have been modeling the effects of heterogeneous linear and non-linear sorption in heterogeneous aquifers (e.g. Burr et al., 1994; Brusseau, 1995; Bosma et al., 1996). They have found that sorption can enhance longitudinal dispersion. Transverse dispersion, however, does not seem to be affected as much.

Burr et al. (1994) performed a limited Monte Carlo analysis with geostatistical parameters similar to the Borden aquifer. The aim of the study was to examine the effects of linear sorption in which the distribution coefficient was assumed to be negatively correlated with hydraulic conductivity. This indicates the solute will be strongly sorbed in areas of low hydraulic conductivity. This correlation was chosen because it would maximize field-scale nonequilibrium effects on solute movement; there is, however, no evidence to suggest such a correlation exists at the Borden site (Burr et al., 1994). The researchers found that the longitudinal macrodispersivity was more than 3 times greater for the reactive tracer than that of a conservative tracer. In the horizontal and vertical transverse directions, dispersivities were only slightly greater.

Bosma et al. (1996) performed a number of two-dimensional Monte Carlo simulations in aquifers with homogeneous and heterogeneous flow fields and Freundlich isotherms. They performed simulations with random hydraulic conductivity fields of different variances and different Freundlich isotherm parameters. In addition, they performed simulations where the Freundlich sorption coefficient was heterogeneous; that is, the sorption coefficient was treated as a random variable with a given natural log mean and variance. In the heterogeneous flow fields with homogeneous sorption, Bosma et al. found the longitudinal and horizontal transverse variances increased with increasing non-linearity of the Freundlich isotherm. As stated above, the Freundlich exponent can take on values between 0 and 1. They found that exponent values as large as 0.8 produced enhanced longitudinal variance relative to the linear model (n = 1 in the Freundlich isotherm). Chemical heterogeneity only made a small difference in longitudinal variance, and virtually no difference in the transverse variance. The authors did not, however, compare the results to a conservative tracer.

Brusseau (1995) examined the effects of non-linear sorption and rate-limited transformation on the transport of contaminants through a porous medium. Numerical simulations that take into account non-linear sorption and rate-limited transformation were performed in one dimension. Breakthrough curves were derived from the simulations to assess the effects of sorption and rate-limited transformation of a contaminant as it moves past a point in the system. The study compared non-linear sorption and rate-limited transformation relative to that of linear sorption. The results of the study indicated that rate-limited transformation and transport of non-linearly sorbing solutes with exponents less than 0.9 cannot be accurately simulated with a linear sorption isotherm model.

Apparently, none of the studies to date has compared the effects of weakly non-linear sorption relative to that of a conservative tracer. Generally, researchers have compared non-linear sorption to linear sorption (Brusseau, 1995; Bosma et al., 1996), or linear sorption relative to a conservative tracer (Burr et al., 1994). In addition, many previous studies considered sorption isotherms which were designed to show the effects of varying the sorption coefficients, exponents, and chemical heterogeneity; the sorption isotherms were not experimentally derived (Burr, et al., 1994; Brusseau, 1995; Bosma et al., 1996). Most of the sorption isotherms used in previous studies have been moderately strong. Burr et al. (1994) calculated a retardation factor of approximately 4; Bosma et al. (1996) calculated values as large as 26 (numerous simulations were performed with varying degrees of sorption and retardation).

In contrast to the work reviewed above, the aim of this research was to quantify the effects of a tracer undergoing sorption according to a weakly non-linear, experimentally derived Freundlich isotherm relative to a conservative tracer.

## Recent Modeling Trend

Many researchers have performed Monte Carlo simulations with stationary random hydraulic conductivity fields (e.g. Burr et al., 1994; Bosma et al., 1996). This assumes that the statistical parameters do not vary spatially. Webb and Anderson (1996) argue that the problem with this assumption is that the presence of high conductivity pathways in a random field are not correlated to any known geologic structures; they are a function of the variability of the statistical distribution.

Recently, researchers have been generating geometric hydraulic conductivity fields in three dimensions which more realistically represent a given geologic system and its depositional environments (Webb and Anderson, 1996; Scheibe and Freyberg, 1995). Webb and Anderson (1996) argue that the use of a random hydraulic conductivity field underutilizes the existing knowledge of geologic systems. They proposed a method for modeling a braided stream system which takes into account the geometry of features common to the braided stream depositional environment. The subsurface features used in the model were inferred from surface topographical features.

Scheibe and Freyberg (1995) performed a similar study on point bar sediments of the Wabash River in the midwestern United States. They generated a model with aquifer parameters of features at the microform to macroform scale. The microforms include such small-scale features as current ripples; the macroforms are large features which represent the cumulative effect of multiple events over long periods of time, such as point bar deposits. The grid spacing of the model was 0.00381 m to insure that the resolution of the model was sufficient for the smallest-scale features. The resulting high-resolution model was said to accurately characterize the depositional features found in a point bar system.

# METHODS

This study utilized the groundwater modeling programs SUTRA (Voss, 1984) and WATSUTRA (VanderKwaak et al., 1996) to perform a limited Monte Carlo analysis. The Fast Fourier Transform (FFT) method of random field generation (Gutjahr et al., 1995) was used to generate random hydraulic conductivity fields with given covariance parameters. The numerical models were tested to confirm they worked properly. Apparent dispersivities were calculated by the method of moments. The ensemble mean estimates for various simulation cases were tested for significance using null hypothesis testing with a standard t-test.

## Transport Modeling Using SUTRA and WATUSTRA

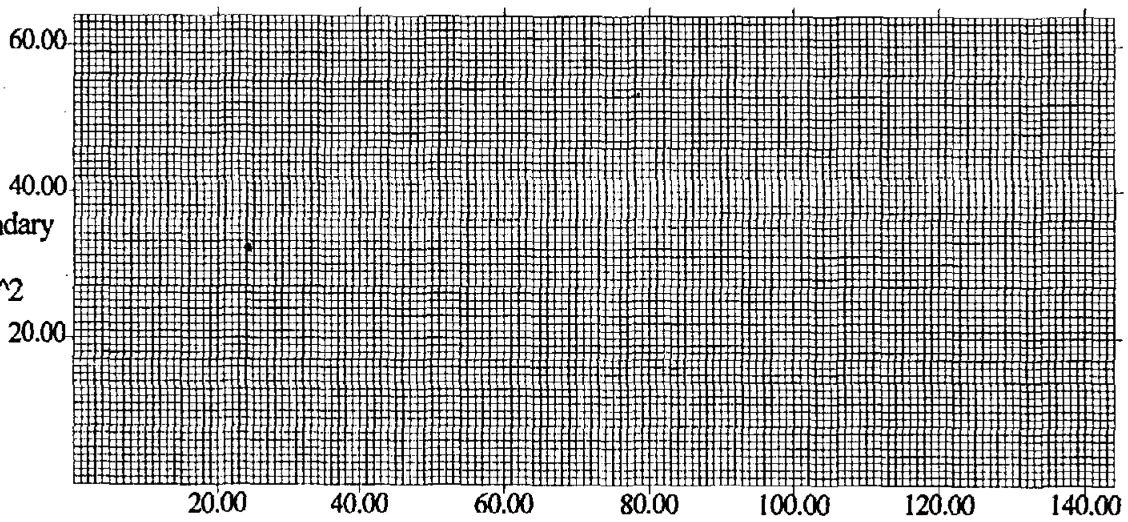
The numerical simulations in this study were done using SUTRA and WATSUTRA. SUTRA, an acronym for Saturated-Unsaturated TRAnsport, is a United States Geological Survey finite element, two-dimensional simulation model. This program simulates fluid movement and the transport of either energy or dissolved substances in the saturated or unsaturated zones. SUTRA also contains routines for modeling sorption, including the Freundlich isotherm. WATSUTRA is a modified version of SUTRA with an iterative sparse matrix solver, WATSOLVE (VanderKwaak et al., 1995), which speeds up calculations and conserves memory. The codes for SUTRA and WATSUTRA were written in ANSI-Standard FORTRAN-77.

WATSUTRA was found to be about 15 times faster than SUTRA for simulations requiring an iterative solution. WATSUTRA performed the simulations reported herein in approximately 20 hours. The iterative solution is required to resolve non-linearities, such as for a non-linear sorption isotherm. The conservative runs were done using SUTRA with a non-iterative solution. The simulations were performed on 100 and 120 megahertz (MHz) Pentium PCs, both equipped with 32 megabytes (Mb) of random access memory (RAM). The simulations were run on FORTRAN Powerstation version 1.0 for Windows.

## Model Parameters

The simulations in this study were designed to replicate natural gradient tracer tests in two different flow fields, weakly and strongly heterogeneous. Figure 3 shows the basic model design used in all simulations in this study. The model consisted of 9425 nodes and 9216 elements (145 by 65 nodes, 144 by 64 elements). This size was chosen because it was big enough to facilitate a large amount of plume spreading without loosing tracer mass through the constant-pressure boundaries. Each element was 1 m by 1 m and was of unit thickness. All model boundaries were constant-pressure (head). The left and right sides had constant pressure nodes of 103524.7 $kg/m*s^2$ and 97886.4 $kg/m*s^2$, respectively. The top and bottom constant pressure nodes decreased at a constant rate from the left to right sides. This gave a uniform hydraulic gradient from left to right of 0.004. Other researchers (e.g. Burr et al., 1994; Bosma et al., 1996) have modeled with no-flow boundaries on the top and bottom to allow flow parallel to the x-axis. The constant head boundaries were chosen to better represent a field situation. All elements had a porosity of 0.35. The experimentally derived Freundlich isotherm in Eq. (1) was used over the entire model domain for the reactive simulations (i.e. chemically homogeneous). A chemically homogeneous model was used in this study because there is little sorption data available at the Savannah River Site to model chemical heterogeneity.

Constant Head Boundary
Pressure = 103524.7 kg/m*s^2 - (39.1549)*(J)
where J is the distance in meters from the left boundary



Constant Head Boundary
Pressure =
103524.7 kg/m*s^2

Constant Head Boundary
Pressure =
97886.4 kg/m*s^2

Injection Node
x = 24 m, y = 32 m

Constant Head Boundary
Pressure = 103524.7 kg/m*s^2 - (39.1549)*(J)
where J is the distance in meters from the left boundary

Figure 3. Two-dimensional model used for all simulations in this study.

Local dispersivity values (model input values which represent pore-scale dispersivity) in the longitudinal and horizontal transverse directions were 0.6 m and 0.03 m, respectively, for all simulations. The local dispersivity values used in this study are larger than those used by other researchers (e.g. Burr et al., 1994 used 0.1 m and 0.005 m, respectively). The local dispersivity values were chosen to facilitate enough plume spreading so that the plume front covered a minimum of five elements, a discretization rule of thumb for SUTRA (Voss, 1984, p. 231). It was also found that large discrepancies occurred in the moment calculations between using all concentrations and only those greater than 0.1 ppm when local dispersivity values were small. For example, realization 1 in a weakly heterogeneous flow field was simulated using local longitudinal and horizontal transverse dispersivities of 0.2 m and 0.001 m, respectively. The zeroth and second moment calculations using concentrations greater than 0.1 ppm were found to be as much as twice as large as the same calculations using all concentrations. When the local longitudinal and horizontal transverse dispersivities were given values of 0.6 m and 0.03 m, respectively, the zeroth and second moment calculations using all concentrations and only those above 0.1 ppm generally agreed within a few percent. The larger local dispersivity values will not affect the results of this study because the same values were used in the reactive and conservative cases.

The user must specify the convergence parameters for pressure and concentration in SUTRA and WATSUTRA for simulations requiring an iterative solution. The simulations in this study were designed to quantify the effects of the Freundlich isotherm in Eq. (1) on apparent dispersivities. The concentration convergence parameter should be small enough so that all significant figures in the Freundlich isotherm are utilized. In addition, the convergence criteria should be accurate enough to facilitate sorption of the smallest concentration values used in the dispersivity calculations (detection limit set at 0.1 ppm). A convergence parameter of $1.00 \times 10^{-8}$ was found to accurately characterize the Freundlich isotherm in Eq. (1) for the concentrations used in this study. This value is small enough to include all significant figures in the Freundlich isotherm and will accommodate sorption of the smallest concentration values used in this study. The same value was used for pressure convergence. Thus, the change in concentration or pressure from the previous to the current iteration had to be less than or equal to $1.00 \times 10^{-8}$ at all nodes for convergence.

The permeability values were generated for each element using a FFT random field generator (Gutjahr, et al., 1995). This random field generator uses the turning bands method of field generation. The turning bands method generates the random field along lines in space rather than synthesizing the multidimensional field directly (Bras and Rodriguez-Iturbe, 1985, p. 310). This is an efficient method of generating a random field. The fields on average are of mean zero, with the variance specified by the user (Gutjahr, et al., 1995).

The random ln K fields generated in this study were stationary; that is, the covariance parameters did not vary spatially. The input parameters in the FFT random field generator consisted of a ln K variance, correlation lengths in the x and y directions, spectral model type, size and length of the field in the x and y directions, and a seed number. The input parameters were chosen to be similar to the Borden and Columbus aquifer parameters to represent two extreme aquifer conditions, weakly and strongly heterogeneous, respectively. The variance of the weakly and strongly heterogeneous flow fields, 0.35 and 3.5, respectively, were chosen to differ by an order of magnitude. Both fields had the same correlation length of 5 m in the x and y directions. The anisotropic exponential covariance model (spectral model) was chosen in the random field generator because the statistical characterization of hydraulic conductivities at the Borden and Columbus sites assumed an exponential covariance function (Sudicky, 1986; Woodbury and Sudicky, 1991; Rehfeldt et al., 1992). In addition, Monte Carlo simulations with the geostatistical characteristics of the Borden aquifer performed by Burr et al. (1994) also used an exponential covariance function in generating random hydraulic conductivity fields. The size of the random field was chosen to be 256 by 64, in the x and y directions, respectively, because the random field generator required the number of values in the x and y directions to be a power of 2. The field was therefore truncated to attain the model dimensions of 144 by 64. Finally, the seed number tells the random field generator where to begin the random field generation. Holding all other input parameters constant, a unique seed number will generate a unique realization. Each realization generated by the random field generator can therefore be replicated by using the same input parameters. The mean and variance of the entire field and truncated field, and the seed numbers used are shown in Tables 1 and 2 for the weakly and strongly heterogeneous fields, respectively.

A FORTRAN program was written to shift the ln K mean from about 0 to about -5, convert ln K to permeability, and print the results in the proper format for SUTRA's input files (see appendix E). The mean hydraulic conductivity value used in both fields was $6.74 \times 10^{-3}$ cm/s (ln K = -5). This value is characteristic of a clean sand (Freeze and Cherry, 1979, p. 29) and is the approximate mean value found at the Borden and Columbus sites.

Ten random hydraulic conductivity fields were generated in this study; five weakly heterogeneous and five strongly heterogeneous. Each of the ten realizations was used for four simulations: conservative tracer with 1 kg of bromide, reactive tracer with 1 kg of bromide, conservative tracer with 0.1 kg of bromide, and reactive tracer with 0.1 kg of bromide. Forty simulations were performed. Each simulation consisted of three smaller simulations: injection (600 s time-steps), first 100 hours of simulation (200 s time-steps, a size necessary for convergence when implementing the Freundlich isotherm), and the two year simulation (8640 s time-steps).

Table 1. Random field generator input and output parameters for a weakly heterogeneous flow field.

| Realization Number | Seed Number | Output Variance | Truncated Variance | Output Mean | Truncated Mean |
|---|---|---|---|---|---|
| 1 | 267913 | 0.335 | 0.317 | 0.059 | 2.71E-04 |
| 2 | 70269 | 0.316 | 0.317 | -0.095 | -0.075 |
| 3 | 392279 | 0.322 | 0.346 | 0.088 | 0.102 |
| 4 | 693471 | 0.373 | 0.410 | -0.035 | -0.040 |
| 5 | 7779433 | 0.327 | 0.272 | -0.018 | 0.012 |
| Average | na* | 0.335 | 0.333 | -3.34E-04 | -9.68E-05 |

* denotes not applicable

Table 2. Random field generator input and output parameters for a strongly heterogeneous flow field.

| Realization Number | Seed Number | Output Variance | Truncated Variance | Output Mean | Truncated Mean |
|---|---|---|---|---|---|
| 1 | 70269 | 3.161 | 3.173 | -0.300 | -0.237 |
| 2 | 112643 | 3.332 | 3.733 | -0.335 | -0.398 |
| 3 | 11262 | 3.157 | 3.102 | -0.247 | -0.349 |
| 4 | 267913 | 3.355 | 3.166 | 0.185 | 0.001 |
| 5 | 693471 | 3.735 | 4.105 | -0.110 | -0.125 |
| Average | na* | 3.348 | 3.456 | -0.161 | -0.222 |

* denotes not applicable

The ensemble means were estimated by averaging the apparent longitudinal or horizontal transverse dispersivities in the five realizations for each simulation case. As stated in the Background section, Burr et al. (1994) found this number to be sufficient to provide a good estimate of the ensemble mean in a weakly heterogeneous flow field. This estimate will probably not be as good in the strongly heterogeneous flow field because plume variance is much greater. This number of realizations will, however, give some insight into the effects of the Freundlich isotherm in Eq. (1) on apparent dispersivities.

The following simplifying assumptions were used in this study:

1) Sorption according to the Freundlich isotherm was assumed to be a reversible equilibrium process. Thus, desorption followed the same isotherm as adsorption, only with decreasing concentrations, and both adsorption and desorption were rapid in comparison to advective flow.

2) The Freundlich isotherm was constant throughout the model domain.

3) The groundwater model employed was two-dimensional; vertical heterogeneity was not represented.

## Model Testing

Model testing in solute transport is crucial in determining if the output parameters are reasonable. A homogeneous simulation can be used to test the local dispersivity values put into the modeling program; the local dispersivity values should be equal to the calculated dispersivity values. Heterogeneous models can be tested for grid spacing and time-step size. If the grid spacing and time-step size are too large, a phenomenon called numerical dispersion will cause the dispersivity values to be overestimated.

A homogeneous natural gradient tracer simulation was performed with SUTRA. The homogeneous model had a single value of permeability, $1.025 \times 10^{-11}$ m$^2$, throughout the model domain. The model had dimensions of 316 m by 20 m in the x and y directions, respectively, with a grid spacing of 1 m. A local longitudinal dispersivity value of 4.000 m was used in SUTRA; the value calculated by the method of moments, 3.979 m, was within 0.5 percent of the local dispersivity value (see Appendix F for spatial moment estimates). A local horizontal transverse dispersivity value of 0.1000 m was put into SUTRA and an apparent horizontal transverse dispersivity value of 0.1005 m was calculated by the method of moments. Again, the calculated value was with 0.5 percent of the local value. Therefore SUTRA was performing as expected.

The type of comparison outlined above cannot be performed in heterogeneous aquifers because the heterogeneities in the flow field enhance dispersivity. Therefore the heterogeneous model was tested for spatial and temporal discretization. Discretization is a measure of the fineness of the grid spacing and the size of the time steps. An inadequate model discretization may lead to numerical dispersion. Numerical dispersion is a result of difficulties in solving the advection-dispersion equation (Eq. 5) numerically (Anderson and Woessner, 1992, p. 327). It is minimized by using a fine grid size and small time steps (dx and dt, respectively, in Eq. 5). Increased accuracy must be balanced with the increased CPU time required for the simulations. A finer grid size and smaller time steps will require more calculations for a given simulation time.

A peclet number can be calculated to estimate a grid spacing that minimizes numerical dispersion. The peclet number for grid spacing is defined as the length of the node spacing divided by the characteristic dispersivity value, $\Delta L/\alpha$. Acceptable solutions may be obtained with peclet numbers as high as 10 (Huyakorn and Pinder, 1983). Burr et al. (1994) found that using a grid spacing in the x and y directions of 0.5 m and a horizontal transverse dispersivity of 0.005 m (peclet number of 100) appeared to accurately characterize dispersivities. The length of the node spacing for the model used in this research was 1 m, the characteristic dispersivity was 0.03 m (the local horizontal transverse dispersivity). The peclet number was therefore 33.3.

A more direct way to test the effect of grid spacing on numerical dispersion for a specific model is to increase the number of nodes, repeat the simulation, and compare the dispersivity values (Sudicky, 1996, personal communication). If numerical dispersion is occurring, the dispersivity values will be larger in the model with a smaller number of nodes.

The grid size discretization was tested by breaking each element into four elements of the same permeability (see Appendix E for the FORTRAN program written to do this). The number of nodes and elements was increased by a factor of four, to 37,281 nodes and 36,864 elements. This test was performed on a simulation where plume dispersion was small, a reactive simulation in the weakly heterogeneous flow field (realization 1 with 1 kg of bromide). Numerical dispersion is maximized in cases where the plume occupies a minimum number of nodes.

The grid size test was run on WATSUTRA. The CPU run-time for the grid size test was 93 hours using a 100 MHz Pentium PC equipped with 56 Mb of RAM. Using all concentrations in the moment calculations, the simulation with the finer discretization yielded dispersivity values 5.7 percent smaller in the longitudinal direction and 3.0 percent smaller in the horizontal transverse direction than the 9425 node model (see Appendix E for grid-size test moment programs and Appendix F for moment calculations). Because numerical dispersion apparently accounted for a relatively small amount of the dispersivity, the original model of 9425 nodes was assumed to be adequate to compare the spreading of the plumes of conservative tracers to weakly adsorbed tracers.

The Courant number can be calculated to estimate a time step size that minimizes numerical dispersion. The Courant number is defined as the average velocity times the time step divided by the node spacing, $v_i \Delta t / \Delta L$. The Courant number should be less than or equal to one (Anderson and Woessner, 1992, p. 327). Using the largest time step in the simulations (8640 seconds) and the largest value of velocity ($7.5 \times 10^{-7}$ m/s), the Courant number was $6.48 \times 10^{-3}$, which is $\leq 1$. Thus, the time-step size of 8640 seconds was small enough to minimize numerical dispersion.

The temporal discretization was also tested by running a 7-day simulation and examining the concentration at a given node as the time step size was decreased. At some point, the concentration at the node should level off as the time step size is decreased, thus converging on the true value. This test was simulated with realization 1 in a strongly heterogeneous flow field with dimensions of 196 m by 36 m, respectively, in the x and y directions. The 8640 second time step was chosen to be sufficiently small (see Table 3).

Table 3. The effects of time step size on concentration values at a given node for a 1 week simulation in a strongly heterogeneous flow field.

| Time-step size (s) | Number of time steps | Concentration at node 574 (mass fraction) |
|---|---|---|
| $6.048 \times 10^{5}$ | 1 | $4.847 \times 10^{-5}$ |
| $8.640 \times 10^{4}$ | 7 | $4.553 \times 10^{-5}$ |
| $4.320 \times 10^{4}$ | 14 | $4.521 \times 10^{-5}$ |
| $1.728 \times 10^{4}$ | 35 | $4.502 \times 10^{-5}$ |
| $8.640 \times 10^{3}$ | 70 | $4.495 \times 10^{-5}$ |
| $4.320 \times 10^{3}$ | 140 | $4.492 \times 10^{-5}$ |

The reactive simulations were performed using WATSUTRA. This modified version of SUTRA has only been tested for transient solute transport and flow (VanderKwaak, 1996, personal communication). WATSUTRA was tested to confirm it would provide the same solute solution as SUTRA. Details are given in Appendix F.

## Method of Moments

Calculations of dispersivity and velocity were done using the method of moments. The method of moments can be used to estimate many parameters describing the solute plume through time: total mass of solute in solution, average linear velocity, longitudinal and horizontal transverse dispersivities, skewness, and kurtosis. These parameters are important in quantifying how the solute plume changes through time. The moments, zeroth through fourth, were calculated using a FORTRAN program (see Appendix E).

The general spatial moment equation for the zeroth and first moment in two dimensions is (Freyberg, 1986):

$$M_{ij}(t) = \int\int n\, C(x,y,t)\, x^i\, y^j\, dx\, dy \tag{6}$$

where C(x,y,t) is the mass concentration of the solute at a given node at time t, x and y are the spatial coordinates, and $0 \leq i + j \leq 1$ are integers that define the moment. The zeroth moment, $M_{00}$, is obtained when $i + j = 0$ and is the total mass of solute in solution. The first moment is defined when $i + j = 1$. When normalized by the total solute mass in solution, $M_{00}$, this represents the location of the center of mass of the plume in the x-direction, $x_c$, or y-direction, $y_c$:

$$x_c = M_{10} / M_{00} \qquad y_c = M_{01} / M_{00} \tag{7}$$

Average linear velocity in the x-direction (direction of flow) can be estimated from the rate of change of the center of mass with respect to time:

$$v = dx_c / dt \tag{8}$$

The average velocity can be estimated by plotting $x_c$ as a function of time. A linear regression can then be performed to find the slope of the best-fit line through the points.

The retardation factor for a reactive simulation can be calculated from the average linear velocities of the conservative and reactive cases for a given realization. The retardation factor, R, is the ratio of the conservative velocity to the reactive velocity:

$$R = v_c / v_r \tag{9}$$

where $v_c$ is the average linear velocity of the conservative plume and $v_r$ is the average linear velocity of the reactive plume. The larger the retardation factor, the slower the reactive plume moves relative to the conservative plume.

The generic spatial moment equation for the second and higher moments in two dimensions is (Farrell et al., 1994):

$$M_{ij}(t) = \int\int n\, C(x,y,t)\, (x-x_c)^i\, (y-y_c)^j\, dx\, dy \tag{10}$$

The second spatial moment is defined when $i + j = 2$. When normalized by the total mass in solution, the spatial variance about the center of mass is obtained:

$$\sigma^2_{xx} = M_{20} / M_{00} \qquad \sigma^2_{yy} = M_{02} / M_{00} \tag{11}$$

Apparent dispersivities in the longitudinal ($A_L$) and horizontal transverse ($A_T$) directions can be obtained from the following relationships (Freyberg, 1986):

$$A_L = (1 / |2v|)(d\sigma^2_{xx} / dt) \qquad A_T = (1 / |2v|)(d\sigma^2_{yy} / dt) \tag{12}$$

The quantity $d\sigma^2/dt$ in Eq. (12) can be estimated by plotting $d\sigma^2$ as a function of time. A linear regression can then be performed to find the slope of the best fit line through the points. As will be discussed later, however, many of the plots were not linear. Freyberg (1986) coined the term "apparent dispersivity" because the relationships in Eq. (12) only produce a true dispersivity value for a Gaussian (normal) solute distribution. When the solute distribution is not normal, the relationships in Eq. (12) are only estimates of true dispersivities. Loaiciga (1988) pointed out the relationship in Eq. (12), without the velocity term, was originally derived by Einstein (1905) to describe Brownian motion of particles immersed in a fluid solution. Equivalent equations for longitudinal and horizontal transverse dispersivities are (Garabedian et al., 1991; Adams and Gelhar, 1992):

$$A_L = (1/2)(d\sigma^2{}_{xx} / dx_c) \qquad A_T = (1/2)(d\sigma^2{}_{yy} / dx_c) \qquad (13)$$

since average velocity, v, is defined as $dx_c/dt$ (the dt terms cancel out). This is a more straightforward way to calculate apparent dispersivities because only one linear regression is required.

The third moment is obtained when $i + j = 3$. The coefficient of skewness of the plume in the x and y directions can be estimated from the third moment through the following equations:

$$SK_x = M_{30} / (M_{00}(\sigma^2{}_{xx})^{3/2}) \qquad SK_y = M_{03} / (M_{00}(\sigma^2{}_{yy})^{3/2}) \qquad (14)$$

The coefficient of skewness is a unitless measure of asymmetry (Yevjevich, 1972, p. 110). The coefficient of skewness, because it is an odd-valued moment, can have positive or negative values. A value of zero indicates the plume is symmetrical. A positive skewness indicates tailing to the right of the mode (in a down-gradient direction); a negative skewness indicates tailing to the left of the mode (in an up-gradient direction) (Haan, 1977, p. 51).

The fourth moment is obtained when $i + j = 4$. The kurtosis of the concentration distribution in the x and y directions can be estimated using the forth moment in the following equations:

$$KR_x = M_{40} / (M_{00}(\sigma^2{}_{xx})^2) \qquad KR_y = M_{04} / (M_{00}(\sigma^2{}_{yy})^2) \tag{15}$$

The kurtosis of a concentration distribution is a measure of peakedness or flatness. A value of 3 indicates a normal distribution (Haan, 1977, p. 51). A kurtosis value greater than three indicates a distribution more peaked than a normal distribution. The value of kurtosis, because it is based on positive moments, will always be positive (Yevjevich, 1972, p. 109).

Values for skewness and kurtosis are susceptible to error because they are based on quantities raised to the third or fourth power. Thus, a small error in concentration values due to numerical dispersion will be magnified when it is multiplied by a moment arm raised to the third or fourth power.

## Moment Program Testing

The FORTRAN programs written to calculate the spatial moments were tested for each of the moments. The zeroth moment was tested by comparing its value to that of the mass of bromide injected. A nearly identical mass was obtained. The first moment was tested by plotting the bromide plume in SURFER (Golden Software, 1994) and estimating the center of mass. The plume in the homogeneous simulation was symmetrical and it was therefore easy to determine its center of mass. The calculated and visual center of mass were found to be in agreement.

The second moment was tested in a homogeneous aquifer by calculating the longitudinal and horizontal transverse dispersivities and comparing them against those put into SUTRA. In homogeneous sediments dispersivities are simply a result of the local dispersivity values put into SUTRA. As stated earlier, the input and calculated values of longitudinal and horizontal transverse dispersivities agreed within 0.5 percent. The weakness in this method of verification is that the second moment calculations were tested simultaneously with the performance of SUTRA. The second moment equation, however, is straightforward and has the same basic form as the higher-order moments.

The third and fourth moments were tested by inserting concentrations of $1 \times 10^{-4}$ at 41 nodes in a symmetrical diamond-shaped pattern. All arrays and parameters in the moment program were declared as double-precision (14 significant figures). The skewness values in the x and y directions were found to be approximately zero ($-0.4 \times 10^{-13}$ and $-0.6 \times 10^{-13}$, respectively). The kurtosis values in the x and y directions had a value of 2.5. This seemed reasonable since the pattern looked similar to a normal distribution (kurtosis of 3). In addition, the center of mass of the plume in the x and y directions was found to be in the exact middle of the diamond-shaped pattern. The plume variances in the x and y direction were equal, as would be expected for a symmetrical pattern. It was concluded that the moment programs accurately calculated the moments.

## Null Hypothesis Testing

Null hypothesis testing can be employed to test if the ensemble mean estimates are significantly different. The null hypothesis states the two ensemble means are equal: the mean of the population from which the first sample was drawn is the same as the mean of the parent population of the second sample. The ensemble mean estimates can be tested with a standard two-tailed t-test. This test uses the difference between the means and a pooled standard deviation to calculate the t value. If the calculated t value is greater than the table value for a given number of degrees of freedom, the null hypothesis is rejected.

There are three assumptions in using the t-test (Davis, 1986, p. 66). The first is that both samples were selected at random. This assumption is believed to hold for this study because the results are based on randomly generated hydraulic conductivity fields. The second assumption is that the populations from which the samples were drawn is normally distributed. This assumption is impossible to test with a limited number (i.e. five) of realizations. The third assumption is that the two samples have the same variance. This can be tested with an F-test and confirmed before the t-test is employed.

It was concluded that, based on tests previously described, SUTRA and the method of moments FORTRAN program were giving acceptable results for the tasks required for this research.

# RESULTS AND DISCUSSION

Forty simulations were performed in this study for eight cases. Five realizations were performed for each case. The eight cases were:

strongly heterogeneous flow field with

(1) conservative simulations with 1 kg of bromide;
(2) reactive simulations with 1 kg of bromide;
(3) conservative simulations with 0.1 kg of bromide;
(4) reactive simulations with 0.1 kg of bromide;

weakly heterogeneous flow field with

(5) conservative simulations with 1 kg of bromide;
(6) reactive simulations with 1 kg of bromide;
(7) conservative simulations with 0.1 kg of bromide;
(8) reactive simulations with 0.1 kg of bromide.

Each realization was simulated for two years (with two exceptions). All four cases in the weakly heterogeneous flow field were performed with the same five generated hydraulic conductivity fields. Similarly, all four cases in the strongly heterogeneous flow field were performed with each of the five generated hydraulic conductivity fields. This allowed direct comparisons between the reactive and conservative simulations, and the 0.1 and 1 kg simulations. In addition, the moment calculations were performed two ways for each case, using (1) all concentrations and (2) only those above the detection level (set at 0.1 ppm).

## Simulations with 1 kg of Bromide

### Weakly Heterogeneous Flow Field

Ten simulations were performed in the weakly heterogeneous flow field with 1 kg of bromide, five conservative and five reactive. SURFER contour plots of plume "snapshots" are given to provide a visual perspective of plume behavior (see Appendix B). All contour plots of the plumes were done using concentrations greater than 0.1 ppm. The reactive simulations are only shown at T = 2 years (with two exceptions) because the plumes are similar to the conservative simulations at T = 1 year. SURFER contour plots of the weakly heterogeneous natural log hydraulic conductivity fields, given in Appendix C, are of the same scale as the plume "snapshots" and can be overlaid to examine the effects of heterogeneities on plume spreading.

### Spatial Moment Estimates of Plume Behavior

Mass of Bromide in Solution. Moment calculations, zeroth through fourth, are given in Appendix A. In all conservative realizations, the zeroth moments are reasonably close to 1 kg. As expected, there is a slight difference (a few percent) between using all concentrations and omitting those below 0.1 ppm. The zeroth moments for the reactive simulations showed a steady decline in mass through time. This was predominantly a result of concentration mass loss through adsorption according to the Freundlich isotherm in Eq. (1). At 2 years about 42 percent of the bromide injected was adsorbed onto the aquifer sediments.

Center of Mass. The first moments, when normalized by the total mass in solution, yields the plume center of mass. Plots of the center of mass in the x-direction as a function of time are shown in Appendix D. The average linear velocity for each realization was calculated from the slope of a best-fit line through the points on the graph.

Table 4. Dispersivities, velocities, and retardation factors for simulations in a weakly heterogeneous flow field with 1 kg of bromide.

| Simulation | AL (m) | AT (m) | V (m/yr) | Retardation Factor |
|---|---|---|---|---|
| Case 9 = 1.0 kg, all concentrations, conservative | | | | |
| 9.1 | 0.429 | 0.069 | 23.243 | na |
| 9.2 | 0.276 | 0.094 | 22.377 | na |
| 9.3 | 0.634 | 0.052 | 18.063 | na |
| 9.4 | 0.464 | 0.090 | 24.959 | na |
| 9.5 | 0.661 | 0.036 | 22.777 | na |
| Ensemble mean* | 0.493 | 0.068 | 22.284 | na |
| Case 10 = 1.0 kg, all concentrations, reactive | | | | |
| 10.1 | 0.402 | 0.066 | 13.910 | 1.671 |
| 10.2 | 0.300 | 0.076 | 13.640 | 1.641 |
| 10.3 | 0.529 | 0.048 | 10.808 | 1.671 |
| 10.4 | 0.474 | 0.077 | 14.781 | 1.689 |
| 10.5 | 0.607 | 0.032 | 13.598 | 1.675 |
| Ensemble mean* | 0.462 | 0.060 | 13.347 | 1.669 |
| Case 11 = 1.0 kg, concentrations > 0.1 ppm, conservative | | | | |
| 11.1 | 0.448 | 0.074 | 23.096 | na |
| 11.2 | 0.298 | 0.094 | 22.256 | na |
| 11.3 | 0.641 | 0.057 | 17.931 | na |
| 11.4 | 0.482 | 0.094 | 24.776 | na |
| 11.5 | 0.670 | 0.039 | 22.697 | na |
| Ensemble mean* | 0.508 | 0.072 | 22.151 | na |
| Case 12 = 1.0 kg, concentrations > 0.1 ppm, reactive | | | | |
| 12.1 | 0.387 | 0.068 | 13.949 | 1.656 |
| 12.2 | 0.294 | 0.075 | 13.641 | 1.632 |
| 12.3 | 0.536 | 0.052 | 10.772 | 1.665 |
| 12.4 | 0.461 | 0.078 | 14.790 | 1.675 |
| 12.5 | 0.615 | 0.039 | 13.643 | 1.664 |
| Ensemble mean* | 0.459 | 0.062 | 13.359 | 1.658 |

* denotes estimate

'na' denotes not applicable

heterogeneous flow field will be discussed in the Strongly Heterogeneous Flow Field section.

The graphs of longitudinal and horizontal transverse variances as a function of center of mass (x-coordinate) for realization 2, using all concentrations in the calculations, are shown in Figures 4 and 5, respectively. Figures 6 and 7 are the same graphs with only concentrations greater than detection limit (0.1 ppm) used in the calculations. The conservative and reactive curves in Figures 4-7 are similar. In all cases, the conservative variance was slightly greater than the reactive variance. This indicates the spreading of the conservative plumes was slightly greater than that of the reactive plume.

Apparent dispersivities for all simulations were calculated using Eq. (13) and the slope of the best-fit line through the points in the graph of variance as a function of center of mass (x-coordinate). It is evident from these graphs that the conservative simulation plumes traveled a greater distance than the reactive plumes. The scale effect of dispersivity suggests that as a plume travels longer distances, more heterogeneities are encountered, and the macrodispersivity of the formation increases. The main goal of this study was to quantify the effects of the Freundlich isotherm in Eq. (1) relative to a conservative tracer. Thus, the best fit line used to calculate the apparent dispersivities only included data points common to both the reactive and conservative simulations. It was found in all simulations that the center of mass of the reactive plume after 2 years had traveled the same distance as the conservative plume after it had traveled from 1 to 1.25 years. Linear interpolation was performed on the conservative data to provide an overlap with the reactive data. Data points from 0 and 0.0114 years were not used in the dispersivity calculations because the grid-size test, described earlier, revealed a significant amount of numerical dispersion at these times (compare Appendices A and F).

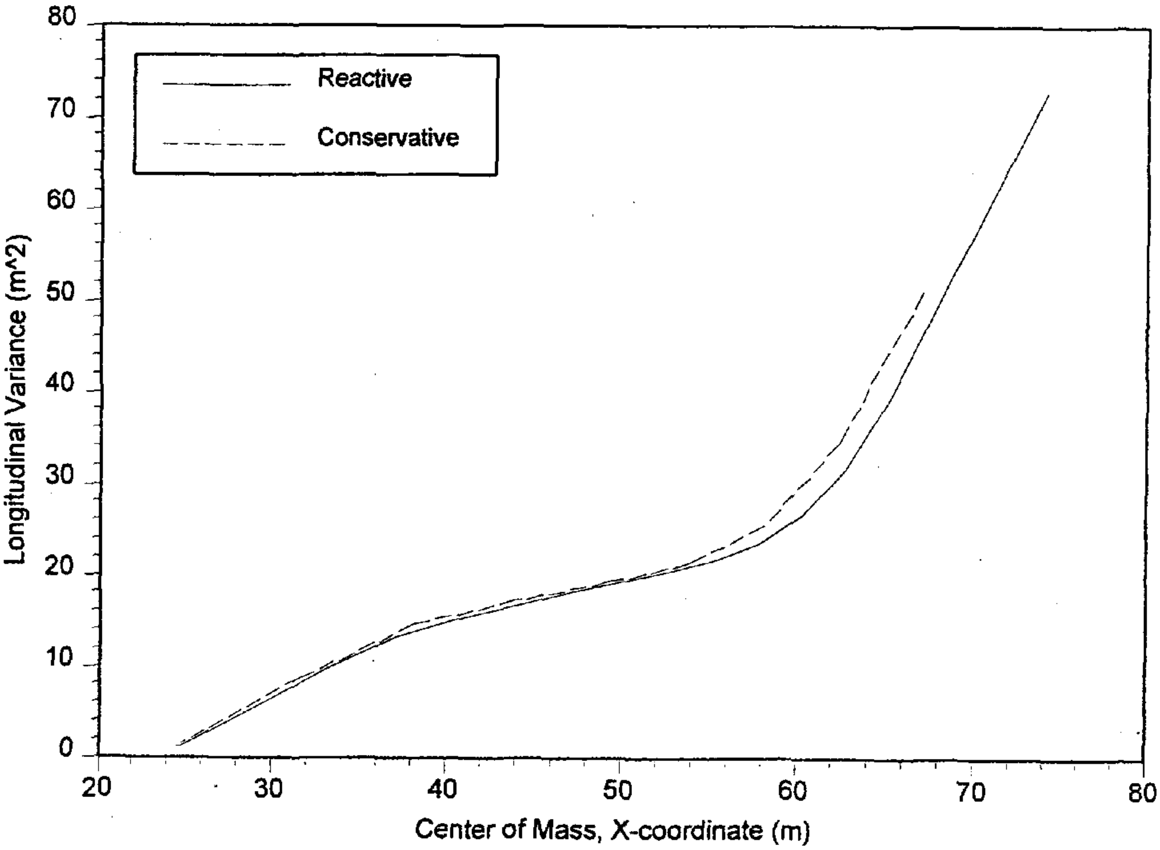


Figure 4. Reactive and conservative curves for realization 2 in a weakly heterogeneous flow field with 1 kg of bromide. All concentrations used in calculations.

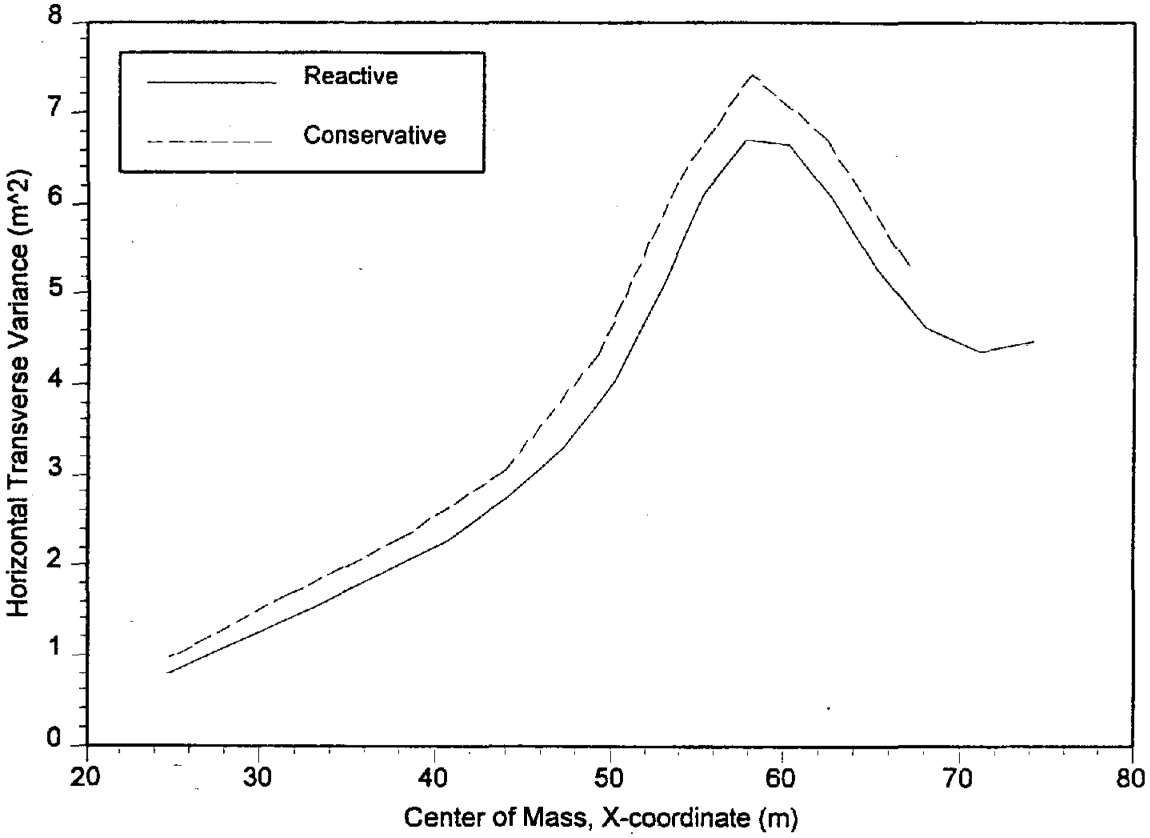


Figure 5. Reactive and conservative curves for realization 2 in a weakly heterogeneous flow field with 1 kg of bromide. All concentrations used in calculations.

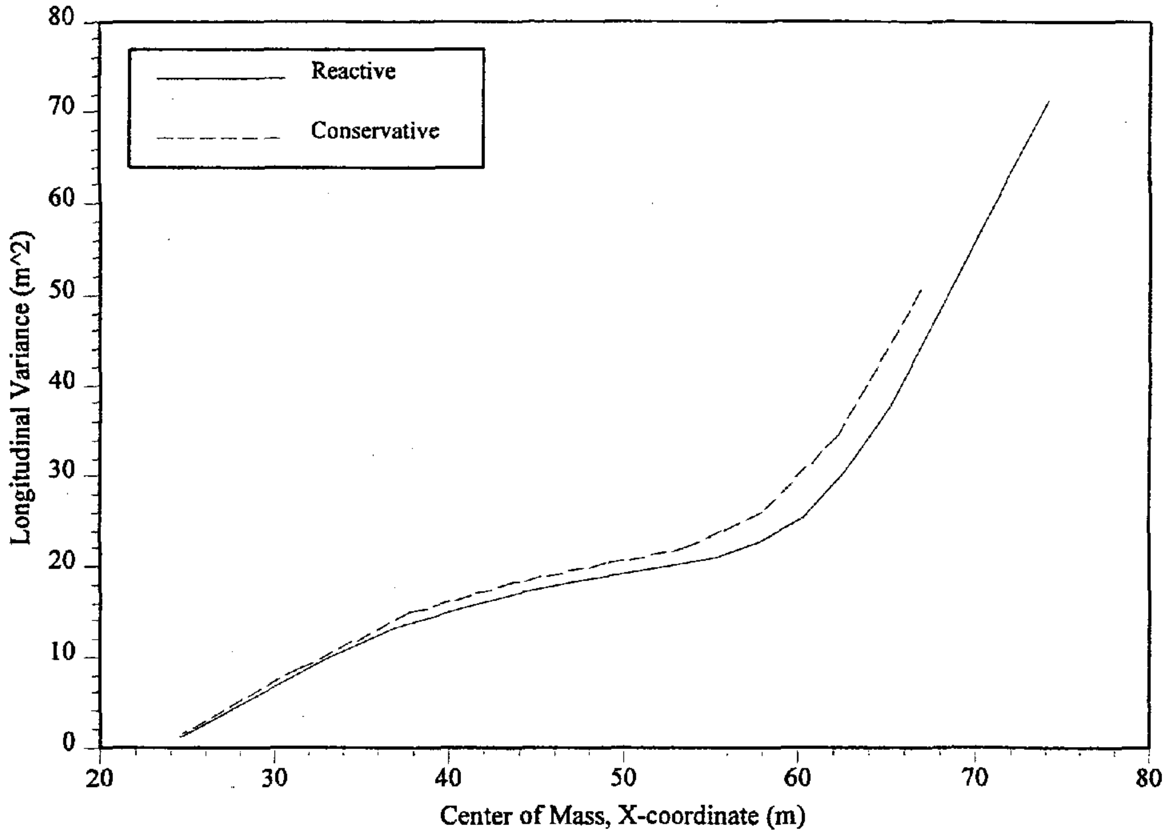


Figure 6. Reactive and conservative curves for realization 2 in a weakly heterogeneous flow field with 1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.

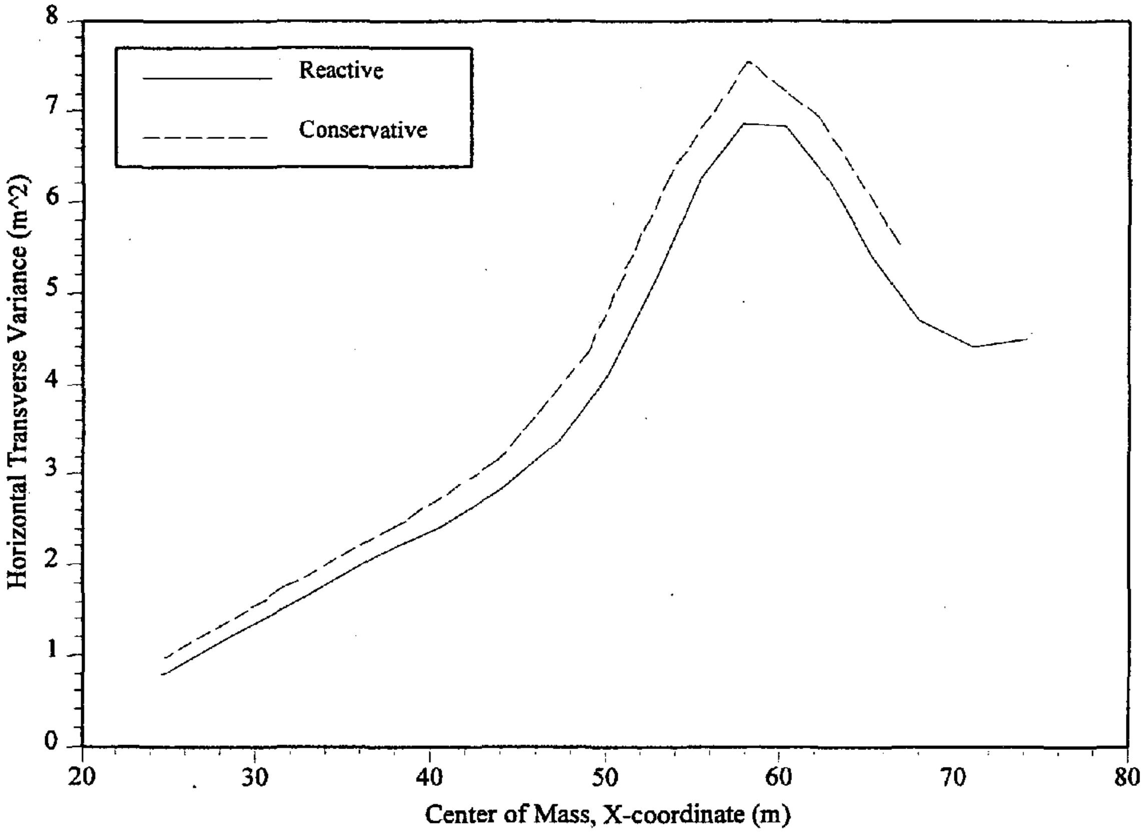


Figure 7. Reactive and conservative curves for realization 2 in a weakly heterogeneous flow field with 1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.

Apparent dispersivities for simulations in a weakly heterogeneous flow field with 1 kg of bromide are shown in Table 4. The apparent longitudinal dispersivity values for conservative simulations using all concentrations ranged from 0.276 m to 0.661 m. The same calculations performed on concentrations greater than 0.1 ppm ranged from 0.298 m to 0.670 m.

The ensemble mean estimates were calculated by averaging the dispersivity values for the five realizations in each case. Null hypothesis testing was employed to test if the ensemble mean estimates were significantly different. The null hypothesis in all cases states the two ensemble means are equal: the mean of the population from which the first sample was drawn is the same as the mean of the parent population of the second sample. A significance level of 5 percent was used in all statistical tests. This indicates there is a 5 percent chance of rejecting a true hypothesis (type I error). Results of increasing the significance level are discussed at the end of the Results and Discussion section.

The null hypothesis tests were set up in such a way as to isolate the affects of the parameter in question. For example, when testing the affects of the Freundlich isotherm, ensemble means with identical simulations and calculations for the reactive and conservative cases were compared. The ensemble mean estimate in a weakly heterogeneous flow field with a conservative tracer and 1 kg of bromide using all concentrations was tested with the ensemble mean estimate in a weakly heterogeneous flow field with a reactive tracer and 1 kg of bromide using all concentrations.

The ensemble mean estimates of apparent longitudinal dispersivities for the conservative simulations using all concentrations and those greater than 0.1 ppm were 0.493 m and 0.508 m, respectively. The null hypothesis was not rejected (see Table 5). The ensemble mean estimate of apparent longitudinal dispersivities for the reactive

Table 5. Statistics for hypothesis testing of ensemble means using all concentrations and omitting concentrations below 0.1 ppm. The significance level was 5 percent.

| Cases tested | Test F | Table F | Null Hyp. | Test t | Table t | Null Hyp. |
|---|---|---|---|---|---|---|
| 1,3 AL* | 1.099 | 6.39 | not rej. | -0.031 | +/- 2.306 | not rej. |
| 2,4 AL | 1.048 | 6.39 | not rej. | 0.103 | +/- 2.306 | not rej. |
| 5,7 AL | 1.180 | 6.39 | not rej. | -0.163 | +/- 2.306 | not rej. |
| 6,8 AL | 1.398 | 6.39 | not rej. | 0.309 | +/- 2.306 | not rej. |
| 9,11 AL | 1.085 | 6.39 | not rej. | 0.153 | +/- 2.306 | not rej. |
| 10,12 AL | 1.129 | 6.39 | not rej. | -0.049 | +/- 2.306 | not rej. |
| 13,15 AL | 1.093 | 6.39 | not rej. | -0.007 | +/- 2.306 | not rej. |
| 14,16 AL | 2.175 | 6.39 | not rej. | -0.782 | +/- 2.306 | not rej. |
| 1,3 AT** | 1.014 | 6.39 | not rej. | 0.043 | +/- 2.306 | not rej. |
| 2,4 AT | 1.018 | 6.39 | not rej. | 0.037 | +/- 2.306 | not rej. |
| 5,7 AT | 1.054 | 6.39 | not rej. | -0.055 | +/- 2.306 | not rej. |
| 6,8 AT | 1.203 | 6.39 | not rej. | -0.130 | +/- 2.306 | not rej. |
| 9,11 AT | 1.068 | 6.39 | not rej. | 0.221 | +/- 2.306 | not rej. |
| 10,12 AT | 1.385 | 6.39 | not rej. | 0.228 | +/- 2.306 | not rej. |
| 13,15 AT | 1.449 | 6.39 | not rej. | -0.225 | +/- 2.306 | not rej. |
| 14,16 AT | 4.104 | 6.39 | not rej. | -0.337 | +/- 2.306 | not rej. |

Key: Case 1 = 1.0 kg, strongly heterogeneous, all concentrations, conservative
Case 2 = 1.0 kg, strongly heterogeneous, all concentrations, reactive
Case 3 = 1.0 kg, strongly heterogeneous, concentrations > 0.1 ppm, conservative
Case 4 = 1.0 kg, strongly heterogeneous, concentrations > 0.1 ppm, reactive
Case 5 = 0.1 kg, strongly heterogeneous, all concentrations, conservative
Case 6 = 0.1 kg, strongly heterogeneous, all concentrations, reactive
Case 7 = 0.1 kg, strongly heterogeneous, concentrations > 0.1 ppm, conservative
Case 8 = 0.1 kg, strongly heterogeneous, concentrations > 0.1 ppm, reactive
Case 9 = 1.0 kg, weakly heterogeneous, all concentrations, conservative
Case 10 = 1.0 kg, weakly heterogeneous, all concentrations, reactive
Case 11 = 1.0 kg, weakly heterogeneous, concentrations > 0.1 ppm, conservative
Case 12 = 1.0 kg, weakly heterogeneous, concentrations > 0.1 ppm, reactive
Case 13 = 0.1 kg, weakly heterogeneous, all concentrations, conservative
Case 14 = 0.1 kg, weakly heterogeneous, all concentrations, reactive
Case 15 = 0.1 kg, weakly heterogeneous, concentrations > 0.1 ppm, conservative
Case 16 = 0.1 kg, weakly heterogeneous, concentrations > 0.1 ppm, reactive

* denotes apparent longitudinal dispersivity

** denotes apparent horizontal transverse dispersivity

simulations using all concentrations and those greater than 0.1 ppm were 0.462 m and 0.459 m, respectively. Again, the null hypothesis was not rejected (see Table 5).

The null hypothesis was also not rejected for the horizontal transverse dispersivities in the reactive and conservative cases. Therefore, with the assumptions and limited number of realizations used in this study, omitting concentrations below 0.1 ppm did not have a significant effect on apparent dispersivity values in a weakly heterogeneous flow field.

Hypothesis testing was also performed on the reactive and conservative runs. None of the null hypotheses was rejected (see Table 6). It was concluded, with the assumptions and limited number of realizations used in this study, that the Freundlich isotherm in Eq. (1) did not have a significant effect on apparent dispersivity values in a weakly heterogeneous flow field when compared to a conservative plume.

The reactive simulation for realization 2, as discussed above, was simulated for an additional 2 years. All data from the 2 year conservative simulation were used in the apparent dispersivity calculations. The apparent dispersivities in the longitudinal and horizontal transverse direction for the conservative simulation using concentrations greater than 0.1 ppm were 0.487 m and 0.078 m, respectively. The same calculations for the reactive simulation were 0.397 m and 0.073 m, respectively. Thus, the similarities in apparent longitudinal and horizontal transverse dispersivities between the conservative and reactive simulations were also observed for a longer plume travel distance in a weakly heterogeneous flow field.

Skewness and Kurtosis. The significance of skewness and kurtosis is that they are measures of how close a concentration distribution is to a Gaussian distribution. The skewness and kurtosis values through time for each simulation are listed in Appendix A.

Table 6. Statistics for hypothesis testing of reactive and conservative ensemble means. The significance level was 5 percent.

| Cases tested | Test F | Table F | Null Hyp. | Test t | Table t | Null Hyp. |
|---|---|---|---|---|---|---|
| 1,2 AL* | 1.068 | 6.39 | not rej. | -1.673 | +/- 2.306 | not rej. |
| 3,4 AL | 1.231 | 6.39 | not rej. | -1.553 | +/- 2.306 | not rej. |
| 5,6 AL | 1.199 | 6.39 | not rej. | -1.034 | +/- 2.306 | not rej. |
| 7,8 AL | 1.011 | 6.39 | not rej. | -0.472 | +/- 2.306 | not rej. |
| 9,10 AL | 1.804 | 6.39 | not rej. | -0.345 | +/- 2.306 | not rej. |
| 11,12 AL | 1.473 | 6.39 | not rej. | -0.559 | +/- 2.306 | not rej. |
| 13,14 AL | 3.928 | 6.39 | not rej. | 0.397 | +/- 2.306 | not rej. |
| 15,16 AL | 1.653 | 6.39 | not rej. | -0.205 | +/- 2.306 | not rej. |
| 1,2 AT** | 1.156 | 6.39 | not rej. | -0.079 | +/- 2.306 | not rej. |
| 3,4 AT | 1.161 | 6.39 | not rej. | -0.082 | +/- 2.306 | not rej. |
| 5,6 AT | 1.261 | 6.39 | not rej. | -0.306 | +/- 2.306 | not rej. |
| 7,8 AT | 1.438 | 6.39 | not rej. | -0.386 | +/- 2.306 | not rej. |
| 9,10 AT | 1.618 | 6.39 | not rej. | -0.598 | +/- 2.306 | not rej. |
| 11,12 AT | 2.098 | 6.39 | not rej. | -0.708 | +/- 2.306 | not rej. |
| 13,14 AT | 1.256 | 6.39 | not rej. | -0.859 | +/- 2.306 | not rej. |
| 15,16 AT | 3.557 | 6.39 | not rej. | -1.269 | +/- 2.306 | not rej. |

Key: Case 1 = 1.0 kg, strongly heterogeneous, all concentrations, conservative
Case 2 = 1.0 kg, strongly heterogeneous, all concentrations, reactive
Case 3 = 1.0 kg, strongly heterogeneous, concentrations > 0.1 ppm, conservative
Case 4 = 1.0 kg, strongly heterogeneous, concentrations > 0.1 ppm, reactive
Case 5 = 0.1 kg, strongly heterogeneous, all concentrations, conservative
Case 6 = 0.1 kg, strongly heterogeneous, all concentrations, reactive
Case 7 = 0.1 kg, strongly heterogeneous, concentrations > 0.1 ppm, conservative
Case 8 = 0.1 kg, strongly heterogeneous, concentrations > 0.1 ppm, reactive
Case 9 = 1.0 kg, weakly heterogeneous, all concentrations, conservative
Case 10 = 1.0 kg, weakly heterogeneous, all concentrations, reactive
Case 11 = 1.0 kg, weakly heterogeneous, concentrations > 0.1 ppm, conservative
Case 12 = 1.0 kg, weakly heterogeneous, concentrations > 0.1 ppm, reactive
Case 13 = 0.1 kg, weakly heterogeneous, all concentrations, conservative
Case 14 = 0.1 kg, weakly heterogeneous, all concentrations, reactive
Case 15 = 0.1 kg, weakly heterogeneous, concentrations > 0.1 ppm, conservative
Case 16 = 0.1 kg, weakly heterogeneous, concentrations > 0.1 ppm, reactive

* denotes apparent longitudinal dispersivity

** denotes apparent horizontal transverse dispersivity

The skewness and kurtosis values vary, but are relatively close to that of a normal distribution. This indicates that the apparent dispersivities are probably close to true dispersivities.

When using all concentrations in the calculations, the last three kurtosis values in the y-direction are negative for the reactive simulation of realization 5. As discussed earlier, kurtosis values are always positive because every term in Eq. (15) is positive or is raised to an even power. SUTRA and WATSUTRA provide non-zero concentration values for all nodes in the model domain. The majority of the values outside the plume are given extremely small negative numbers. Clearly, negative concentration values are not possible. These numbers are important because the bromide plume only occupies a small percentage of nodes in the model domain. The method of moments FORTRAN program uses all concentration values in the model domain (see Appendix E). When higher-order moments are calculated, such as third or fourth order, the solute concentration at a given node is multiplied by the third or fourth power of the quantity ($x-x_c$) or ($y-y_c$) (see Eq. 10). In addition, the concentration is multiplied by the density of water (998.23 kg/m$^3$) to convert mass fraction (kg/kg) to mass since each element has a volume of 1 m$^3$ (the moment programs take porosity into account). Clearly, if the quantity ($x-x_c$) or ($y-y_c$) is large, the fourth power of the quantity may produce a significant number when multiplied by the small negative concentration. Therefore the negative values for kurtosis are likely a result of the small negative concentrations. This interpretation is reinforced by the absence of negative kurtosis values when concentrations below 0.1 ppm are omitted.

It is not clear why SUTRA and WATSUTRA have small negative concentrations at many of the nodes when this model is simulated. It may be a result of numerical dispersion.

As a result of the negative concentration numbers at many of the nodes in the model domain, it is probably best to examine the moment calculations when the values below detection limit are omitted. One must exercise caution when interpreting the differences between moment values with and without omitting concentrations below detection limit. The presence of small negative values may only be a phenomenon observed in SUTRA and WATSUTRA or in similar finite-element programs. Thus, the findings may not apply to all solute transport modeling programs.

## Strongly Heterogeneous Flow Field

Ten simulations were performed in the strongly heterogeneous flow field with 1 kg of bromide, five conservative and five reactive. SURFER contour plots of the plumes are given in Appendix B. SURFER contour plots of the strongly heterogeneous natural log hydraulic conductivity fields are given in Appendix C. The difference in plume spreading between the weakly and strongly heterogeneous flow fields is striking. The strong heterogeneities caused enhanced spreading in the longitudinal and horizontal transverse directions.

### Spatial Moment Estimates of Plume Behavior

Mass of Bromide. Moment calculations, zeroth through fourth, are given in Appendix A. The same basic trends of tracer mass for the weakly heterogeneous flow field are observed in the strongly heterogeneous flow field. Again, about 42% of the tracer is adsorbed onto the sediments in the reactive simulations at 2 years.

Center of Mass. Graphs of center of mass as a function of time are shown in Appendix D. The average linear velocities show more variability than those for the weakly heterogeneous flow field; the velocities varied by as much as a factor of 2 (see Table 7). A greater range of velocities is expected for a greater variance in the hydraulic conductivity field. The retardation factor averaged approximately 1.7.

Table 7. Dispersivities, velocities, and retardation factors for simulations in a strongly heterogeneous flow field with 1 kg of bromide.

| Simulation | AL (m) | AT (m) | V (m/yr) | Retardation Factor |
|---|---|---|---|---|
| Case 1 = 1.0 kg, all concentrations, conservative | | | | |
| 1.1 | 1.919 | 0.701 | 14.198 | na |
| 1.2 | 1.230 | 0.477 | 10.181 | na |
| 1.3 | 1.188 | 0.168 | 17.538 | na |
| 1.4 | 1.430 | 0.118 | 22.266 | na |
| 1.5 | 1.555 | 0.301 | 19.889 | na |
| Ensemble mean* | 1.464 | 0.353 | 16.814 | na |
| Case 2 = 1.0 kg, all concentrations, reactive | | | | |
| 2.1 | 1.447 | 0.722 | 8.140 | 1.744 |
| 2.2 | 0.682 | 0.468 | 5.966 | 1.706 |
| 2.3 | 1.113 | 0.143 | 10.400 | 1.686 |
| 2.4 | 1.099 | 0.098 | 13.159 | 1.692 |
| 2.5 | 1.395 | 0.272 | 11.705 | 1.699 |
| Ensemble mean* | 1.147 | 0.341 | 9.874 | 1.705 |
| Case 3 = 1.0 kg, concentrations > 0.1 ppm, conservative | | | | |
| 3.1 | 1.850 | 0.708 | 14.121 | na |
| 3.2 | 1.151 | 0.484 | 10.086 | na |
| 3.3 | 1.222 | 0.175 | 17.332 | na |
| 3.4 | 1.520 | 0.117 | 21.780 | na |
| 3.5 | 1.551 | 0.314 | 19.761 | na |
| Ensemble mean* | 1.459 | 0.360 | 16.616 | na |
| Case 4 = 1.0 kg, concentrations > 0.1 ppm, reactive | | | | |
| 4.1 | 1.418 | 0.733 | 8.134 | 1.736 |
| 4.2 | 0.653 | 0.472 | 5.963 | 1.691 |
| 4.3 | 1.137 | 0.146 | 10.314 | 1.680 |
| 4.4 | 1.220 | 0.103 | 12.940 | 1.683 |
| 4.5 | 1.408 | 0.279 | 11.659 | 1.695 |
| Ensemble mean* | 1.167 | 0.347 | 9.802 | 1.697 |

* denotes estimate
'na' denotes not applicable

Plume Variance. Graphs of plume variance in the longitudinal and horizontal transverse directions as a function of center of mass (x-coordinate) are given in Appendix D. Note the scales for the reactive and conservative simulations are the same. The curves for the reactive simulations are similar to the conservative simulation curves. In most cases, the conservative simulations exhibited slightly enhanced plume variance.

The reactive simulation of realization 4 was run for an addition two years to see if the plume variance similarities hold for longer travel distances. The longitudinal and horizontal transverse variance as a function of center of mass using all concentrations are shown in Figures 8 and 9, respectively. The same quantities are graphed in Figures 10 and 11, respectively, using concentrations greater than 0.1 ppm in the calculations. These graphs indicate the reactive and conservative curves are similar. The conservative plume variances were slightly greater than the reactive variances.

Apparent dispersivities were calculated after performing a linear interpolation as previously described. The apparent dispersivities for the 1 kg simulations in a strongly heterogeneous flow field are given in Table 7. The values are approximately 2 to 3 times larger than those in the weakly heterogeneous flow field. This is the result of greater heterogeneity in the flow fields.

The ensemble mean estimates of apparent longitudinal dispersivities for the conservative simulations using all concentrations and only those greater than 0.1 ppm were 1.464 m and 1.459 m, respectively. Null hypothesis testing was employed to test if they were significantly different. The null hypothesis was not rejected (see Table 5). The same hypothesis test was performed on the ensemble mean estimates of the apparent horizontal transverse dispersivities. Again, the null hypothesis was not rejected.

The ensemble mean estimates of apparent longitudinal dispersivities for the reactive simulations using all concentrations and only those greater than 0.1 ppm were 1.147 m and 1.167 m, respectively. The null hypothesis was not rejected. The same

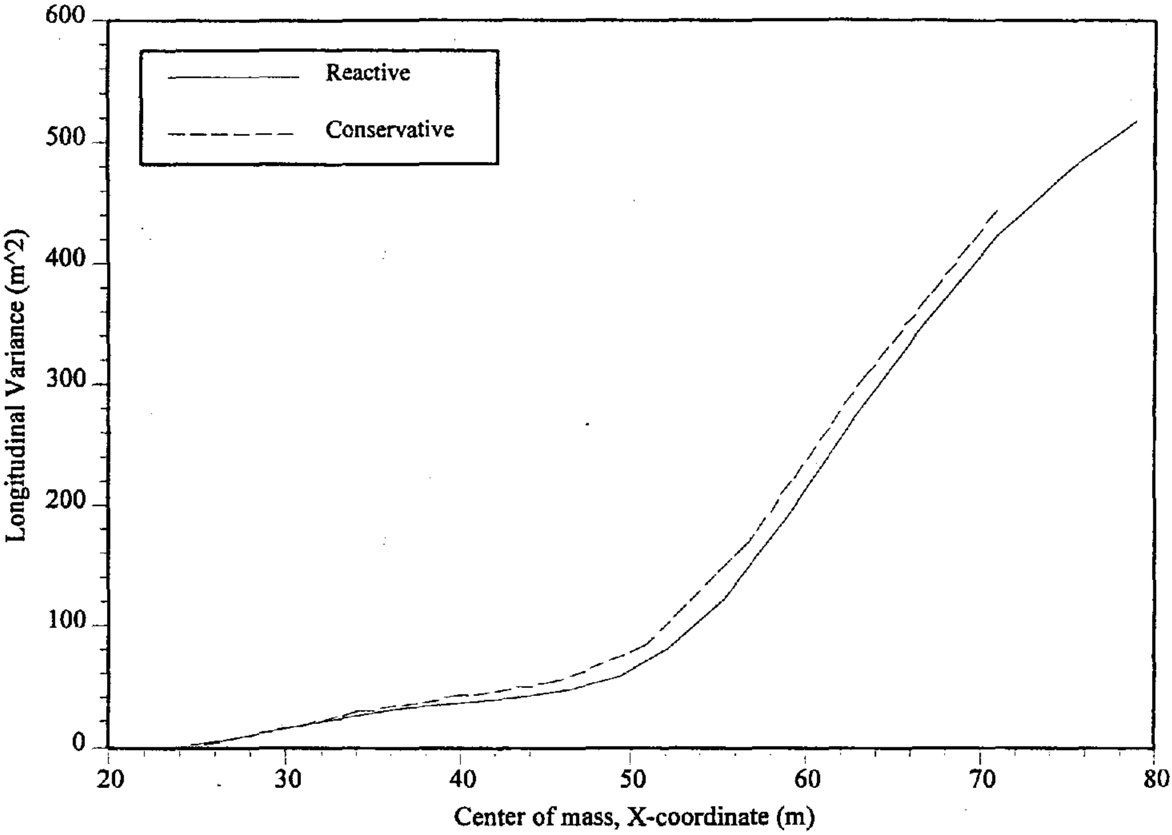


Figure 8. Reactive and conservative curves for realization 4 in a strongly heterogeneous flow field with 1 kg of bromide. All concentrations were used in calculations.

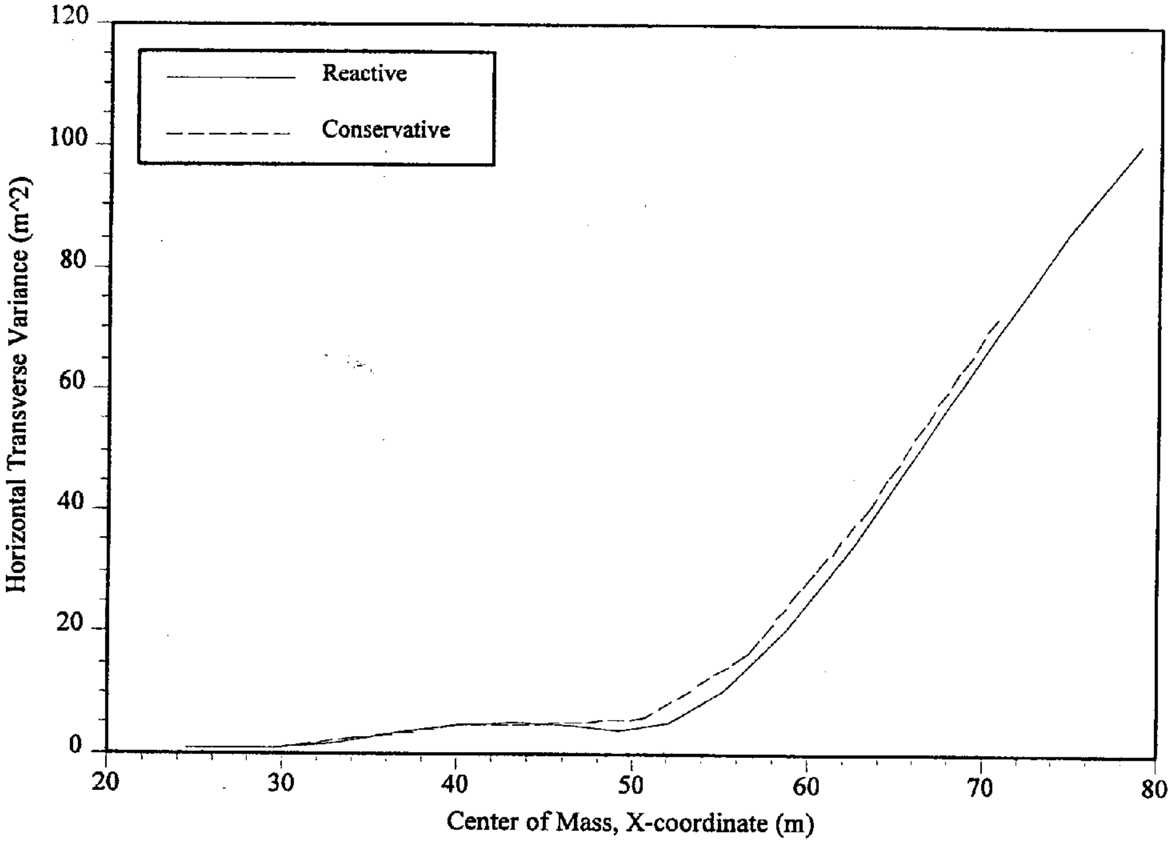


Figure 9. Reactive and conservative curves for realization 4 in a strongly heterogeneous flow field with 1 kg of bromide. All concentrations were used in calculations.

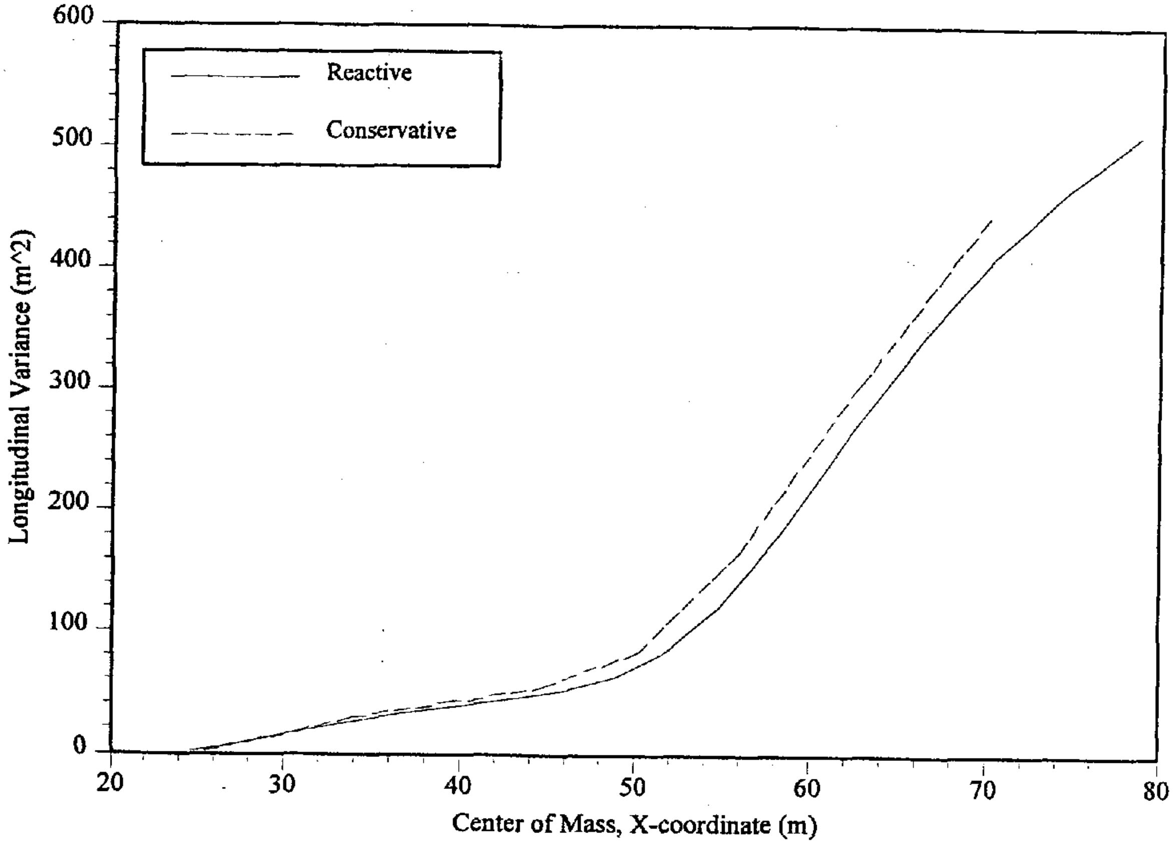


Figure 10. Reactive and conservative curves for realization 4 in a strongly heterogeneous flow field with 1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.

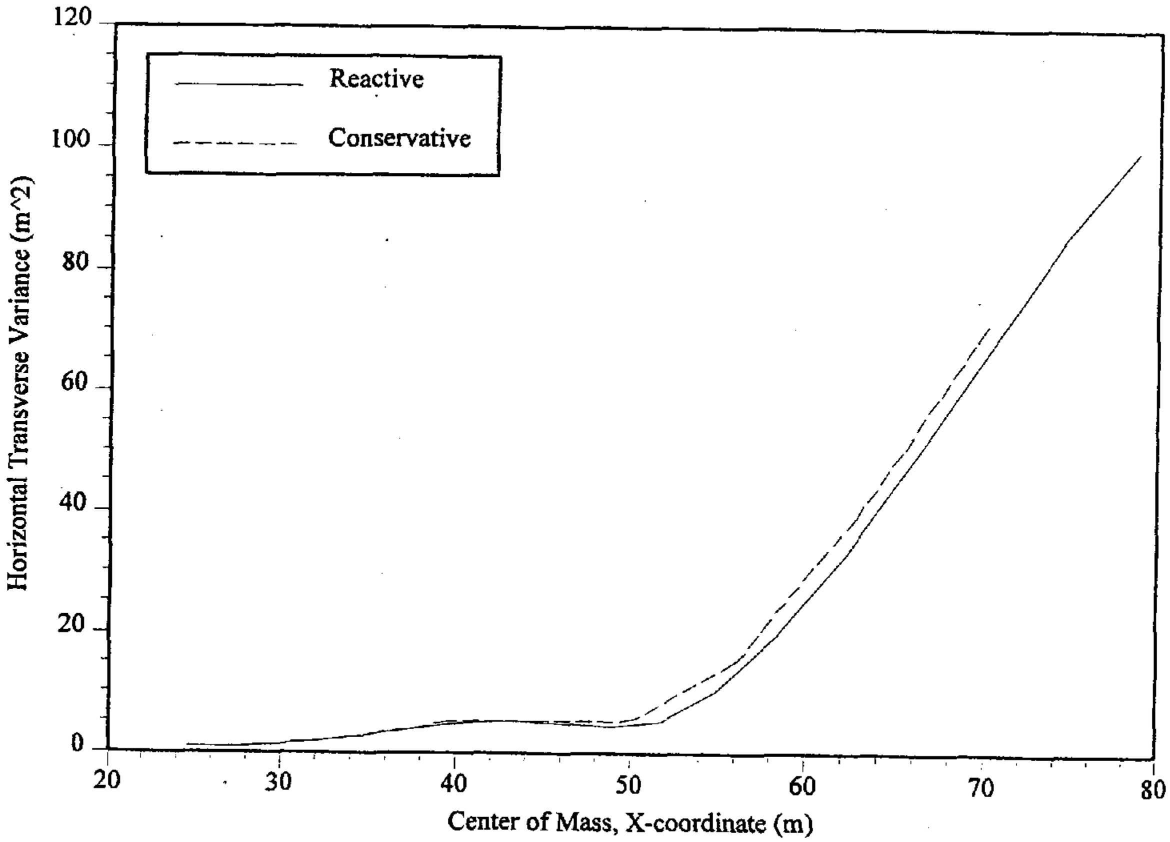


Figure 11. Reactive and conservative curves for realization 4 in a strongly heterogeneous flow field with 1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.

hypothesis test was performed on the ensemble mean estimates of the horizontal transverse dispersivities. It was not rejected. This indicates that, with the assumptions and limited number of realizations used in this study, there is no significant difference between the apparent dispersivity ensemble mean estimates using all concentrations and only those greater than 0.1 ppm in a strongly heterogeneous flow field.

The ensemble mean estimates for the reactive simulations were compared to those with the same parameters for the conservative simulations. Again, none of the null hypotheses was rejected. Thus, with the assumptions and limited number of realizations used in this study, there was no significant difference between the apparent dispersivity ensemble mean estimates of the conservative and reactive simulations in a strongly heterogeneous flow field.

As stated above, the reactive simulation of realization 4 was run for an additional two years to see if the similarities between the reactive and conservative cases hold for longer travel distances. All data from the 2 year conservative simulation were used in the apparent dispersivity calculations. The apparent longitudinal and horizontal transverse dispersivities for the conservative simulation using concentrations greater than 0.1 ppm were 5.018 m and 0.744 m, respectively. The same calculations for the reactive simulation yielded 4.274 m and 0.622 m, respectively. Thus, the similarities between the reactive and conservative apparent longitudinal and horizontal transverse dispersivities were observed for a longer plume travel distance in a strongly heterogeneous flow field.

Skewness and Kurtosis. The values of skewness and kurtosis through time for the strongly heterogeneous flow field are given in Appendix A. In contrast to the weakly heterogeneous flow field, the skewness and kurtosis values in many simulations indicate concentration distributions much different than a Gaussian distribution.

## Simulations with 0.1 kg of Bromide

The purpose of performing simulations with 0.1 kg of bromide was to examine the effects of tracer mass on apparent dispersivities. The only difference between the simulations with 0.1 kg of bromide and those with 1 kg was the injection time. The injection time for the 0.1 kg simulations was 1/10 that of the 1 kg simulations; the injection rate and bromide concentration in the injected water were unchanged. The simulations in the weakly and strongly heterogeneous flow fields will be discussed together because most of the same trends are observed in both flow fields.

SURFER contour plots of plumes using 0.1 kg of bromide are shown in Appendix B. For comparison, the contour intervals in the 0.1 kg plots were exactly one order of magnitude smaller than the 1 kg plots. The plumes with 0.1 kg of bromide were similar to the 1 kg plumes. In most cases the 0.1 kg plumes were slightly smaller than the 1 kg plumes, but the same general characteristics are present.

### Spatial Moment Estimates of Plume Behavior

Mass of Bromide. The same basic trends of tracer mass in the 1 kg simulations were observed in the 0.1 kg simulations. The main difference between them is that the reactive 0.1 kg simulations experience more mass loss due to adsorption. Approximately 48 to 50 percent of the total tracer mass was lost due to adsorption at 2 years; the reactive 1 kg simulations lost about 42 percent to adsorption.

Center of Mass. Graphs of center of mass as a function of time are given in Appendix D. Average linear velocities for the weakly and strongly heterogeneous flow fields are given in Tables 8 and 9, respectively. In all cases, with the exception of the strongly heterogeneous conservative cases, the ensemble mean velocities are slightly smaller in the 0.1 kg simulations than the equivalent 1 kg simulations. The retardation factor averaged approximately 1.85 in the weakly and strongly heterogeneous flow fields.

Table 8. Dispersivities, velocities, and retardation factors for simulations in a weakly heterogeneous flow field with 0.1 kg of bromide.

| Simulation | AL (m) | AT (m) | V (m/yr) | Retardation Factor |
|---|---|---|---|---|
| Case 13 = 0.1 kg, all concentrations, conservative | | | | |
| 13.1 | 0.379 | 0.073 | 23.782 | na |
| 13.2 | 0.227 | 0.079 | 23.393 | na |
| 13.3 | 0.596 | 0.055 | 18.240 | na |
| 13.4 | 0.494 | 0.086 | 25.389 | na |
| 13.5 | 0.737 | 0.033 | 22.657 | na |
| Ensemble mean* | 0.487 | 0.065 | 22.692 | na |
| Case 14 = 0.1 kg, all concentrations, reactive | | | | |
| 14.1 | 0.470 | 0.064 | 12.659 | 1.879 |
| 14.2 | 0.381 | 0.061 | 12.655 | 1.848 |
| 14.3 | 0.585 | 0.042 | 9.592 | 1.902 |
| 14.4 | 0.567 | 0.076 | 13.208 | 1.922 |
| 14.5 | 0.625 | 0.028 | 11.928 | 1.899 |
| Ensemble mean* | 0.526 | 0.054 | 12.008 | 1.890 |
| Case 15 = 0.1 kg, concentrations > 0.1 ppm, conservative | | | | |
| 15.1 | 0.350 | 0.073 | 23.536 | na |
| 15.2 | 0.263 | 0.073 | 23.000 | na |
| 15.3 | 0.633 | 0.054 | 17.810 | na |
| 15.4 | 0.472 | 0.077 | 25.040 | na |
| 15.5 | 0.711 | 0.035 | 22.453 | na |
| Ensemble mean* | 0.486 | 0.062 | 22.368 | na |
| Case 16 = 0.1 kg, concentrations > 0.1 ppm, reactive | | | | |
| 16.1 | 0.354 | 0.059 | 12.839 | 1.833 |
| 16.2 | 0.286 | 0.053 | 12.772 | 1.801 |
| 16.3 | 0.588 | 0.045 | 9.663 | 1.843 |
| 16.4 | 0.467 | 0.060 | 13.361 | 1.874 |
| 16.5 | 0.625 | 0.038 | 12.130 | 1.851 |
| Ensemble mean* | 0.464 | 0.051 | 12.153 | 1.840 |

* denotes estimate
'na' denotes not applicable

Table 9. Dispersivities, velocities, and retardation factors for simulations in a strongly heterogeneous flow field with 0.1 kg of bromide.

| Simulation | AL (m) | AT (m) | V (m/yr) | Retardation Factor |
|---|---|---|---|---|
| Case 5 = 0.1 kg, all concentrations, conservative | | | | |
| 5.1 | 1.397 | 0.555 | 13.644 | na |
| 5.2 | 0.562 | 0.480 | 10.075 | na |
| 5.3 | 1.100 | 0.150 | 18.034 | na |
| 5.4 | 1.069 | 0.127 | 22.686 | na |
| 5.5 | 1.608 | 0.267 | 18.781 | na |
| Ensemble mean* | 1.147 | 0.316 | 16.644 | na |
| Case 6 = 0.1 kg, all concentrations, reactive | | | | |
| 6.1 | 0.904 | 0.517 | 7.260 | 1.879 |
| 6.2 | 0.283 | 0.402 | 5.790 | 1.740 |
| 6.3 | 1.168 | 0.141 | 9.302 | 1.939 |
| 6.4 | 0.999 | 0.123 | 11.974 | 1.895 |
| 6.5 | 1.144 | 0.219 | 9.722 | 1.932 |
| Ensemble mean* | 0.900 | 0.280 | 8.810 | 1.877 |
| Case 7 = 0.1 kg, concentrations > 0.1 ppm, conservative | | | | |
| 7.1 | 1.258 | 0.532 | 13.373 | na |
| 7.2 | 0.388 | 0.480 | 9.849 | na |
| 7.3 | 1.160 | 0.144 | 17.473 | na |
| 7.4 | 1.173 | 0.125 | 21.770 | na |
| 7.5 | 1.544 | 0.265 | 18.498 | na |
| Ensemble mean* | 1.105 | 0.309 | 16.193 | na |
| Case 8 = 0.1 kg, concentrations > 0.1 ppm, reactive | | | | |
| 8.1 | 1.115 | 0.448 | 7.464 | 1.792 |
| 8.2 | 0.241 | 0.419 | 5.526 | 1.782 |
| 8.3 | 1.119 | 0.121 | 9.192 | 1.901 |
| 8.4 | 1.054 | 0.129 | 11.684 | 1.863 |
| 8.5 | 1.355 | 0.217 | 9.856 | 1.877 |
| Ensemble mean* | 0.977 | 0.267 | 8.744 | 1.843 |

* denotes estimate

'na' denotes not applicable

Plume Variance. The graphs of plume variances versus center of mass for the 0.1 kg simulations are shown in Appendix D. The variances in the 0.1 kg simulations follow the same trends as the 1 kg simulations, but are slightly smaller.

Apparent dispersivities for the 0.1 kg simulations in the weakly and strongly heterogeneous flow fields are given in Tables 8 and 9, respectively. Note the total mass of tracer does not affect the apparent dispersivity calculations since the second moment is normalized by the total mass of tracer (see Appendix E). All ensemble mean estimates in the strongly heterogeneous flow field were smaller than the 1 kg simulations. The ensemble mean estimates for the 0.1 kg simulations in the weakly heterogeneous flow field were mixed; most were smaller than the equivalent 1 kg ensemble means, but a few were greater. The reason for this finding is unclear, but may be partly due to small numerical errors in SUTRA and WATSUTRA.

The ensemble mean estimates of the longitudinal and horizontal transverse dispersivities for the 0.1 kg simulations were tested against the same simulations with 1 kg of bromide. The results of the null hypothesis testing are shown in Table 10. None of the hypotheses was rejected. Therefore, with the assumptions and limited number of realizations used in this study, there is no evidence to suggest tracer mass has any significant effect on apparent dispersivities in weakly and strongly heterogeneous flow fields.

Skewness and Kurtosis. The skewness and kurtosis values for the 0.1 kg simulations differed from the 1 kg simulations, especially kurtosis values in the reactive simulations using all concentrations in the calculations. Many of the kurtosis values for the reactive simulations using all concentrations were negative. This result is probably due to the small negative concentrations in the model domain, as previously discussed. This is supported by the observation that negative kurtosis values only occur in the moment calculations using all concentrations.

Table 10. Statistics for hypothesis testing of tracer mass ensemble means. The significance level was 5 percent.

| Cases tested | Test F | Table F | Null Hyp. | Test t | Table t | Null Hyp. |
|---|---|---|---|---|---|---|
| 1,5 AL* | 1.801 | 6.39 | not rej. | -1.438 | +/- 2.306 | not rej. |
| 2,6 AL | 1.406 | 6.39 | not rej. | -1.172 | +/- 2.306 | not rej. |
| 3,7 AL | 2.334 | 6.39 | not rej. | -1.543 | +/- 2.306 | not rej. |
| 4,8 AL | 1.876 | 6.39 | not rej. | -0.805 | +/- 2.306 | not rej. |
| 9,13 AL | 1.535 | 6.39 | not rej. | -0.055 | +/- 2.306 | not rej. |
| 10,14 AL | 1.419 | 6.39 | not rej. | 0.919 | +/- 2.306 | not rej. |
| 11,15 AL | 1.524 | 6.39 | not rej. | -0.204 | +/- 2.306 | not rej. |
| 12,16 AL | 1.358 | 6.39 | not rej. | 0.063 | +/- 2.306 | not rej. |
| 1,5 AT** | 1.527 | 6.39 | not rej. | -0.270 | +/- 2.306 | not rej. |
| 2,6 AT | 2.226 | 6.39 | not rej. | -0.435 | +/- 2.306 | not rej. |
| 3,7 AT | 1.633 | 6.39 | not rej. | -0.369 | +/- 2.306 | not rej. |
| 4,8 AT | 2.727 | 6.39 | not rej. | -0.588 | +/- 2.306 | not rej. |
| 9,13 AT | 1.338 | 6.39 | not rej. | -0.205 | +/- 2.306 | not rej. |
| 10,14 AT | 1.039 | 6.39 | not rej. | -0.460 | +/- 2.306 | not rej. |
| 11,15 AT | 1.815 | 6.39 | not rej. | -0.691 | +/- 2.306 | not rej. |
| 12,16 AT | 3.077 | 6.39 | not rej. | -1.342 | +/- 2.306 | not rej. |

Key: Case 1 = 1.0 kg, strongly heterogeneous, all concentrations, conservative
Case 2 = 1.0 kg, strongly heterogeneous, all concentrations, reactive
Case 3 = 1.0 kg, strongly heterogeneous, concentrations > 0.1 ppm, conservative
Case 4 = 1.0 kg, strongly heterogeneous, concentrations > 0.1 ppm, reactive
Case 5 = 0.1 kg, strongly heterogeneous, all concentrations, conservative
Case 6 = 0.1 kg, strongly heterogeneous, all concentrations, reactive
Case 7 = 0.1 kg, strongly heterogeneous, concentrations > 0.1 ppm, conservative
Case 8 = 0.1 kg, strongly heterogeneous, concentrations > 0.1 ppm, reactive
Case 9 = 1.0 kg, weakly heterogeneous, all concentrations, conservative
Case 10 = 1.0 kg, weakly heterogeneous, all concentrations, reactive
Case 11 = 1.0 kg, weakly heterogeneous, concentrations > 0.1 ppm, conservative
Case 12 = 1.0 kg, weakly heterogeneous, concentrations > 0.1 ppm, reactive
Case 13 = 0.1 kg, weakly heterogeneous, all concentrations, conservative
Case 14 = 0.1 kg, weakly heterogeneous, all concentrations, reactive
Case 15 = 0.1 kg, weakly heterogeneous, concentrations > 0.1 ppm, conservative
Case 16 = 0.1 kg, weakly heterogeneous, concentrations > 0.1 ppm, reactive

* denotes apparent longitudinal dispersivity

** denotes apparent horizontal transverse dispersivity

## Significance Levels of Null Hypothesis Testing

A 5 percent significance level was used in all null hypothesis testing in this study. This significance level was chosen because it is widely used in statistics. A 5 percent significance level for 8 degrees of freedom corresponds to a table t value of 2.306. A total of 48 null hypothesis were tested in this study (see Tables 5, 6, and 10). None of the hypotheses was rejected.

The significance level was increased to see at what point the hypotheses would be rejected. A 10 percent significance level for 8 degrees of freedom corresponds to a table t value of 1.860. None of the hypotheses was rejected at this level. A 20 percent significance level corresponds to a table t value of 1.397. Only 4 of the 48 hypotheses were rejected at this level.

The acceptance of the null hypotheses in this study is reasonable because the significance level must be increased to 20 percent in order to reject some of the hypotheses (4 out of 48). At a 20 percent significance level there is a 20 percent chance of rejecting a true hypothesis (type I error).

## Practical Application of the Results

Bromide is commonly used as a tracer because it is inexpensive, easily detected, and is commonly believed to behave conservatively. In recent years, however, bromide has been found to be non-conservative in anion-sorbing sediments. This study has shown, with several assumptions and a limited number of realizations, that bromide is a suitable groundwater tracer for macrodispersivity experiments in anion-sorbing sediments.

One of the assumptions used in this study is that the adsorption and desorption isotherms are equal. There are apparently no data on desorption rates for bromide. If, for example, desorption follows a more strongly non-linear isotherm than adsorption, the apparent longitudinal dispersivity would be overestimated because of plume "tailing".

Testing the desorption isotherm with column studies would, however, be difficult and costly to perform.

Another assumption used in this study is that the aquifer is chemically homogeneous. There are not enough data available at the present time to model chemical heterogeneity. Adsorption of bromide at the Savannah River Site is primarily a function of the iron oxide content of the sediments (Seaman et al., 1996) and has apparently no correlation with hydraulic conductivity. Chemical heterogeneity has been examined by several researchers. Bosma et al. (1996) found the effects of chemical heterogeneity in strongly non-linear sorbing solutes to be small on plume variance. It has apparently not been explored in weakly sorbing solutes. A more sophisticated model than SUTRA and WATSUTRA would be required to perform such modeling.

Recently, researchers have been using dissolved noble gases as tracers because they are truly conservative (Sanford et al., 1996). Dissolved gas tracers, in contrast to bromide, are cumbersome and expensive to sample and analyze. However, researchers are developing simplified sampling and analyzing techniques for dissolved gas tracers to lower these costs (e.g. Sanford et al., 1996).

The results of this study are encouraging for the use of bromide as a groundwater tracer in anion-sorbing sediments. The desorption isotherm, however, needs to be examined before one can definitively conclude that bromide can be used as a tracer for macrodispersivity experiments in anion-sorbing sediments.

# SUMMARY AND CONCLUSIONS

A weakly non-linear, experimentally derived Freundlich sorption isotherm was found to describe bromide adsorption in sediments from the Savannah River Site in South Carolina. The aim of this research was to quantify the effects of this sorption isotherm on apparent dispersivities relative to a conservative tracer. In addition, the effects of an order-of-magnitude difference in tracer mass injected into the simulated aquifer and omitting concentrations below detection level (set at 0.1 ppm) were evaluated.

Monte Carlo simulations were performed using SUTRA and WATSUTRA. The models were developed to simulate natural gradient tracer tests. Two different hydraulic conductivity fields were modeled; a weakly heterogeneous field with physical parameters similar to the Borden aquifer in Ontario, Canada and a strongly heterogeneous field with physical parameters similar to the Columbus aquifer in Mississippi. The variance of the natural log transformed hydraulic conductivity was chosen to differ by an order-of-magnitude. These hydraulic conductivity fields represent two extremes in aquifer conditions.

Forty simulations were performed in this study for eight cases. Five realizations were performed for each case; each realization was simulated for 2 years (with two exceptions). Apparent dispersivities were calculated by the method of moments. Ensemble means were estimated by averaging the five realizations for each case. Null hypothesis testing was performed with a standard t-test to test the significance between the ensemble mean estimates for various cases.

The following simplifying assumptions were used in this research:

1) Sorption according to the Freundlich isotherm was assumed to be a reversible equilibrium process. Thus, desorption followed the same isotherm as adsorption, only with decreasing concentrations, and both adsorption and desorption were rapid in comparison to advective flow.

2) The Freundlich isotherm was constant throughout the model domain.

3) The groundwater model employed was two-dimensional; vertical heterogeneity was not represented.

With the above assumptions and the limited number of realizations used in this study, the following conclusions can be drawn:

1) The Freundlich isotherm did not significantly affect apparent dispersivity values; thus, tracers which are adsorbed following a Freundlich isotherm similar to the one used in this study are not unsuitable as groundwater tracers.

2) An order-of-magnitude difference in tracer mass did not significantly affect apparent dispersivity values.

3) Omitting concentrations below detection limit did not significantly affect apparent dispersivity values.

4) In numerical simulations, moment calculations should be performed with concentrations above detection level because using all concentrations can have adverse effects on higher-order moments. This finding may, however, be unique to SUTRA and WATSUTRA or to similar finite-element programs. Omitting low concentrations is reasonable because numerical studies are meant to replicate field studies.

The results of this study are encouraging for the use of bromide as a groundwater tracer in anion-sorbing sediments. The desorption isotherm, however, needs to be examined before one can definitively conclude that bromide can be used as a tracer for macrodispersivity experiments in anion-sorbing sediments.

# APPENDICES

# APPENDIX A

# MOMENT CALCULATIONS

Weakly Heterogeneous
Realization 1
1 Kilogram of Bromide
All Concentrations Used in Calculations

*************************************************************************************

Conservative Run

*************************************************************************************

| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 1.0001 | 24.5665 | 32.0971 | 1.2214 | 0.9216 | 0.5494 | 0.0923 | 3.4211 | 2.8443 |
| 0.0114 | 1.0001 | 24.8011 | 32.1255 | 1.5614 | 0.8995 | 0.6812 | 0.0942 | 3.4981 | 2.8221 |
| 0.2614 | 1.0001 | 31.0896 | 32.3770 | 11.6149 | 1.0121 | 0.6800 | 0.1422 | 3.0487 | 3.1483 |
| 0.5113 | 1.0001 | 37.8965 | 32.3370 | 18.2535 | 1.9780 | -0.0015 | 0.0529 | 3.0266 | 3.9360 |
| 0.7613 | 1.0001 | 43.8887 | 32.0349 | 20.7139 | 3.1311 | 0.4685 | -0.5231 | 3.0548 | 3.9826 |
| 1.0113 | 1.0001 | 49.1625 | 31.5683 | 25.1115 | 3.8143 | 1.4815 | -1.1464 | 3.2990 | 3.2473 |
| 1.2612 | 1.0001 | 54.2330 | 31.1266 | 34.7925 | 3.8319 | 3.5578 | -0.7456 | 3.9337 | 2.7762 |
| 1.5112 | 1.0001 | 59.6777 | 30.9365 | 55.4922 | 3.9826 | 5.1825 | 1.0769 | 3.4503 | 4.6405 |
| 1.7612 | 1.0001 | 65.9357 | 31.3664 | 83.0534 | 6.2282 | 3.8587 | 3.1753 | 2.7429 | 5.4858 |
| 2.0114 | 1.0001 | 72.7905 | 32.4377 | 103.0710 | 9.6304 | 1.1864 | 3.0417 | 2.6234 | 3.7905 |

*************************************************************************************

Reactive Run

*************************************************************************************

| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.6574 | 24.3978 | 32.0631 | 0.9055 | 0.7668 | 0.3537 | 0.0658 | 3.2124 | 2.8273 |
| 0.0114 | 0.6545 | 24.5454 | 32.0823 | 1.1002 | 0.7570 | 0.4525 | 0.0763 | 3.3010 | 2.7868 |
| 0.2614 | 0.6229 | 28.3377 | 32.3356 | 6.8112 | 0.7072 | 0.4469 | 0.1631 | 2.8130 | 2.1765 |
| 0.5113 | 0.6059 | 32.5868 | 32.3748 | 12.3618 | 0.9783 | -0.1720 | 0.1393 | 2.9529 | 2.9817 |
| 0.7613 | 0.5971 | 36.7364 | 32.3462 | 16.1052 | 1.5366 | -0.8912 | 0.0274 | 3.0662 | 3.4222 |
| 1.0113 | 0.5916 | 40.4959 | 32.2255 | 18.1348 | 2.1781 | -1.3121 | -0.1099 | 3.2945 | 3.5129 |
| 1.2612 | 0.5885 | 43.8592 | 32.0111 | 19.9494 | 2.6992 | -1.3642 | -0.4867 | 3.3862 | 3.3650 |
| 1.5112 | 0.5858 | 46.9701 | 31.7508 | 22.1862 | 3.1453 | -1.3491 | -0.9201 | 3.4109 | 3.0674 |
| 1.7612 | 0.5836 | 49.9294 | 31.4872 | 24.7929 | 3.5176 | -1.2188 | -0.9692 | 3.5039 | 2.8885 |
| 2.0114 | 0.5816 | 52.8136 | 31.2133 | 28.5866 | 3.6094 | -0.4644 | -0.6897 | 3.6699 | 2.7628 |

*************************************************************************************

Key: XC and YC are the center of mass values in the x and y directions, respectively
Var X and Var Y are the plume variances in the x and y directions, respectively
SKX and SKY are the plume skewness values in the x and y directions, respectively
KRX and KRY are the plume kurtosis values in the x and y directions, respectively

Weakly Heterogeneous
Realization 2
1 Kilogram of Bromide
All Concentrations Used in Calculations

********************************************************************************

Conservative Run

********************************************************************************

| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 1.0001 | 24.7014 | 31.9337 | 1.2126 | 0.9598 | 0.5369 | -0.0622 | 3.3521 | 2.9688 |
| 0.0114 | 1.0001 | 25.0255 | 31.9340 | 1.5930 | 0.9910 | 0.5687 | -0.0938 | 3.2899 | 3.0097 |
| 0.2614 | 1.0001 | 31.6779 | 32.1099 | 8.6523 | 1.6780 | 0.8432 | 0.2081 | 3.2255 | 3.1882 |
| 0.5113 | 1.0001 | 38.0680 | 33.1034 | 14.5517 | 2.3131 | 0.3725 | 0.5461 | 2.9758 | 2.6179 |
| 0.7613 | 1.0001 | 43.9162 | 33.3759 | 17.2021 | 3.0528 | 0.6745 | 0.2212 | 2.9847 | 2.9339 |
| 1.0113 | 1.0001 | 49.1518 | 33.4190 | 19.1857 | 4.3149 | 0.9602 | 0.6268 | 2.8192 | 3.5682 |
| 1.2612 | 1.0001 | 53.8699 | 33.9824 | 21.3472 | 6.2377 | 1.5744 | 1.3574 | 3.1475 | 3.6383 |
| 1.5112 | 1.0001 | 58.2344 | 34.8836 | 25.5015 | 7.4140 | 2.8823 | 1.1386 | 3.8119 | 2.8907 |
| 1.7612 | 1.0001 | 62.5090 | 35.6643 | 34.4842 | 6.7100 | 4.8180 | 0.5034 | 4.1806 | 2.3870 |
| 2.0114 | 1.0001 | 67.0663 | 36.0747 | 50.9757 | 5.3197 | 5.7660 | 0.1897 | 3.5566 | 2.3296 |

********************************************************************************

Reactive Run

********************************************************************************

| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.6574 | 24.4979 | 31.9508 | 0.8965 | 0.7810 | 0.3844 | -0.0349 | 3.2112 | 2.9031 |
| 0.0114 | 0.6533 | 24.7111 | 31.9542 | 1.1367 | 0.7998 | 0.4270 | -0.0514 | 3.1920 | 2.9186 |
| 0.2614 | 0.6195 | 29.0534 | 31.9319 | 5.3541 | 1.1630 | 0.2460 | -0.0624 | 3.1377 | 2.7195 |
| 0.5113 | 0.6086 | 33.0779 | 32.3388 | 9.5860 | 1.5189 | 0.2530 | 0.4893 | 2.9785 | 2.4602 |
| 0.7613 | 0.6013 | 37.0259 | 33.0140 | 13.1244 | 1.9143 | -0.4320 | 0.6555 | 2.9305 | 2.2171 |
| 1.0113 | 0.5960 | 40.7136 | 33.3661 | 15.0496 | 2.2624 | -0.7923 | 0.4128 | 3.2347 | 2.5197 |
| 1.2612 | 0.5918 | 44.1096 | 33.3758 | 16.6516 | 2.7389 | -0.8016 | 0.1415 | 3.2564 | 2.7556 |
| 1.5112 | 0.5886 | 47.2537 | 33.3457 | 18.0814 | 3.2866 | -1.0085 | 0.1566 | 3.2176 | 2.8771 |
| 1.7612 | 0.5857 | 50.1717 | 33.4918 | 19.2188 | 4.0409 | -1.2471 | 0.5293 | 3.3184 | 3.2158 |
| 2.0114 | 0.5832 | 52.8938 | 33.8540 | 20.3486 | 5.0747 | -1.3560 | 1.0285 | 3.4756 | 3.4548 |
| 2.2614 | 0.5808 | 55.4588 | 34.3653 | 21.6658 | 6.1187 | -1.2877 | 1.2344 | 3.6235 | 3.2224 |
| 2.5113 | 0.5787 | 57.9102 | 34.9199 | 23.4893 | 6.7200 | -0.9338 | 1.0327 | 3.7520 | 2.7808 |
| 2.7613 | 0.5768 | 60.3105 | 35.4224 | 26.4807 | 6.6519 | -0.1801 | 0.6249 | 3.8081 | 2.4493 |
| 3.0113 | 0.5751 | 62.7461 | 35.8127 | 31.5074 | 6.0633 | 0.8623 | 0.2349 | 3.7098 | 2.2927 |
| 3.2612 | 0.5736 | 65.3098 | 36.0591 | 39.2814 | 5.2804 | 1.8032 | -0.0443 | 3.4284 | 2.2590 |
| 3.5112 | 0.5720 | 68.0753 | 36.1591 | 49.7830 | 4.6247 | 2.1583 | -0.2033 | 3.0147 | 2.2713 |
| 3.7612 | 0.5704 | 71.0607 | 36.1286 | 61.7203 | 4.3440 | 1.6367 | -0.3146 | 2.6055 | 2.3700 |
| 4.0114 | 0.5688 | 74.2276 | 36.0111 | 72.9324 | 4.4894 | 0.2902 | -0.3434 | 2.3329 | 2.5734 |

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Weakly Heterogeneous
Realization 3
1 Kilogram of Bromide
All Concentrations Used in Calculations

* * *

Conservative Run

* * *

| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) |  | (Unitless values) |  |  |
| 0 | 1.0001 | 24.3185 | 31.8779 | 1.0567 | 1.0856 | 0.3917 | -0.0540 | 3.1358 | 3.0304 |
| 0.0114 | 1.0001 | 24.5242 | 31.8719 | 1.2717 | 1.1360 | 0.4370 | -0.0808 | 3.2164 | 3.0719 |
| 0.2614 | 1.0001 | 28.7287 | 31.7802 | 6.5568 | 1.4412 | 1.5151 | -0.1327 | 3.5965 | 2.7972 |
| 0.5113 | 1.0001 | 33.3194 | 31.9527 | 15.1665 | 1.6861 | 1.1503 | -0.0869 | 2.6183 | 4.2749 |
| 0.7613 | 1.0001 | 38.0788 | 31.9892 | 19.8447 | 2.6462 | -0.4115 | -0.1776 | 2.9459 | 4.0656 |
| 1.0113 | 1.0001 | 42.4145 | 31.8365 | 22.6142 | 3.1226 | 0.8669 | -0.3466 | 4.0686 | 3.2065 |
| 1.2612 | 1.0001 | 46.6807 | 31.6709 | 32.6010 | 2.8532 | 4.3840 | -0.4499 | 4.5220 | 2.6254 |
| 1.5112 | 1.0001 | 51.5336 | 31.5743 | 55.1046 | 2.3926 | 6.2521 | -0.2585 | 3.6632 | 2.4466 |
| 1.7612 | 1.0001 | 57.3352 | 31.5730 | 86.7325 | 2.2627 | 5.2197 | 0.2315 | 2.7930 | 3.0361 |
| 2.0114 | 1.0001 | 63.9836 | 31.6617 | 116.7307 | 2.5747 | 2.7153 | 0.6647 | 2.5312 | 3.6982 |

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Reactive Run

* * *

| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) |  | (Unitless values) |  |  |
| 0 | 0.6567 | 24.2030 | 31.9029 | 0.8290 | 0.8539 | 0.2451 | -0.0359 | 3.0058 | 2.9839 |
| 0.0114 | 0.6538 | 24.3367 | 31.9011 | 0.9651 | 0.8824 | 0.2885 | 0.0494 | 3.0704 | 3.0190 |
| 0.2614 | 0.6276 | 26.9964 | 31.8166 | 3.5852 | 1.1707 | 0.6704 | -0.1490 | 3.2930 | 2.7167 |
| 0.5113 | 0.6173 | 29.5784 | 31.8370 | 7.2842 | 1.1214 | 1.1821 | -0.0489 | 3.1925 | 2.1380 |
| 0.7613 | 0.6080 | 32.4083 | 31.9699 | 12.4877 | 1.2147 | 0.9499 | 0.1170 | 2.5982 | 2.8852 |
| 1.0113 | 0.6007 | 35.3710 | 32.0540 | 16.5561 | 1.6549 | -0.3381 | 0.1863 | 2.4154 | 3.6747 |
| 1.2612 | 0.5943 | 38.1989 | 32.0323 | 18.1604 | 2.1787 | -1.4284 | 0.0920 | 2.8529 | 3.4128 |
| 1.5112 | 0.5906 | 40.7868 | 31.9481 | 18.9043 | 2.5325 | -1.5648 | -0.0487 | 3.3744 | 2.9556 |
| 1.7612 | 0.5885 | 43.2230 | 31.8488 | 20.7064 | 2.6443 | -0.6655 | -0.2007 | 3.6935 | 2.6512 |
| 2.0114 | 0.5868 | 45.6771 | 31.7555 | 25.2417 | 2.5616 | 1.0118 | -0.3062 | 3.7664 | 2.5605 |

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Weakly Heterogeneous
Realization 4
1 Kilogram of Bromide
All Concentrations Used in Calculations

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Conservative Run

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| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 1.0001 | 24.5255 | 31.9387 | 1.2325 | 0.9237 | 0.5364 | 0.0437 | 3.3341 | 2.8758 |
| 0.0114 | 1.0001 | 24.7905 | 31.9704 | 1.5686 | 0.9335 | 0.6120 | 0.0598 | 3.3389 | 2.8840 |
| 0.2614 | 1.0001 | 30.7025 | 32.7252 | 9.5570 | 1.2316 | 0.9900 | 0.4702 | 3.1483 | 2.9705 |
| 0.5113 | 1.0001 | 37.0674 | 33.8865 | 20.2732 | 1.8332 | 1.2673 | 1.1681 | 3.0226 | 3.4015 |
| 0.7613 | 1.0001 | 43.8226 | 34.9987 | 28.7955 | 2.8739 | -0.0533 | 1.3600 | 2.7789 | 4.2744 |
| 1.0113 | 1.0001 | 49.9215 | 35.8246 | 29.6833 | 4.4048 | -0.3514 | 1.2607 | 3.2908 | 3.7884 |
| 1.2612 | 1.0001 | 55.1106 | 36.5624 | 32.2449 | 5.6833 | 1.5111 | 0.5012 | 3.6051 | 3.2312 |
| 1.5112 | 1.0001 | 59.9408 | 36.9820 | 40.0071 | 7.0379 | 2.9189 | -0.5826 | 3.5617 | 3.2356 |
| 1.7612 | 1.0001 | 64.6715 | 36.9478 | 49.6706 | 8.1167 | 3.8709 | -0.8359 | 3.7613 | 2.8937 |
| 2.0114 | 1.0001 | 69.3119 | 36.6297 | 62.8012 | 7.9397 | 5.9715 | -0.3317 | 4.2149 | 2.4860 |

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Reactive Run

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| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.6573 | 24.3579 | 31.9432 | 0.9167 | 0.7645 | 0.3521 | 0.0203 | 3.1807 | 2.8414 |
| 0.0114 | 0.6540 | 24.5288 | 31.9647 | 1.1197 | 0.7720 | 0.4229 | 0.0337 | 3.2211 | 2.8361 |
| 0.2614 | 0.6222 | 28.2513 | 32.4166 | 5.5346 | 0.9205 | 0.5121 | 0.3123 | 2.9985 | 2.5078 |
| 0.5113 | 0.6087 | 31.9682 | 32.9566 | 10.4568 | 1.1187 | 0.3993 | 0.6519 | 2.9009 | 2.5645 |
| 0.7613 | 0.5990 | 35.8333 | 33.6933 | 16.4218 | 1.5036 | 0.3177 | 0.9857 | 2.9260 | 2.9551 |
| 1.0113 | 0.5916 | 39.8614 | 34.4554 | 22.9693 | 1.9756 | -0.2747 | 1.0076 | 2.7566 | 3.4322 |
| 1.2612 | 0.5870 | 43.8273 | 35.0451 | 27.1938 | 2.6313 | -1.4505 | 1.0169 | 2.8395 | 3.9086 |
| 1.5112 | 0.5836 | 47.4702 | 35.5326 | 28.2635 | 3.4056 | -2.3453 | 1.1465 | 3.2340 | 3.7965 |
| 1.7612 | 0.5811 | 50.7090 | 36.0163 | 28.1018 | 4.1141 | -2.4624 | 1.0810 | 3.6241 | 3.2532 |
| 2.0114 | 0.5793 | 53.6520 | 36.4891 | 28.7334 | 4.7387 | -1.8666 | 0.6913 | 3.7759 | 2.7810 |

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Weakly Heterogeneous

Realization 5

1 Kilogram of Bromide

*All Concentrations Used in Calculations*

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Conservative Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 1.0001 | 24.6342 | 31.8751 | 1.2954 | 0.9306 | 0.6270 | -0.0662 | 3.4826 | 2.8993 |
| 0.0114 | 1.0001 | 24.9910 | 31.8421 | 1.7537 | 0.9533 | 0.7087 | -0.1011 | 3.4130 | 2.9902 |
| 0.2614 | 1.0001 | 32.1609 | 31.4260 | 8.1997 | 2.6431 | 0.3067 | -0.2825 | 3.3005 | 3.2935 |
| 0.5113 | 1.0001 | 37.6702 | 32.2051 | 13.7678 | 3.2853 | 1.3779 | 1.1126 | 3.2480 | 2.6728 |
| 0.7613 | 1.0001 | 43.1958 | 33.5891 | 23.0628 | 4.0064 | 1.3951 | 0.7823 | 3.0308 | 2.6101 |
| 1.0113 | 1.0001 | 49.1041 | 34.6100 | 31.7245 | 3.9321 | 0.6257 | 0.5527 | 2.9064 | 2.5197 |
| 1.2612 | 1.0001 | 54.9706 | 34.8276 | 35.8996 | 4.3929 | -0.1582 | 0.1082 | 2.9869 | 2.7981 |
| 1.5112 | 1.0001 | 60.4190 | 34.5522 | 37.0424 | 5.3742 | 0.2259 | -0.4641 | 3.3737 | 2.8135 |
| 1.7612 | 1.0001 | 65.4908 | 34.1566 | 41.2988 | 5.9095 | 2.2458 | -0.4725 | 3.5998 | 2.5924 |
| 2.0114 | 1.0001 | 70.5739 | 33.8998 | 52.7726 | 5.9384 | 3.8321 | 0.0756 | 3.3107 | 2.7435 |

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Reactive Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.6570 | 24.4295 | 31.9101 | 0.9346 | 0.7670 | 0.4180 | -0.0461 | 3.2930 | 2.8442 |
| 0.0114 | 0.6527 | 24.6572 | 31.8873 | 1.2059 | 0.7765 | 0.4974 | -0.0563 | 3.2985 | 2.8448 |
| 0.2614 | 0.6156 | 29.4571 | 31.5118 | 5.9141 | 1.6262 | -0.1519 | -0.7476 | 2.8911 | 3.6570 |
| 0.5113 | 0.6025 | 33.2531 | 31.5257 | 7.9238 | 2.2312 | -0.1185 | 0.4467 | 3.2614 | 2.0005 |
| 0.7613 | 0.5967 | 36.4824 | 31.9880 | 10.8013 | 2.5554 | 0.2382 | 1.0398 | 2.9945 | 1.9709 |
| 1.0113 | 0.5925 | 39.6755 | 32.7706 | 15.1210 | 3.1116 | 0.2315 | 0.9803 | 2.8091 | 1.9284 |
| 1.2612 | 0.5885 | 43.0268 | 33.6584 | 20.4603 | 3.4169 | -0.0506 | 1.0191 | 2.7266 | 0.8364 |
| 1.5112 | 0.5852 | 46.5126 | 34.3722 | 25.7618 | 3.2714 | -0.5896 | 1.3547 | 2.7170 | -1.3911 |
| 1.7612 | 0.5820 | 50.0369 | 34.7699 | 29.9933 | 3.0734 | -1.2925 | 1.7984 | 2.7394 | -3.5859 |
| 2.0114 | 0.5793 | 53.4833 | 34.8759 | 32.5293 | 3.2820 | -2.1461 | 1.6399 | 2.7792 | -2.6667 |

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Weakly Heterogeneous

*Realization 1*

1 Kilogram of Bromide

Only Concentrations Greater than 0.1 ppm Used in Calculations

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Conservative Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 1.0002 | 24.5650 | 32.0972 | 1.2190 | 0.9206 | 0.5320 | 0.0929 | 3.3641 | 2.8365 |
| 0.0114 | 1.0001 | 24.7998 | 32.1253 | 1.5555 | 0.9013 | 0.6620 | 0.0925 | 3.4230 | 2.8177 |
| 0.2614 | 1.0162 | 31.0191 | 32.3710 | 11.6889 | 1.1085 | 0.6393 | 0.0832 | 2.9609 | 3.3187 |
| 0.5113 | 1.0229 | 37.7214 | 32.3361 | 19.0946 | 2.0918 | -0.3219 | 0.1156 | 2.9613 | 3.6916 |
| 0.7613 | 1.0223 | 43.6802 | 32.0459 | 22.0251 | 3.2795 | -0.3200 | -0.3909 | 3.1429 | 3.8732 |
| 1.0113 | 1.0210 | 48.9598 | 31.5878 | 26.2434 | 4.0740 | 0.5177 | -0.9232 | 3.3045 | 3.4657 |
| 1.2612 | 1.0174 | 54.0406 | 31.1383 | 35.1399 | 4.0926 | 2.7005 | -0.6385 | 3.6869 | 2.9555 |
| 1.5112 | 1.0145 | 59.4781 | 30.9321 | 55.2603 | 4.1459 | 4.5371 | 0.7875 | 3.2629 | 4.0273 |
| 1.7612 | 1.0131 | 65.7145 | 31.3478 | 82.6696 | 6.2863 | 3.3751 | 2.7933 | 2.6347 | 4.9552 |
| 2.0114 | 1.0105 | 72.5541 | 32.4079 | 102.5586 | 9.6419 | 0.6849 | 2.8137 | 2.5172 | 3.6358 |

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Reactive Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.6574 | 24.3967 | 32.0628 | 0.9041 | 0.7662 | 0.3409 | 0.0624 | 3.1742 | 2.8111 |
| 0.0114 | 0.6545 | 24.5444 | 32.0815 | 1.0967 | 0.7563 | 0.4419 | 0.0696 | 3.2558 | 2.7810 |
| 0.2614 | 0.6321 | 28.3023 | 32.3279 | 6.7853 | 0.8072 | 0.4518 | 0.0404 | 2.7623 | 3.1102 |
| 0.5113 | 0.6233 | 32.4651 | 32.3653 | 12.5884 | 1.1373 | -0.1506 | 0.1078 | 2.8448 | 3.4194 |
| 0.7613 | 0.6127 | 36.5847 | 32.3423 | 16.6705 | 1.6958 | -0.9823 | 0.0998 | 2.9645 | 3.5140 |
| 1.0113 | 0.6047 | 40.3534 | 32.2287 | 18.7527 | 2.3449 | -1.4814 | -0.0051 | 3.2168 | 3.5788 |
| 1.2612 | 0.5987 | 43.7431 | 32.0168 | 20.4055 | 2.8908 | -1.5347 | -0.3754 | 3.3158 | 3.6954 |
| 1.5112 | 0.5936 | 46.8980 | 31.7559 | 22.2081 | 3.4021 | -1.3627 | -0.7971 | 3.2367 | 3.6640 |
| 1.7612 | 0.5892 | 49.8910 | 31.4891 | 24.4428 | 3.7719 | -1.1571 | -0.8993 | 3.2785 | 3.3664 |
| 2.0114 | 0.5850 | 52.7969 | 31.2068 | 27.9337 | 3.7797 | -0.2921 | -0.7255 | 3.4070 | 3.0169 |

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Weakly Heterogeneous

Realization 2

1 Kilogram of Bromide

Only Concentrations Greater than 0.1 ppm Used in Calculations

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Conservative Run

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| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 1.0004 | 24.6993 | 31.9334 | 1.2108 | 0.9600 | 0.5189 | -0.0582 | 3.2932 | 2.9481 |
| 0.0114 | 1.0001 | 25.0241 | 31.9339 | 1.5868 | 0.9911 | 0.5515 | -0.0921 | 3.2247 | 3.0002 |
| 0.2614 | 1.0088 | 31.6313 | 32.1070 | 8.7334 | 1.7535 | 0.7638 | 0.1356 | 3.1444 | 3.3052 |
| 0.5113 | 1.0111 | 37.9747 | 33.0916 | 14.9573 | 2.4249 | 0.1515 | 0.3641 | 2.9295 | 2.8744 |
| 0.7613 | 1.0113 | 43.7866 | 33.3662 | 18.0770 | 3.1418 | 0.1250 | 0.1316 | 3.0509 | 2.8657 |
| 1.0113 | 1.0097 | 49.0082 | 33.4132 | 20.2036 | 4.3569 | 0.0973 | 0.5324 | 2.9461 | 3.3351 |
| 1.2612 | 1.0081 | 53.7280 | 33.9759 | 22.1761 | 6.2980 | 0.5022 | 1.2654 | 3.1490 | 3.5417 |
| 1.5112 | 1.0070 | 58.1001 | 34.8734 | 25.9198 | 7.5389 | 1.7511 | 1.0552 | 3.5431 | 2.9368 |
| 1.7612 | 1.0057 | 62.3809 | 35.6558 | 34.3747 | 6.9106 | 3.8322 | 0.4248 | 3.8596 | 2.5961 |
| 2.0114 | 1.0052 | 66.9377 | 36.0697 | 50.4426 | 5.5353 | 5.0468 | 0.0822 | 3.3631 | 2.6331 |

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Reactive Run

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| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.6575 | 24.4963 | 31.9505 | 0.8956 | 0.7809 | 0.3721 | -0.0355 | 3.1722 | 2.8869 |
| 0.0114 | 0.6534 | 24.7099 | 31.9540 | 1.1325 | 0.7994 | 0.4159 | -0.0538 | 3.1442 | 2.9172 |
| 0.2614 | 0.6263 | 29.0196 | 31.9280 | 5.3795 | 1.2582 | 0.2298 | -0.1132 | 3.0675 | 3.2133 |
| 0.5113 | 0.6168 | 33.0165 | 32.3301 | 9.6775 | 1.6607 | 0.2251 | 0.2829 | 2.9075 | 3.1707 |
| 0.7613 | 0.6096 | 36.9431 | 32.9991 | 13.3192 | 2.0849 | -0.4431 | 0.3876 | 2.8322 | 2.8716 |
| 1.0113 | 0.6038 | 40.6181 | 33.3521 | 15.3408 | 2.4149 | -0.8267 | 0.2692 | 3.0891 | 2.7864 |
| 1.2612 | 0.5978 | 44.0186 | 33.3706 | 16.9681 | 2.8342 | -0.8624 | 0.1169 | 3.1166 | 2.7713 |
| 1.5112 | 0.5935 | 47.1735 | 33.3404 | 18.3236 | 3.3721 | -1.0376 | 0.1267 | 3.0464 | 2.8555 |
| 1.7612 | 0.5890 | 50.1167 | 33.4832 | 19.1488 | 4.1160 | -1.1525 | 0.4335 | 3.0438 | 3.1584 |
| 2.0114 | 0.5854 | 52.8557 | 33.8412 | 19.9433 | 5.1594 | -1.1387 | 0.8943 | 3.0752 | 3.4259 |
| 2.2614 | 0.5822 | 55.4352 | 34.3509 | 20.9668 | 6.2228 | -0.9559 | 1.1105 | 3.1097 | 3.2681 |
| 2.5113 | 0.5793 | 57.8999 | 34.9089 | 22.5838 | 6.8578 | -0.5438 | 0.9685 | 3.2120 | 2.9372 |
| 2.7613 | 0.5771 | 60.3122 | 35.4190 | 25.4197 | 6.8371 | 0.2438 | 0.6300 | 3.2945 | 2.7012 |
| 3.0113 | 0.5751 | 62.7566 | 35.8147 | 30.2946 | 6.2384 | 1.2854 | 0.2926 | 3.2861 | 2.6040 |
| 3.2612 | 0.5732 | 65.3255 | 36.0674 | 37.8731 | 5.4171 | 2.2151 | 0.0735 | 3.1222 | 2.6138 |
| 3.5112 | 0.5712 | 68.0944 | 36.1691 | 48.2472 | 4.7056 | 2.5402 | -0.0403 | 2.8077 | 2.6319 |
| 3.7612 | 0.5695 | 71.0834 | 36.1390 | 60.0471 | 4.3977 | 2.0297 | -0.1217 | 2.4572 | 2.7462 |
| 4.0114 | 0.5676 | 74.2608 | 36.0232 | 71.1852 | 4.4939 | 0.7076 | -0.1371 | 2.2238 | 2.9654 |

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Weakly Heterogeneous
Realization 3
1 Kilogram of Bromide
Only Concentrations Greater than 0.1 ppm Used in Calculations

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Conservative Run

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| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 1.0001 | 24.3169 | 31.8781 | 1.0553 | 1.0838 | 0.3742 | -0.0505 | 3.0832 | 3.0103 |
| 0.0114 | 0.9999 | 24.5234 | 31.8718 | 1.2678 | 1.1349 | 0.4247 | -0.0792 | 3.1624 | 3.0560 |
| 0.2614 | 1.0052 | 28.7091 | 31.7798 | 6.5092 | 1.4997 | 1.4331 | -0.1245 | 3.4697 | 2.9686 |
| 0.5113 | 1.0113 | 33.2696 | 31.9518 | 15.1130 | 1.7892 | 1.0809 | -0.1207 | 2.5626 | 4.1804 |
| 0.7613 | 1.0151 | 37.9814 | 31.9891 | 19.8872 | 2.7686 | -0.5580 | -0.1935 | 2.8169 | 4.0055 |
| 1.0113 | 1.0147 | 42.2918 | 31.8374 | 22.7102 | 3.2999 | 0.4180 | -0.3102 | 3.7836 | 3.3501 |
| 1.2612 | 1.0132 | 46.5432 | 31.6704 | 32.3860 | 3.0797 | 3.7046 | -0.3741 | 4.1836 | 3.0354 |
| 1.5112 | 1.0116 | 51.3891 | 31.5728 | 54.3600 | 2.6140 | 5.6868 | -0.2500 | 3.4517 | 2.9599 |
| 1.7612 | 1.0098 | 57.1682 | 31.5688 | 85.4977 | 2.4247 | 4.8033 | 0.1306 | 2.6544 | 3.1798 |
| 2.0114 | 1.0077 | 63.7836 | 31.6568 | 115.1971 | 2.6508 | 2.2424 | 0.5186 | 2.4072 | 3.4136 |

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Reactive Run

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| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.6567 | 24.2016 | 31.9027 | 0.8286 | 0.8528 | 0.2313 | -0.0384 | 2.9712 | 2.9564 |
| 0.0114 | 0.6535 | 24.3361 | 31.9012 | 0.9618 | 0.8801 | 0.2794 | -0.0478 | 3.0262 | 3.0010 |
| 0.2614 | 0.6305 | 26.9853 | 31.8163 | 3.5698 | 1.2202 | 0.6300 | -0.1520 | 3.1984 | 3.0374 |
| 0.5113 | 0.6225 | 29.5579 | 31.8372 | 7.2451 | 1.2180 | 1.1304 | -0.0805 | 3.1248 | 2.9520 |
| 0.7613 | 0.6158 | 32.3731 | 31.9685 | 12.4517 | 1.3427 | 0.9175 | -0.0113 | 2.5738 | 3.7065 |
| 1.0113 | 0.6092 | 35.3149 | 32.0550 | 16.5577 | 1.7956 | -0.3718 | 0.0634 | 2.3892 | 4.1702 |
| 1.2612 | 0.6044 | 38.1202 | 32.0302 | 18.2412 | 2.3488 | -1.4220 | 0.0152 | 2.8067 | 3.7908 |
| 1.5112 | 0.5994 | 40.7007 | 31.9436 | 19.1124 | 2.7285 | -1.6474 | -0.0662 | 3.3305 | 3.3887 |
| 1.7612 | 0.5954 | 43.1527 | 31.8456 | 20.8686 | 2.8446 | -0.7908 | -0.1605 | 3.6908 | 3.1335 |
| 2.0114 | 0.5922 | 45.6185 | 31.7500 | 25.3039 | 2.7467 | 0.8658 | -0.2712 | 3.7898 | 3.0278 |

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Weakly Heterogeneous

Realization 4

1 Kilogram of Bromide

Only Concentrations Greater than 0.1 ppm Used in Calculations

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Conservative Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 1.0001 | 24.5239 | 31.9387 | 1.2303 | 0.9228 | 0.5176 | 0.0441 | 3.2767 | 2.8626 |
| 0.0114 | 1.0000 | 24.7896 | 31.9703 | 1.5635 | 0.9333 | 0.5977 | 0.0572 | 3.2858 | 2.8772 |
| 0.2614 | 1.0126 | 30.6546 | 32.7086 | 9.5729 | 1.3320 | 0.9221 | 0.2911 | 3.0484 | 3.2463 |
| 0.5113 | 1.0214 | 36.9359 | 33.8421 | 20.5697 | 2.0259 | 1.1232 | 0.7680 | 2.9364 | 3.4809 |
| 0.7613 | 1.0230 | 43.6307 | 34.9415 | 29.5482 | 3.0696 | -0.3153 | 0.9899 | 2.7241 | 4.0490 |
| 1.0113 | 1.0210 | 49.7077 | 35.7693 | 30.7724 | 4.6020 | -0.9928 | 1.0551 | 3.2363 | 3.6585 |
| 1.2612 | 1.0173 | 54.9401 | 36.5142 | 32.6324 | 5.9494 | 0.7977 | 0.3672 | 3.4878 | 3.1669 |
| 1.5112 | 1.0149 | 59.7941 | 36.9459 | 39.5921 | 7.3705 | 2.3047 | -0.6111 | 3.3579 | 3.1596 |
| 1.7612 | 1.0120 | 64.5352 | 36.9284 | 48.5561 | 8.4341 | 3.2349 | -0.8279 | 3.4573 | 2.9002 |
| 2.0114 | 1.0094 | 69.1830 | 36.6206 | 61.1276 | 8.3064 | 5.2173 | -0.3013 | 3.8768 | 2.6718 |

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Reactive Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.6572 | 24.3564 | 31.9430 | 0.9154 | 0.7628 | 0.3381 | 0.0185 | 3.1469 | 2.8083 |
| 0.0114 | 0.6539 | 24.5276 | 31.9646 | 1.1150 | 0.7705 | 0.4068 | 0.0317 | 3.1520 | 2.8220 |
| 0.2614 | 0.6295 | 28.2228 | 32.4029 | 5.5173 | 1.0103 | 0.4859 | 0.1493 | 2.9345 | 3.0769 |
| 0.5113 | 0.6210 | 31.8988 | 32.9301 | 10.4980 | 1.2800 | 0.3698 | 0.3582 | 2.8305 | 3.2654 |
| 0.7613 | 0.6137 | 35.7244 | 33.6491 | 16.5428 | 1.7215 | 0.3045 | 0.5846 | 2.8502 | 3.3449 |
| 1.0113 | 0.6052 | 39.7452 | 34.4055 | 23.0840 | 2.1951 | -0.2848 | 0.5990 | 2.6926 | 3.5149 |
| 1.2612 | 0.5980 | 43.7200 | 35.0017 | 27.1916 | 2.8053 | -1.4344 | 0.7332 | 2.7592 | 3.7513 |
| 1.5112 | 0.5925 | 47.3860 | 35.4911 | 28.1232 | 3.5860 | -2.3234 | 0.8952 | 3.1195 | 3.7533 |
| 1.7612 | 0.5874 | 50.6574 | 35.9841 | 27.7661 | 4.3215 | -2.4569 | 0.8998 | 3.4812 | 3.3649 |
| 2.0114 | 0.5835 | 53.6279 | 36.4694 | 27.9893 | 4.9526 | -1.8024 | 0.6176 | 3.5530 | 2.9621 |

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Weakly Heterogeneous

Realization 5

1 Kilogram of Bromide

Only Concentrations Greater than 0.1 ppm Used in Calculations

Conservative Run

| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 1.0006 | 24.6312 | 31.8747 | 1.2938 | 0.9329 | 0.5988 | -0.0624 | 3.4036 | 2.8824 |
| 0.0114 | 1.0012 | 24.9874 | 31.8413 | 1.7492 | 0.9607 | 0.6807 | -0.1010 | 3.3334 | 3.0033 |
| 0.2614 | 1.0178 | 32.0923 | 31.4080 | 8.2861 | 2.8097 | 0.1847 | -0.3922 | 3.1830 | 3.3869 |
| 0.5113 | 1.0208 | 37.5736 | 32.1638 | 13.9128 | 3.6459 | 1.0794 | 0.5999 | 3.0999 | 3.1832 |
| 0.7613 | 1.0188 | 43.0746 | 33.5447 | 23.1841 | 4.3633 | 1.1284 | 0.3339 | 2.9083 | 2.9405 |
| 1.0113 | 1.0162 | 48.9616 | 34.5727 | 32.0508 | 4.2854 | 0.3290 | 0.0560 | 2.8095 | 3.2418 |
| 1.2612 | 1.0128 | 54.8234 | 34.8100 | 36.3911 | 4.6957 | -0.5816 | -0.2217 | 2.9103 | 3.5075 |
| 1.5112 | 1.0098 | 60.2779 | 34.5465 | 37.3722 | 5.6574 | -0.4182 | -0.6122 | 3.2679 | 3.2386 |
| 1.7612 | 1.0072 | 65.3641 | 34.1575 | 41.1136 | 6.1792 | 1.4840 | -0.5507 | 3.4240 | 2.9120 |
| 2.0114 | 1.0061 | 70.4427 | 33.9018 | 52.0813 | 6.1791 | 3.0866 | -0.0526 | 3.1318 | 2.9587 |

Reactive Run

| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.6573 | 24.4276 | 31.9097 | 0.9352 | 0.7680 | 0.4018 | -0.0461 | 3.2620 | 2.8409 |
| 0.0114 | 0.6532 | 24.6549 | 31.8866 | 1.2042 | 0.7810 | 0.4828 | -0.0610 | 3.2644 | 2.8801 |
| 0.2614 | 0.6260 | 29.4149 | 31.4994 | 5.9202 | 1.7641 | -0.1713 | -0.7692 | 2.8321 | 3.8365 |
| 0.5113 | 0.6156 | 33.1961 | 31.5013 | 8.0562 | 2.5573 | -0.1907 | -0.0127 | 3.1833 | 3.2172 |
| 0.7613 | 0.6089 | 36.4414 | 31.9534 | 10.9872 | 2.9629 | 0.2099 | 0.4676 | 2.9671 | 3.1940 |
| 1.0113 | 0.6026 | 39.6492 | 32.7395 | 15.4279 | 3.4916 | 0.3323 | 0.4908 | 2.8461 | 2.9114 |
| 1.2612 | 0.5970 | 43.0114 | 33.6208 | 20.8760 | 3.8464 | 0.1132 | 0.2448 | 2.7637 | 2.7766 |
| 1.5112 | 0.5917 | 46.5108 | 34.3341 | 26.2016 | 3.7581 | -0.3985 | 0.0931 | 2.7506 | 2.8298 |
| 1.7612 | 0.5871 | 50.0495 | 34.7328 | 30.4424 | 3.6252 | -1.0559 | 0.1327 | 2.7943 | 2.9723 |
| 2.0114 | 0.5831 | 53.5093 | 34.8435 | 33.0080 | 3.8112 | -1.8114 | 0.1536 | 2.8844 | 2.9786 |

Strongly Heterogeneous

Realization 1

1 Kilogram of Bromide

All Concentrations Used in Calculations

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Conservative Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 1.0001 | 24.8139 | 31.6708 | 1.1525 | 1.0193 | 0.5189 | -0.4007 | 3.2702 | 3.4637 |
| 0.0114 | 1.0001 | 25.1470 | 31.5712 | 1.4665 | 1.1782 | 0.5016 | -0.6011 | 3.1785 | 3.8109 |
| 0.2614 | 1.0001 | 30.3676 | 29.8174 | 5.8701 | 5.4237 | 1.7517 | -2.4155 | 4.0764 | 4.5921 |
| 0.5113 | 1.0001 | 34.3059 | 29.4057 | 13.9741 | 13.7167 | 2.5575 | -3.0027 | 3.4013 | 3.3978 |
| 0.7613 | 1.0001 | 37.8555 | 29.0756 | 25.1664 | 21.0076 | 3.5156 | -3.2834 | 3.8932 | 2.6015 |
| 1.0113 | 1.0001 | 41.2363 | 28.8377 | 42.6498 | 22.5423 | 5.1986 | -2.8632 | 4.2241 | 2.3082 |
| 1.2612 | 1.0003 | 44.4694 | 29.0222 | 64.7651 | 23.2109 | 6.3768 | -1.7201 | 4.1187 | 2.5893 |
| 1.5112 | 1.0004 | 47.5164 | 29.6311 | 90.6536 | 26.7601 | 7.3464 | 0.4111 | 3.8880 | 3.1473 |
| 1.7612 | 1.0004 | 50.4920 | 30.5089 | 123.6033 | 33.4786 | 8.3854 | 2.2194 | 3.6198 | 3.1655 |
| 2.0114 | 1.0004 | 53.5500 | 31.4322 | 167.5898 | 41.5332 | 9.3993 | 2.7412 | 3.3439 | 2.8205 |

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Reactive Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.6585 | 24.5934 | 31.7687 | 0.8675 | 0.7944 | 0.4033 | -0.2309 | 3.1434 | 3.1419 |
| 0.0114 | 0.6535 | 24.8210 | 31.7112 | 1.0806 | 0.8709 | 0.4224 | -0.3469 | 3.1017 | 3.3592 |
| 0.2614 | 0.6137 | 28.5980 | 30.4080 | 3.5269 | 2.8367 | 0.5991 | -1.6094 | 3.4362 | 4.2035 |
| 0.5113 | 0.6017 | 31.2150 | 29.8550 | 6.7433 | 5.0668 | 1.5400 | -1.7735 | 3.5723 | 3.5185 |
| 0.7613 | 0.5942 | 33.5272 | 29.7291 | 11.3770 | 9.4240 | 1.5110 | -2.0776 | 2.1918 | 3.1828 |
| 1.0113 | 0.5885 | 35.6363 | 29.6160 | 16.0266 | 14.6001 | 0.8933 | -2.8908 | 1.3270 | 2.9949 |
| 1.2612 | 0.5839 | 37.5842 | 29.3816 | 21.3858 | 18.3261 | 0.9009 | -3.3973 | 1.5086 | 2.7528 |
| 1.5112 | 0.5798 | 39.4513 | 29.1425 | 28.2821 | 20.1993 | 1.2834 | -3.4886 | 1.9368 | 2.5457 |
| 1.7612 | 0.5758 | 41.2668 | 29.0158 | 36.5955 | 20.9133 | 1.6788 | -3.2378 | 2.2889 | 2.3707 |
| 2.0114 | 0.5719 | 43.0204 | 29.0481 | 45.9365 | 21.3254 | 2.0984 | -2.7109 | 2.5973 | 2.3138 |

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Strongly Heterogeneous

Realization 2

1 Kilogram of Bromide

All Concentrations Used in Calculations

Conservative Run

| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 1.0001 | 24.3087 | 32.0510 | 1.0621 | 1.0961 | 0.4120 | -0.0559 | 3.2416 | 2.9995 |
| 0.0114 | 1.0001 | 24.4333 | 32.1192 | 1.2283 | 1.1256 | 0.5398 | -0.0271 | 3.4373 | 2.9490 |
| 0.2614 | 1.0001 | 27.7548 | 33.0043 | 6.2312 | 1.4894 | 0.5584 | 0.0627 | 2.6681 | 3.3587 |
| 0.5113 | 1.0001 | 31.0098 | 33.3241 | 8.4257 | 3.0756 | 0.2262 | 0.4208 | 4.1312 | 3.9662 |
| 0.7613 | 1.0001 | 33.5665 | 33.7597 | 10.8693 | 6.0091 | 3.8887 | 0.9050 | 7.9335 | 3.0784 |
| 1.0113 | 1.0001 | 35.7230 | 34.3738 | 19.2552 | 8.7946 | 10.0032 | 1.1767 | 12.0611 | 2.5915 |
| 1.2612 | 1.0001 | 37.9197 | 35.0619 | 41.4495 | 10.6894 | 17.2670 | 1.1580 | 12.6780 | 2.3879 |
| 1.5112 | 1.0001 | 40.5060 | 35.6720 | 88.3845 | 11.8399 | 23.0354 | 1.0046 | 9.4975 | 2.3086 |
| 1.7612 | 1.0001 | 43.6102 | 36.0930 | 166.2334 | 12.8736 | 26.4021 | 0.6407 | 6.7305 | 2.4012 |
| 2.0114 | 1.0000 | 47.1862 | 36.2954 | 276.0819 | 14.3475 | 28.7077 | -0.2982 | 5.2242 | 3.0223 |

Reactive Run

| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.6568 | 24.1902 | 32.0443 | 0.8237 | 0.8664 | 0.2502 | -0.0223 | 3.0653 | 2.9706 |
| 0.0114 | 0.6548 | 24.2679 | 32.0889 | 0.9119 | 0.8920 | 0.3330 | 0.0080 | 3.2191 | 2.9559 |
| 0.2614 | 0.6310 | 26.2882 | 32.8143 | 3.8427 | 1.1447 | 0.8576 | 0.0423 | 2.8095 | 2.7276 |
| 0.5113 | 0.6178 | 28.5330 | 33.1376 | 6.4202 | 1.4136 | -0.0846 | 0.2237 | 2.5255 | 3.3870 |
| 0.7613 | 0.6088 | 30.5365 | 33.3264 | 7.2552 | 2.3087 | -0.7638 | 0.4306 | 3.1937 | 3.8864 |
| 1.0113 | 0.6030 | 32.1783 | 33.5631 | 7.5225 | 3.8862 | -0.2581 | 0.6046 | 4.4738 | 3.4308 |
| 1.2612 | 0.5988 | 33.5387 | 33.8496 | 8.4822 | 5.7996 | 1.5473 | 0.8093 | 5.9155 | 2.9013 |
| 1.5112 | 0.5952 | 34.7304 | 34.1722 | 10.7869 | 7.6623 | 3.8928 | 0.9912 | 6.8844 | 2.5866 |
| 1.7612 | 0.5918 | 35.8468 | 34.5303 | 14.9895 | 9.2370 | 6.3578 | 1.0795 | 7.7091 | 2.4191 |
| 2.0114 | 0.5881 | 36.9709 | 34.9182 | 22.1449 | 10.4076 | 9.3926 | 1.0761 | 8.9653 | 2.3211 |

Strongly Heterogeneous

Realization 3

1 Kilogram of Bromide

All Concentrations Used in Calculations

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Conservative Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) |  | (Unitless values) |  |  |
| 0 | 1.0001 | 24.4630 | 31.9121 | 1.1409 | 1.0042 | 0.3787 | -0.2129 | 3.1336 | 3.0753 |
| 0.0114 | 1.0001 | 24.5748 | 31.8671 | 1.2690 | 1.0292 | 0.4382 | -0.2515 | 3.1889 | 3.1243 |
| 0.2614 | 1.0001 | 27.1275 | 30.8872 | 5.4109 | 1.3626 | 2.1869 | -0.1155 | 4.6711 | 2.7098 |
| 0.5113 | 1.0001 | 30.6175 | 31.1846 | 16.7618 | 2.5248 | 3.0754 | 1.3121 | 3.3461 | 3.9358 |
| 0.7613 | 1.0001 | 35.1706 | 32.5381 | 30.9994 | 4.3883 | 2.0776 | 0.9293 | 3.0171 | 2.9466 |
| 1.0113 | 1.0001 | 40.0072 | 34.0128 | 40.9598 | 5.4209 | 1.4315 | 1.0892 | 3.2101 | 3.6700 |
| 1.2612 | 1.0001 | 44.3581 | 35.5647 | 44.2034 | 7.3733 | 1.7052 | 1.7714 | 3.5778 | 3.5267 |
| 1.5112 | 1.0001 | 47.7724 | 37.2660 | 45.0055 | 9.8518 | 3.9803 | 1.4474 | 4.2515 | 2.7474 |
| 1.7612 | 1.0001 | 50.4368 | 38.9796 | 51.4292 | 11.2645 | 7.4386 | 0.5042 | 4.7886 | 2.4221 |
| 2.0114 | 1.0001 | 52.9298 | 40.5023 | 67.5162 | 11.1569 | 9.5718 | -0.3284 | 4.5569 | 2.5441 |

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Reactive Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) |  | (Unitless values) |  |  |
| 0 | 0.6571 | 24.3355 | 31.9696 | 0.8782 | 0.7989 | 0.2661 | -0.1221 | 3.0650 | 2.9744 |
| 0.0114 | 0.6554 | 24.4088 | 31.9429 | 0.9602 | 0.8127 | 0.3094 | -0.1477 | 3.0995 | 2.9987 |
| 0.2614 | 0.6334 | 26.0016 | 31.2299 | 2.7664 | 1.1231 | 0.8078 | -0.4044 | 3.5241 | 2.6449 |
| 0.5113 | 0.6204 | 27.7133 | 30.7495 | 6.1308 | 1.1754 | 1.9920 | 0.0089 | 3.9659 | 2.3681 |
| 0.7613 | 0.6081 | 29.8751 | 30.9696 | 12.5942 | 1.8865 | 2.3458 | 1.1071 | 3.0622 | 4.0196 |
| 1.0113 | 0.5970 | 32.4976 | 31.7325 | 20.5298 | 3.2518 | 1.6002 | 1.2043 | 2.6071 | 3.0950 |
| 1.2612 | 0.5894 | 35.3669 | 32.6322 | 27.7786 | 4.0715 | 0.7944 | 0.6706 | 2.7391 | 2.6996 |
| 1.5112 | 0.5840 | 38.2867 | 33.4667 | 33.7583 | 4.3834 | 0.3520 | 0.4727 | 2.9629 | 3.0981 |
| 1.7612 | 0.5797 | 41.0957 | 34.2882 | 37.9064 | 4.9564 | 0.0828 | 0.8326 | 3.1265 | 3.5477 |
| 2.0114 | 0.5763 | 43.6267 | 35.1849 | 39.7290 | 6.1542 | 0.0195 | 1.2318 | 3.3373 | 3.4365 |

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Strongly Heterogeneous
Realization 4
1 Kilogram of Bromide
All Concentrations Used in Calculations

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Conservative Run

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| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 1.0001 | 24.6657 | 32.0905 | 1.2748 | 0.8626 | 0.6566 | 0.1443 | 3.6938 | 2.7816 |
| 0.0114 | 1.0001 | 24.7894 | 32.1040 | 1.5096 | 0.8340 | 0.8229 | 0.1280 | 3.8733 | 2.7439 |
| 0.2614 | 1.0001 | 28.7187 | 32.3177 | 12.5055 | 0.8126 | 2.0385 | 0.5717 | 3.2965 | 4.2947 |
| 0.5113 | 1.0001 | 34.1884 | 32.9527 | 29.4587 | 2.4653 | 1.3341 | 1.8522 | 2.7746 | 4.6815 |
| 0.7613 | 1.0001 | 40.0053 | 33.9561 | 42.2776 | 4.8103 | 0.3102 | 1.4601 | 2.9903 | 2.7270 |
| 1.0113 | 1.0001 | 45.4969 | 34.4380 | 53.8106 | 5.0338 | 2.9150 | 0.7105 | 4.0165 | 2.8289 |
| 1.2612 | 1.0001 | 50.8024 | 34.3418 | 85.2176 | 5.8781 | 11.4516 | 3.3705 | 5.8600 | 9.6845 |
| 1.5112 | 1.0000 | 56.6938 | 34.8208 | 170.6140 | 16.4549 | 19.8898 | 8.7768 | 5.3342 | 8.6222 |
| 1.7612 | 0.9992 | 63.5846 | 36.3979 | 309.7285 | 41.0308 | 20.2738 | 9.3432 | 3.2971 | 4.2334 |
| 2.0114 | 0.9941 | 70.8837 | 38.5874 | 444.5628 | 71.9351 | 15.0073 | 7.8423 | 2.1241 | 2.5599 |

* * *

Reactive Run

* * *

| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.6584 | 24.4852 | 32.0393 | 0.9192 | 0.7332 | 0.4178 | 0.0994 | 3.3776 | 2.7793 |
| 0.0114 | 0.6568 | 24.5587 | 32.0481 | 1.0353 | 0.7171 | 0.5100 | 0.0908 | 3.4692 | 2.7367 |
| 0.2614 | 0.6308 | 26.7009 | 32.2002 | 5.9570 | 0.5237 | 1.4432 | 0.1245 | 3.0275 | 1.4384 |
| 0.5113 | 0.6135 | 29.6480 | 32.3467 | 13.9395 | 0.8142 | 1.2350 | 0.7133 | 2.9155 | 4.1596 |
| 0.7613 | 0.5989 | 33.0856 | 32.7415 | 23.3795 | 1.6846 | 0.7603 | 1.4592 | 2.7623 | 4.6327 |
| 1.0113 | 0.5902 | 36.6703 | 33.3598 | 31.4702 | 3.1898 | -0.2108 | 1.8221 | 2.7022 | 3.6997 |
| 1.2612 | 0.5842 | 40.1453 | 34.0128 | 37.1346 | 4.5846 | -0.8404 | 1.4847 | 2.9182 | 2.6274 |
| 1.5112 | 0.5794 | 43.3975 | 34.4301 | 41.5726 | 4.9288 | -0.4373 | 0.9340 | 3.2560 | 2.2252 |
| 1.7612 | 0.5756 | 46.4124 | 34.4844 | 47.9712 | 4.4504 | 1.4704 | 0.5622 | 3.5775 | 2.3504 |
| 2.0114 | 0.5727 | 49.2845 | 34.2941 | 59.9831 | 3.9329 | 4.5431 | 0.5114 | 3.8632 | 3.3579 |
| 2.2614 | 0.5693 | 52.1786 | 34.1740 | 82.7090 | 5.0255 | 8.7818 | 3.0997 | 4.4130 | 9.3675 |
| 2.5113 | 0.5652 | 55.3095 | 34.4097 | 124.3444 | 10.3420 | 13.9232 | 6.9092 | 4.8324 | 9.5177 |
| 2.7613 | 0.5607 | 58.8176 | 35.0439 | 189.8753 | 20.6248 | 17.7377 | 8.3383 | 4.3681 | 6.0570 |
| 3.0113 | 0.5562 | 62.6720 | 35.9757 | 270.4983 | 34.7306 | 18.4577 | 8.4741 | 3.4380 | 4.0714 |
| 3.2612 | 0.5512 | 66.7147 | 37.1158 | 350.6550 | 51.4707 | 16.5728 | 8.1029 | 2.6451 | 3.0481 |
| 3.5112 | 0.5454 | 70.8260 | 38.4182 | 420.5270 | 69.4004 | 13.2609 | 7.3077 | 2.1220 | 2.4314 |
| 3.7612 | 0.5382 | 74.9496 | 39.8394 | 476.8072 | 86.3054 | 9.2701 | 6.0513 | 1.8145 | 2.0227 |
| 4.0114 | 0.5289 | 79.0435 | 41.3195 | 518.6431 | 100.0927 | 4.9434 | 4.4164 | 1.6599 | 1.7636 |

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Strongly Heterogeneous
Realization 5
1 Kilogram of Bromide
All Concentrations Used in Calculations

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Conservative Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 1.0001 | 24.4826 | 31.7554 | 1.3514 | 0.8243 | 0.5705 | 0.0224 | 3.4158 | 2.8348 |
| 0.0114 | 1.0001 | 24.7155 | 31.7969 | 1.6523 | 0.8385 | 0.6539 | 0.0398 | 3.3972 | 2.8460 |
| 0.2614 | 1.0001 | 29.4282 | 33.0220 | 9.4973 | 1.1083 | 1.6447 | 0.6941 | 3.3526 | 2.5894 |
| 0.5113 | 1.0001 | 34.0508 | 34.4884 | 24.6371 | 1.8372 | 2.5247 | 1.5976 | 3.0659 | 4.5194 |
| 0.7613 | 1.0001 | 39.1165 | 36.1270 | 44.0461 | 4.7009 | 1.6027 | 2.2770 | 2.5976 | 5.0638 |
| 1.0113 | 1.0001 | 44.2890 | 38.0652 | 59.3952 | 9.4440 | -0.2230 | 2.0606 | 2.7044 | 3.1516 |
| 1.2612 | 1.0001 | 49.1355 | 39.9262 | 66.8584 | 12.2138 | -1.6990 | 0.5607 | 3.3114 | 2.4826 |
| 1.5112 | 1.0001 | 53.4863 | 41.2840 | 69.1851 | 12.4011 | -1.7597 | -0.1700 | 4.4026 | 2.5223 |
| 1.7612 | 1.0001 | 57.4433 | 42.1896 | 72.0681 | 13.1180 | 0.9583 | -0.1236 | 6.4432 | 2.5251 |
| 2.0114 | 1.0001 | 61.1802 | 42.8298 | 79.8718 | 15.9681 | 7.1712 | -0.3562 | 9.8525 | 2.8605 |

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Reactive Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.6579 | 24.3199 | 31.7904 | 0.9799 | 0.6989 | 0.3657 | -0.0072 | 3.2624 | 2.7867 |
| 0.0114 | 0.6551 | 24.4707 | 31.8183 | 1.1609 | 0.7097 | 0.4415 | 0.0074 | 3.2786 | 2.7882 |
| 0.2614 | 0.6247 | 27.5306 | 32.5003 | 5.1084 | 0.8800 | 0.8362 | 0.4945 | 3.0490 | 2.3634 |
| 0.5113 | 0.6106 | 30.2093 | 33.3802 | 10.4661 | 1.0016 | 1.3983 | 0.8851 | 2.9594 | 2.0239 |
| 0.7613 | 0.6016 | 32.9072 | 34.2403 | 18.4842 | 1.3885 | 1.7092 | 1.1121 | 2.8094 | 3.4139 |
| 1.0113 | 0.5949 | 35.7717 | 35.1562 | 28.3491 | 2.4057 | 1.5314 | 1.2624 | 2.5792 | 4.2576 |
| 1.2612 | 0.5899 | 38.8001 | 36.1773 | 38.5346 | 4.1497 | 0.6828 | 1.8611 | 2.3642 | 4.4305 |
| 1.5112 | 0.5835 | 41.9042 | 37.3585 | 47.5833 | 6.8196 | -0.6177 | 2.4235 | 2.3159 | 3.5868 |
| 1.7612 | 0.5780 | 44.9494 | 38.6118 | 54.1740 | 9.5922 | -2.1805 | 1.9636 | 2.4270 | 2.5597 |
| 2.0114 | 0.5739 | 47.8258 | 39.7587 | 57.9371 | 11.1326 | -3.7428 | 1.0484 | 2.6839 | 2.1023 |

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Strongly Heterogeneous

Realization 1

1 Kilogram of Bromide

Only Concentrations Greater than 0.1 ppm Used in Calculations

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Conservative Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 1.0005 | 24.8122 | 31.6704 | 1.1518 | 1.0203 | 0.5056 | -0.3923 | 3.2277 | 3.4171 |
| 0.0114 | 1.0004 | 25.1452 | 31.5715 | 1.4637 | 1.1778 | 0.4861 | -0.5840 | 3.1412 | 3.7292 |
| 0.2614 | 1.0138 | 30.3054 | 29.8360 | 5.9936 | 5.4678 | 1.5056 | -2.2133 | 3.8943 | 4.2157 |
| 0.5113 | 1.0119 | 34.2251 | 29.4184 | 13.7761 | 13.8914 | 2.1396 | -3.0568 | 2.8453 | 3.4246 |
| 0.7613 | 1.0078 | 37.7677 | 29.0843 | 24.3126 | 21.2452 | 2.8546 | -3.3706 | 3.1658 | 2.6392 |
| 1.0113 | 1.0067 | 41.1287 | 28.8393 | 41.1865 | 22.8278 | 4.5318 | -3.0132 | 3.7754 | 2.3465 |
| 1.2612 | 1.0056 | 44.3207 | 29.0080 | 62.3537 | 23.2611 | 5.6724 | -2.0271 | 3.8370 | 2.4925 |
| 1.5112 | 1.0049 | 47.3347 | 29.6097 | 87.0589 | 26.7032 | 6.5216 | 0.0074 | 3.6361 | 3.0145 |
| 1.7612 | 1.0038 | 50.2730 | 30.4750 | 118.1014 | 33.1930 | 7.4029 | 1.6674 | 3.3771 | 3.0673 |
| 2.0114 | 1.0028 | 53.2591 | 31.3936 | 159.0339 | 40.9364 | 8.1992 | 2.1824 | 3.0816 | 2.8076 |

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Reactive Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.6587 | 24.5923 | 31.7683 | 0.8677 | 0.7955 | 0.3951 | -0.2269 | 3.1215 | 3.1202 |
| 0.0114 | 0.6537 | 24.8194 | 31.7121 | 1.0783 | 0.8708 | 0.4068 | -0.3320 | 3.0713 | 3.3192 |
| 0.2614 | 0.6217 | 28.5537 | 30.4222 | 3.6407 | 2.9043 | 0.4264 | -1.4617 | 3.4496 | 4.0255 |
| 0.5113 | 0.6120 | 31.1576 | 29.8793 | 6.8337 | 5.3030 | 1.4481 | -1.8314 | 3.5759 | 3.8071 |
| 0.7613 | 0.6020 | 33.4927 | 29.7373 | 11.5692 | 9.7631 | 1.8293 | -2.3213 | 2.8218 | 3.5141 |
| 1.0113 | 0.5939 | 35.6160 | 29.6298 | 16.3164 | 14.9018 | 1.5825 | -3.0928 | 2.3879 | 3.2292 |
| 1.2612 | 0.5876 | 37.5630 | 29.3993 | 21.5455 | 18.6131 | 1.5290 | -3.5846 | 2.2871 | 2.9647 |
| 1.5112 | 0.5825 | 39.4185 | 29.1590 | 28.1556 | 20.5209 | 1.6074 | -3.6521 | 2.2802 | 2.7155 |
| 1.7612 | 0.5782 | 41.2160 | 29.0243 | 36.1224 | 21.3338 | 1.7608 | -3.4047 | 2.3932 | 2.5368 |
| 2.0114 | 0.5734 | 42.9538 | 29.0446 | 45.1148 | 21.7264 | 2.0368 | -2.9618 | 2.6153 | 2.4656 |

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Strongly Heterogeneous
Realization 2
1 Kilogram of Bromide
Only Concentrations Greater than 0.1 ppm Used in Calculations

Conservative Run

| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.9998 | 24.3077 | 32.0511 | 1.0584 | 1.0934 | 0.3968 | -0.0537 | 3.1811 | 2.9702 |
| 0.0114 | 0.9998 | 24.4327 | 32.1192 | 1.2247 | 1.1220 | 0.5276 | -0.0248 | 3.3799 | 2.9183 |
| 0.2614 | 1.0050 | 27.7349 | 32.9987 | 6.2443 | 1.5132 | 0.5030 | 0.0051 | 2.6064 | 3.3436 |
| 0.5113 | 1.0094 | 30.9528 | 33.3109 | 8.5278 | 3.1086 | -0.0916 | 0.3610 | 3.8029 | 3.8541 |
| 0.7613 | 1.0089 | 33.4920 | 33.7398 | 10.7877 | 6.0530 | 2.8595 | 0.8422 | 6.4030 | 3.0450 |
| 1.0113 | 1.0071 | 35.6300 | 34.3440 | 18.0750 | 8.8764 | 7.8679 | 1.0989 | 8.7548 | 2.5862 |
| 1.2612 | 1.0054 | 37.8192 | 35.0316 | 38.5900 | 10.7604 | 15.3207 | 1.0980 | 11.1424 | 2.3853 |
| 1.5112 | 1.0047 | 40.3640 | 35.6446 | 82.2951 | 11.8690 | 21.3558 | 1.0005 | 8.8735 | 2.2907 |
| 1.7612 | 1.0036 | 43.3973 | 36.0772 | 155.0772 | 12.7780 | 24.6470 | 0.7677 | 6.2276 | 2.2650 |
| 2.0114 | 1.0013 | 46.8234 | 36.3053 | 254.8609 | 14.0198 | 26.3174 | 0.0887 | 4.6579 | 2.5943 |

Reactive Run

| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.6567 | 24.1892 | 32.0443 | 0.8213 | 0.8653 | 0.2365 | -0.0209 | 3.0087 | 2.9570 |
| 0.0114 | 0.6547 | 24.2674 | 32.0889 | 0.9101 | 0.8897 | 0.3250 | 0.0084 | 3.1835 | 2.9281 |
| 0.2614 | 0.6343 | 26.2747 | 32.8111 | 3.8523 | 1.1709 | 0.8271 | -0.0160 | 2.7836 | 2.8578 |
| 0.5113 | 0.6244 | 28.4928 | 33.1268 | 6.4999 | 1.4628 | -0.1487 | 0.1426 | 2.5125 | 3.3849 |
| 0.7613 | 0.6167 | 30.4700 | 33.3128 | 7.4661 | 2.3549 | -0.9597 | 0.3354 | 3.1246 | 3.7531 |
| 1.0113 | 0.6100 | 32.1114 | 33.5485 | 7.7571 | 3.9375 | -0.6404 | 0.5250 | 4.2943 | 3.8310 |
| 1.2612 | 0.6039 | 33.4758 | 33.8313 | 8.6036 | 5.8551 | 0.9761 | 0.7266 | 5.5222 | 2.8863 |
| 1.5112 | 0.5990 | 34.6819 | 34.1499 | 10.7280 | 7.7434 | 3.2572 | 0.9099 | 6.2115 | 2.5864 |
| 1.7612 | 0.5946 | 35.8078 | 34.5085 | 14.6665 | 9.3130 | 5.5643 | 1.0203 | 6.6208 | 2.4138 |
| 2.0114 | 0.5904 | 36.9368 | 34.8970 | 21.2775 | 10.4705 | 8.1548 | 1.0382 | 7.2848 | 2.3099 |

Strongly Heterogeneous
Realization 3
1 Kilogram of Bromide
Only Concentrations Greater than 0.1 ppm Used in Calculations

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Conservative Run

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| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.9999 | 24.4620 | 31.9127 | 1.1380 | 1.0018 | 0.3641 | -0.2057 | 3.0836 | 3.0427 |
| 0.0114 | 0.9998 | 24.5740 | 31.8674 | 1.2661 | 1.0267 | 0.4264 | -0.2438 | 3.1479 | 3.0758 |
| 0.2614 | 1.0071 | 27.1125 | 30.8940 | 5.3949 | 1.4125 | 2.0302 | -0.0825 | 4.4284 | 2.8152 |
| 0.5113 | 1.0175 | 30.5782 | 31.1755 | 16.5752 | 2.6194 | 2.9377 | 1.1614 | 3.2305 | 3.7241 |
| 0.7613 | 1.0243 | 35.0562 | 32.4851 | 30.7419 | 4.4966 | 1.9954 | 0.7238 | 2.9243 | 2.8357 |
| 1.0113 | 1.0244 | 39.8311 | 33.9307 | 41.2984 | 5.5982 | 1.2936 | 0.8062 | 3.1001 | 3.4944 |
| 1.2612 | 1.0206 | 44.1585 | 35.4695 | 44.9554 | 7.6021 | 1.2180 | 1.4741 | 3.4176 | 3.4333 |
| 1.5112 | 1.0152 | 47.5930 | 37.1754 | 45.5015 | 10.1069 | 3.0916 | 1.2270 | 4.0170 | 2.7376 |
| 1.7612 | 1.0107 | 50.2803 | 38.9018 | 51.1893 | 11.4912 | 6.3660 | 0.3327 | 4.4706 | 2.4086 |
| 2.0114 | 1.0067 | 52.7886 | 40.4410 | 65.9300 | 11.3258 | 8.5922 | -0.4769 | 4.2240 | 2.4996 |

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Reactive Run

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| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.6570 | 24.3346 | 31.9699 | 0.8760 | 0.7977 | 0.2551 | -0.1192 | 3.0248 | 2.9536 |
| 0.0114 | 0.6553 | 24.4085 | 31.9430 | 0.9576 | 0.8108 | 0.3028 | -0.1446 | 3.0713 | 2.9753 |
| 0.2614 | 0.6370 | 25.9887 | 31.2382 | 2.7826 | 1.1641 | 0.7040 | -0.3273 | 3.4196 | 2.8480 |
| 0.5113 | 0.6298 | 27.6967 | 30.7650 | 6.1049 | 1.2937 | 1.8579 | 0.0620 | 3.8298 | 2.7988 |
| 0.7613 | 0.6227 | 29.8450 | 30.9713 | 12.4896 | 2.0349 | 2.2676 | 0.9468 | 3.0052 | 3.8014 |
| 1.0113 | 0.6149 | 32.4340 | 31.7025 | 20.3194 | 3.3815 | 1.5677 | 1.0070 | 2.5684 | 2.9999 |
| 1.2612 | 0.6076 | 35.2553 | 32.5742 | 27.6613 | 4.2202 | 0.8043 | 0.4904 | 2.6813 | 2.6785 |
| 1.5112 | 0.5998 | 38.1487 | 33.3932 | 33.8936 | 4.5494 | 0.3376 | 0.2605 | 2.8825 | 3.0230 |
| 1.7612 | 0.5927 | 40.9552 | 34.2142 | 38.3230 | 5.1240 | 0.0085 | 0.5949 | 3.0356 | 3.4312 |
| 2.0114 | 0.5865 | 43.4968 | 35.1124 | 40.2342 | 6.2830 | -0.1689 | 0.9939 | 3.2386 | 3.3289 |

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Strongly Heterogeneous
Realization 4
1 Kilogram of Bromide
Only Concentrations Greater than 0.1 ppm Used in Calculations

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Conservative Run

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| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.9999 | 24.6652 | 32.0904 | 1.2722 | 0.8614 | 0.6469 | 0.1429 | 3.6476 | 2.7738 |
| 0.0114 | 0.9999 | 24.7886 | 32.1041 | 1.5039 | 0.8326 | 0.8042 | 0.1283 | 3.7924 | 2.7419 |
| 0.2614 | 1.0147 | 28.6898 | 32.3193 | 12.3432 | 0.8947 | 1.9877 | 0.4485 | 3.2292 | 4.1888 |
| 0.5113 | 1.0267 | 34.0128 | 32.9265 | 29.7251 | 2.5733 | 1.3282 | 1.6784 | 2.6952 | 4.4273 |
| 0.7613 | 1.0257 | 39.7193 | 33.9125 | 43.9741 | 4.9583 | -0.0395 | 1.3785 | 2.8562 | 2.6857 |
| 1.0113 | 1.0250 | 45.0887 | 34.3925 | 56.5190 | 5.1739 | 1.1967 | 0.5925 | 3.5360 | 2.5391 |
| 1.2612 | 1.0216 | 50.2968 | 34.2935 | 85.7572 | 5.6428 | 7.7277 | 2.4200 | 4.6771 | 7.3812 |
| 1.5112 | 1.0202 | 56.1151 | 34.7447 | 168.8713 | 15.4344 | 17.3892 | 7.9217 | 5.0609 | 7.8764 |
| 1.7612 | 1.0181 | 62.9614 | 36.2939 | 306.7125 | 39.3595 | 19.0822 | 8.9987 | 3.3136 | 4.1361 |
| 2.0114 | 1.0117 | 70.2471 | 38.4707 | 443.6142 | 70.7171 | 14.4995 | 7.9109 | 2.1744 | 2.6040 |

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Reactive Run

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| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.6582 | 24.4845 | 32.0386 | 0.9148 | 0.7313 | 0.4050 | 0.0924 | 3.3046 | 2.7535 |
| 0.0114 | 0.6569 | 24.5590 | 32.0485 | 1.0382 | 0.7186 | 0.5175 | 0.0954 | 3.5110 | 2.7469 |
| 0.2614 | 0.6402 | 26.6935 | 32.1963 | 5.8912 | 0.6174 | 1.4056 | 0.0267 | 2.9688 | 2.9206 |
| 0.5113 | 0.6310 | 29.5716 | 32.3374 | 13.8139 | 0.9530 | 1.2794 | 0.5421 | 2.8825 | 4.2143 |
| 0.7613 | 0.6205 | 32.8903 | 32.7055 | 23.7277 | 1.8509 | 0.8374 | 1.2468 | 2.6804 | 4.3793 |
| 1.0113 | 0.6102 | 36.3911 | 33.3058 | 32.7369 | 3.3877 | -0.2701 | 1.6558 | 2.6019 | 3.6181 |
| 1.2612 | 0.6027 | 39.8074 | 33.9528 | 39.5872 | 4.8429 | -1.1883 | 1.3784 | 2.8178 | 2.6730 |
| 1.5112 | 0.5964 | 43.0227 | 34.3774 | 45.1289 | 5.2438 | -1.2633 | 0.8700 | 3.1931 | 2.3435 |
| 1.7612 | 0.5900 | 46.0444 | 34.4525 | 52.0296 | 4.7596 | 0.1110 | 0.5793 | 3.5676 | 2.4960 |
| 2.0114 | 0.5842 | 48.9159 | 34.2685 | 63.2680 | 4.1159 | 2.5317 | 0.4156 | 3.7062 | 2.9728 |
| 2.2614 | 0.5791 | 51.8243 | 34.1456 | 84.3861 | 4.9569 | 6.4866 | 2.4321 | 4.0316 | 7.6063 |
| 2.5113 | 0.5728 | 54.9703 | 34.3684 | 122.9311 | 9.8799 | 11.8358 | 6.3535 | 4.4920 | 9.0178 |
| 2.7613 | 0.5668 | 58.4809 | 34.9803 | 185.6970 | 19.6474 | 16.3858 | 7.9742 | 4.2823 | 5.9277 |
| 3.0113 | 0.5604 | 62.3325 | 35.8799 | 264.0420 | 33.1567 | 17.7685 | 8.1694 | 3.4626 | 3.9703 |
| 3.2612 | 0.5539 | 66.3923 | 37.0107 | 342.2943 | 49.8069 | 16.2447 | 7.9265 | 2.6723 | 3.0009 |
| 3.5112 | 0.5465 | 70.5330 | 38.3194 | 410.8095 | 67.9949 | 13.2583 | 7.2518 | 2.1383 | 2.4231 |
| 3.7612 | 0.5379 | 74.6934 | 39.7598 | 466.7721 | 85.4241 | 9.4041 | 6.0746 | 1.8153 | 2.0273 |
| 4.0114 | 0.5276 | 78.8320 | 41.2734 | 509.5995 | 99.7803 | 5.1196 | 4.4479 | 1.6508 | 1.7644 |

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Strongly Heterogeneous

Realization 5

1 Kilogram of Bromide

Only Concentrations Greater than 0.1 ppm Used in Calculations

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Conservative Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.9998 | 24.4817 | 31.7551 | 1.3467 | 0.8220 | 0.5566 | 0.0181 | 3.3609 | 2.8063 |
| 0.0114 | 0.9999 | 24.7147 | 31.7968 | 1.6461 | 0.8374 | 0.6376 | 0.0387 | 3.3349 | 2.8339 |
| 0.2614 | 1.0134 | 29.3943 | 32.9825 | 9.4551 | 1.2289 | 1.5249 | 0.3435 | 3.2170 | 3.1242 |
| 0.5113 | 1.0197 | 33.9758 | 34.4171 | 24.3186 | 2.0340 | 2.3668 | 1.0227 | 2.9686 | 4.2686 |
| 0.7613 | 1.0194 | 39.0182 | 36.0499 | 43.5169 | 4.8872 | 1.3448 | 2.0451 | 2.4849 | 4.7997 |
| 1.0113 | 1.0194 | 44.1565 | 37.9629 | 58.8478 | 9.8050 | -0.6964 | 1.8526 | 2.5444 | 3.1201 |
| 1.2612 | 1.0195 | 48.9710 | 39.7962 | 66.3742 | 12.8804 | -2.5134 | 0.2925 | 3.0679 | 2.5293 |
| 1.5112 | 1.0162 | 53.2752 | 41.1590 | 68.0212 | 13.1633 | -3.5126 | -0.5610 | 3.7650 | 2.6509 |
| 1.7612 | 1.0102 | 57.1551 | 42.1000 | 68.8642 | 13.5972 | -2.7304 | -0.5522 | 4.7760 | 2.6873 |
| 2.0114 | 1.0057 | 60.7776 | 42.7700 | 71.2557 | 16.0947 | -0.7257 | -0.6139 | 5.5518 | 2.8677 |

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Reactive Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.6578 | 24.3194 | 31.7904 | 0.9777 | 0.6984 | 0.3573 | -0.0070 | 3.2259 | 2.7687 |
| 0.0114 | 0.6550 | 24.4702 | 31.8182 | 1.1567 | 0.7093 | 0.4298 | 0.0065 | 3.2240 | 2.7768 |
| 0.2614 | 0.6320 | 27.5105 | 32.4708 | 5.1263 | 0.9709 | 0.7717 | 0.2173 | 3.0184 | 3.0214 |
| 0.5113 | 0.6259 | 30.1604 | 33.3104 | 10.3860 | 1.2071 | 1.2916 | 0.2817 | 2.8906 | 3.1589 |
| 0.7613 | 0.6148 | 32.8571 | 34.1710 | 18.3050 | 1.5883 | 1.5976 | 0.5518 | 2.7539 | 3.7067 |
| 1.0113 | 0.6059 | 35.7299 | 35.0949 | 28.0947 | 2.5414 | 1.3904 | 0.9646 | 2.5255 | 3.9554 |
| 1.2612 | 0.5993 | 38.7468 | 36.1183 | 38.3135 | 4.2793 | 0.5004 | 1.6351 | 2.3048 | 4.2460 |
| 1.5112 | 0.5926 | 41.8336 | 37.2871 | 47.6073 | 7.0848 | -0.8173 | 2.1242 | 2.2524 | 3.6289 |
| 1.7612 | 0.5869 | 44.8462 | 38.5282 | 54.2872 | 9.9511 | -2.4440 | 1.6883 | 2.3499 | 2.6663 |
| 2.0114 | 0.5819 | 47.7186 | 39.6789 | 58.2733 | 11.5249 | -4.0086 | 0.8154 | 2.6077 | 2.2283 |

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Weakly Heterogeneous
Realization 1
0.1 Kilogram of Bromide
All Concentrations Used in Calculations

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Conservative Run

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| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.1003 | 24.0832 | 32.0109 | 0.3985 | 0.3862 | 0.1827 | 0.0267 | 2.9466 | 2.8026 |
| 0.0114 | 0.1003 | 24.3017 | 32.0327 | 0.6831 | 0.3894 | 0.5071 | 0.0773 | 3.7969 | 2.7401 |
| 0.2614 | 0.1003 | 30.5664 | 32.3266 | 10.3335 | 0.7665 | 0.5869 | 0.0706 | 3.1047 | 3.7219 |
| 0.5113 | 0.1003 | 37.4771 | 32.3044 | 16.6069 | 1.7066 | 0.1974 | -0.0119 | 3.0806 | 4.2019 |
| 0.7613 | 0.1003 | 43.5077 | 32.0083 | 19.2034 | 2.8097 | 0.7482 | -0.6043 | 2.9738 | 4.1469 |
| 1.0113 | 0.1003 | 48.7633 | 31.5447 | 23.9195 | 3.4570 | 1.3932 | -1.3352 | 3.2561 | 3.3065 |
| 1.2612 | 0.1003 | 53.7912 | 31.1070 | 33.1011 | 3.5148 | 3.1614 | -0.9237 | 3.9904 | 2.7447 |
| 1.5112 | 0.1003 | 59.1493 | 30.8867 | 52.7506 | 3.5693 | 5.0201 | 0.8998 | 3.5598 | 4.6698 |
| 1.7612 | 0.1003 | 65.3205 | 31.2515 | 80.1170 | 5.5776 | 3.9321 | 3.1874 | 2.7904 | 5.9430 |
| 2.0114 | 0.1003 | 72.1358 | 32.2773 | 100.9021 | 8.9329 | 1.2820 | 3.1600 | 2.6264 | 4.0181 |

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Reactive Run

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| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.0642 | 24.0486 | 32.0061 | 0.3347 | 0.3276 | 0.1280 | 0.0170 | 2.4937 | 2.4268 |
| 0.0114 | 0.0635 | 24.1756 | 32.0184 | 0.4882 | 0.3298 | 0.3522 | 0.0542 | 3.4032 | 2.3588 |
| 0.2614 | 0.0550 | 27.5965 | 32.2760 | 5.5969 | 0.3959 | 0.4755 | 0.1186 | 2.7171 | -0.5375 |
| 0.5113 | 0.0531 | 31.4300 | 32.3473 | 10.8688 | 0.6496 | -0.3219 | 0.0110 | 2.9516 | 1.7499 |
| 0.7613 | 0.0528 | 35.1600 | 32.3482 | 15.1896 | 1.0778 | -1.0532 | -0.0894 | 3.0819 | 2.9192 |
| 1.0113 | 0.0527 | 38.5749 | 32.2667 | 18.2966 | 1.6170 | -1.8085 | -0.1786 | 3.3325 | 3.1158 |
| 1.2612 | 0.0526 | 41.6637 | 32.1147 | 20.5885 | 2.0511 | -2.2345 | -0.3557 | 3.5751 | 2.8009 |
| 1.5112 | 0.0525 | 44.5212 | 31.9064 | 22.7510 | 2.4071 | -2.4345 | -0.7349 | 3.7023 | 2.4430 |
| 1.7612 | 0.0523 | 47.2276 | 31.6837 | 25.0383 | 2.7981 | -2.6037 | -0.9416 | 3.7688 | 2.5970 |
| 2.0114 | 0.0522 | 49.8347 | 31.4560 | 27.3609 | 3.1393 | -2.6521 | -0.8502 | 3.8581 | 2.8135 |

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Weakly Heterogeneous

Realization 2

0.1 Kilogram of Bromide

All Concentrations Used in Calculations

`******************************************************************************`

Conservative Run

`******************************************************************************`

| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.1003 | 24.1047 | 31.9880 | 0.3973 | 0.3857 | 0.2274 | -0.0247 | 2.9407 | 2.8168 |
| 0.0114 | 0.1003 | 24.4493 | 32.0060 | 0.8060 | 0.4218 | 0.5022 | -0.0079 | 3.5276 | 3.0217 |
| 0.2614 | 0.1003 | 31.3631 | 32.2113 | 7.8565 | 0.9914 | 0.8664 | 0.6134 | 3.2192 | 3.6783 |
| 0.5113 | 0.1003 | 37.9670 | 33.2445 | 13.4047 | 1.6244 | 0.2937 | 1.2054 | 3.0574 | 2.6477 |
| 0.7613 | 0.1003 | 43.9776 | 33.5434 | 14.9847 | 2.4710 | 1.0881 | 0.1738 | 3.0268 | 3.3794 |
| 1.0113 | 0.1003 | 49.2690 | 33.5608 | 16.6404 | 3.6130 | 1.6351 | 0.6049 | 2.6829 | 3.9469 |
| 1.2612 | 0.1003 | 53.9866 | 34.1488 | 19.0083 | 5.2656 | 2.0418 | 1.6871 | 3.2041 | 4.0204 |
| 1.5112 | 0.1003 | 58.3194 | 35.0978 | 23.4166 | 6.1613 | 3.0523 | 1.6856 | 4.0317 | 2.8857 |
| 1.7612 | 0.1003 | 62.5364 | 35.8997 | 32.5463 | 5.3390 | 4.8305 | 1.1485 | 4.3843 | 1.8628 |
| 2.0114 | 0.1003 | 67.0265 | 36.2973 | 49.3916 | 4.1113 | 5.7248 | 0.7146 | 3.6538 | 1.6206 |

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Reactive Run

`******************************************************************************`

| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.0643 | 24.0611 | 31.9929 | 0.3339 | 0.3271 | 0.1605 | -0.0183 | 2.4848 | 2.4249 |
| 0.0114 | 0.0627 | 24.2701 | 32.0103 | 0.5707 | 0.3402 | 0.3910 | 0.0214 | 3.3190 | 2.4516 |
| 0.2614 | 0.0549 | 28.4338 | 32.0689 | 4.5855 | 0.4960 | 0.1644 | 0.5434 | 3.1053 | -3.8318 |
| 0.5113 | 0.0539 | 32.0983 | 32.3506 | 8.8320 | 0.6605 | -0.0374 | 1.7817 | 3.0045 | -4.7059 |
| 0.7613 | 0.0531 | 35.7531 | 32.9696 | 12.9211 | 1.0930 | -0.8926 | 1.6093 | 2.9936 | 0.1438 |
| 1.0113 | 0.0529 | 39.2017 | 33.4196 | 15.2979 | 1.5412 | -1.7114 | 0.7517 | 3.4206 | 2.2215 |
| 1.2612 | 0.0524 | 42.3770 | 33.5402 | 17.0525 | 1.8888 | -2.0356 | 0.2294 | 3.7715 | 2.3927 |
| 1.5112 | 0.0523 | 45.2848 | 33.4949 | 18.9325 | 2.2320 | -2.2955 | 0.0901 | 3.8356 | 2.1227 |
| 1.7612 | 0.0521 | 47.9894 | 33.5224 | 20.5867 | 2.6215 | -2.6854 | 0.4006 | 3.9262 | 2.2077 |
| 2.0114 | 0.0520 | 50.5092 | 33.7162 | 22.0512 | 3.1962 | -3.0413 | 0.9914 | 4.0689 | 2.7692 |

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Weakly Heterogeneous
Realization 3
0.1 Kilogram of Bromide
All Concentrations Used in Calculations

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Conservative Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) |  | (Unitless values) |  |  |
| 0 | 0.1003 | 24.0345 | 31.9750 | 0.3900 | 0.3960 | 0.0872 | -0.0472 | 2.8706 | 2.8889 |
| 0.0114 | 0.1003 | 24.2462 | 31.9791 | 0.6294 | 0.4225 | 0.3425 | -0.0534 | 3.4385 | 3.1445 |
| 0.2614 | 0.1003 | 28.3510 | 31.9281 | 5.5290 | 0.5648 | 1.5340 | -0.1365 | 3.7740 | 1.3935 |
| 0.5113 | 0.1003 | 32.8064 | 32.1001 | 14.3972 | 0.8609 | 1.5315 | 0.3898 | 2.6617 | 6.5859 |
| 0.7613 | 0.1003 | 37.6120 | 32.1907 | 20.0780 | 1.6737 | -0.4089 | 0.2377 | 2.7549 | 4.8189 |
| 1.0113 | 0.1003 | 42.0243 | 32.0719 | 22.3165 | 2.0814 | 0.3463 | -0.0272 | 3.9861 | 2.8924 |
| 1.2612 | 0.1003 | 46.3062 | 31.9115 | 30.9101 | 1.9194 | 4.0003 | -0.1720 | 4.6102 | 1.6854 |
| 1.5112 | 0.1003 | 51.1486 | 31.7944 | 51.9961 | 1.6419 | 6.1989 | -0.0221 | 3.7428 | 1.5913 |
| 1.7612 | 0.1003 | 56.9693 | 31.7559 | 82.2673 | 1.6656 | 5.2555 | 0.3834 | 2.8159 | 3.1092 |
| 2.0114 | 0.1003 | 63.6787 | 31.8086 | 110.1756 | 2.0740 | 2.7987 | 0.7210 | 2.5479 | 4.0902 |

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Reactive Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) |  | (Unitless values) |  |  |
| 0 | 0.0642 | 24.0195 | 31.9850 | 0.3290 | 0.3326 | 0.0549 | -0.0373 | 2.4560 | 2.4853 |
| 0.0114 | 0.0634 | 24.1451 | 31.9883 | 0.4691 | 0.3460 | 0.2578 | -0.0324 | 3.1750 | 2.6472 |
| 0.2614 | 0.0561 | 26.5985 | 31.9687 | 2.7863 | 0.2711 | 0.5900 | -0.1921 | 3.3093 | -22.1321 |
| 0.5113 | 0.0544 | 28.7922 | 31.9660 | 5.6795 | 0.2260 | 1.0647 | 0.7502 | 3.2839 | -54.6425 |
| 0.7613 | 0.0537 | 31.1546 | 32.0799 | 10.3290 | 0.3215 | 1.2992 | 1.9205 | 2.8532 | -31.3147 |
| 1.0113 | 0.0527 | 33.7388 | 32.2069 | 15.4866 | 0.5400 | 0.3642 | 2.4218 | 2.2893 | -16.5518 |
| 1.2612 | 0.0523 | 36.3154 | 32.2562 | 18.6252 | 0.8204 | -1.1390 | 2.3679 | 2.3213 | -11.6469 |
| 1.5112 | 0.0523 | 38.7108 | 32.2251 | 19.7961 | 1.0950 | -2.3348 | 1.9843 | 2.6443 | -8.1605 |
| 1.7612 | 0.0523 | 40.9390 | 32.1617 | 20.2513 | 1.3282 | -3.0061 | 1.4800 | 2.7369 | -4.7656 |
| 2.0114 | 0.0522 | 43.0902 | 32.0849 | 21.3565 | 1.5227 | -3.1058 | 0.9148 | 2.2380 | -1.4019 |

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Weakly Heterogeneous
Realization 4
0.1 Kilogram of Bromide
All Concentrations Used in Calculations

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Conservative Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.1003 | 24.0699 | 31.9825 | 0.3984 | 0.3859 | 0.1614 | -0.0293 | 2.9607 | 2.7902 |
| 0.0114 | 0.1003 | 24.3359 | 32.0201 | 0.7231 | 0.4037 | 0.4733 | 0.0513 | 3.6469 | 2.8838 |
| 0.2614 | 0.1003 | 30.2382 | 32.7856 | 8.3620 | 0.8027 | 1.0904 | 0.8778 | 3.1847 | 3.0865 |
| 0.5113 | 0.1003 | 36.5508 | 33.9180 | 18.5653 | 1.5129 | 1.4217 | 1.4863 | 3.0427 | 3.7144 |
| 0.7613 | 0.1003 | 43.2704 | 35.0752 | 27.2691 | 2.5941 | 0.2409 | 1.4601 | 2.7366 | 4.5107 |
| 1.0113 | 0.1003 | 49.3693 | 35.9411 | 28.4225 | 3.9672 | -0.1956 | 1.4636 | 3.2214 | 3.9557 |
| 1.2612 | 0.1003 | 54.5373 | 36.7114 | 30.7446 | 5.0162 | 1.5023 | 0.7807 | 3.5818 | 3.2318 |
| 1.5112 | 0.1003 | 59.3308 | 37.1974 | 37.8856 | 6.0871 | 2.7791 | -0.3831 | 3.5369 | 3.3198 |
| 1.7612 | 0.1003 | 64.0098 | 37.2193 | 46.3926 | 7.0476 | 3.5648 | -0.8203 | 3.7562 | 3.0292 |
| 2.0114 | 0.1003 | 68.5613 | 36.9007 | 57.5580 | 7.0633 | 5.5993 | -0.4527 | 4.3419 | 2.4909 |

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Reactive Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.0642 | 24.0405 | 31.9893 | 0.3337 | 0.3274 | 0.1093 | -0.0258 | 2.5033 | 2.4173 |
| 0.0114 | 0.0631 | 24.1982 | 32.0157 | 0.5179 | 0.3341 | 0.3448 | 0.0522 | 3.3478 | 2.4101 |
| 0.2614 | 0.0547 | 27.6192 | 32.4806 | 4.4518 | 0.4063 | 0.5164 | 1.3177 | 3.0180 | -4.4263 |
| 0.5113 | 0.0534 | 30.8517 | 32.9389 | 8.9641 | 0.6136 | 0.4413 | 1.2699 | 2.8366 | -0.8048 |
| 0.7613 | 0.0527 | 34.1574 | 33.5291 | 14.3070 | 1.0396 | 0.2866 | 1.1751 | 2.8248 | 2.8376 |
| 1.0113 | 0.0525 | 37.5890 | 34.1956 | 20.3783 | 1.6736 | 0.0223 | 0.7872 | 2.7758 | 3.7006 |
| 1.2612 | 0.0524 | 41.0879 | 34.7985 | 25.6763 | 2.2420 | -0.8296 | 0.6645 | 2.7117 | 3.8857 |
| 1.5112 | 0.0522 | 44.4643 | 35.3023 | 28.3676 | 2.7268 | -2.0020 | 0.9872 | 2.9257 | 3.8565 |
| 1.7612 | 0.0521 | 47.5699 | 35.7454 | 28.7066 | 3.2531 | -2.9041 | 1.1981 | 3.3598 | 3.5173 |
| 2.0114 | 0.0520 | 50.3843 | 36.1819 | 28.2241 | 3.7687 | -3.2844 | 1.0957 | 3.7719 | 2.8332 |

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Weakly Heterogeneous

Realization 5

0.1 Kilogram of Bromide

All Concentrations Used in Calculations

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Conservative Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.1003 | 24.0826 | 31.9809 | 0.3970 | 0.3852 | 0.1923 | -0.0392 | 2.9850 | 2.7985 |
| 0.0114 | 0.1003 | 24.4313 | 31.9374 | 0.8232 | 0.4101 | 0.5483 | -0.1248 | 3.7036 | 2.9179 |
| 0.2614 | 0.1003 | 31.6991 | 31.4884 | 7.2110 | 1.7213 | 0.3205 | -0.0532 | 3.3346 | 3.4698 |
| 0.5113 | 0.1003 | 37.1390 | 32.1598 | 12.6585 | 2.3058 | 1.5227 | 1.7271 | 3.1729 | 2.6506 |
| 0.7613 | 0.1003 | 42.6258 | 33.5397 | 22.7023 | 3.1130 | 1.3493 | 1.5373 | 2.9806 | 2.1952 |
| 1.0113 | 0.1003 | 48.6017 | 34.6496 | 31.9128 | 2.9145 | 0.4061 | 1.5345 | 2.9204 | 0.9046 |
| 1.2612 | 0.1003 | 54.5710 | 34.9218 | 35.8093 | 3.1720 | -0.4321 | 0.8157 | 3.0519 | 1.6105 |
| 1.5112 | 0.1003 | 60.1012 | 34.6569 | 35.9565 | 4.1032 | 0.0207 | -0.2275 | 3.4423 | 2.3369 |
| 1.7612 | 0.1003 | 65.1963 | 34.2585 | 39.0141 | 4.6812 | 2.3415 | -0.3947 | 3.6432 | 2.2629 |
| 2.0114 | 0.1003 | 70.2530 | 33.9843 | 49.6706 | 4.7468 | 4.1676 | 0.1620 | 3.3141 | 2.5929 |

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Reactive Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.0643 | 24.0477 | 31.9888 | 0.3324 | 0.3274 | 0.1300 | -0.0289 | 2.5014 | 2.4092 |
| 0.0114 | 0.0627 | 24.2553 | 31.9545 | 0.5719 | 0.3315 | 0.4000 | -0.1182 | 3.4251 | 2.2863 |
| 0.2614 | 0.0538 | 28.7366 | 31.5402 | 5.1388 | 0.6754 | -0.1612 | -0.7534 | 2.8556 | -0.7598 |
| 0.5113 | 0.0532 | 32.1603 | 31.4914 | 7.1901 | 1.1006 | -0.7469 | 0.9603 | 3.2085 | -5.7646 |
| 0.7613 | 0.0529 | 34.9667 | 31.7560 | 9.4935 | 1.2484 | -0.8595 | 1.2147 | 2.5041 | -5.8248 |
| 1.0113 | 0.0529 | 37.6993 | 32.3299 | 12.8805 | 1.6920 | -1.1282 | 1.2942 | 1.8227 | -2.3367 |
| 1.2612 | 0.0527 | 40.5842 | 33.1260 | 17.3098 | 2.1541 | -1.3850 | 1.8082 | 1.7397 | -3.5767 |
| 1.5112 | 0.0525 | 43.6243 | 33.9133 | 22.2715 | 2.2058 | -1.8119 | 2.5730 | 1.8026 | -9.3375 |
| 1.7612 | 0.0522 | 46.7823 | 34.5113 | 26.6550 | 1.8926 | -2.5757 | 4.0820 | 1.8286 | -22.2444 |
| 2.0114 | 0.0519 | 49.9529 | 34.8373 | 29.9011 | 1.6770 | -3.6287 | 5.3684 | 1.7426 | -34.2540 |

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Weakly Heterogeneous

Realization 1

0.1 Kilogram of Bromide

Only Concentrations Greater than 0.1 ppm Used in Calculations

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Conservative Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.1001 | 24.0811 | 32.0100 | 0.3941 | 0.3814 | 0.1607 | 0.0164 | 2.8214 | 2.6839 |
| 0.0114 | 0.1002 | 24.2992 | 32.0318 | 0.6689 | 0.3883 | 0.4660 | 0.0619 | 3.5089 | 2.7598 |
| 0.2614 | 0.1052 | 30.3360 | 32.3075 | 10.3453 | 0.9072 | 0.4493 | 0.0503 | 2.8007 | 3.4213 |
| 0.5113 | 0.1034 | 37.1308 | 32.2942 | 17.3890 | 1.7306 | -0.5264 | 0.0688 | 2.8960 | 3.3836 |
| 0.7613 | 0.1027 | 43.0978 | 32.0249 | 20.2569 | 2.7671 | -0.7298 | -0.3310 | 3.0345 | 3.6360 |
| 1.0113 | 0.1017 | 48.3908 | 31.5886 | 23.0447 | 3.5893 | -0.1677 | -0.9397 | 2.8805 | 3.4644 |
| 1.2612 | 0.1011 | 53.3648 | 31.1285 | 29.8779 | 3.6791 | 1.2933 | -0.7489 | 3.2021 | 2.9410 |
| 1.5112 | 0.1005 | 58.6250 | 30.8401 | 46.7236 | 3.3723 | 3.1836 | 0.0526 | 2.9381 | 3.0094 |
| 1.7612 | 0.0997 | 64.6939 | 31.1610 | 71.8787 | 4.8945 | 2.4840 | 2.0327 | 2.4122 | 4.2966 |
| 2.0114 | 0.0985 | 71.4281 | 32.1614 | 91.7358 | 7.8439 | 0.0552 | 2.3105 | 2.3350 | 3.2734 |

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Reactive Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.0642 | 24.0472 | 32.0059 | 0.3313 | 0.3268 | 0.1087 | 0.0140 | 2.3656 | 2.3824 |
| 0.0114 | 0.0635 | 24.1737 | 32.0175 | 0.4813 | 0.3304 | 0.3190 | 0.0408 | 3.1665 | 2.4070 |
| 0.2614 | 0.0587 | 27.4487 | 32.2511 | 5.4270 | 0.6066 | 0.5096 | 0.0414 | 2.5481 | 3.3636 |
| 0.5113 | 0.0562 | 31.1777 | 32.3138 | 10.7794 | 0.8699 | -0.2876 | -0.0034 | 2.6907 | 3.3727 |
| 0.7613 | 0.0544 | 34.9330 | 32.3230 | 14.9189 | 1.2125 | -1.0283 | -0.0056 | 2.7959 | 3.2613 |
| 1.0113 | 0.0534 | 38.4275 | 32.2594 | 17.2342 | 1.7201 | -1.7033 | -0.0204 | 3.0037 | 3.2878 |
| 1.2612 | 0.0526 | 41.5947 | 32.1224 | 18.5421 | 2.0991 | -1.8139 | -0.1677 | 3.1078 | 3.2393 |
| 1.5112 | 0.0520 | 44.5259 | 31.9232 | 19.7963 | 2.4883 | -1.6520 | -0.5317 | 3.0670 | 3.4209 |
| 1.7612 | 0.0514 | 47.2752 | 31.7067 | 21.1897 | 2.8485 | -1.5499 | -0.8140 | 2.9452 | 3.4403 |
| 2.0114 | 0.0510 | 49.9014 | 31.4702 | 22.5527 | 3.1953 | -1.4887 | -0.8580 | 2.9071 | 3.2806 |

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Weakly Heterogeneous
Realization 2
0.1 Kilogram of Bromide
Only Concentrations Greater than 0.1 ppm Used in Calculations

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Conservative Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.1002 | 24.1037 | 31.9885 | 0.3955 | 0.3816 | 0.2181 | -0.0186 | 2.8753 | 2.6787 |
| 0.0114 | 0.1001 | 24.4455 | 32.0071 | 0.7877 | 0.4188 | 0.4554 | 0.0016 | 3.2418 | 2.9506 |
| 0.2614 | 0.1048 | 31.1286 | 32.1700 | 8.1907 | 1.1433 | 0.5813 | 0.2574 | 2.9436 | 3.4112 |
| 0.5113 | 0.1052 | 37.5366 | 33.1579 | 14.8528 | 1.9124 | -0.4521 | 0.5565 | 2.8366 | 2.9623 |
| 0.7613 | 0.1041 | 43.4710 | 33.4799 | 17.3084 | 2.5734 | -0.6662 | 0.0512 | 3.1462 | 2.8245 |
| 1.0113 | 0.1030 | 48.7726 | 33.5002 | 18.6196 | 3.5115 | -0.4401 | 0.2034 | 2.8399 | 3.0138 |
| 1.2612 | 0.1020 | 53.4973 | 34.0644 | 19.6471 | 5.1602 | -0.2542 | 1.1577 | 2.8214 | 3.4906 |
| 1.5112 | 0.1011 | 57.8212 | 34.9945 | 22.1459 | 6.2930 | 0.4453 | 1.1948 | 2.9617 | 2.9284 |
| 1.7612 | 0.1006 | 62.0118 | 35.8123 | 28.7901 | 5.7831 | 2.1662 | 0.6176 | 3.1912 | 2.5224 |
| 2.0114 | 0.0998 | 66.4297 | 36.2422 | 42.9053 | 4.4117 | 3.7731 | 0.2363 | 3.0336 | 2.4346 |

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Reactive Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.0642 | 24.0593 | 31.9931 | 0.3300 | 0.3262 | 0.1375 | -0.0165 | 2.3261 | 2.3720 |
| 0.0114 | 0.0628 | 24.2642 | 32.0075 | 0.5569 | 0.3430 | 0.3401 | 0.0114 | 3.0270 | 2.5068 |
| 0.2614 | 0.0582 | 28.2748 | 32.0194 | 4.5938 | 0.7677 | 0.1441 | -0.0494 | 2.8137 | 3.3039 |
| 0.5113 | 0.0569 | 31.8990 | 32.2820 | 8.6501 | 1.0521 | 0.0180 | 0.3579 | 2.7304 | 3.4601 |
| 0.7613 | 0.0559 | 35.5166 | 32.8856 | 12.6333 | 1.5130 | -0.6725 | 0.5397 | 2.6612 | 3.0810 |
| 1.0113 | 0.0549 | 38.9710 | 33.3607 | 14.8182 | 1.8217 | -1.3859 | 0.4593 | 2.9772 | 2.8285 |
| 1.2612 | 0.0538 | 42.1723 | 33.4966 | 16.0012 | 2.0852 | -1.6049 | 0.1729 | 3.2062 | 2.7494 |
| 1.5112 | 0.0528 | 45.1786 | 33.4594 | 16.8131 | 2.3720 | -1.4517 | -0.0273 | 3.0638 | 2.7149 |
| 1.7612 | 0.0521 | 47.9492 | 33.4795 | 17.4322 | 2.7077 | -1.3429 | 0.0269 | 2.8650 | 2.7084 |
| 2.0114 | 0.0515 | 50.5276 | 33.6543 | 17.8761 | 3.2265 | -1.4806 | 0.3274 | 2.8433 | 2.9339 |

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Weakly Heterogeneous

Realization 3

0.1 Kilogram of Bromide

*Only Concentrations Greater than* 0.1 ppm Used in Calculations

## Conservative Run

| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.1001 | 24.0323 | 31.9758 | 0.3849 | 0.3890 | 0.0625 | -0.0362 | 2.7417 | 2.6988 |
| 0.0114 | 0.1001 | 24.2442 | 31.9782 | 0.6163 | 0.4177 | 0.3192 | -0.0628 | 3.2202 | 3.0280 |
| 0.2614 | 0.1057 | 28.1730 | 31.9169 | 5.4249 | 0.7738 | 1.1495 | -0.0655 | 3.1966 | 3.2763 |
| 0.5113 | 0.1065 | 32.4526 | 32.0708 | 14.5871 | 1.0461 | 1.2179 | 0.1763 | 2.4948 | 4.4291 |
| 0.7613 | 0.1056 | 37.1294 | 32.1604 | 21.0789 | 1.7954 | -1.0330 | 0.1397 | 2.5006 | 3.9527 |
| 1.0113 | 0.1042 | 41.5004 | 32.0404 | 23.1800 | 2.2661 | -1.3375 | 0.0344 | 3.3765 | 3.1892 |
| 1.2612 | 0.1025 | 45.8028 | 31.8779 | 29.4415 | 2.1818 | 1.5508 | -0.1761 | 3.8383 | 2.9195 |
| 1.5112 | 0.1015 | 50.5933 | 31.7661 | 47.5587 | 1.8591 | 4.2737 | -0.1756 | 3.1967 | 2.7969 |
| 1.7612 | 0.1005 | 56.2840 | 31.7300 | 75.1787 | 1.7212 | 3.7292 | 0.1284 | 2.4230 | 2.8266 |
| 2.0114 | 0.1000 | 62.8792 | 31.7752 | 102.1359 | 1.9815 | 1.1087 | 0.4752 | 2.2202 | 3.1370 |

## Reactive Run

| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.0642 | 24.0187 | 31.9853 | 0.3276 | 0.3313 | 0.0444 | -0.0338 | 2.3814 | 2.4124 |
| 0.0114 | 0.0634 | 24.1436 | 31.9888 | 0.4646 | 0.3427 | 0.2455 | -0.0240 | 3.0559 | 2.4956 |
| 0.2614 | 0.0601 | 26.4811 | 31.9543 | 2.7605 | 0.5800 | 0.4890 | -0.1280 | 2.9120 | 3.1097 |
| 0.5113 | 0.0590 | 28.6238 | 31.9269 | 5.6852 | 0.6423 | 0.8471 | -0.1417 | 2.9749 | 3.3291 |
| 0.7613 | 0.0577 | 30.9490 | 32.0270 | 10.2452 | 0.7200 | 1.0966 | 0.0027 | 2.7050 | 3.8367 |
| 1.0113 | 0.0561 | 33.4996 | 32.1470 | 15.3192 | 0.9508 | 0.2638 | 0.1636 | 2.2234 | 4.1933 |
| 1.2612 | 0.0549 | 36.0981 | 32.1758 | 18.8086 | 1.2871 | -1.1542 | 0.1894 | 2.3421 | 3.9081 |
| 1.5112 | 0.0542 | 38.5595 | 32.1391 | 20.0766 | 1.5994 | -2.1871 | 0.1465 | 2.8149 | 3.3024 |
| 1.7612 | 0.0535 | 40.8658 | 32.0746 | 20.5314 | 1.8246 | -2.5600 | 0.1257 | 3.3019 | 2.9751 |
| 2.0114 | 0.0529 | 43.0923 | 32.0149 | 21.4856 | 1.9169 | -2.0606 | 0.0851 | 3.6273 | 2.8288 |

Weakly Heterogeneous

Realization 4

0.1 Kilogram of Bromide

Only Concentrations Greater than 0.1 ppm Used in Calculations

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Conservative Run

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| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.1001 | 24.0678 | 31.9828 | 0.3937 | 0.3808 | 0.1391 | -0.0275 | 2.8415 | 2.6812 |
| 0.0114 | 0.1002 | 24.3339 | 32.0204 | 0.7097 | 0.4024 | 0.4435 | 0.0534 | 3.4050 | 2.8598 |
| 0.2614 | 0.1055 | 30.0302 | 32.7024 | 8.3230 | 1.0286 | 0.8441 | 0.2661 | 2.8517 | 3.5483 |
| 0.5113 | 0.1048 | 36.2039 | 33.8002 | 18.4876 | 1.8296 | 0.8517 | 0.5382 | 2.7749 | 3.6068 |
| 0.7613 | 0.1038 | 42.8014 | 34.9479 | 27.7389 | 2.7457 | -0.4347 | 0.6663 | 2.5601 | 3.7464 |
| 1.0113 | 0.1019 | 48.9375 | 35.8508 | 27.9422 | 3.8734 | -1.5035 | 1.0437 | 3.0027 | 3.4432 |
| 1.2612 | 0.1008 | 54.1458 | 36.6675 | 27.9431 | 4.8750 | -0.2125 | 0.6491 | 3.0636 | 2.8214 |
| 1.5112 | 0.1000 | 58.9140 | 37.1810 | 32.6953 | 5.9306 | 1.0965 | -0.4336 | 2.8104 | 2.9351 |
| 1.7612 | 0.0995 | 63.5523 | 37.2193 | 39.5655 | 6.9485 | 1.4631 | -0.9002 | 2.8722 | 2.8924 |
| 2.0114 | 0.0987 | 68.0172 | 36.9230 | 46.9191 | 6.9914 | 2.5328 | -0.4695 | 3.2003 | 2.6040 |

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Reactive Run

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| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.0642 | 24.0391 | 31.9894 | 0.3306 | 0.3264 | 0.0906 | -0.0251 | 2.3795 | 2.3768 |
| 0.0114 | 0.0631 | 24.1961 | 32.0152 | 0.5092 | 0.3336 | 0.3101 | 0.0361 | 3.1200 | 2.4391 |
| 0.2614 | 0.0588 | 27.4704 | 32.3910 | 4.3494 | 0.7053 | 0.4570 | 0.1530 | 2.7560 | 3.4447 |
| 0.5113 | 0.0570 | 30.6657 | 32.8247 | 8.5828 | 0.9690 | 0.3171 | 0.1625 | 2.6244 | 3.4130 |
| 0.7613 | 0.0554 | 33.9735 | 33.4095 | 13.5381 | 1.4059 | 0.1283 | 0.2549 | 2.6247 | 3.6330 |
| 1.0113 | 0.0540 | 37.4415 | 34.1105 | 19.0927 | 1.8817 | -0.1011 | 0.2623 | 2.5905 | 3.5258 |
| 1.2612 | 0.0528 | 40.9862 | 34.7550 | 23.5520 | 2.2260 | -0.8024 | 0.3635 | 2.5016 | 3.4310 |
| 1.5112 | 0.0517 | 44.4297 | 35.2732 | 25.4198 | 2.5058 | -1.8243 | 0.6659 | 2.6708 | 3.2154 |
| 1.7612 | 0.0513 | 47.6015 | 35.7254 | 25.2065 | 3.0097 | -2.5049 | 0.9141 | 2.9973 | 3.1217 |
| 2.0114 | 0.0508 | 50.4684 | 36.1735 | 23.9358 | 3.5439 | -2.4575 | 0.8913 | 3.1795 | 2.8813 |

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Weakly Heterogeneous

Realization 5

0.1 Kilogram of Bromide

Only Concentrations Greater than 0.1 ppm Used in Calculations

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Conservative Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.1002 | 24.0810 | 31.9814 | 0.3937 | 0.3805 | 0.1767 | -0.0308 | 2.8939 | 2.6816 |
| 0.0114 | 0.1002 | 24.4260 | 31.9386 | 0.8002 | 0.4108 | 0.4911 | -0.1208 | 3.3485 | 2.9027 |
| 0.2614 | 0.1055 | 31.4352 | 31.5208 | 7.6589 | 1.9270 | -0.1636 | -0.2866 | 2.9845 | 3.5540 |
| 0.5113 | 0.1047 | 36.8207 | 32.1184 | 12.9066 | 2.6542 | 0.5271 | 0.7844 | 2.8873 | 3.1933 |
| 0.7613 | 0.1036 | 42.2901 | 33.4775 | 22.1373 | 3.4651 | 0.7247 | 0.6818 | 2.6903 | 2.7035 |
| 1.0113 | 0.1027 | 48.1541 | 34.5718 | 31.4587 | 3.2490 | -0.3303 | 0.3573 | 2.6958 | 2.7130 |
| 1.2612 | 0.1017 | 54.1094 | 34.8767 | 35.4901 | 3.4093 | -1.4854 | 0.1617 | 2.8072 | 2.9452 |
| 1.5112 | 0.1006 | 59.6718 | 34.6415 | 34.3906 | 4.2488 | -1.4383 | -0.3943 | 3.0513 | 2.8802 |
| 1.7612 | 0.1001 | 64.7649 | 34.2459 | 35.8918 | 4.8060 | 0.4298 | -0.4914 | 3.1020 | 2.6673 |
| 2.0114 | 0.0994 | 69.7412 | 33.9541 | 44.3272 | 4.7017 | 2.0126 | -0.1773 | 2.7933 | 2.6045 |

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Reactive Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.0642 | 24.0461 | 31.9891 | 0.3289 | 0.3259 | 0.1079 | -0.0260 | 2.3508 | 2.3714 |
| 0.0114 | 0.0628 | 24.2481 | 31.9606 | 0.5562 | 0.3384 | 0.3423 | -0.0792 | 3.0786 | 2.4461 |
| 0.2614 | 0.0583 | 28.5340 | 31.6141 | 5.2582 | 1.0493 | -0.1186 | -0.5804 | 2.5986 | 4.2195 |
| 0.5113 | 0.0562 | 31.9991 | 31.5118 | 7.3846 | 1.6772 | -0.7014 | -0.1362 | 3.0136 | 3.2725 |
| 0.7613 | 0.0551 | 34.9185 | 31.7377 | 9.6974 | 1.9077 | -0.2948 | 0.3468 | 2.9186 | 3.1082 |
| 1.0113 | 0.0542 | 37.7238 | 32.2900 | 13.1357 | 2.2572 | 0.0193 | 0.5968 | 2.7223 | 2.8457 |
| 1.2612 | 0.0535 | 40.6641 | 33.0600 | 17.4903 | 2.8023 | 0.0232 | 0.5038 | 2.5823 | 2.5857 |
| 1.5112 | 0.0529 | 43.7453 | 33.8372 | 22.6545 | 2.9806 | -0.3616 | 0.2854 | 2.5519 | 2.4848 |
| 1.7612 | 0.0522 | 46.8950 | 34.4210 | 27.1973 | 2.7575 | -0.9363 | 0.1016 | 2.6023 | 2.5530 |
| 2.0114 | 0.0516 | 50.0800 | 34.7483 | 30.4543 | 2.5554 | -1.5825 | 0.1641 | 2.7106 | 2.5499 |

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Strongly Heterogeneous

Realization 1

0.1 Kilogram of Bromide

All Concentrations Used in Calculations

Conservative Run

| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.1003 | 24.1305 | 31.9503 | 0.3994 | 0.3836 | 0.2708 | -0.1109 | 2.8912 | 2.8368 |
| 0.0114 | 0.1003 | 24.5097 | 31.8821 | 0.7961 | 0.4825 | 0.5130 | -0.3255 | 3.3885 | 3.6734 |
| 0.2614 | 0.1003 | 30.3498 | 30.3579 | 4.7511 | 2.7441 | 1.9449 | -1.8107 | 3.9363 | 5.3021 |
| 0.5113 | 0.1003 | 34.3672 | 30.3219 | 12.3575 | 7.5473 | 2.2057 | -2.0912 | 2.7481 | 4.1676 |
| 0.7613 | 0.1003 | 37.7812 | 30.3280 | 21.3696 | 12.2836 | 1.6927 | -3.2821 | 2.4963 | 3.7556 |
| 1.0113 | 0.1003 | 40.7858 | 30.0825 | 32.8313 | 14.3335 | 1.7441 | -3.5900 | 2.6785 | 3.5483 |
| 1.2612 | 0.1003 | 43.5550 | 30.0647 | 46.6237 | 16.7357 | 2.1334 | -2.4311 | 3.0956 | 3.6197 |
| 1.5112 | 0.1003 | 46.1944 | 30.4616 | 64.7731 | 21.8977 | 3.6565 | 0.0702 | 3.6486 | 3.8349 |
| 1.7612 | 0.1003 | 48.8632 | 31.2092 | 91.8597 | 29.8972 | 6.0826 | 2.0113 | 3.8795 | 3.5285 |
| 2.0114 | 0.1003 | 51.6896 | 32.1111 | 131.1336 | 38.5751 | 8.3452 | 2.5526 | 3.6997 | 2.9965 |

Reactive Run

| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.0643 | 24.0763 | 31.9710 | 0.3361 | 0.3264 | 0.1954 | -0.0776 | 2.4812 | 2.4153 |
| 0.0114 | 0.0623 | 24.3168 | 31.9382 | 0.5668 | 0.3690 | 0.4374 | -0.1893 | 3.1956 | 2.9453 |
| 0.2614 | 0.0549 | 28.2733 | 30.8510 | 2.8742 | 1.2625 | 0.5424 | -1.0838 | 3.0866 | 2.4097 |
| 0.5113 | 0.0539 | 30.7809 | 30.4214 | 5.4509 | 1.6999 | 1.0132 | 1.7788 | 3.3309 | -16.2163 |
| 0.7613 | 0.0534 | 32.9037 | 30.4485 | 9.2040 | 3.3158 | 0.6196 | 2.6006 | 0.6459 | -9.8325 |
| 1.0113 | 0.0530 | 34.8414 | 30.5829 | 12.5463 | 6.0245 | -1.4291 | 0.4680 | -3.3324 | 1.2195 |
| 1.2612 | 0.0526 | 36.5885 | 30.5748 | 15.2512 | 8.6656 | -4.2499 | -1.6136 | -7.6975 | 1.9851 |
| 1.5112 | 0.0524 | 38.1959 | 30.4227 | 18.3042 | 10.6091 | -6.5994 | -2.8925 | -10.6767 | 3.0243 |
| 1.7612 | 0.0520 | 39.7153 | 30.2384 | 22.2019 | 11.9711 | -7.9463 | -3.4878 | -11.1466 | 3.1660 |
| 2.0114 | 0.0517 | 41.1531 | 30.1046 | 26.5014 | 13.1690 | -9.0030 | -3.6112 | -10.9278 | 3.0986 |

Strongly Heterogeneous
Realization 2
0.1 Kilogram of Bromide
All Concentrations Used in Calculations

Conservative Run

| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.1003 | 24.0291 | 32.0120 | 0.3851 | 0.3969 | 0.0782 | 0.0195 | 2.8618 | 2.9065 |
| 0.0114 | 0.1003 | 24.1478 | 32.0776 | 0.4998 | 0.4492 | 0.3404 | 0.1591 | 3.6257 | 3.1342 |
| 0.2614 | 0.1003 | 27.4915 | 33.0545 | 5.1865 | 1.0059 | 0.7338 | 0.4530 | 2.5885 | 3.3337 |
| 0.5113 | 0.1003 | 30.8505 | 33.4105 | 6.9522 | 2.3360 | -0.3520 | 0.8175 | 3.7315 | 4.4868 |
| 0.7613 | 0.1003 | 33.3516 | 33.8630 | 7.7483 | 5.1743 | 2.4599 | 1.1101 | 7.8781 | 3.3022 |
| 1.0113 | 0.1003 | 35.3346 | 34.4278 | 12.7204 | 8.1674 | 8.2521 | 1.2792 | 13.4464 | 2.6563 |
| 1.2612 | 0.1003 | 37.2638 | 35.0313 | 27.3068 | 10.3275 | 15.4967 | 1.2812 | 15.8779 | 2.3949 |
| 1.5112 | 0.1003 | 39.4895 | 35.5863 | 60.8976 | 11.5648 | 22.1520 | 1.1530 | 12.5335 | 2.2854 |
| 1.7612 | 0.1003 | 42.1883 | 35.9946 | 121.6045 | 12.3592 | 26.4635 | 0.8728 | 8.7240 | 2.3025 |
| 2.0114 | 0.1003 | 45.3626 | 36.2156 | 212.4221 | 13.2549 | 29.3355 | 0.1854 | 6.4961 | 2.6928 |

Reactive Run

| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.0642 | 24.0160 | 32.0073 | 0.3263 | 0.3331 | 0.0467 | 0.0174 | 2.4233 | 2.4964 |
| 0.0114 | 0.0637 | 24.0841 | 32.0447 | 0.3865 | 0.3638 | 0.2169 | 0.1124 | 3.0267 | 2.7552 |
| 0.2614 | 0.0565 | 24.9633 | 32.7867 | 2.6716 | 0.6919 | 1.1986 | 0.6282 | 3.0394 | 1.5341 |
| 0.5113 | 0.0549 | 28.0720 | 33.1392 | 5.2923 | 0.8613 | 0.1734 | 0.7596 | 2.3670 | 2.2766 |
| 0.7613 | 0.0544 | 29.9730 | 33.3110 | 6.3586 | 1.4234 | -0.9318 | 0.9341 | 2.8999 | 3.7129 |
| 1.0113 | 0.0540 | 31.5254 | 33.5207 | 6.4673 | 2.5280 | -1.5064 | 1.0730 | 3.9082 | 3.6963 |
| 1.2612 | 0.0538 | 32.7776 | 33.7767 | 6.4608 | 4.0970 | -1.3091 | 1.0601 | 4.7949 | 3.2393 |
| 1.5112 | 0.0537 | 33.8360 | 34.0277 | 6.9065 | 5.9055 | -0.4051 | 1.0451 | 4.4834 | 2.8570 |
| 1.7612 | 0.0535 | 34.7878 | 34.2770 | 8.1408 | 7.6456 | 0.7391 | 1.0990 | 2.0626 | 2.5986 |
| 2.0114 | 0.0532 | 35.7029 | 34.5482 | 10.4592 | 9.0862 | 2.0251 | 1.1746 | -0.4388 | 2.4365 |

```
Strongly Heterogeneous
Realization 3
0.1 Kilogram of Bromide
All Concentrations Used in Calculations
*******************************************************************************
Conservative Run
*******************************************************************************
Time     Mass     XC       YC       Var X    Var Y    SKX      SKY      KRX      KRY
(yr)     (kg)     (m)      (m)      (m^2)    (m^2)             (Unitless values)
*******************************************************************************
      0   0.1003  24.0730  32.0061   0.3976   0.3859   0.1574  -0.0016   2.9174   2.8366
 0.0114   0.1003  24.1943  31.9759   0.5387   0.3980   0.3384  -0.0874   3.4068   2.9843
 0.2614   0.1003  26.8615  30.9294   4.0002   0.8532   1.8388  -0.7526   4.9532   2.0143
 0.5113   0.1003  30.3409  31.0050  13.8751   1.9380   3.1868   1.5338   3.5160   5.0305
 0.7613   0.1003  35.0390  32.4145  26.8111   3.9856   2.2496   1.1577   3.0626   2.9364
 1.0113   0.1003  40.0800  33.9578  35.1844   4.7510   2.1730   1.2830   3.2587   3.6524
 1.2612   0.1003  44.6129  35.5213  37.8140   6.4405   3.1717   2.1799   3.3748   3.5781
 1.5112   0.1003  48.1201  37.2427  38.8262   8.9254   5.7513   1.8352   3.9107   2.6483
 1.7612   0.1003  50.7665  38.9934  45.8957  10.4065   8.7783   0.7881   4.6419   2.2794
 2.0114   0.1003  53.1932  40.5511  62.6942  10.3237  10.2059  -0.0975   4.5506   2.4032
*******************************************************************************
Reactive Run
*******************************************************************************
Time     Mass     XC       YC       Var X    Var Y    SKX      SKY      KRX      KRY
(yr)     (kg)     (m)      (m)      (m^2)    (m^2)             (Unitless values)
*******************************************************************************
      0   0.0642  24.0430  32.0048   0.3338   0.3273   0.1125   0.0085   2.4916   2.4275
 0.0114   0.0638  24.1151  31.9893   0.4149   0.3321   0.2476  -0.0407   3.0448   2.4988
 0.2614   0.0563  25.7367  31.3335   2.0101   0.5270   0.5620  -1.4915   3.3565   1.5723
 0.5113   0.0540  27.2817  30.7168   4.1944   0.6423   1.6476  -1.3393   4.2382  -1.8377
 0.7613   0.0534  29.1084  30.7115   8.9325   1.0602   2.4391   0.6918   3.4088   4.5933
 1.0113   0.0526  31.3682  31.2952  15.7252   2.2862   1.9321   1.5880   2.6081   4.0884
 1.2612   0.0521  33.9121  32.1357  22.4394   3.3940   0.9933   1.1700   2.5424   2.8385
 1.5112   0.0518  36.5478  32.9343  28.2650   3.8018   0.3943   0.6917   2.7998   2.7488
 1.7612   0.0516  39.1486  33.6428  33.3629   4.0236   0.1044   0.6710   2.9875   3.2532
 2.0114   0.0515  41.6130  34.3639  37.2489   4.6601  -0.1634   1.0400   3.1075   3.6072
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Strongly Heterogeneous

Realization 4

0.1 Kilogram of Bromide

All Concentrations Used in Calculations

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Conservative Run

****************************************************************************************

| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.1003 | 24.1086 | 31.9985 | 0.4009 | 0.3818 | 0.2284 | 0.0086 | 2.9413 | 2.7714 |
| 0.0114 | 0.1003 | 24.2005 | 32.0008 | 0.5328 | 0.3746 | 0.4619 | 0.0135 | 3.8500 | 2.6586 |
| 0.2614 | 0.1003 | 27.5982 | 32.1779 | 9.4017 | 0.5197 | 2.0464 | 0.4135 | 3.3586 | 4.3678 |
| 0.5113 | 0.1003 | 32.9469 | 32.7149 | 25.0817 | 1.8735 | 1.5178 | 1.7857 | 2.9583 | 5.4460 |
| 0.7613 | 0.1003 | 38.8994 | 33.7445 | 37.0593 | 4.3081 | 0.5738 | 1.6943 | 3.0266 | 3.0633 |
| 1.0113 | 0.1003 | 44.5670 | 34.4433 | 45.1065 | 5.0007 | 2.9415 | 0.8054 | 3.8691 | 2.6255 |
| 1.2612 | 0.1003 | 49.8832 | 34.4010 | 67.1620 | 5.1000 | 11.1047 | 2.0577 | 5.8673 | 7.5298 |
| 1.5112 | 0.1003 | 55.5478 | 34.6226 | 136.3299 | 12.5085 | 20.0768 | 8.0238 | 6.0302 | 10.2356 |
| 1.7612 | 0.1002 | 62.2119 | 35.9574 | 266.3285 | 34.3021 | 21.6056 | 9.4801 | 3.7697 | 4.9268 |
| 2.0114 | 0.0999 | 69.5050 | 38.0711 | 407.4573 | 64.8460 | 16.7487 | 8.2405 | 2.3134 | 2.8064 |

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Reactive Run

****************************************************************************************

| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.0643 | 24.0641 | 31.9980 | 0.3364 | 0.3259 | 0.1650 | -0.0018 | 2.5053 | 2.4012 |
| 0.0114 | 0.0639 | 24.1151 | 31.9983 | 0.4027 | 0.3220 | 0.2985 | 0.0026 | 3.1961 | 2.3096 |
| 0.2614 | 0.0578 | 25.7570 | 32.0620 | 3.7254 | 0.2877 | 1.5777 | -0.1068 | 3.4610 | -1.5647 |
| 0.5113 | 0.0545 | 28.2482 | 32.1854 | 10.1853 | 0.4679 | 1.1081 | 0.3163 | 2.7518 | 3.0067 |
| 0.7613 | 0.0530 | 31.2299 | 32.4706 | 18.0048 | 1.0365 | 0.6515 | 1.1263 | 2.8723 | 4.8341 |
| 1.0113 | 0.0524 | 34.4245 | 32.9410 | 25.8832 | 2.0263 | -0.0107 | 1.6463 | 2.8042 | 4.4147 |
| 1.2612 | 0.0520 | 37.6283 | 33.5481 | 32.0411 | 3.4180 | -0.8596 | 1.8103 | 2.8876 | 3.4109 |
| 1.5112 | 0.0517 | 40.6991 | 34.1231 | 36.3214 | 4.5037 | -1.2441 | 1.4434 | 3.1343 | 2.5034 |
| 1.7612 | 0.0514 | 43.5614 | 34.4733 | 40.0114 | 4.7305 | -0.7804 | 0.9518 | 3.4362 | 2.1536 |
| 2.0114 | 0.0512 | 46.2230 | 34.5252 | 45.4859 | 4.3394 | 0.8304 | 0.6093 | 3.7089 | 2.2366 |

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Strongly Heterogeneous

Realization 5

0.1 Kilogram of Bromide

All Concentrations Used in Calculations

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Conservative Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.1003 | 24.0582 | 31.9396 | 0.4038 | 0.3781 | 0.1413 | -0.1095 | 3.0174 | 2.7028 |
| 0.0114 | 0.1003 | 24.2849 | 31.9864 | 0.6804 | 0.4026 | 0.4519 | -0.0062 | 3.6708 | 2.8318 |
| 0.2614 | 0.1003 | 28.6623 | 33.1060 | 7.2124 | 0.7829 | 2.0476 | 1.1340 | 3.7433 | 2.2566 |
| 0.5113 | 0.1003 | 32.7784 | 34.4305 | 19.6326 | 1.4673 | 3.4870 | 1.4538 | 3.5069 | 4.6268 |
| 0.7613 | 0.1003 | 37.4601 | 35.9347 | 36.8650 | 3.7434 | 3.1879 | 2.3380 | 2.8196 | 5.5936 |
| 1.0113 | 0.1003 | 42.5420 | 37.8543 | 52.6208 | 7.7379 | 1.4045 | 2.7571 | 2.4993 | 3.4518 |
| 1.2612 | 0.1003 | 47.5767 | 39.8785 | 60.7425 | 10.3088 | -0.9832 | 1.5920 | 2.6837 | 2.1030 |
| 1.5112 | 0.1003 | 52.2236 | 41.4860 | 61.2783 | 10.0256 | -2.6842 | 1.0575 | 3.3992 | 1.4804 |
| 1.7612 | 0.1003 | 56.4149 | 42.5705 | 59.0495 | 9.9520 | -2.3102 | 1.1657 | 4.9129 | 1.3400 |
| 2.0114 | 0.1003 | 60.2492 | 43.3099 | 58.3035 | 12.0990 | 0.8768 | 0.5236 | 7.6212 | 2.4980 |

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Reactive Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.0642 | 24.0334 | 31.9635 | 0.3364 | 0.3247 | 0.0919 | -0.0903 | 2.5453 | 2.3491 |
| 0.0114 | 0.0633 | 24.1669 | 31.9932 | 0.4925 | 0.3363 | 0.3190 | -0.0010 | 3.3279 | 2.4190 |
| 0.2614 | 0.0554 | 26.8062 | 32.6295 | 3.5706 | 0.4670 | 0.9995 | 1.3747 | 3.2367 | -0.7052 |
| 0.5113 | 0.0542 | 28.8896 | 33.3147 | 6.9196 | 0.7636 | 1.8356 | 1.0319 | 3.4552 | 1.9220 |
| 0.7613 | 0.0539 | 30.9608 | 33.9827 | 11.4854 | 1.1242 | 2.3100 | 0.6099 | 3.2777 | 3.3715 |
| 1.0113 | 0.0538 | 33.2059 | 34.6531 | 16.9673 | 1.7464 | 2.0328 | 0.6210 | 2.8204 | 4.0834 |
| 1.2612 | 0.0533 | 35.6645 | 35.4597 | 23.5038 | 2.5732 | 1.2238 | 1.3546 | 2.1416 | 4.0975 |
| 1.5112 | 0.0528 | 38.2982 | 36.4114 | 30.4530 | 3.9128 | -0.4127 | 2.3934 | 1.1238 | 4.1453 |
| 1.7612 | 0.0522 | 41.0443 | 37.5135 | 36.3509 | 5.9603 | -3.1971 | 3.0944 | -0.2910 | 3.2415 |
| 2.0114 | 0.0516 | 43.7938 | 38.7063 | 40.2236 | 8.0202 | -7.0630 | 2.9961 | -2.0622 | 1.8872 |

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Strongly Heterogeneous

Realization 1

0.1 Kilogram of Bromide

Only Concentrations Greater Than 0.1 ppm Used in Calculations

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Conservative Run

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| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.1002 | 24.1293 | 31.9503 | 0.3959 | 0.3811 | 0.2554 | -0.1057 | 2.7876 | 2.7704 |
| 0.0114 | 0.1003 | 24.5028 | 31.8852 | 0.7870 | 0.4763 | 0.4618 | -0.2743 | 3.1717 | 3.3213 |
| 0.2614 | 0.1040 | 30.1542 | 30.4257 | 5.1310 | 2.8300 | 1.0975 | -1.2617 | 3.7717 | 3.9564 |
| 0.5113 | 0.1020 | 34.1844 | 30.3423 | 12.2176 | 7.4899 | 1.9722 | -1.9241 | 2.6239 | 3.7805 |
| 0.7613 | 0.1009 | 37.5749 | 30.3778 | 20.5280 | 12.0421 | 1.4386 | -3.2673 | 2.2550 | 3.7662 |
| 1.0113 | 0.0993 | 40.5019 | 30.1568 | 30.0311 | 13.9608 | 0.8158 | -3.8900 | 2.0076 | 3.7475 |
| 1.2612 | 0.0980 | 43.0842 | 30.1188 | 39.7027 | 15.8345 | -0.1915 | -3.4588 | 1.8531 | 3.4811 |
| 1.5112 | 0.0960 | 45.3380 | 30.3925 | 49.1570 | 19.3491 | -0.9543 | -2.0249 | 1.8943 | 3.2439 |
| 1.7612 | 0.0938 | 47.5017 | 31.0362 | 63.6224 | 26.5374 | 0.0241 | 0.4130 | 2.3359 | 3.2686 |
| 2.0114 | 0.0923 | 49.7946 | 31.8703 | 89.1476 | 34.7876 | 2.7228 | 1.2385 | 2.8174 | 2.7532 |

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Reactive Run

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| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.0643 | 24.0743 | 31.9717 | 0.3316 | 0.3240 | 0.1697 | -0.0684 | 2.2977 | 2.3471 |
| 0.0114 | 0.0625 | 24.3060 | 31.9402 | 0.5628 | 0.3718 | 0.3635 | -0.1748 | 2.9472 | 2.9195 |
| 0.2614 | 0.0576 | 28.1050 | 30.9153 | 3.1579 | 1.5158 | 0.0360 | -0.7015 | 3.1486 | 3.3014 |
| 0.5113 | 0.0561 | 30.6333 | 30.4203 | 5.4713 | 2.5367 | 0.8191 | -0.8282 | 3.4349 | 3.2986 |
| 0.7613 | 0.0545 | 32.8391 | 30.3694 | 9.1338 | 4.5013 | 1.6968 | -0.9105 | 2.8399 | 3.2759 |
| 1.0113 | 0.0535 | 34.8778 | 30.5357 | 13.4988 | 7.0970 | 1.5388 | -1.3926 | 2.2854 | 3.1661 |
| 1.2612 | 0.0527 | 36.6914 | 30.5474 | 17.6589 | 9.0814 | 1.2072 | -2.1828 | 2.1235 | 3.3051 |
| 1.5112 | 0.0517 | 38.3354 | 30.4451 | 22.0494 | 10.4353 | 1.0575 | -2.9805 | 2.0746 | 3.6036 |
| 1.7612 | 0.0512 | 39.8615 | 30.2929 | 27.1974 | 11.4838 | 0.7658 | -3.5533 | 1.9730 | 3.8079 |
| 2.0114 | 0.0504 | 41.2898 | 30.1902 | 32.3563 | 12.3913 | 0.3456 | -3.8931 | 1.8643 | 3.9243 |

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Strongly Heterogeneous

Realization 2

0.1 Kilogram of Bromide

Only Concentrations Greater Than 0.1 ppm Used in Calculations

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Conservative Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.1001 | 24.0269 | 32.0118 | 0.3806 | 0.3897 | 0.0553 | 0.0170 | 2.7303 | 2.7105 |
| 0.0114 | 0.1001 | 24.1451 | 32.0781 | 0.4876 | 0.4459 | 0.2895 | 0.1644 | 3.2447 | 3.0732 |
| 0.2614 | 0.1046 | 27.3220 | 33.0148 | 5.3947 | 1.1082 | 0.4741 | 0.1532 | 2.4733 | 3.2213 |
| 0.5113 | 0.1035 | 30.6259 | 33.3875 | 7.4841 | 2.3130 | -1.1501 | 0.6153 | 3.2270 | 3.9060 |
| 0.7613 | 0.1023 | 33.0990 | 33.8242 | 7.6934 | 5.0898 | -0.0089 | 0.8869 | 5.1875 | 3.1314 |
| 1.0113 | 0.1009 | 35.0663 | 34.3667 | 10.5545 | 8.0931 | 3.9960 | 1.0721 | 6.6085 | 2.5767 |
| 1.2612 | 0.0999 | 36.8228 | 34.9611 | 17.7126 | 10.2412 | 7.4983 | 1.1322 | 6.8254 | 2.3295 |
| 1.5112 | 0.0984 | 38.5427 | 35.5556 | 32.0896 | 11.5015 | 12.2093 | 1.0251 | 8.5262 | 2.2277 |
| 1.7612 | 0.0971 | 40.7191 | 36.0053 | 69.8959 | 11.9458 | 19.6762 | 0.8655 | 8.7125 | 2.1594 |
| 2.0114 | 0.0960 | 43.1891 | 36.3126 | 127.3922 | 12.2054 | 23.2531 | 0.6796 | 6.4504 | 2.1114 |

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Reactive Run

*************************************************************************************

| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.0642 | 24.0153 | 32.0072 | 0.3246 | 0.3315 | 0.0370 | 0.0165 | 2.3587 | 2.4242 |
| 0.0114 | 0.0636 | 24.0814 | 32.0427 | 0.3806 | 0.3574 | 0.1894 | 0.0818 | 2.8428 | 2.5549 |
| 0.2614 | 0.0605 | 25.8195 | 32.7244 | 2.8440 | 0.8712 | 0.8757 | 0.1224 | 2.9525 | 2.8960 |
| 0.5113 | 0.0583 | 27.8462 | 33.0910 | 5.7295 | 1.0792 | -0.1143 | 0.1468 | 2.3707 | 3.3061 |
| 0.7613 | 0.0568 | 29.7591 | 33.2821 | 6.9575 | 1.5491 | -1.2411 | 0.4521 | 2.8467 | 3.4810 |
| 1.0113 | 0.0556 | 31.3447 | 33.5035 | 7.0128 | 2.5368 | -1.9183 | 0.7405 | 3.7597 | 3.4169 |
| 1.2612 | 0.0545 | 32.6292 | 33.7637 | 6.6411 | 4.0228 | -1.8826 | 0.7998 | 4.6354 | 3.1239 |
| 1.5112 | 0.0539 | 33.7425 | 34.0095 | 6.8306 | 5.8253 | -0.5067 | 0.8069 | 5.3617 | 2.7483 |
| 1.7612 | 0.0532 | 34.6937 | 34.2633 | 7.7111 | 7.4858 | 1.3405 | 0.9130 | 5.5136 | 2.4874 |
| 2.0114 | 0.0524 | 35.6144 | 34.5352 | 9.4161 | 8.9900 | 3.4683 | 1.0568 | 5.4010 | 2.3584 |

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Strongly Heterogeneous
Realization 3
0.1 Kilogram of Bromide
Only Concentrations Greater Than 0.1 ppm Used in Calculations

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Conservative Run

************************************************************************************

| Time (yr) | Mass (kg) | XC (m) | YC (m) | Var X (m^2) | Var Y (m^2) | SKX | SKY (Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.1001 | 24.0715 | 32.0070 | 0.3935 | 0.3807 | 0.1411 | 0.0107 | 2.8147 | 2.6810 |
| 0.0114 | 0.1001 | 24.1917 | 31.9779 | 0.5275 | 0.3926 | 0.2951 | -0.0607 | 3.1386 | 2.8498 |
| 0.2614 | 0.1061 | 26.7342 | 31.0206 | 3.9056 | 1.0920 | 1.4743 | -0.2501 | 4.1249 | 2.8005 |
| 0.5113 | 0.1060 | 30.0577 | 31.0314 | 13.3312 | 2.0565 | 2.5961 | 1.1259 | 3.0237 | 3.9034 |
| 0.7613 | 0.1056 | 34.5465 | 32.3063 | 26.6295 | 3.8972 | 1.4560 | 0.7556 | 2.6588 | 2.6466 |
| 1.0113 | 0.1036 | 39.4873 | 33.7622 | 35.9575 | 4.6897 | 0.6927 | 0.5737 | 2.9196 | 3.0940 |
| 1.2612 | 0.1019 | 44.0395 | 35.3060 | 38.5873 | 6.3302 | 0.8406 | 1.3358 | 3.1674 | 3.1581 |
| 1.5112 | 0.1003 | 47.5419 | 37.0500 | 36.6337 | 8.7810 | 2.3509 | 1.1688 | 3.4188 | 2.4862 |
| 1.7612 | 0.0991 | 50.1256 | 38.8505 | 38.9591 | 10.2624 | 5.0167 | 0.3158 | 3.6947 | 2.2341 |
| 2.0114 | 0.0979 | 52.4583 | 40.4643 | 50.4064 | 9.9578 | 6.3746 | -0.5848 | 3.4221 | 2.3168 |

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Reactive Run

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| Time (yr) | Mass (kg) | XC (m) | YC (m) | Var X (m^2) | Var Y (m^2) | SKX | SKY (Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.0642 | 24.0418 | 32.0050 | 0.3311 | 0.3261 | 0.0963 | 0.0117 | 2.3789 | 2.3761 |
| 0.0114 | 0.0637 | 24.1140 | 31.9900 | 0.4125 | 0.3300 | 0.2328 | -0.0246 | 2.9509 | 2.4018 |
| 0.2614 | 0.0610 | 25.6244 | 31.4405 | 1.9963 | 0.7935 | 0.4341 | -0.4891 | 2.9534 | 3.4066 |
| 0.5113 | 0.0587 | 27.0749 | 30.8502 | 4.0797 | 1.0933 | 1.1633 | -0.0297 | 3.5475 | 3.0338 |
| 0.7613 | 0.0578 | 28.8684 | 30.7849 | 8.7005 | 1.4035 | 2.0032 | 0.6010 | 3.1078 | 3.6265 |
| 1.0113 | 0.0563 | 31.0549 | 31.2781 | 15.2318 | 2.4152 | 1.6038 | 1.1097 | 2.4305 | 3.4223 |
| 1.2612 | 0.0548 | 33.5371 | 32.0455 | 21.8261 | 3.4703 | 0.6183 | 0.8234 | 2.3313 | 2.6935 |
| 1.5112 | 0.0534 | 36.1759 | 32.7955 | 27.6024 | 3.8153 | -0.0172 | 0.3126 | 2.5976 | 2.5711 |
| 1.7612 | 0.0523 | 38.7896 | 33.4897 | 32.3501 | 3.9142 | -0.4669 | 0.1335 | 2.7926 | 2.8795 |
| 2.0114 | 0.0513 | 41.3453 | 34.2099 | 34.7893 | 4.3566 | -0.6752 | 0.4045 | 2.8663 | 3.0925 |

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Strongly Heterogeneous
Realization 4
0.1 Kilogram of Bromide
Only Concentrations Greater Than 0.1 ppm Used in Calculations

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Conservative Run

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| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.1001 | 24.1067 | 31.9976 | 0.3964 | 0.3782 | 0.2070 | -0.0033 | 2.8046 | 2.6761 |
| 0.0114 | 0.1002 | 24.1993 | 31.9996 | 0.5255 | 0.3737 | 0.4300 | -0.0004 | 3.5984 | 2.6653 |
| 0.2614 | 0.1038 | 27.4873 | 32.1835 | 8.8932 | 0.5930 | 1.7862 | 0.3145 | 2.9704 | 3.4947 |
| 0.5113 | 0.1042 | 32.5929 | 32.6633 | 24.7715 | 1.8660 | 1.3345 | 1.4323 | 2.7149 | 4.5919 |
| 0.7613 | 0.1033 | 38.3408 | 33.6596 | 38.3229 | 4.3647 | -0.2855 | 1.6263 | 2.6918 | 2.9708 |
| 1.0113 | 0.1027 | 43.8092 | 34.3783 | 47.8767 | 5.0955 | -0.0481 | 0.8714 | 3.2577 | 2.3268 |
| 1.2612 | 0.1012 | 48.7461 | 34.2858 | 61.5924 | 4.0885 | 3.1541 | 0.5163 | 3.5169 | 2.6904 |
| 1.5112 | 0.0988 | 53.6808 | 34.2228 | 96.7571 | 7.0537 | 9.5305 | 4.8227 | 3.8285 | 9.3355 |
| 1.7612 | 0.0962 | 59.4266 | 35.1944 | 195.4067 | 22.7004 | 17.0575 | 8.1561 | 3.9597 | 5.1892 |
| 2.0114 | 0.0942 | 66.1250 | 37.0093 | 332.0241 | 49.7571 | 16.5235 | 7.8399 | 2.6470 | 2.8511 |

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Reactive Run

*************************************************************************************

| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.0642 | 24.0630 | 31.9985 | 0.3318 | 0.3247 | 0.1450 | -0.0026 | 2.3321 | 2.3566 |
| 0.0114 | 0.0639 | 24.1126 | 31.9978 | 0.3953 | 0.3213 | 0.2637 | -0.0050 | 2.9670 | 2.3284 |
| 0.2614 | 0.0602 | 25.6911 | 32.0983 | 3.5660 | 0.4051 | 1.4759 | 0.1585 | 3.2103 | 2.8789 |
| 0.5113 | 0.0579 | 28.0418 | 32.1792 | 9.5524 | 0.6219 | 0.9896 | 0.2336 | 2.4836 | 3.3507 |
| 0.7613 | 0.0559 | 30.8939 | 32.4170 | 17.6158 | 1.1458 | 0.7146 | 0.7833 | 2.6637 | 4.0503 |
| 1.0113 | 0.0545 | 34.0077 | 32.8477 | 25.9678 | 2.0742 | -0.0274 | 1.3131 | 2.5806 | 3.9512 |
| 1.2612 | 0.0533 | 37.1390 | 33.4522 | 32.8107 | 3.5137 | -1.1192 | 1.6740 | 2.6350 | 3.4058 |
| 1.5112 | 0.0526 | 40.1303 | 34.0299 | 37.7151 | 4.7333 | -1.9095 | 1.3875 | 2.8690 | 2.5818 |
| 1.7612 | 0.0519 | 43.0076 | 34.4222 | 41.1699 | 4.9820 | -1.9964 | 0.9219 | 3.1697 | 2.2545 |
| 2.0114 | 0.0511 | 45.6463 | 34.5223 | 45.2681 | 4.5114 | -0.8402 | 0.6852 | 3.4439 | 2.3295 |

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Strongly Heterogeneous

Realization 5

0.1 Kilogram of Bromide

Only Concentrations Greater Than 0.1 ppm Used in Calculations

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Conservative Run

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| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.1002 | 24.0575 | 31.9403 | 0.4012 | 0.3748 | 0.1322 | -0.1001 | 2.9336 | 2.6072 |
| 0.0114 | 0.1001 | 24.2821 | 31.9853 | 0.6674 | 0.3979 | 0.4176 | -0.0198 | 3.4484 | 2.7242 |
| 0.2614 | 0.1050 | 28.5347 | 32.9795 | 6.9261 | 1.0458 | 1.6644 | 0.1863 | 3.2998 | 3.3631 |
| 0.5113 | 0.1038 | 32.5826 | 34.2881 | 17.8887 | 1.7412 | 2.5526 | 0.3598 | 2.9411 | 4.1872 |
| 0.7613 | 0.1022 | 37.1646 | 35.8078 | 34.0064 | 3.6210 | 2.1803 | 1.7094 | 2.4419 | 4.6250 |
| 1.0113 | 0.1014 | 42.1643 | 37.7159 | 49.8081 | 7.7591 | 0.1855 | 2.4206 | 2.1425 | 3.3721 |
| 1.2612 | 0.1011 | 47.1935 | 39.7223 | 58.7476 | 10.6698 | -2.3194 | 1.1597 | 2.3124 | 2.2077 |
| 1.5112 | 0.1008 | 51.7933 | 41.3101 | 60.3902 | 10.7273 | -4.4994 | 0.0839 | 2.8275 | 2.2058 |
| 1.7612 | 0.1002 | 55.9512 | 42.3944 | 57.4724 | 10.4279 | -5.6928 | -0.1233 | 3.4632 | 2.3168 |
| 2.0114 | 0.0993 | 59.6844 | 43.1464 | 54.3917 | 11.7527 | -5.4260 | -0.3429 | 4.1120 | 2.3528 |

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Reactive Run

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| Time<br>(yr) | Mass<br>(kg) | XC<br>(m) | YC<br>(m) | Var X<br>(m^2) | Var Y<br>(m^2) | SKX | SKY<br>(Unitless values) | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.0642 | 24.0328 | 31.9630 | 0.3320 | 0.3225 | 0.0767 | -0.0909 | 2.4031 | 2.3072 |
| 0.0114 | 0.0633 | 24.1657 | 31.9919 | 0.4859 | 0.3361 | 0.2905 | -0.0176 | 3.1421 | 2.4547 |
| 0.2614 | 0.0590 | 26.7015 | 32.4954 | 3.4793 | 0.7423 | 0.7817 | 0.0657 | 3.0504 | 3.5186 |
| 0.5113 | 0.0569 | 28.8003 | 33.1860 | 6.6254 | 1.0591 | 1.4323 | 0.0110 | 3.1080 | 3.6222 |
| 0.7613 | 0.0558 | 30.9093 | 33.8515 | 10.8983 | 1.3353 | 1.7305 | -0.1973 | 2.8346 | 3.8380 |
| 1.0113 | 0.0550 | 33.1915 | 34.5789 | 16.9367 | 1.7775 | 1.8039 | 0.2503 | 2.7127 | 3.7862 |
| 1.2612 | 0.0539 | 35.6685 | 35.3815 | 24.1157 | 2.4707 | 1.5423 | 0.8638 | 2.4546 | 3.4792 |
| 1.5112 | 0.0531 | 38.3181 | 36.2822 | 32.6130 | 3.7642 | 0.9572 | 1.4284 | 2.2672 | 3.6567 |
| 1.7612 | 0.0524 | 41.1259 | 37.3615 | 41.3313 | 6.1489 | 0.0835 | 2.1884 | 2.1834 | 3.5761 |
| 2.0114 | 0.0518 | 43.9356 | 38.5305 | 48.1416 | 8.5658 | -1.3105 | 1.8898 | 2.1817 | 2.6807 |

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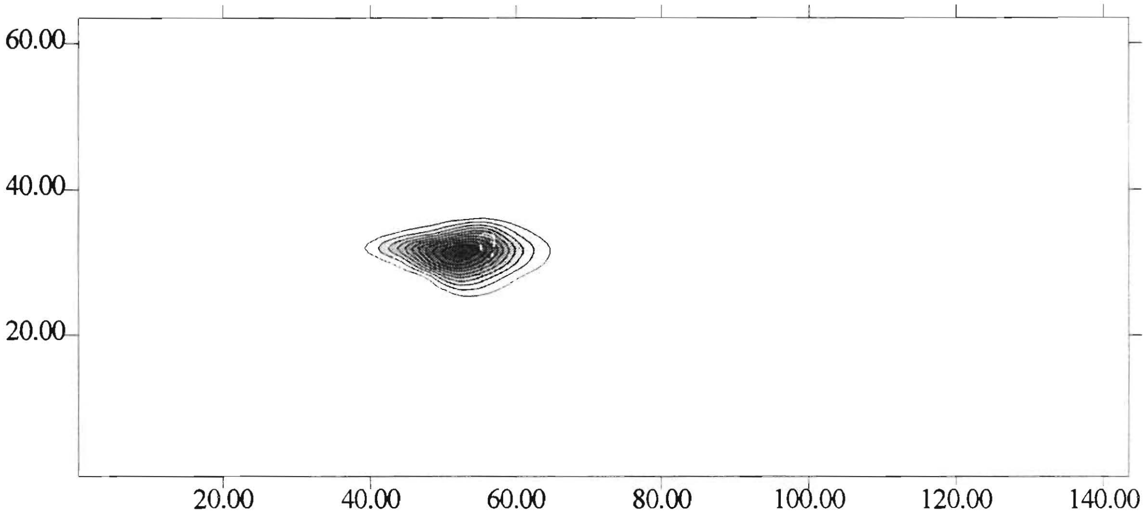
# APPENDIX B

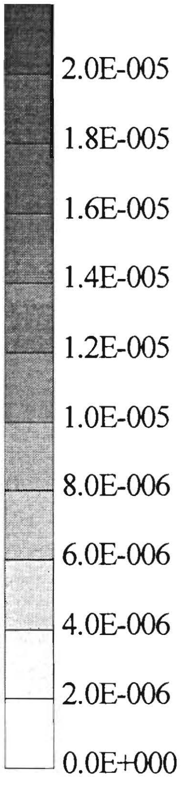
## PLUME "SNAPSHOTS"

Weakly Heterogeneous Flow Field
Realization 1
Reactive Run
1 kg of Bromide

T = 2 Years

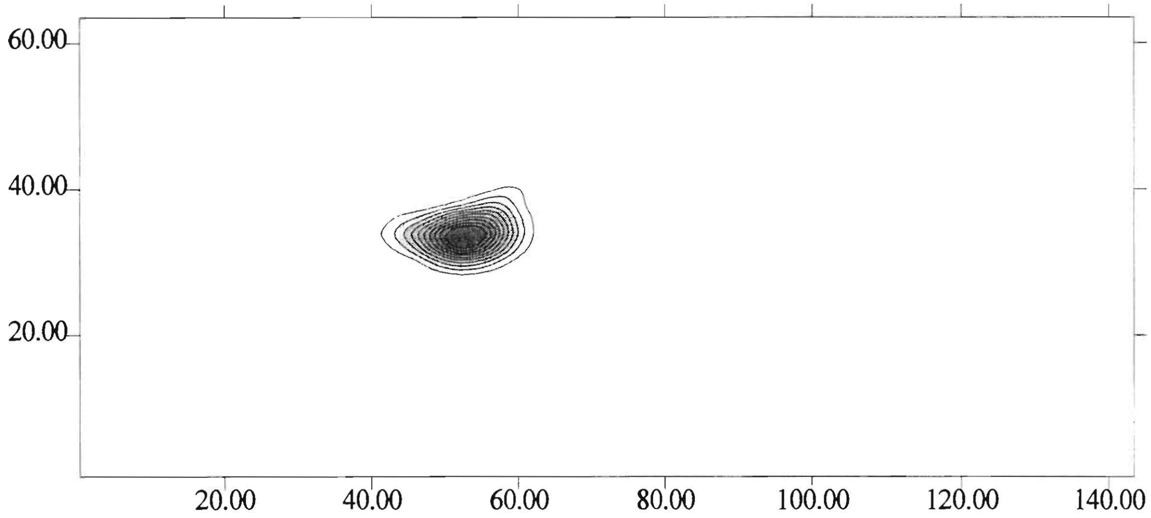


Bromide concentration scale for realizations in a weakly heterogeneous flow field with 1 kg of bromide.

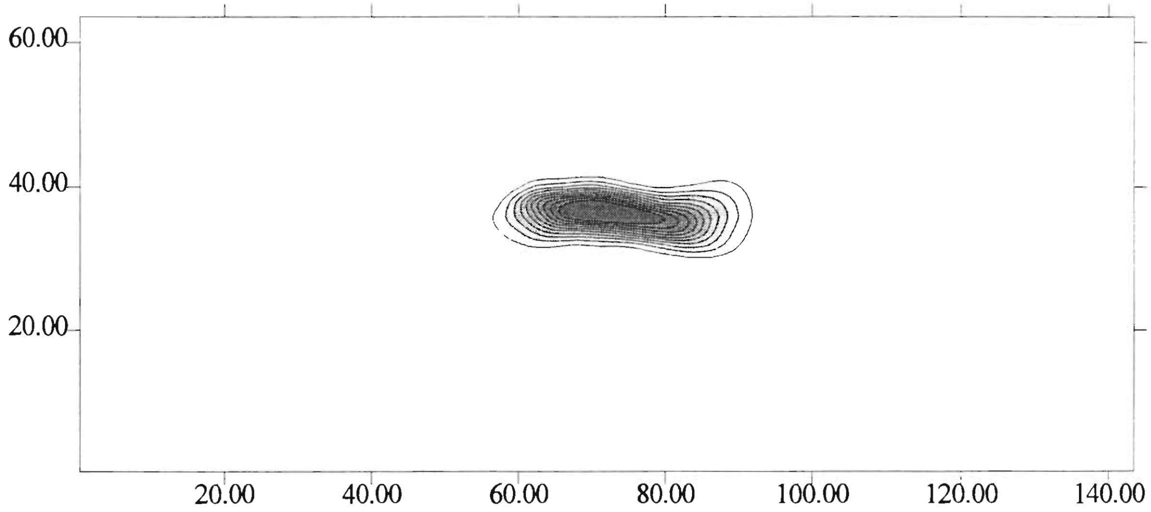


Weakly Heterogeneous Flow Field
Realization 2
Reactive Run
1 kg of Bromide

T = 2 Years



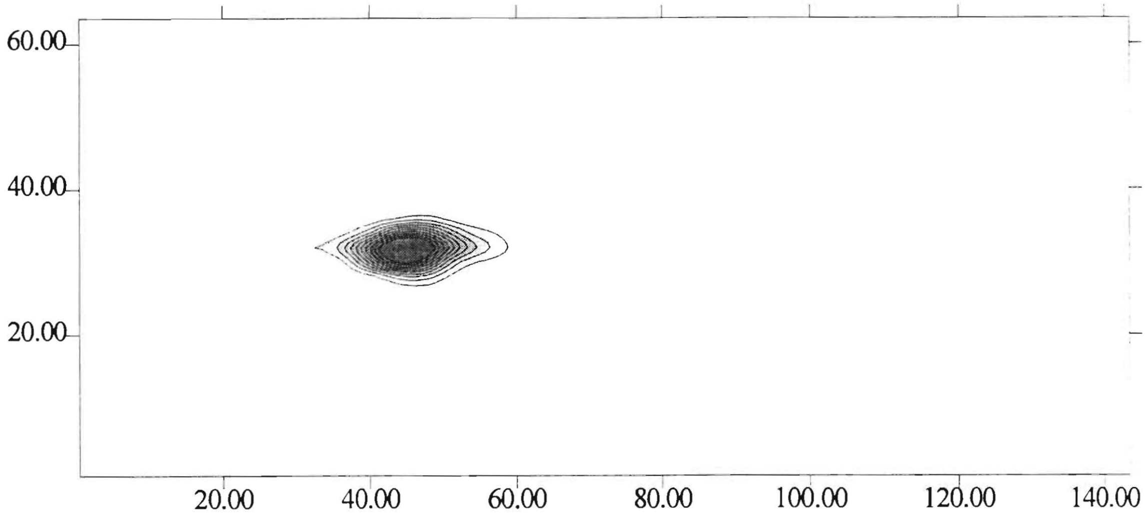
T = 4 Years *



* Contour interval for this plot is 1.0E-006 due
to low concentration values

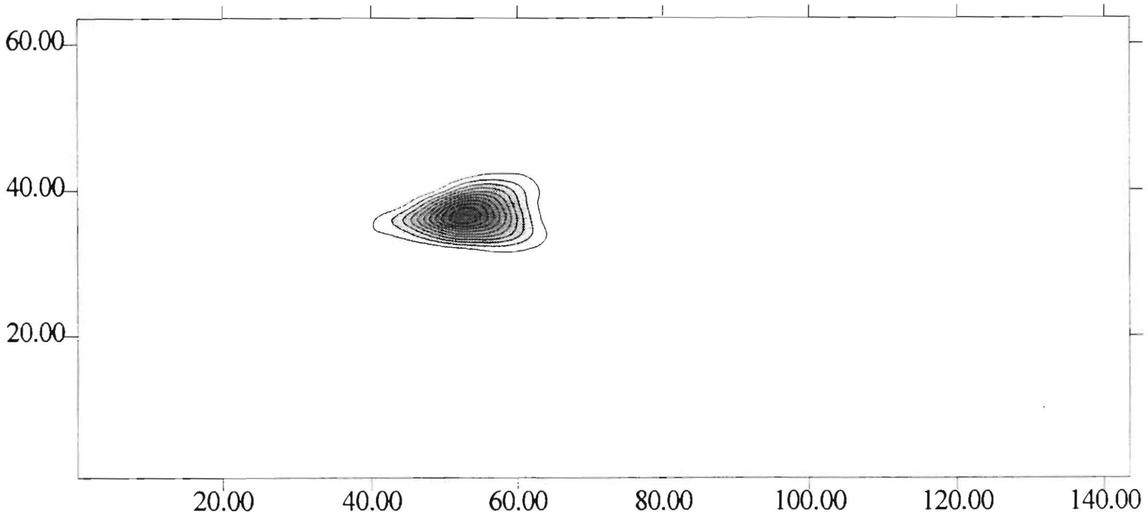
Weakly Heterogeneous Flow Field
Realization 3
Reactive Run
1 kg of Bromide

T = 2 Years



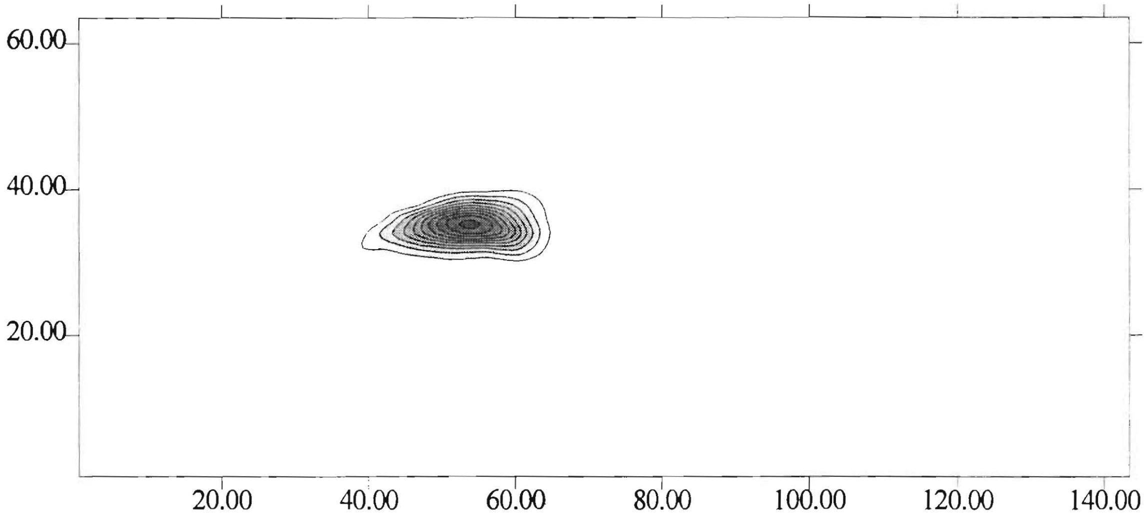
Weakly Heterogeneous Flow Field
Realization 4
Reactive Run
1 kg of Bromide

T = 2 Years



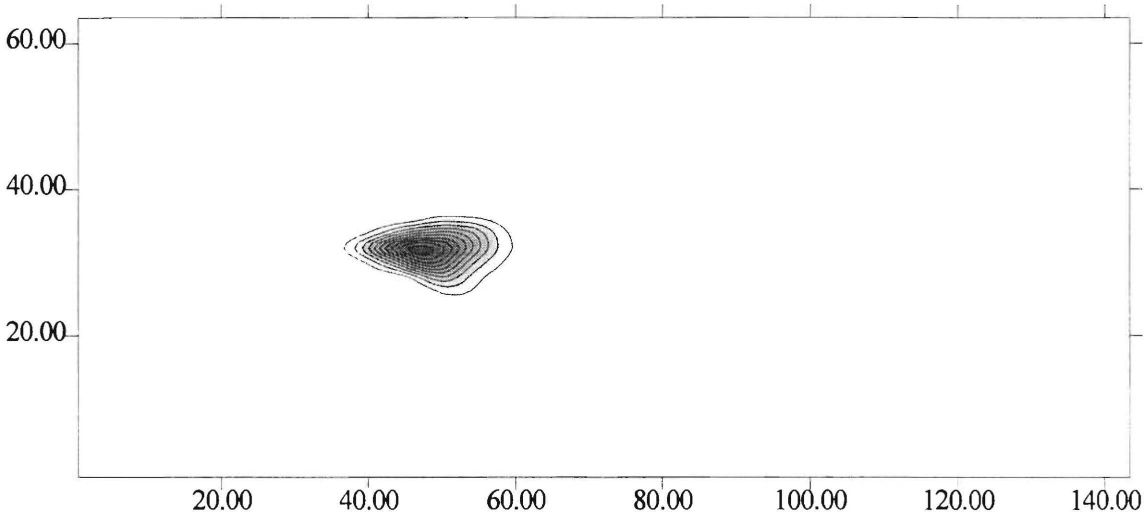
Weakly Heterogeneous Flow Field
Realization 5
Reactive Run
1 kg of Bromide

T = 2 Years

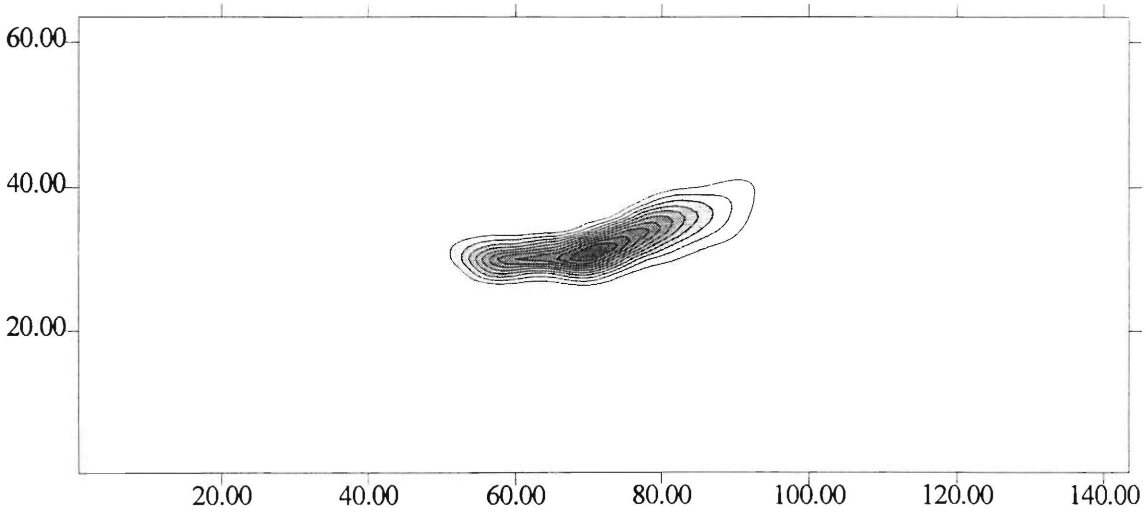


Weakly Heterogeneous Flow Field
Realization 1
Conservatvie Run
1 kg of Bromide

T = 1 Year

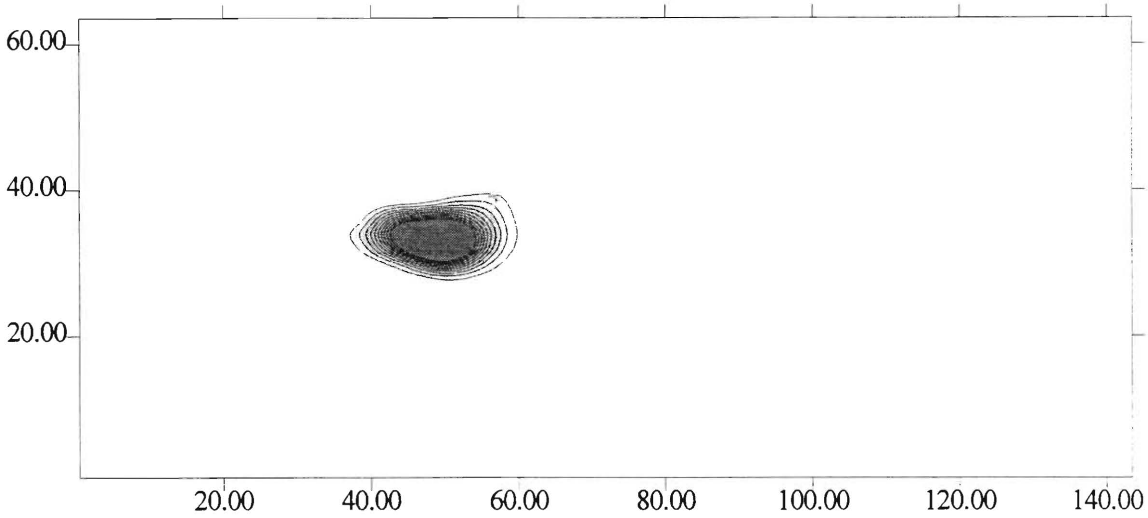


T = 2 Years

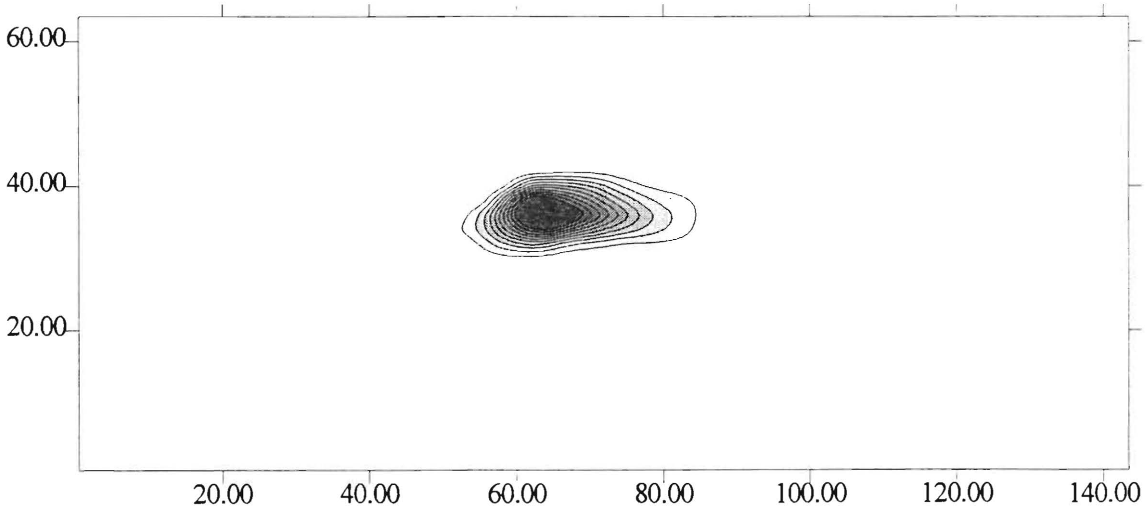


Weakly Heterogeneous Flow Field
Realization 2
Conservative Run
1 kg of Bromide

T = 1 Year

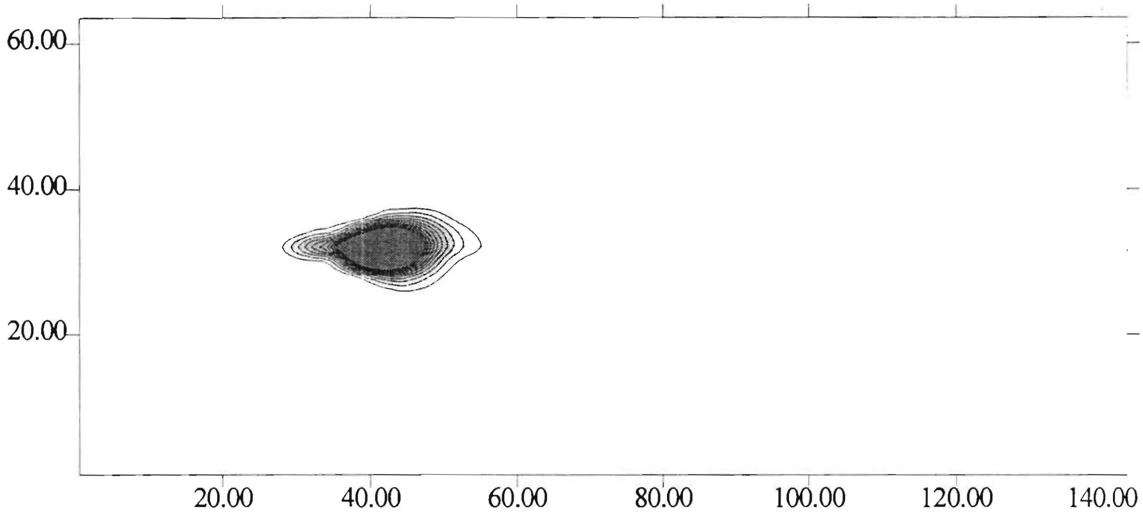


T = 2 Years

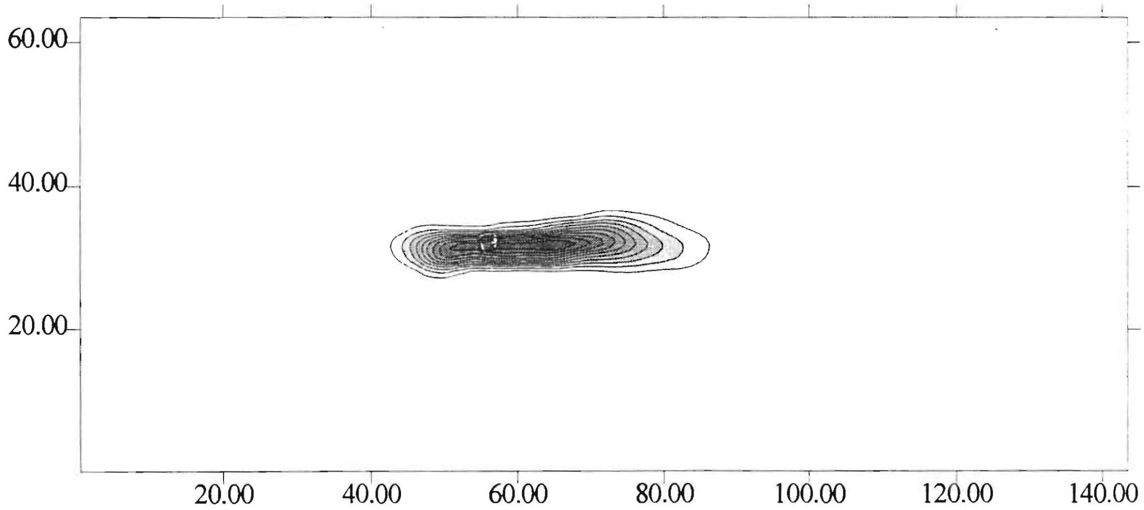


Weakly Heterogeneous Flow Field
Realization 3
Conservative Run
1 kg of Bromide

T = 1 Year

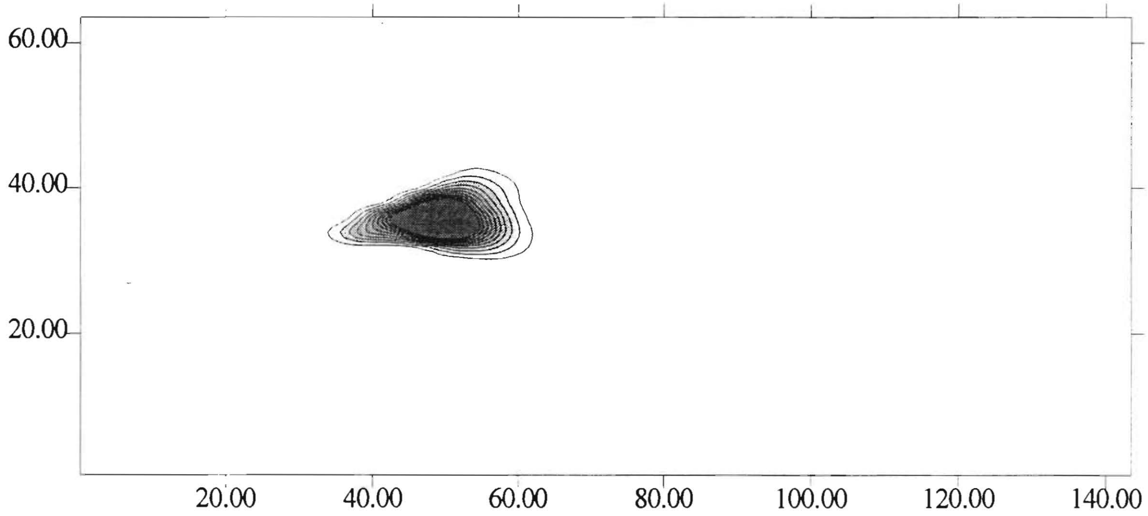


T = 2 Years

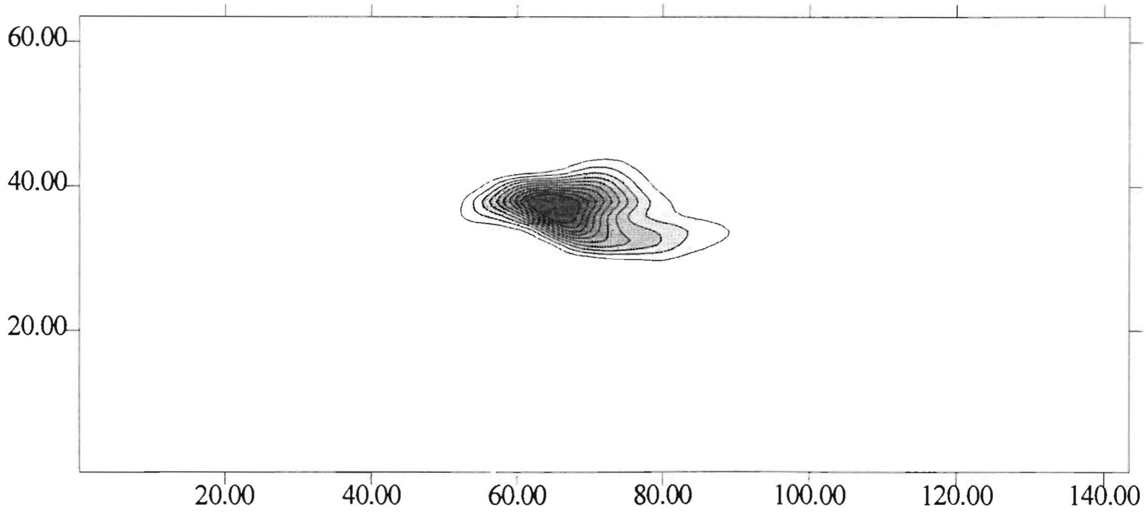


Weakly Heterogeneous Flow Field
Realization 4
Conservative Run
1 kg of Bromide

T = 1 Year

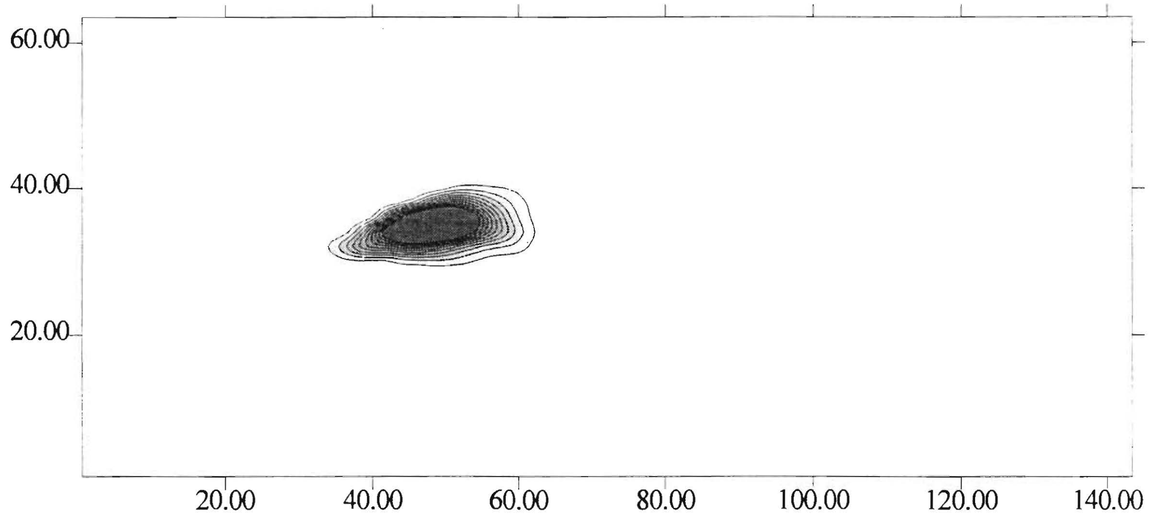


T = 2 Years

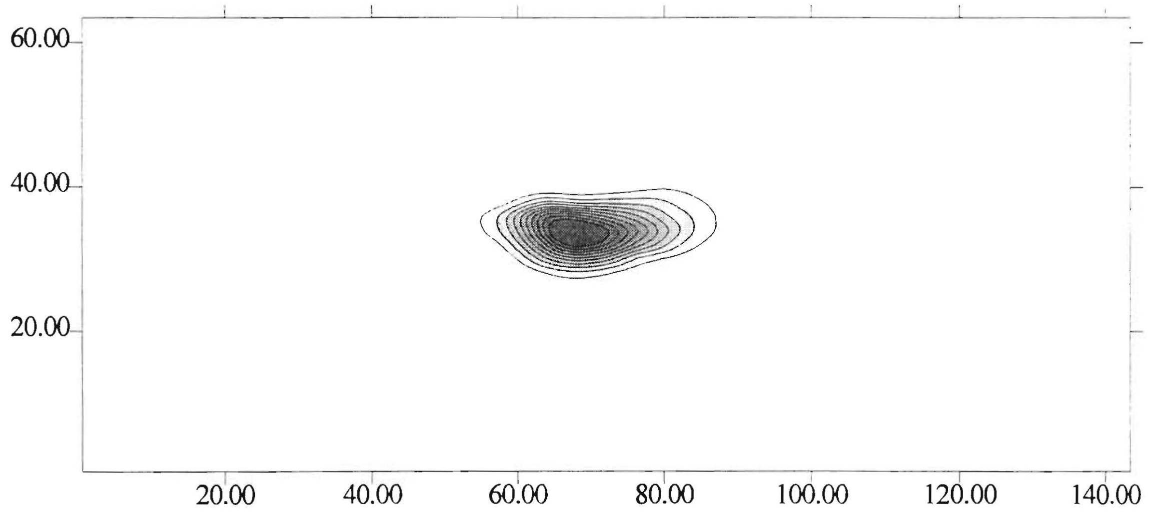


Weakly Heterogeneous Flow Field
Realization 5
Conservative Run
1 kg of Bromide

T = 1 Year

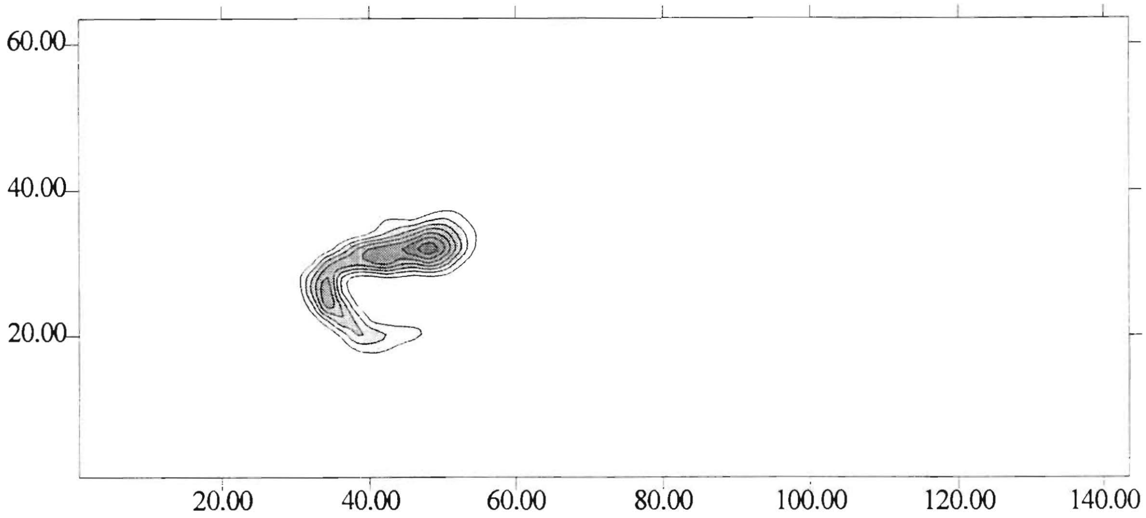


T = 2 Years

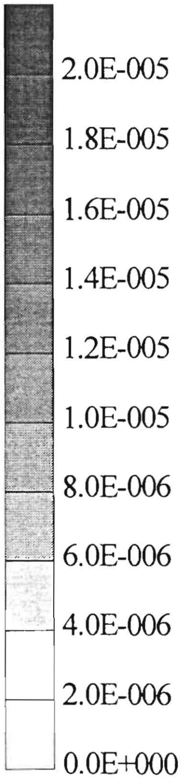


Strongly Heterogeneous Flow Field
Realization 1
Reactive Run
1 kg of Bromide

T = 2 Years

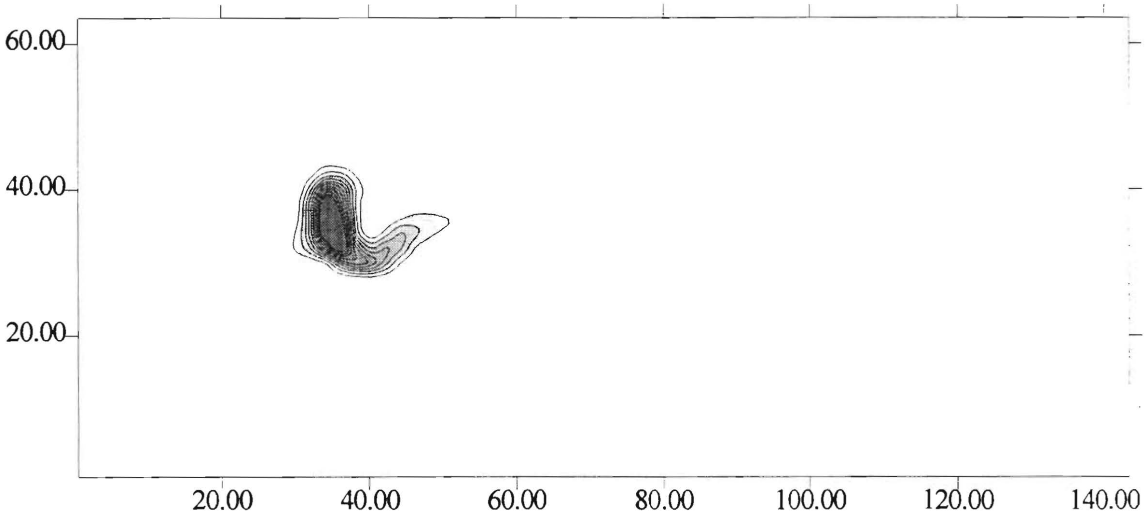


Bromide concentration scale
for realizations in a strongly
heterogeneous flow field with
1 kg of bromide.



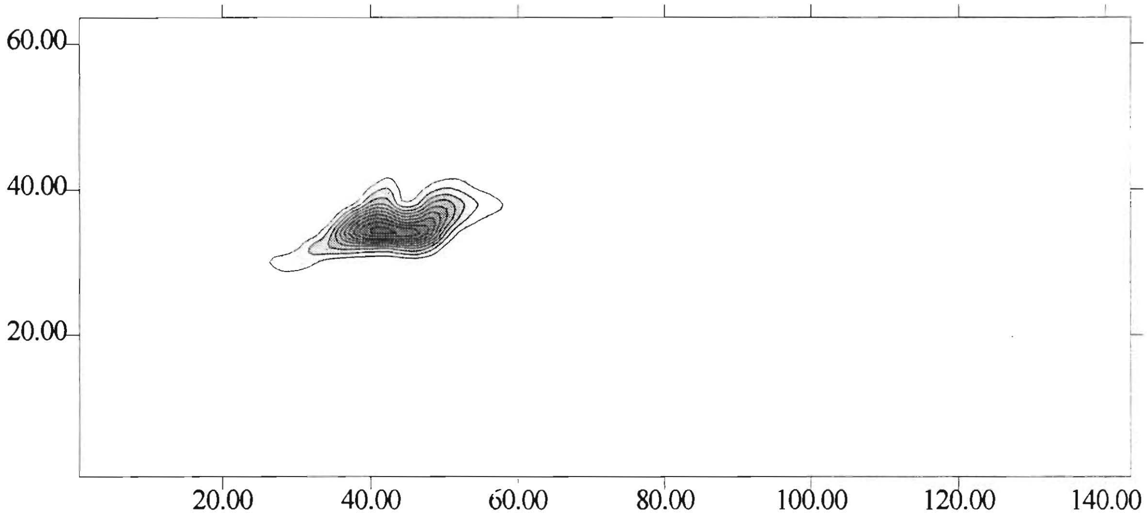
Strongly Heterogeneous Flow Field
Realization 2
Reactive Run
1 kg of Bromide

T = 2 Years



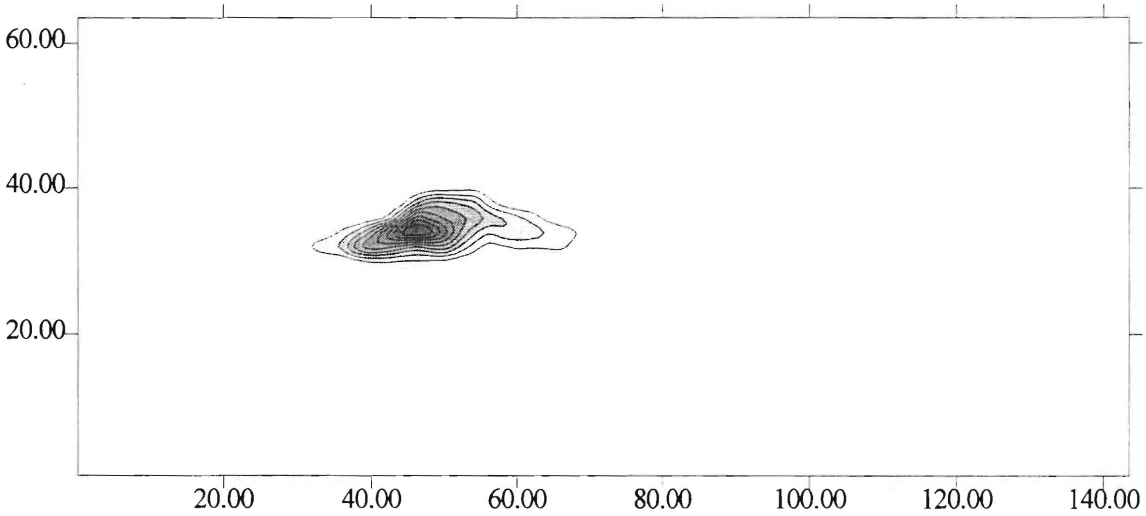
Strongly Heterogeneous Flow Field
Realization 3
Reactive Run
1 kg of Bromide

T = 2 Years

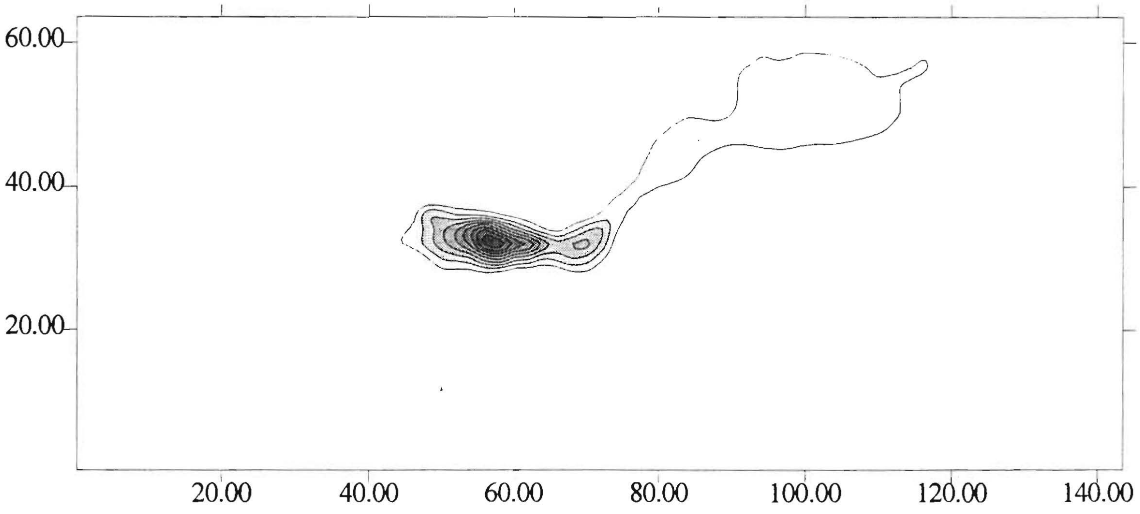


Strongly Heterogeneous Flow Field
Realization 4
Reactive Run
1 kg of Bromide

T = 2 Years



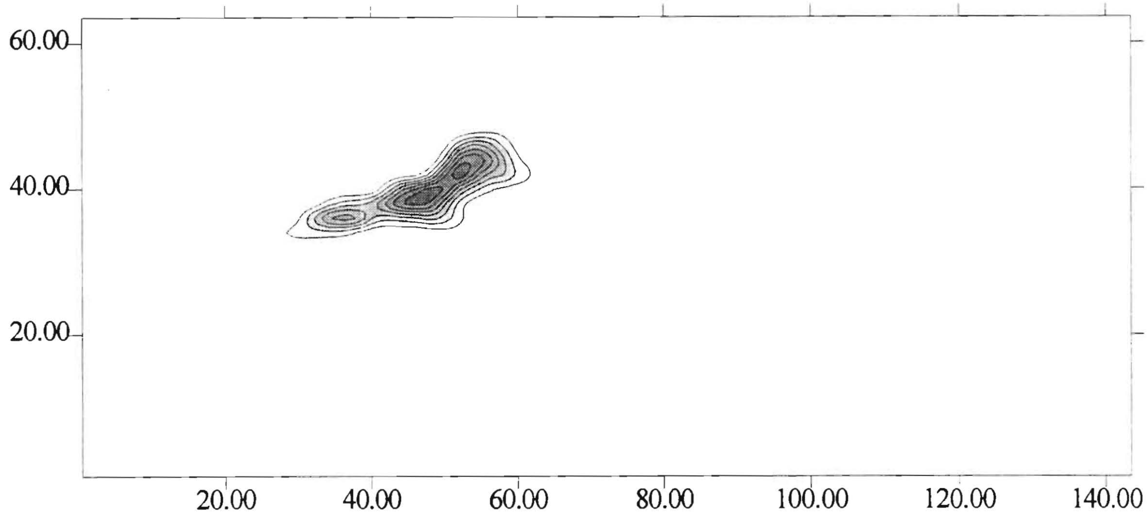
T = 4 Years *



* Concentration interval for this plot is 1.0E-006
due to low bromide concentrations

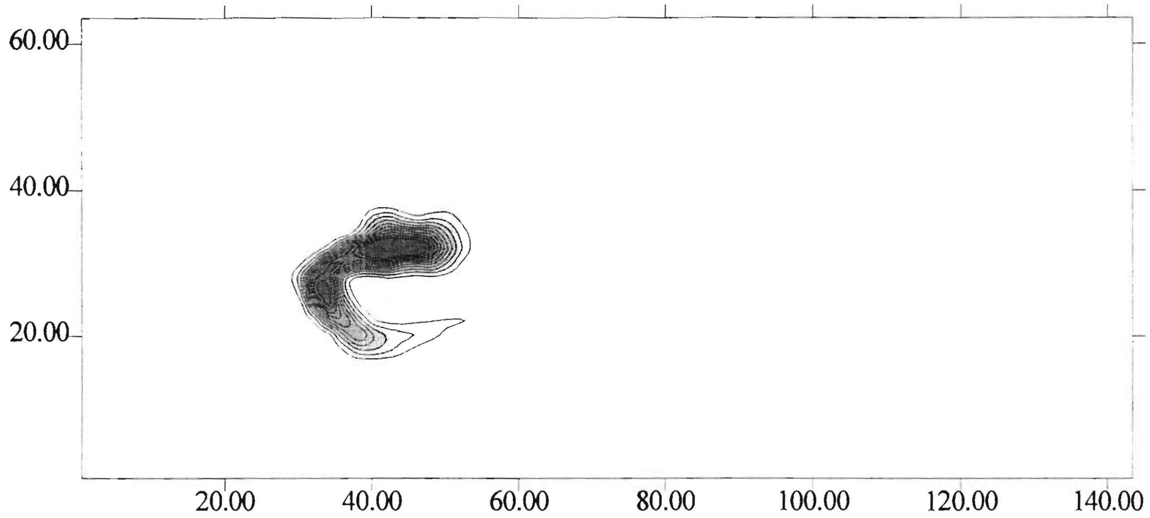
Strongly Heterogeneous Flow Field
Realization 5
Reactive Run
1 kg of Bromide

T = 1 Year

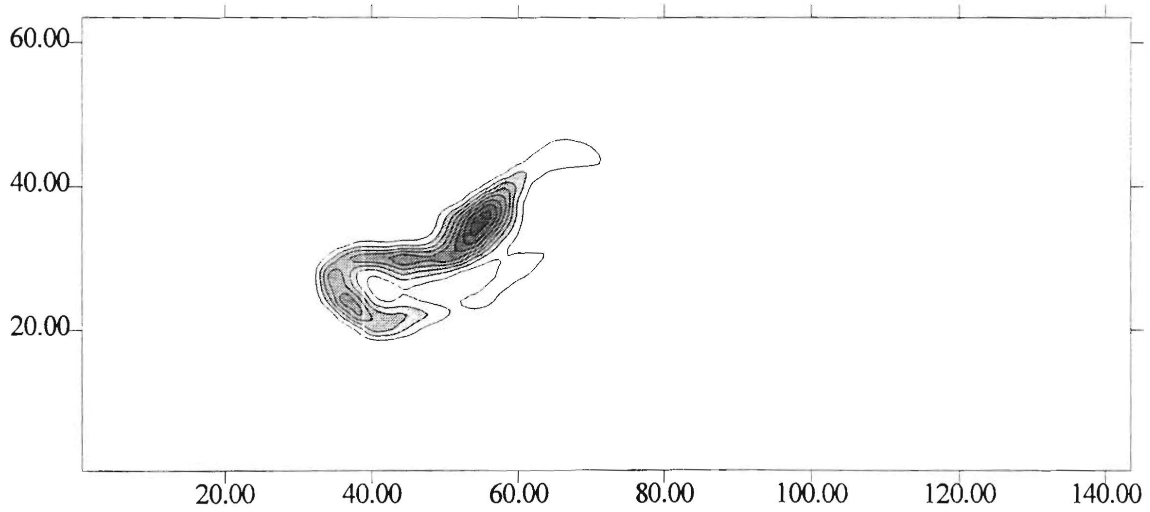


Strongly Heterogeneous Flow Field
Realization 1
Conservative Run
1 kg of Bromide

T = 1 Year

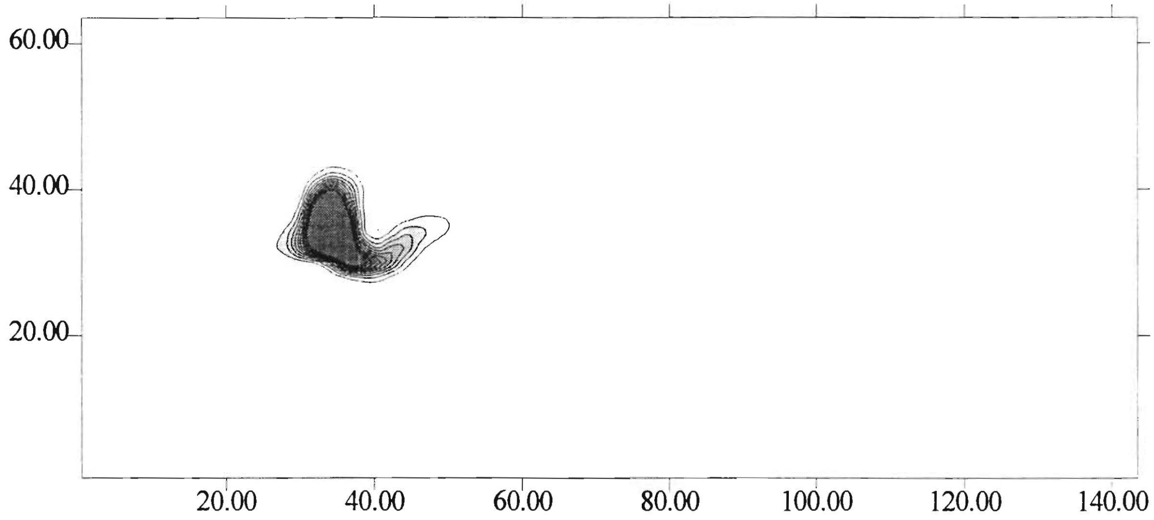


T = 2 Years

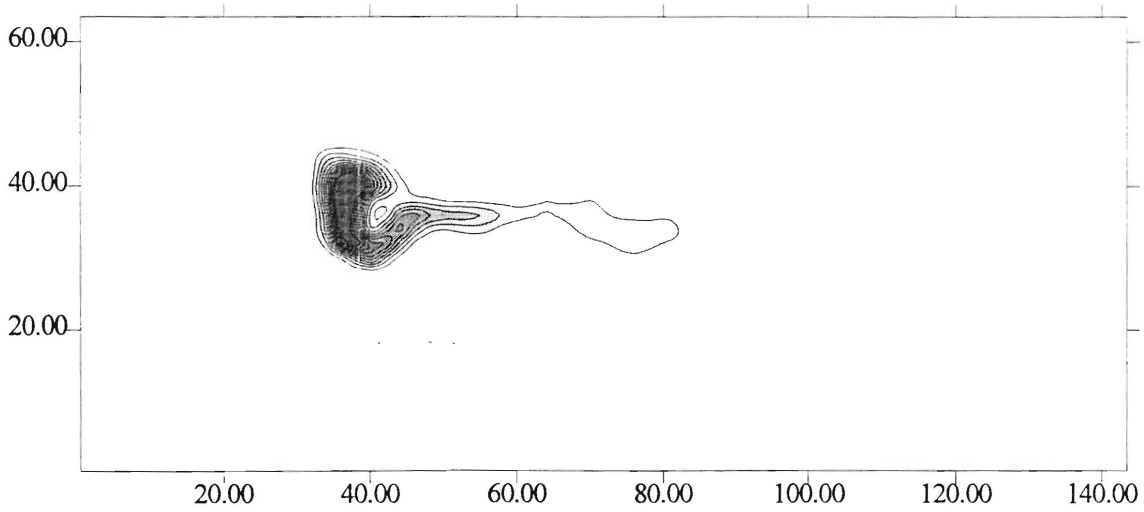


Strongly Heterogeneous Flow Field
Realization 2
Conservative Run
1 kg of Bromide

T = 1 Year

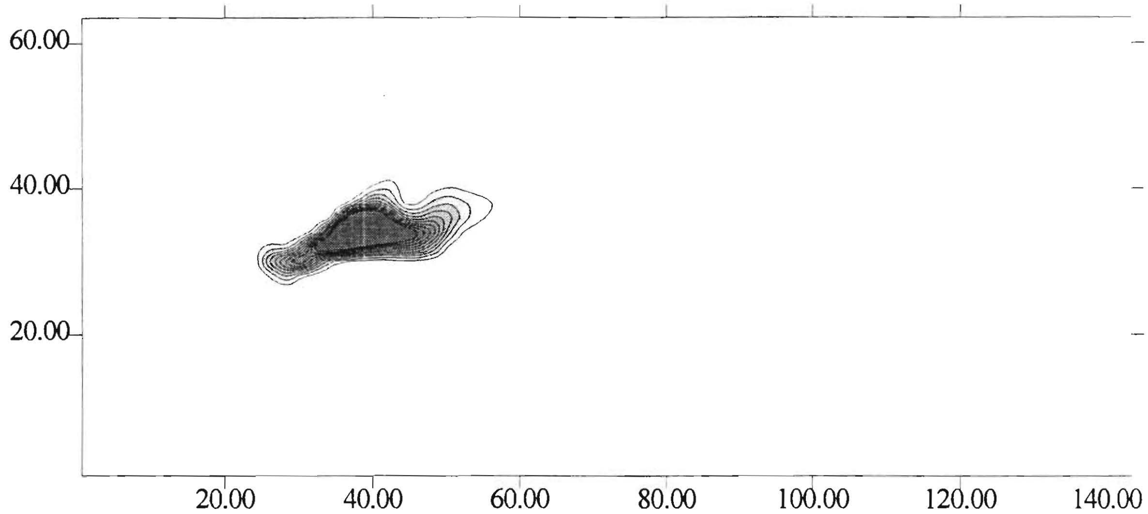


Time = 2 Years

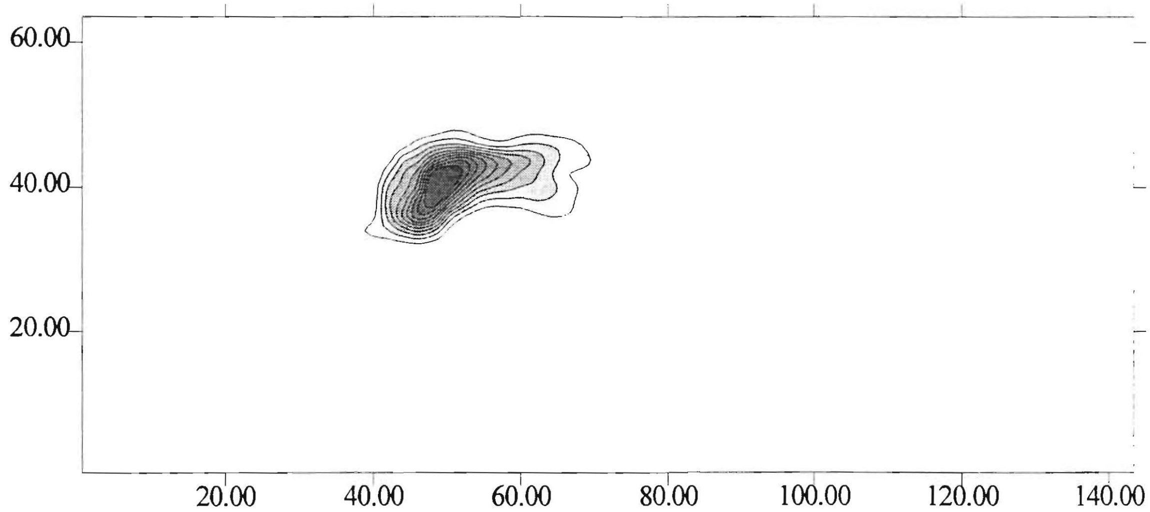


Strongly Heterogeneous Flow Field
Realization 3
Conservative Run
1 kg of Bromide

T = 1 Year

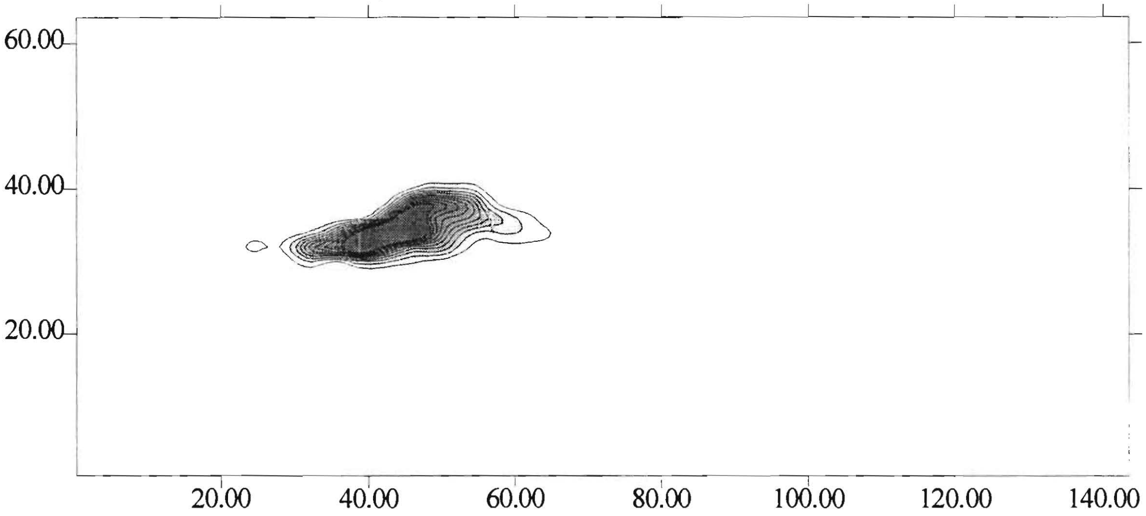


T = 2 Years

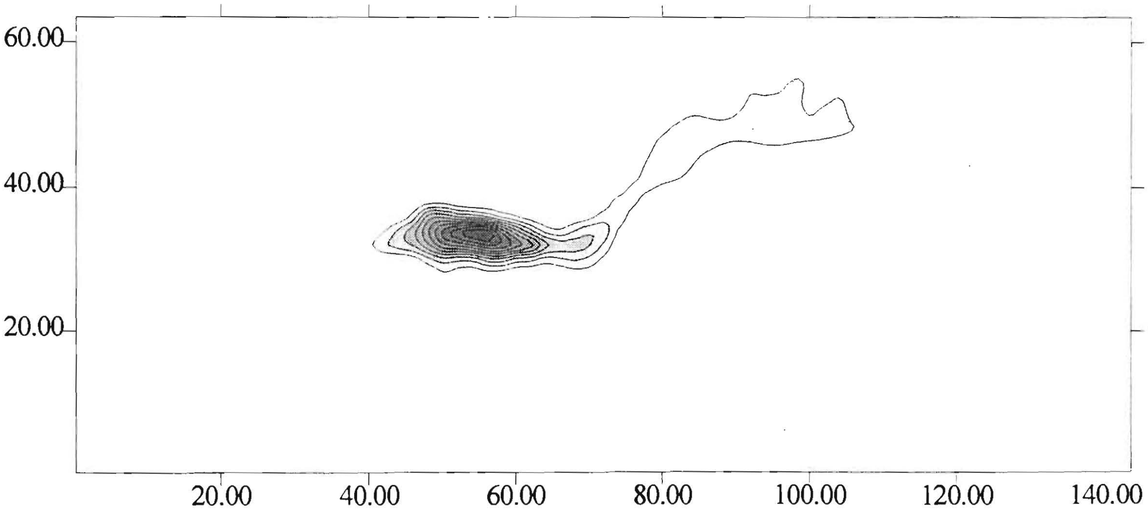


Strongly Heterogeneous Flow Field
Realization 4
Conservative Run
1 kg of Bromide

T = 1 Year

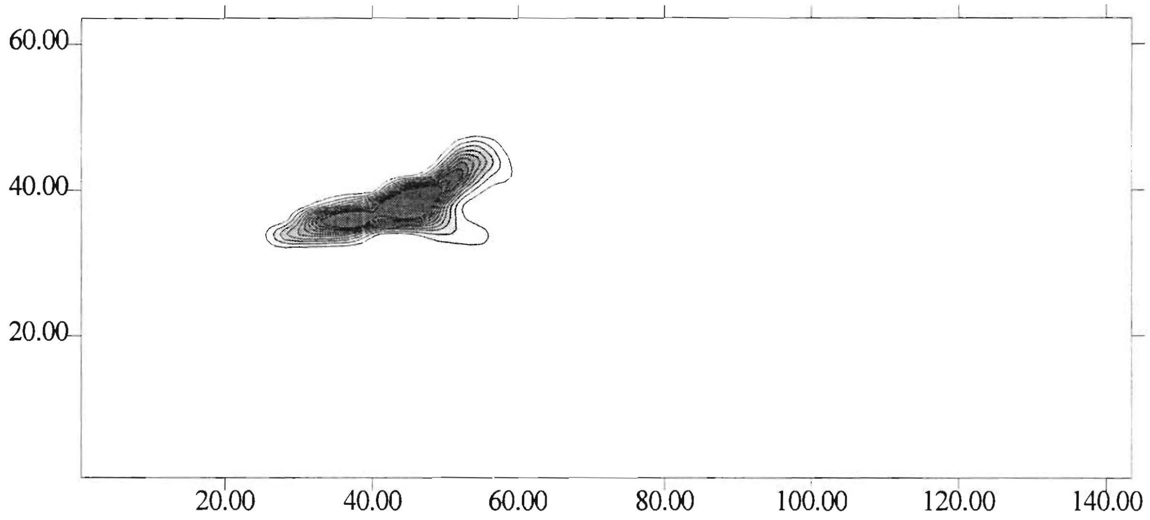


T = 2 Years

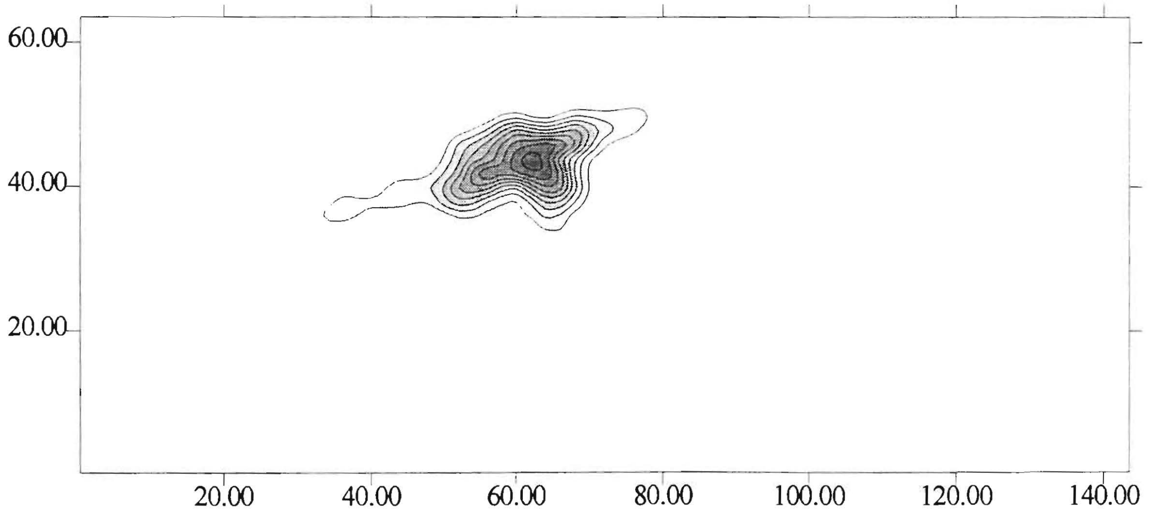


Strongly Heterogeneous Flow Field
Realization 5
Conservative Run
1 kg of Bromide

T = 1 Year

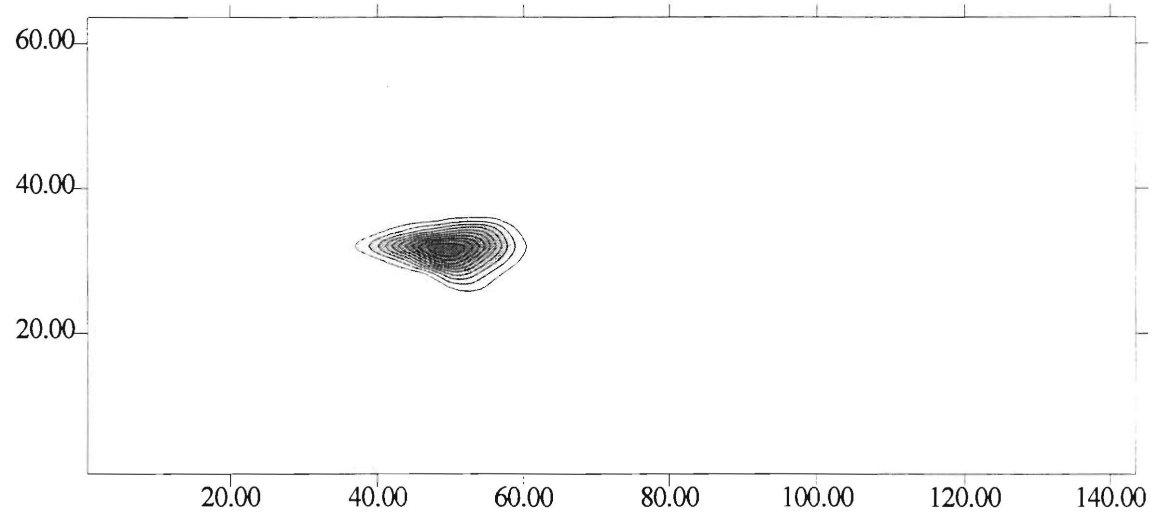


T = 2 Years

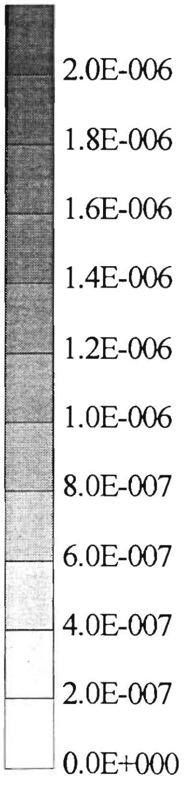


Weakly Heterogeneous Flow Field
Realization 1
Reactive Run
0.1 kg of Bromide

T = 2 Years

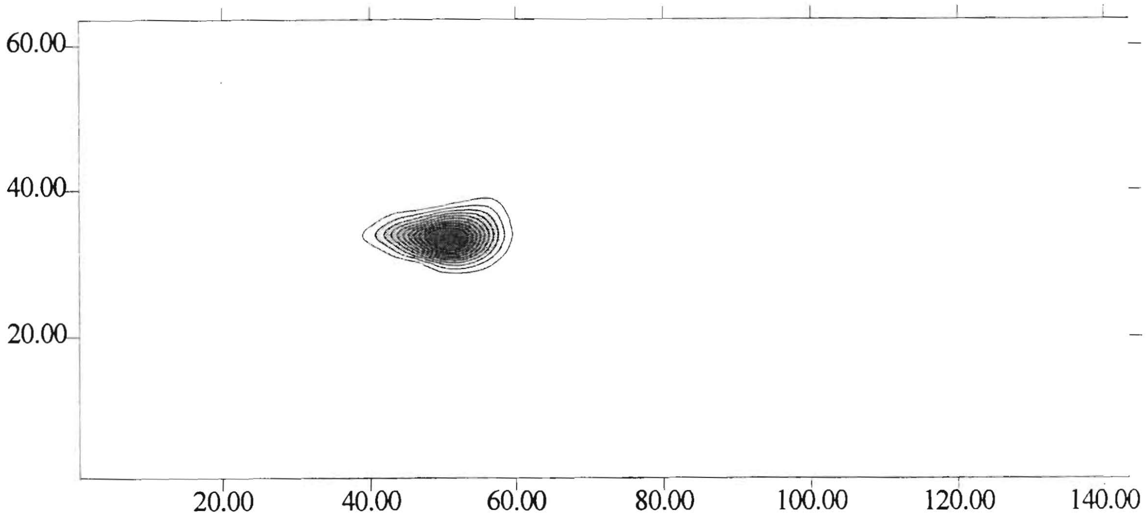


Bromide concentration scale for realizations in a weakly heterogeneous flow field with 0.1 kg of bromide.



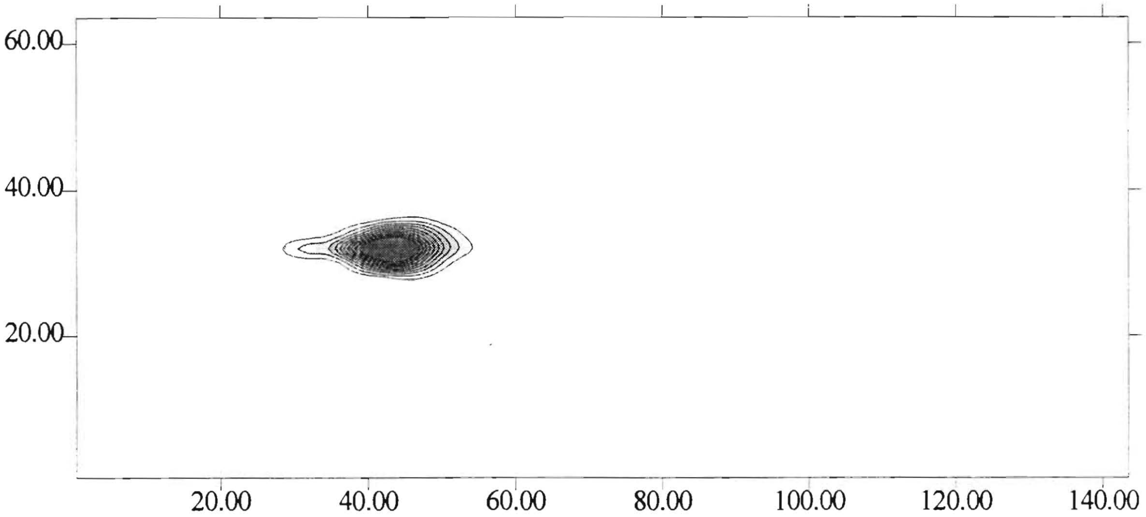
Weakly Heterogeneous Flow Field
Realization 2
Reactive Run
0.1 kg of Bromide

T = 2 Years



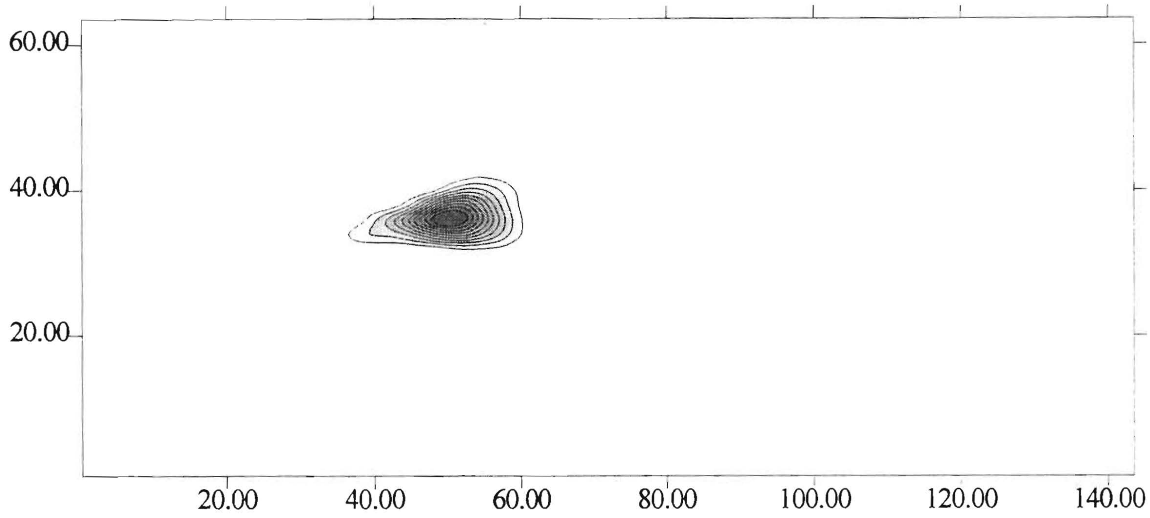
Weakly Heterogeneous Flow Field
Realization 3
Reactive Run
0.1 kg of Bromide

T = 2 Years



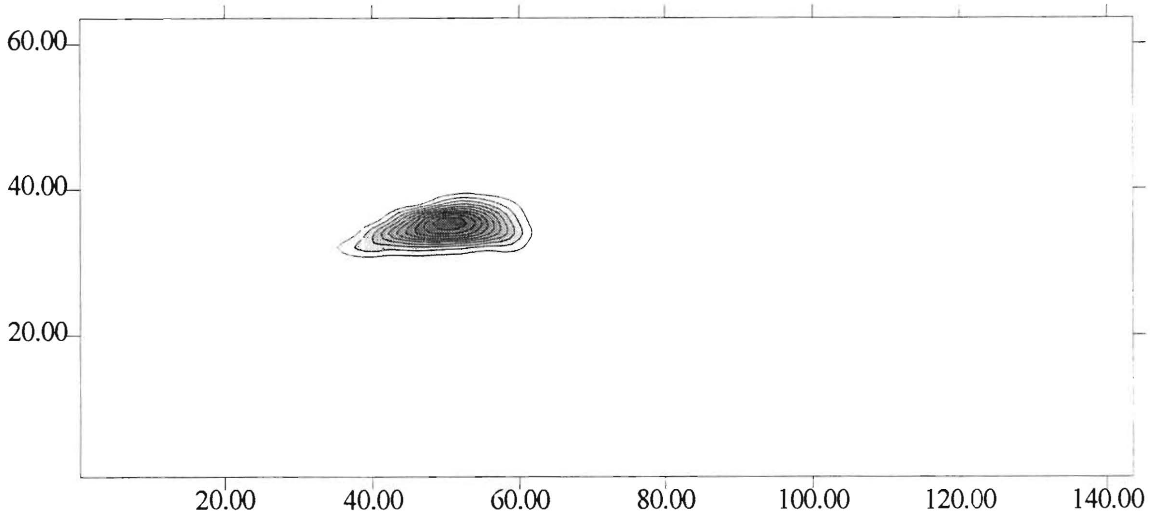
Weakly Heterogeneous Flow Field
Realization 4
Reactive Run
0.1 kg of Bromide

T = 2 Years



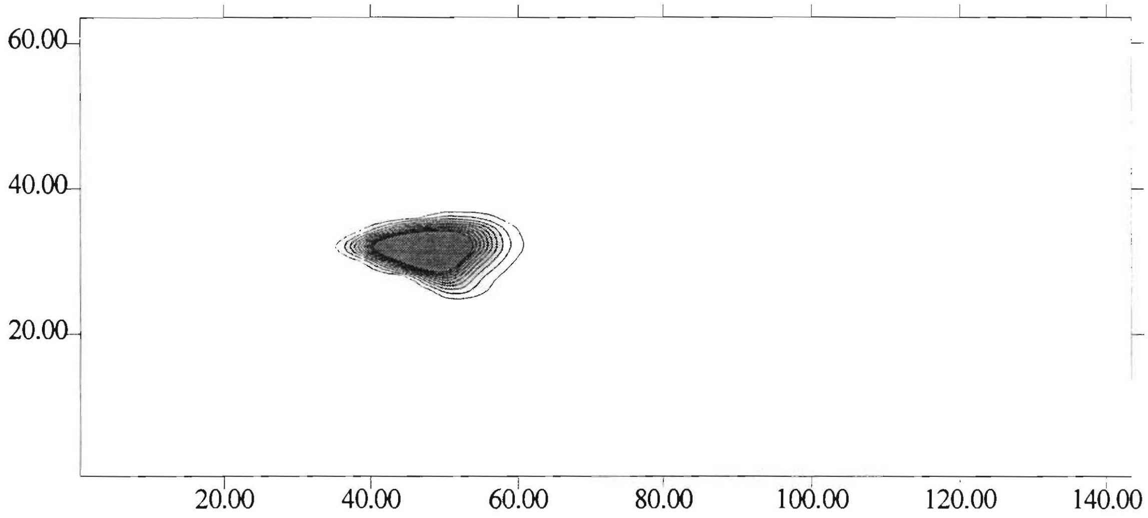
Weakly Heterogeneous Flow Field
Realization 5
Reactive Run
0.1 kg of Bromide

T = 2 Years

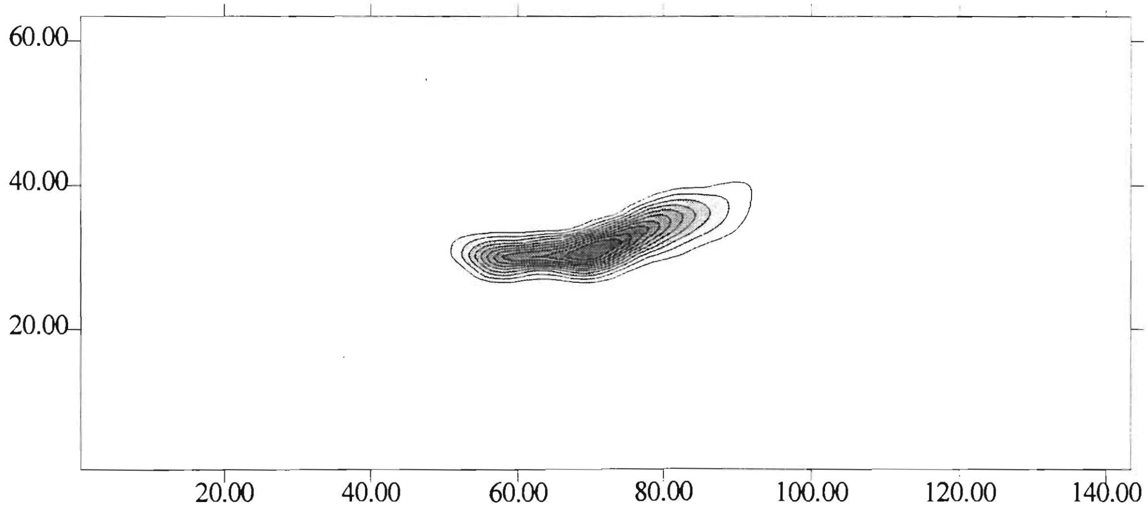


Weakly Heterogeneous Flow Field
Realization 1
Conservative Run
0.1 kg of Bromide

T = 1 Year

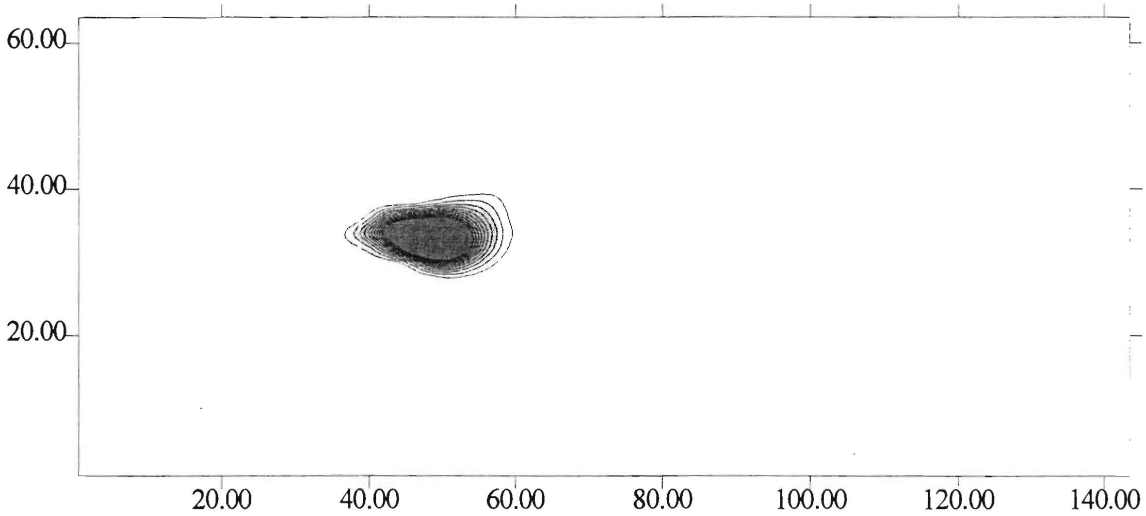


T = 2 Years

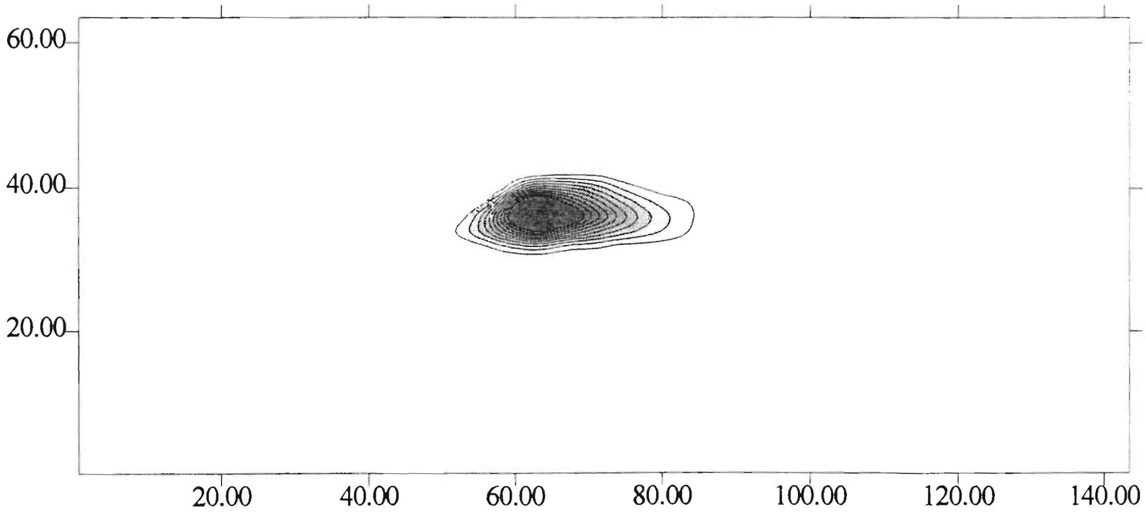


## Weakly Heterogeneous Flow Field
Realization 2
Conservative Run
0.1 kg of Bromide

T = 1 Years

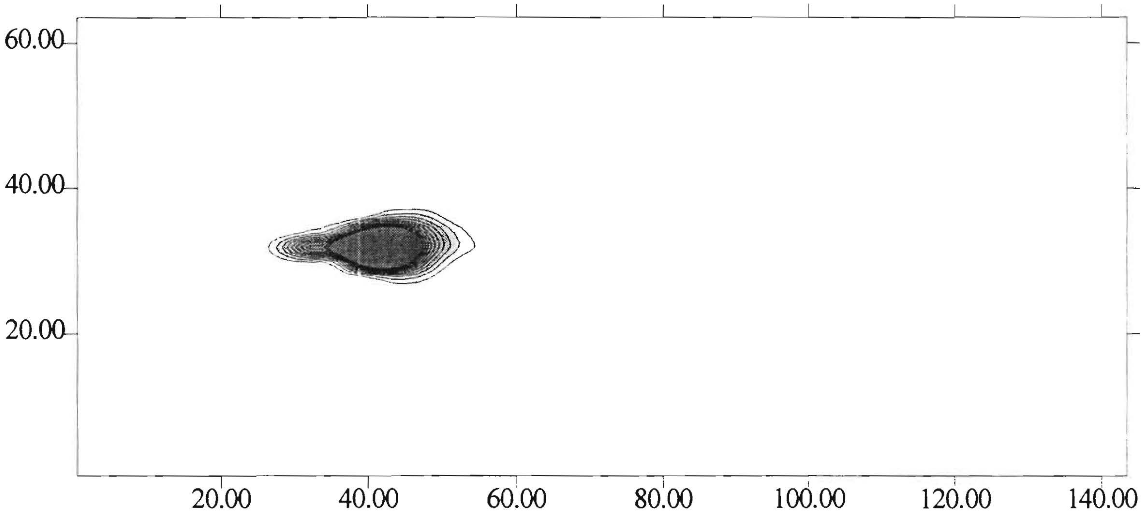


T = 2 Years

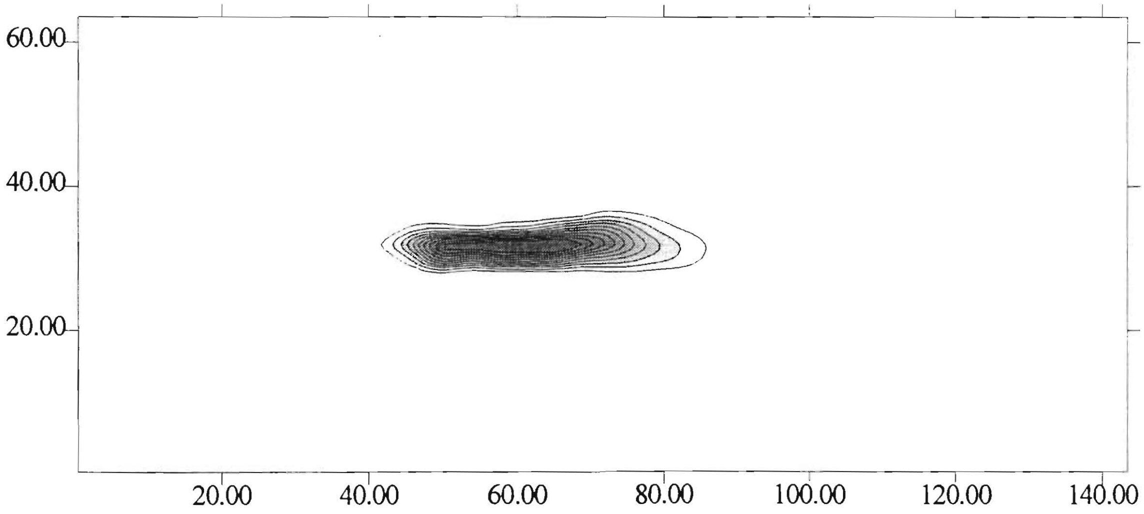


Weakly Heterogeneous Flow Field
Realization 3
Conservative Run
0.1 kg of Bromide

T = 1 Year

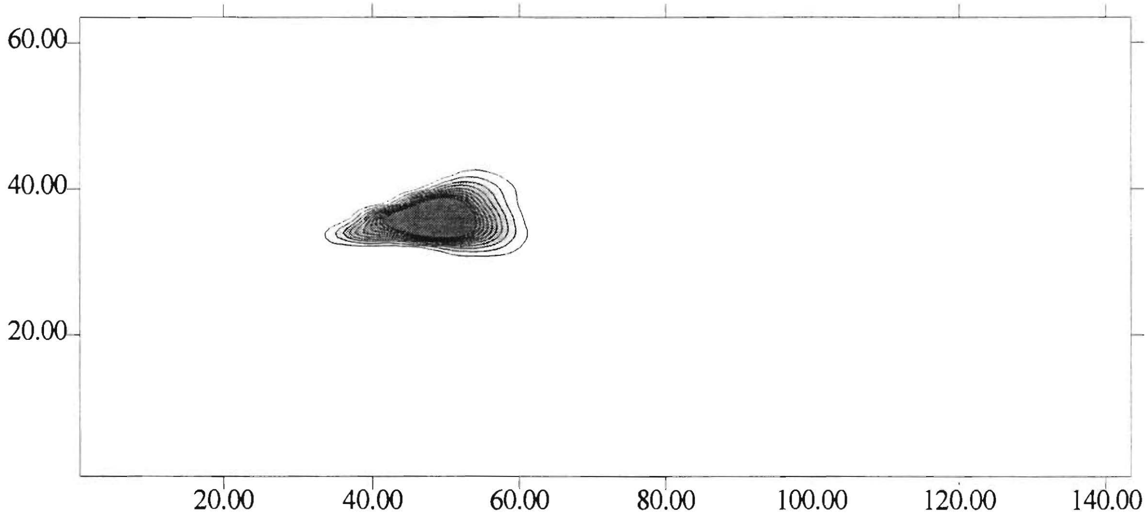


T = 2 Years

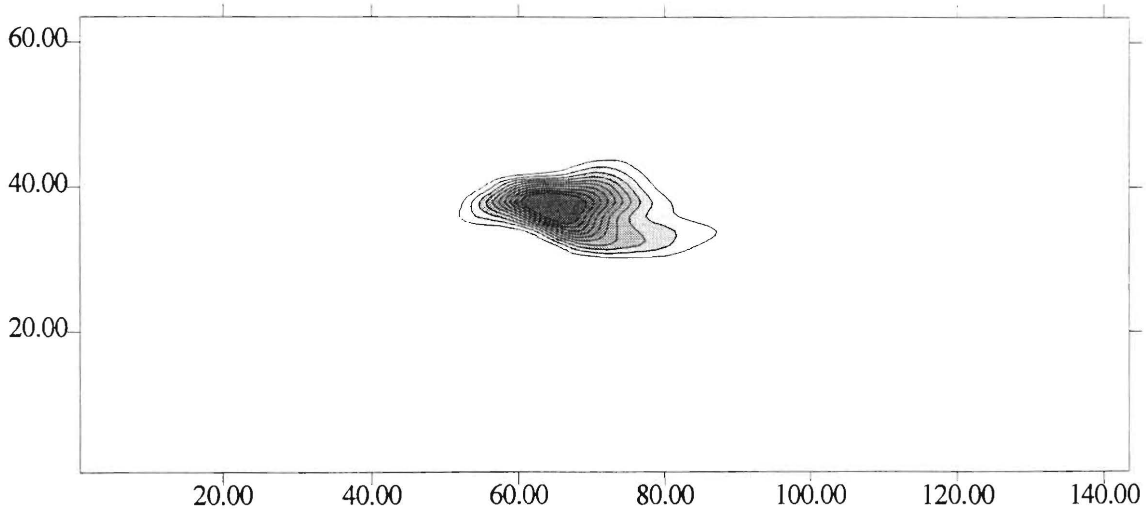


Weakly Heterogeneous Flow Field
Realization 4
Conservative Run
0.1 kg of Bromide

T = 1 Year

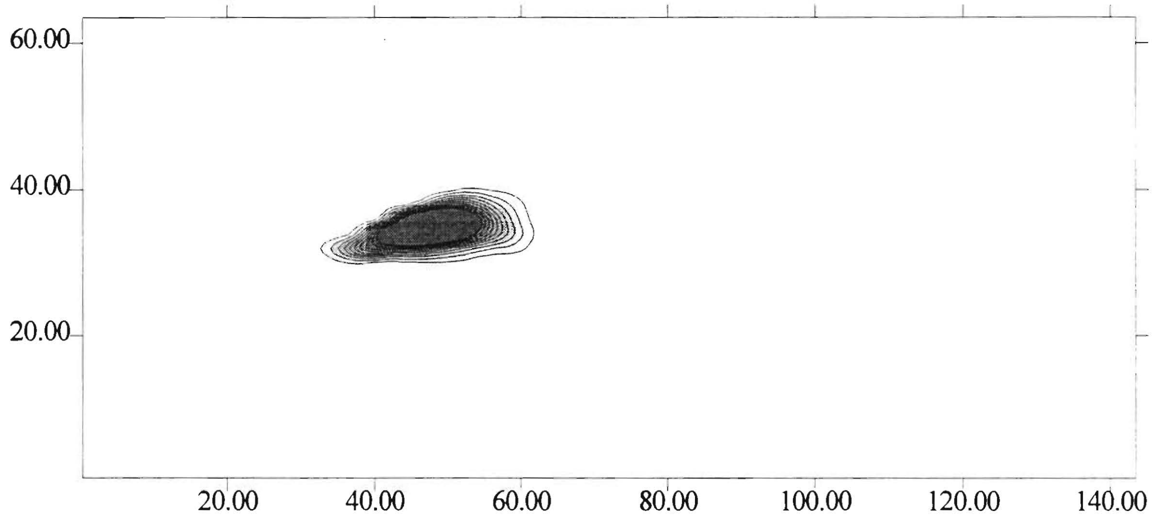


T = 2 Years

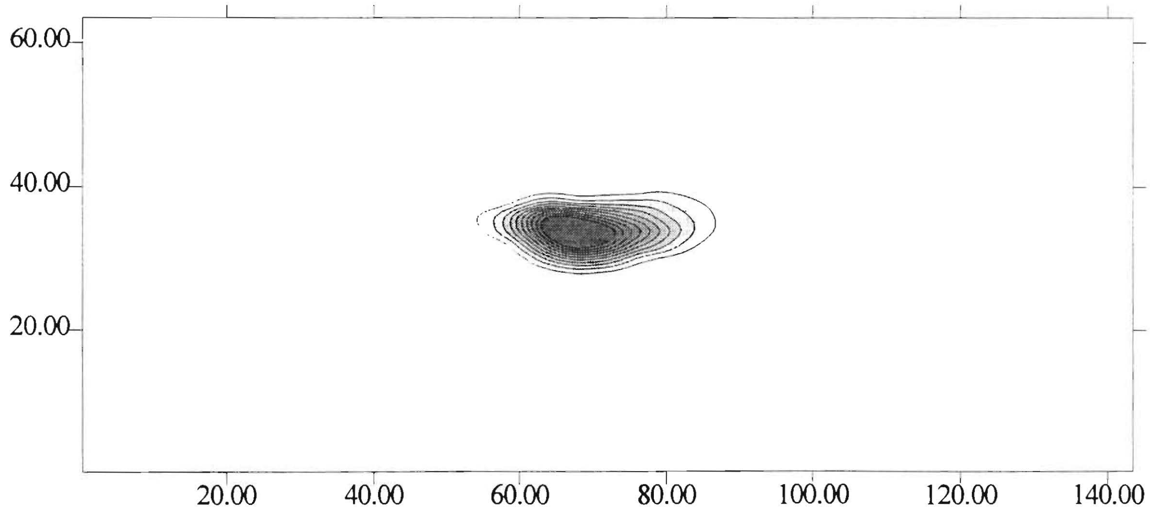


Weakly Heterogeneous Flow Field
Realization 5
Conservative Run
0.1 kg of Bromide

T = 1 Year

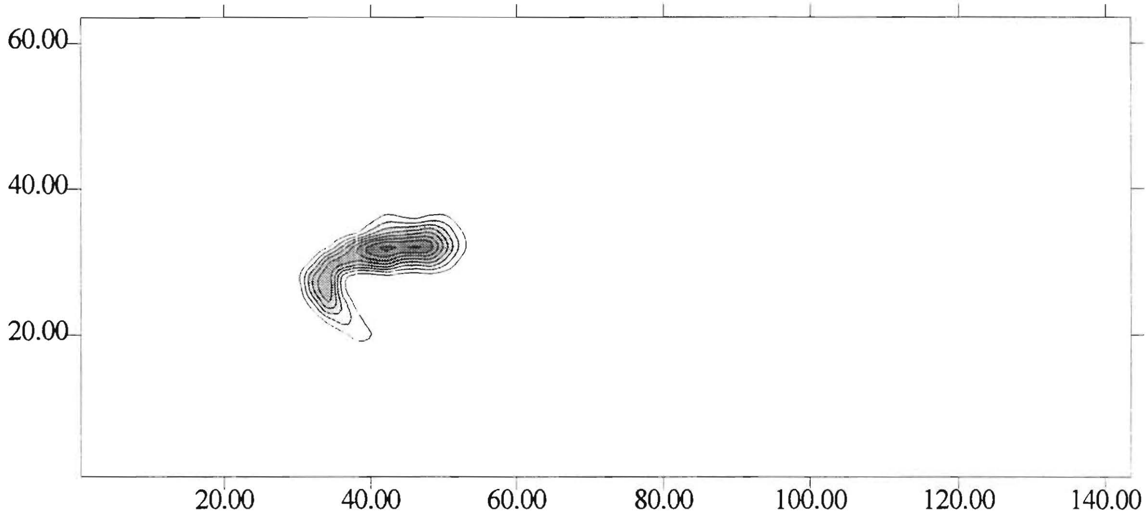


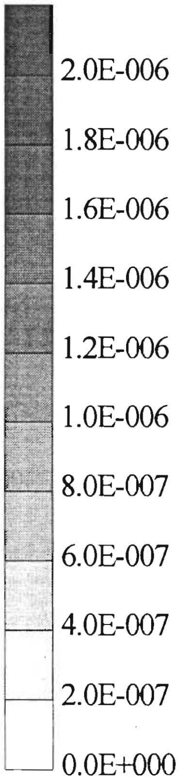
T = 2 Years



Strongly Heterogeneous Flow Field
Realization 1
Reactive Run
0.1 kg of Bromide

T = 2 Years

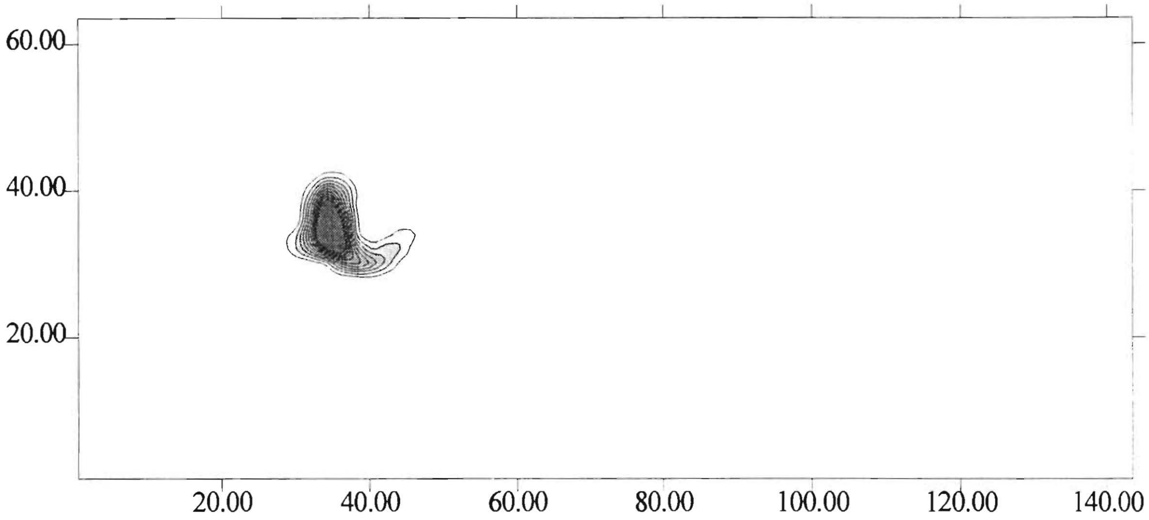




Bromide concentration scale for realizations in a strongly heterogeneous flow field with 0.1 kg of bromide.

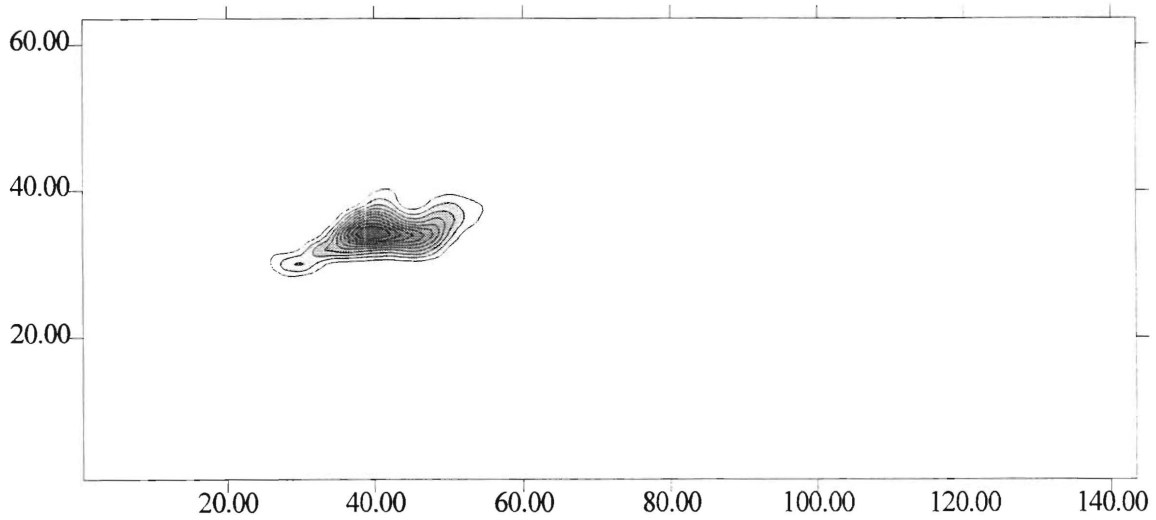
Strongly Heterogeneous Flow Field
Realization 2
Reactive Run
0.1 kg of Bromide

T = 2 Years



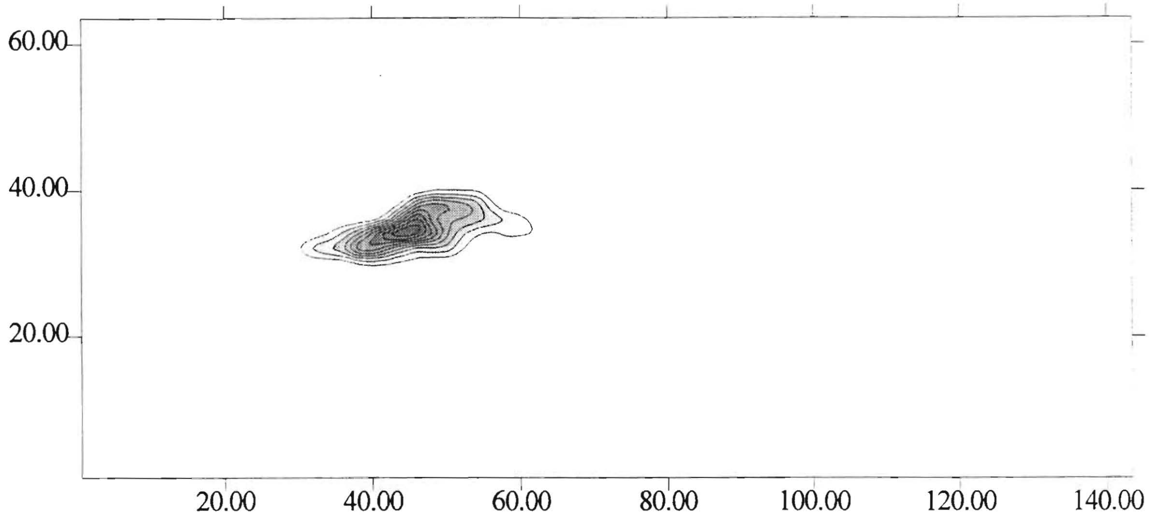
Strongly Heterogeneous Flow Field
Realization 3
Reactive Run
0.1 kg of Bromide

T = 2 Years



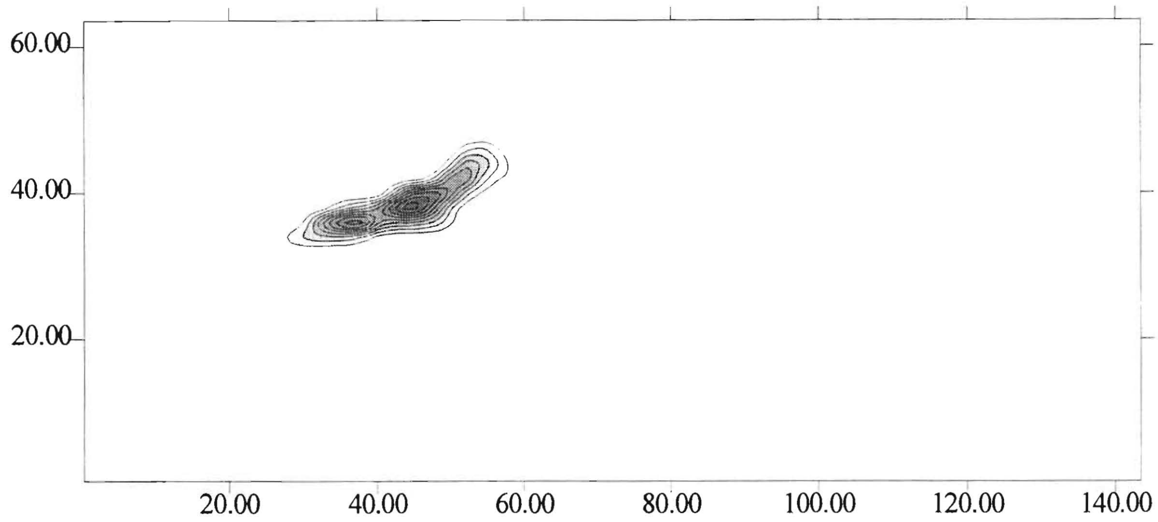
Strongly Heterogeneous Flow Field
Realization 4
Reactive Run
0.1 kg of Bromide

T = 2 Years



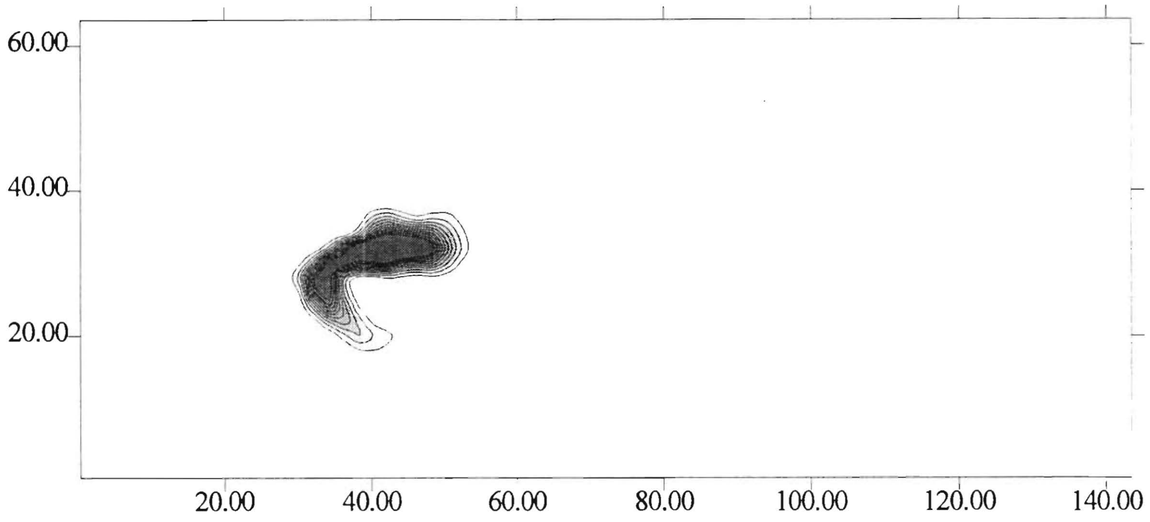
Strongly Heterogeneous Flow Field
Realization 5
Reactive Run
0.1 kg of Bromide

T = 2 Years

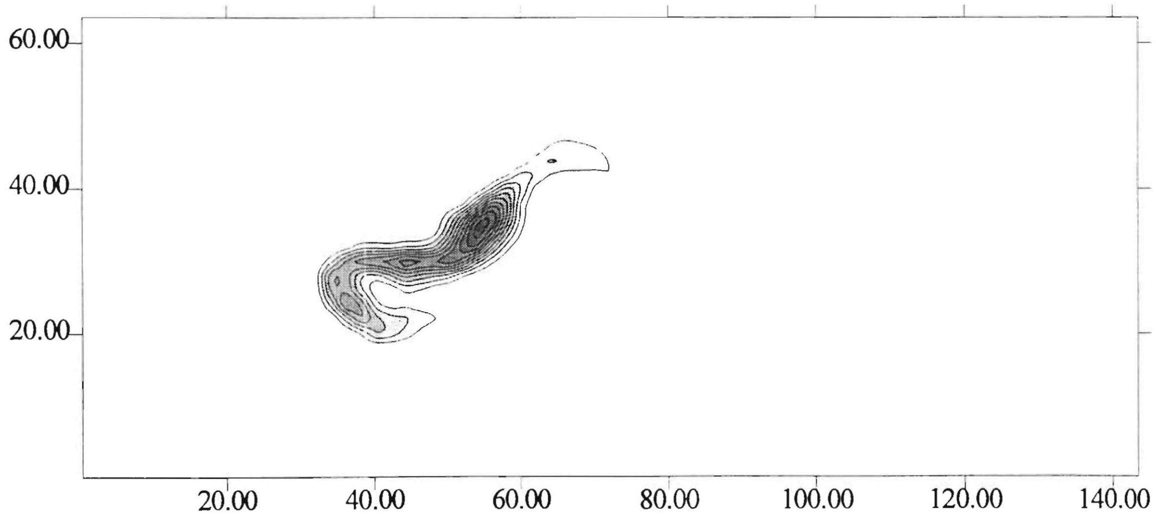


Strongly Heterogeneous Flow Field
Realization 1
Conservative Run
0.1 kg of Bromide

T = 1 Year

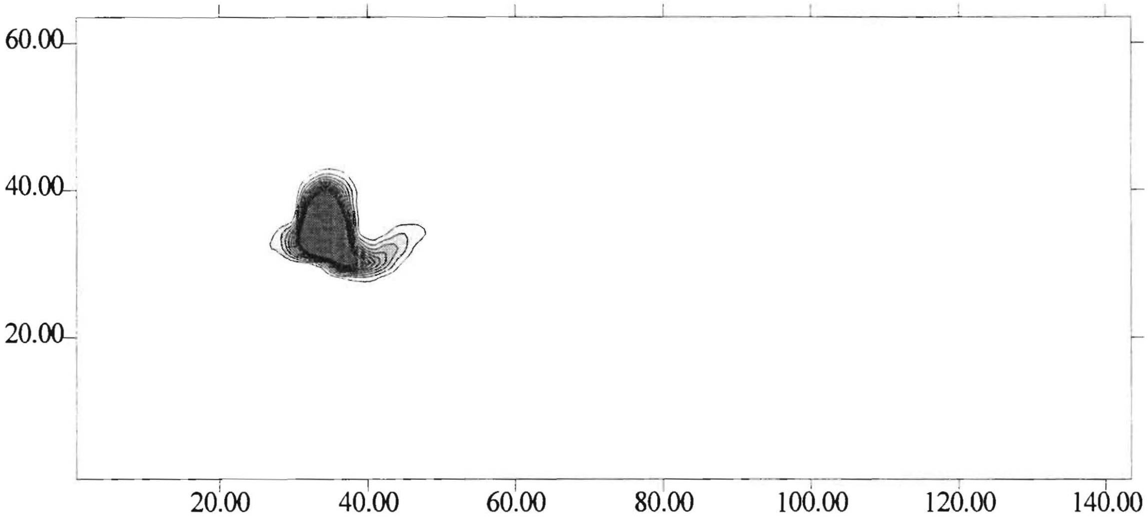


T = 2 Years

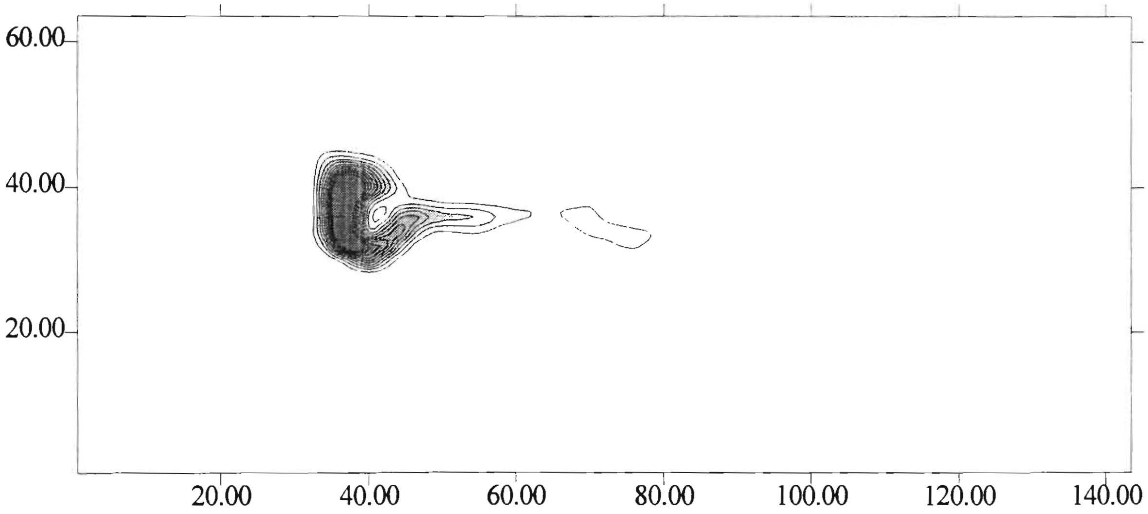


Strongly Heterogeneous Flow Field
Realization 2
Conservative Run
0.1 kg of Bromide

T = 1 Year

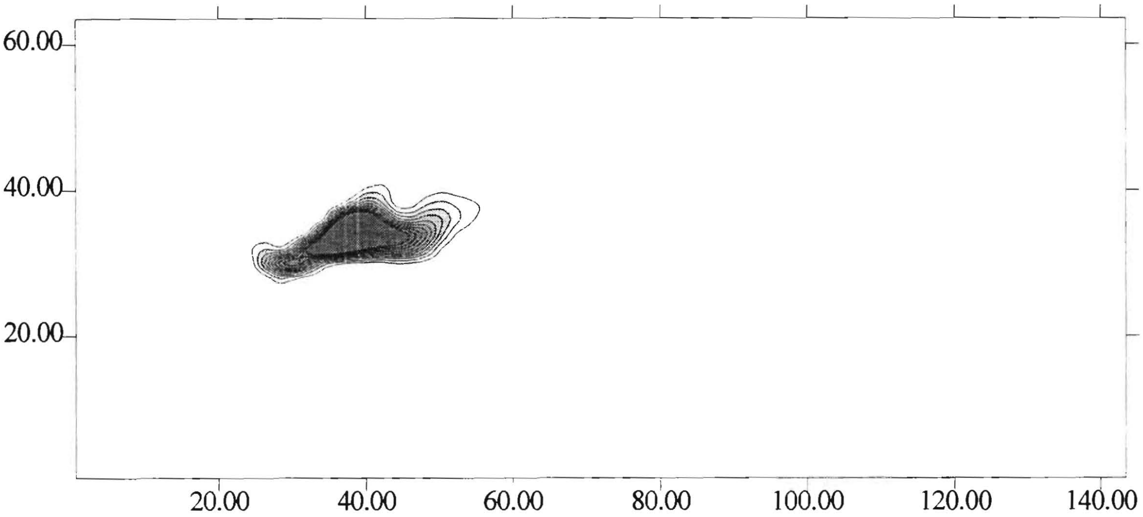


T = 2 Years

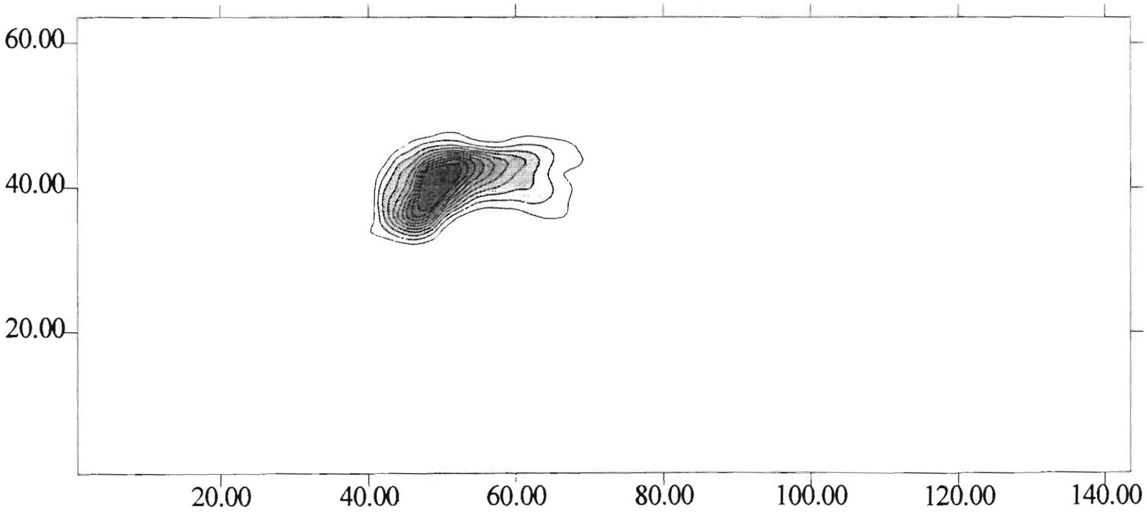


# Strongly Heterogeneous Flow Field
Realization 3
Conservative Run
0.1 kg of Bromide

T = 1 Year

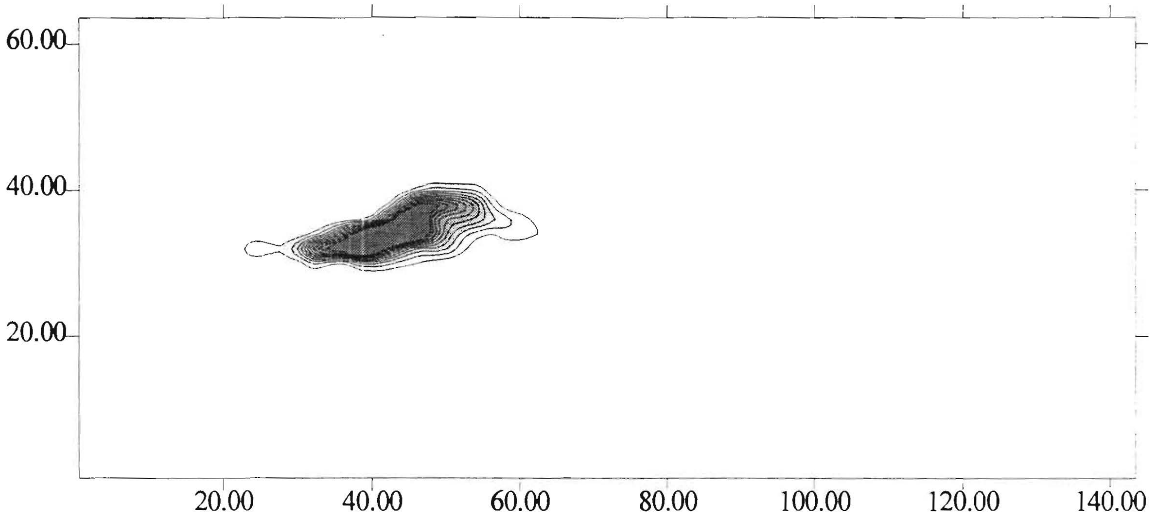


T = 2 Years

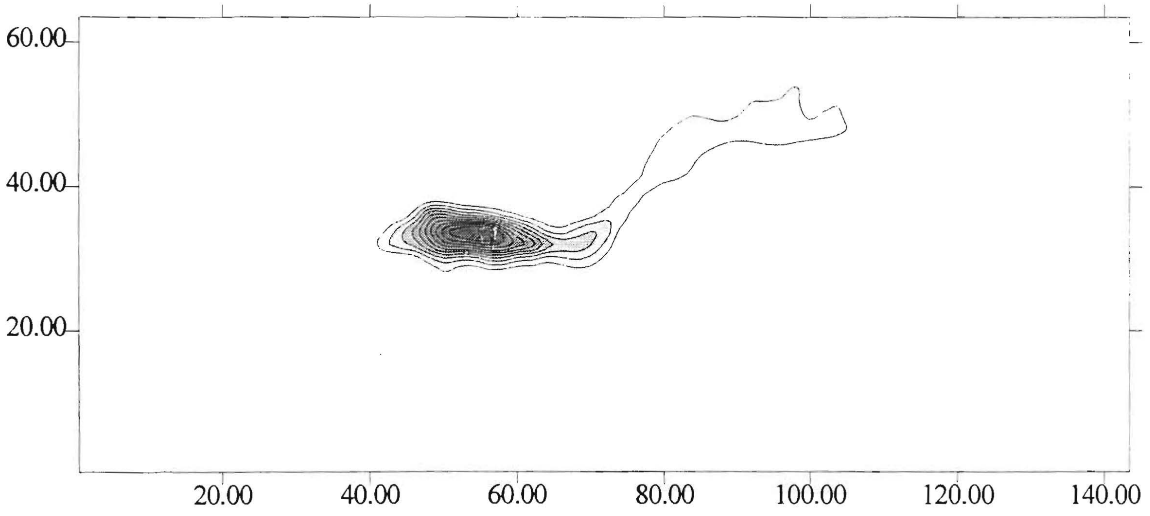


Strongly Heterogeneous Flow Field
Realization 4
Conservative Run
0.1 kg of Bromide

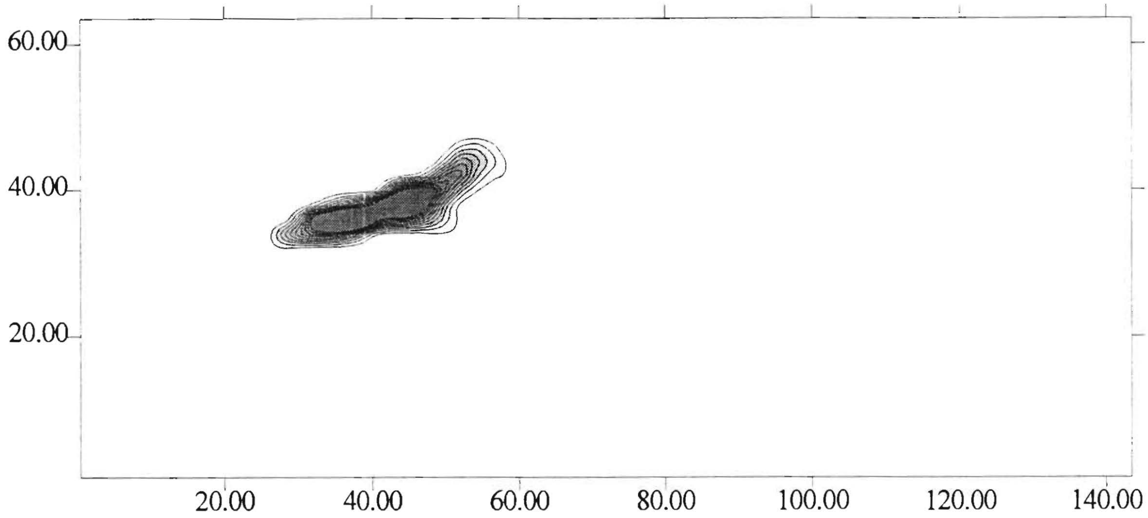
T = 1 Year

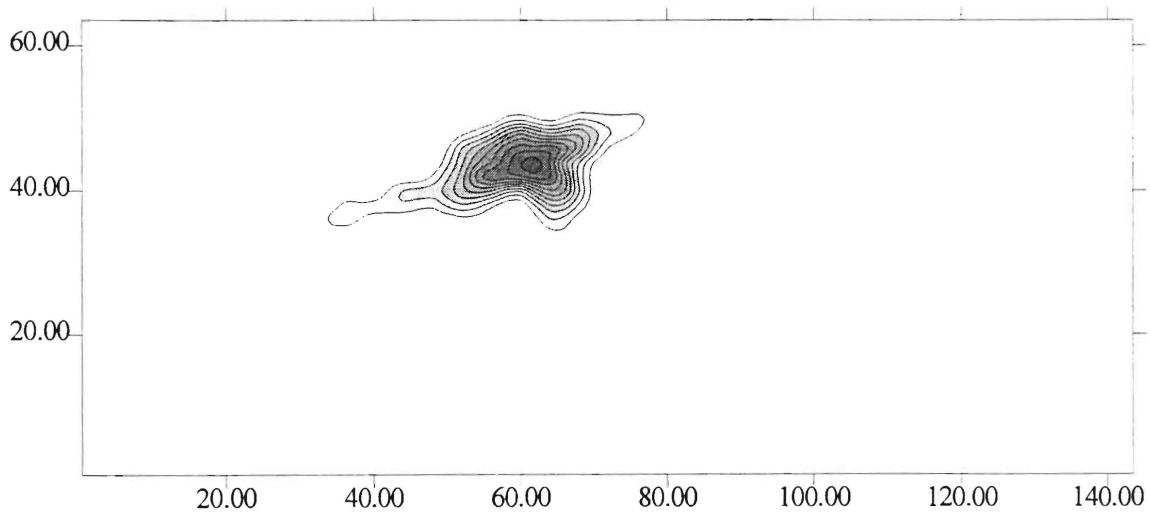


T = 2 Years



## Strongly Heterogeneous Flow Field
Realization 5
Conservative Run
0.1 kg of Bromide


T = 1 Year

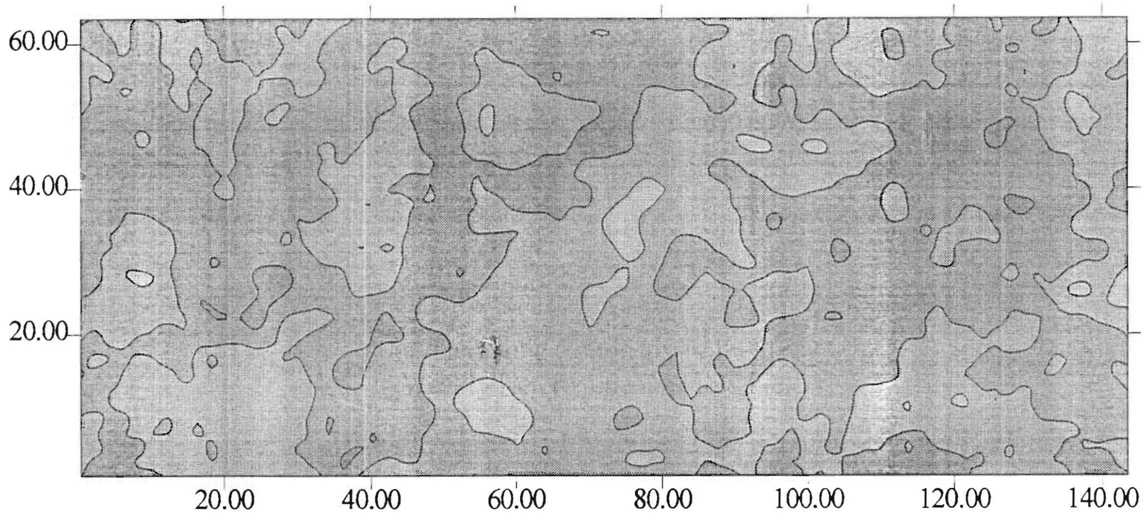

T = 2 Years

# APPENDIX C

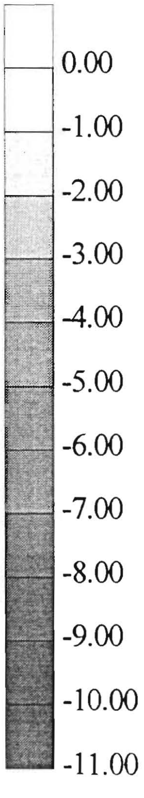
# HYDRAULIC CONDUCTIVITY FIELDS

## Hydraulic Conductivity Field
## Weakly Heterogeneous Flow Field

Realization 1

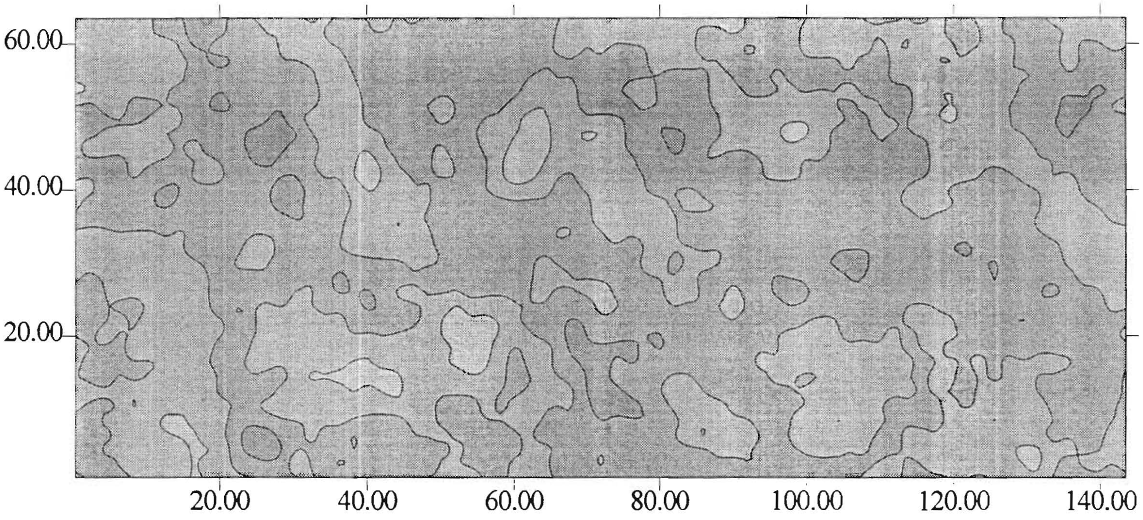


Natural log hydraulic conductivity scale for all realizations.

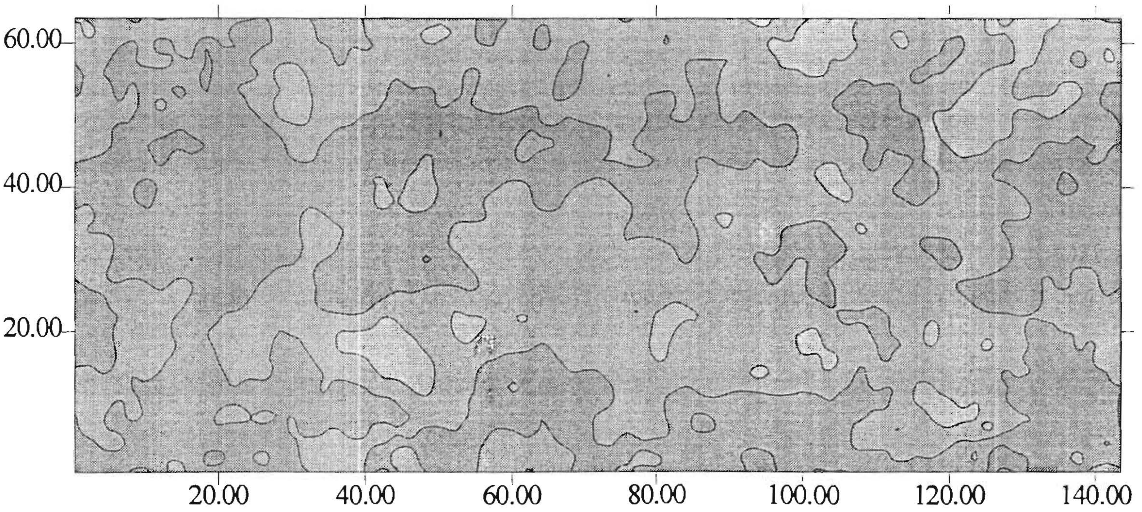


Hydraulic Conductivity Field
Weakly Heterogeneous Flow Field

Realization 2

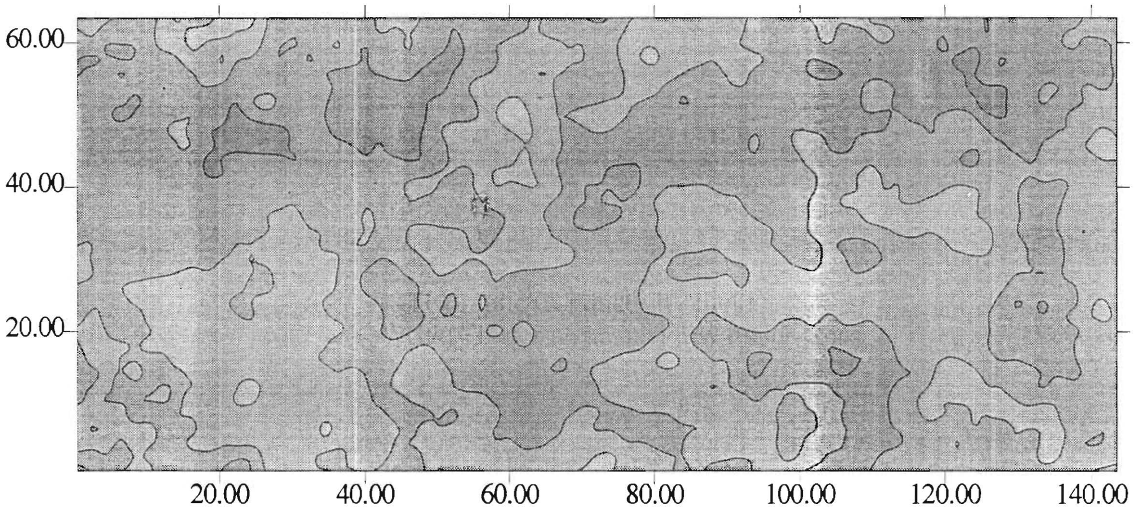


Realization 3

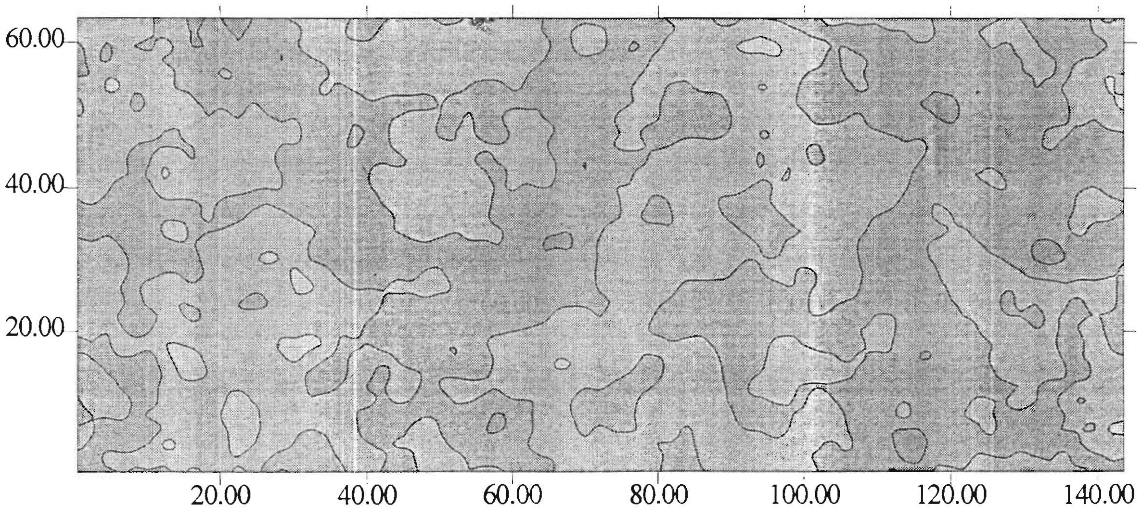


# Hydraulic Conductivity Field
Weakly Heterogeneous Flow Field

Realization 4

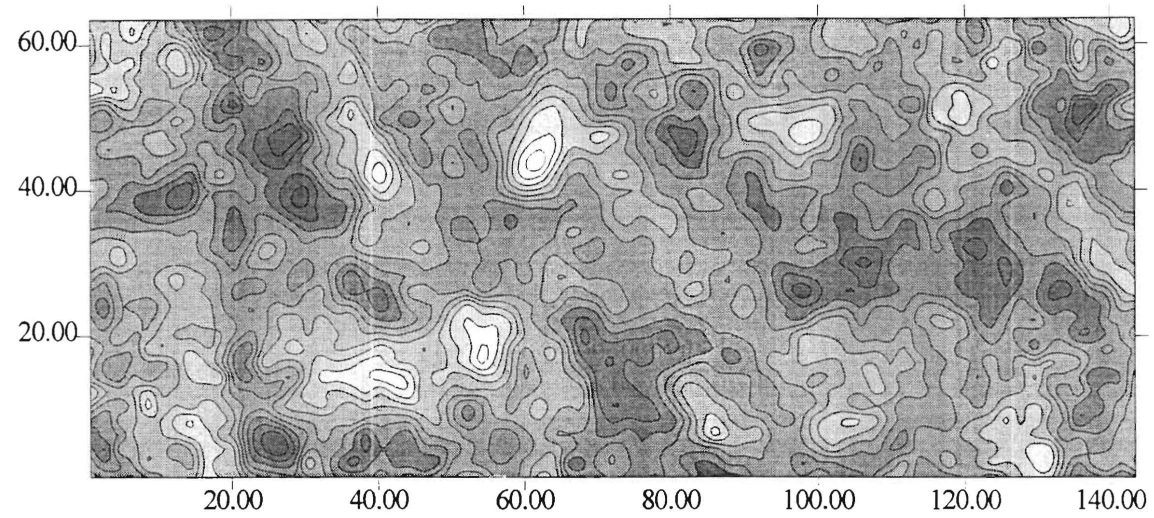


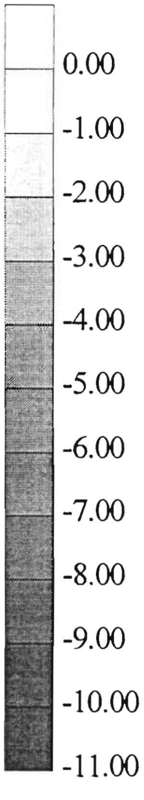
Realization 5



# Hydraulic Conductivity Field Strongly Heterogeneous Flow Field

## Realization 1

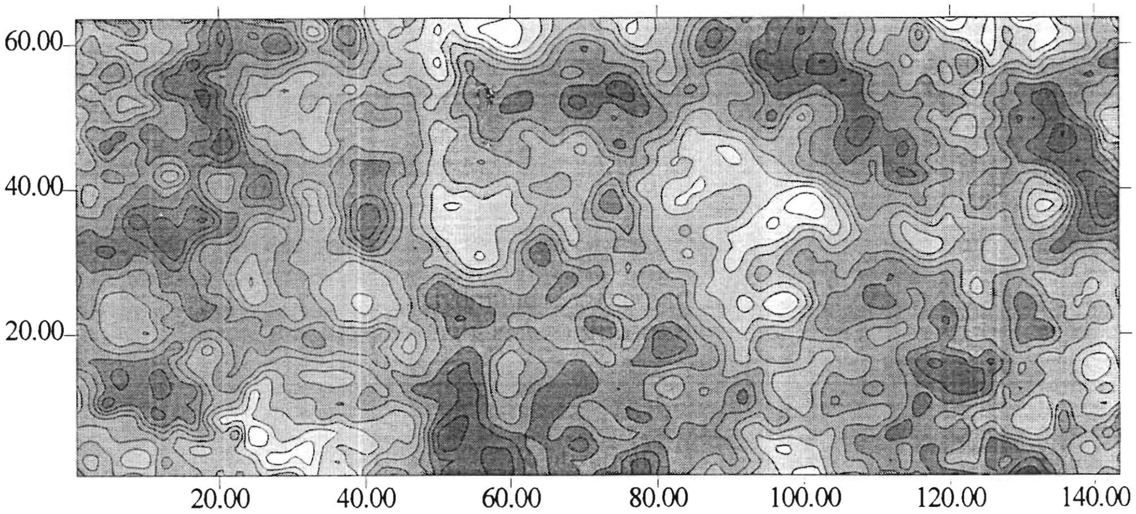




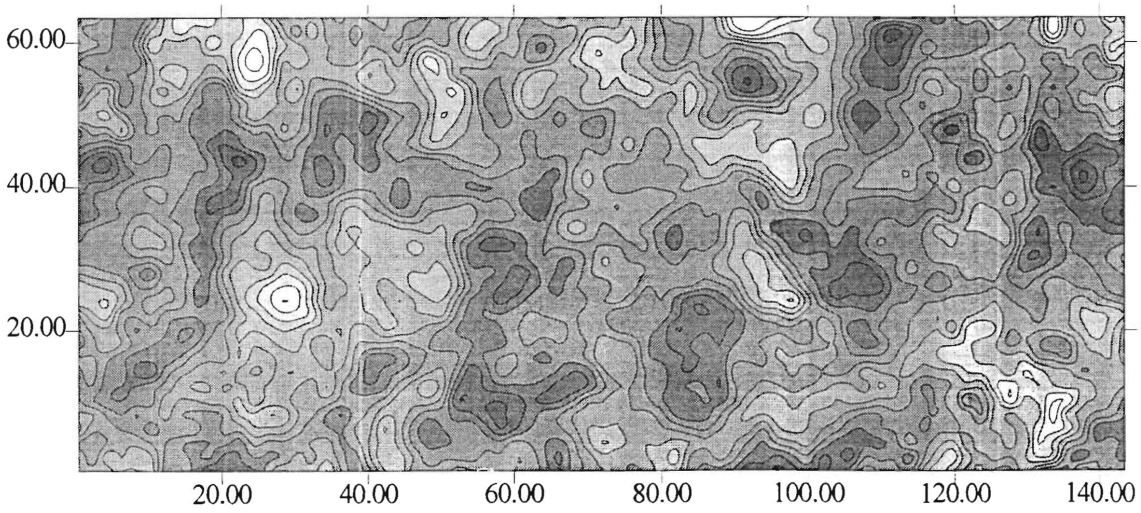
Natural log hydraulic conductivity scale for all realizations.

# Hydraulic Conductivity Field
# Strongly Heterogeneous Flow Field

Realization 2

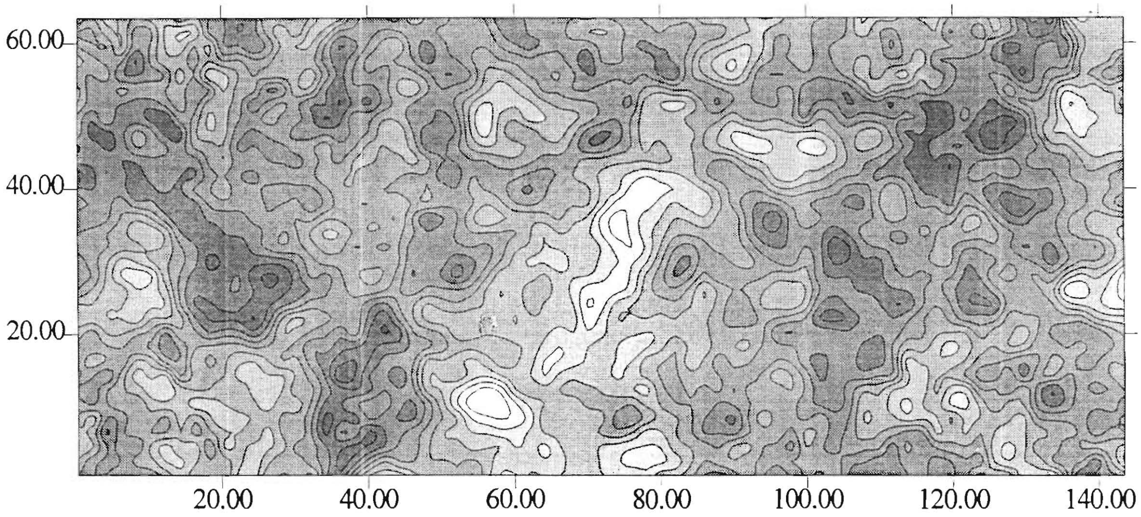


Realization 3

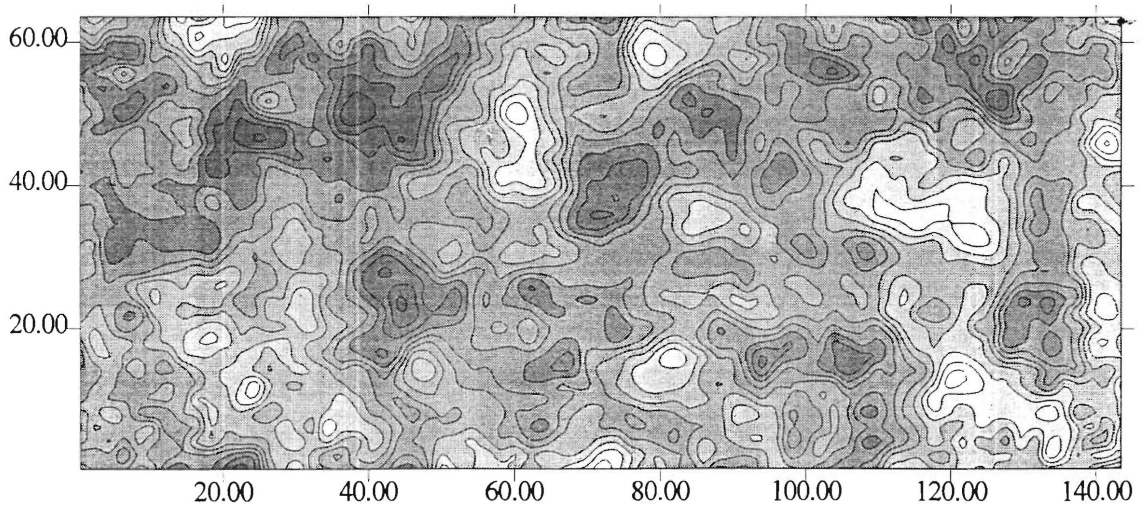


## Hydraulic Conductivity Field
## Strongly Heterogeneous Flow Field

### Realization 4

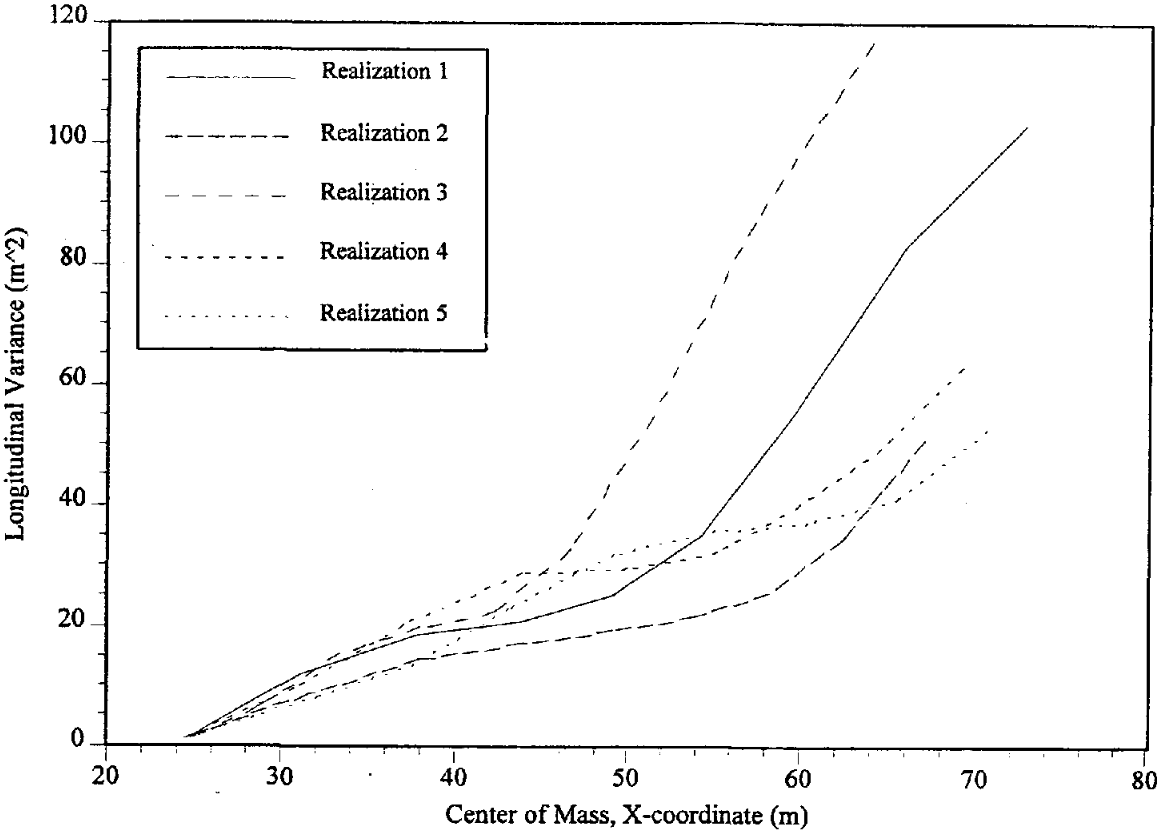


### Realization 5

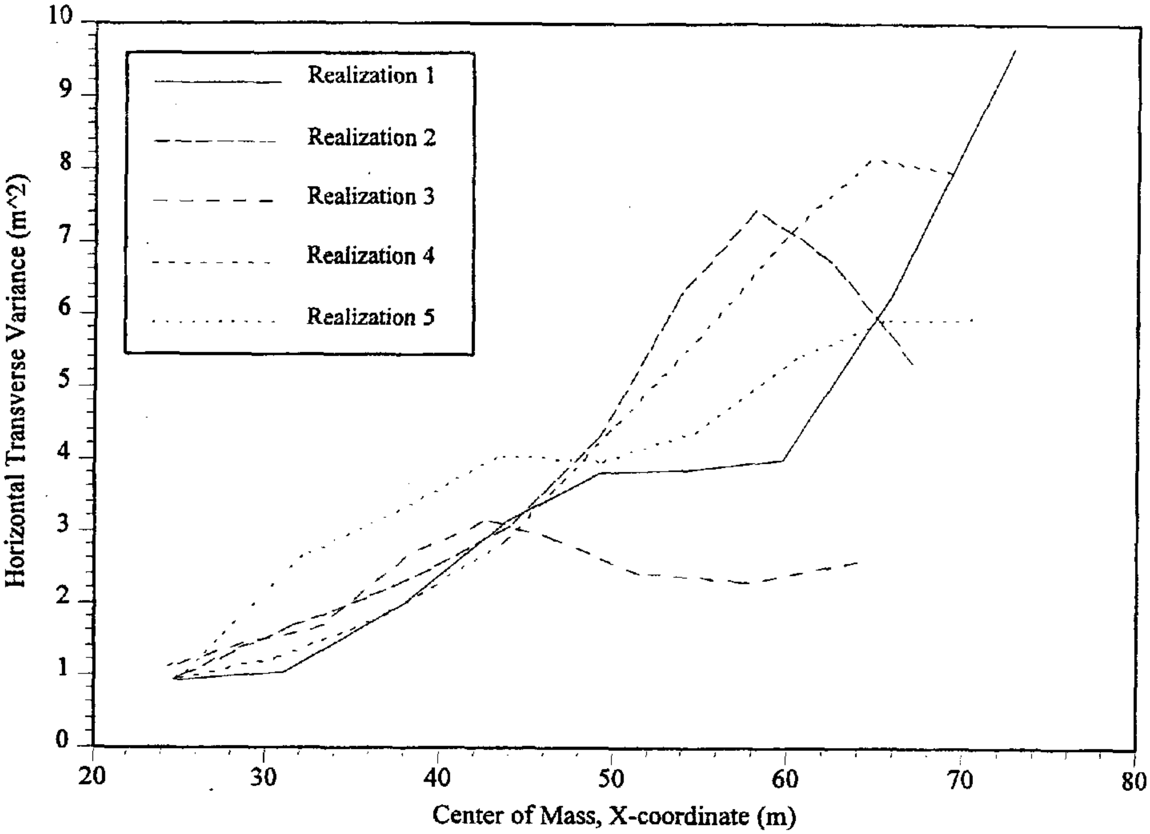


# APPENDIX D

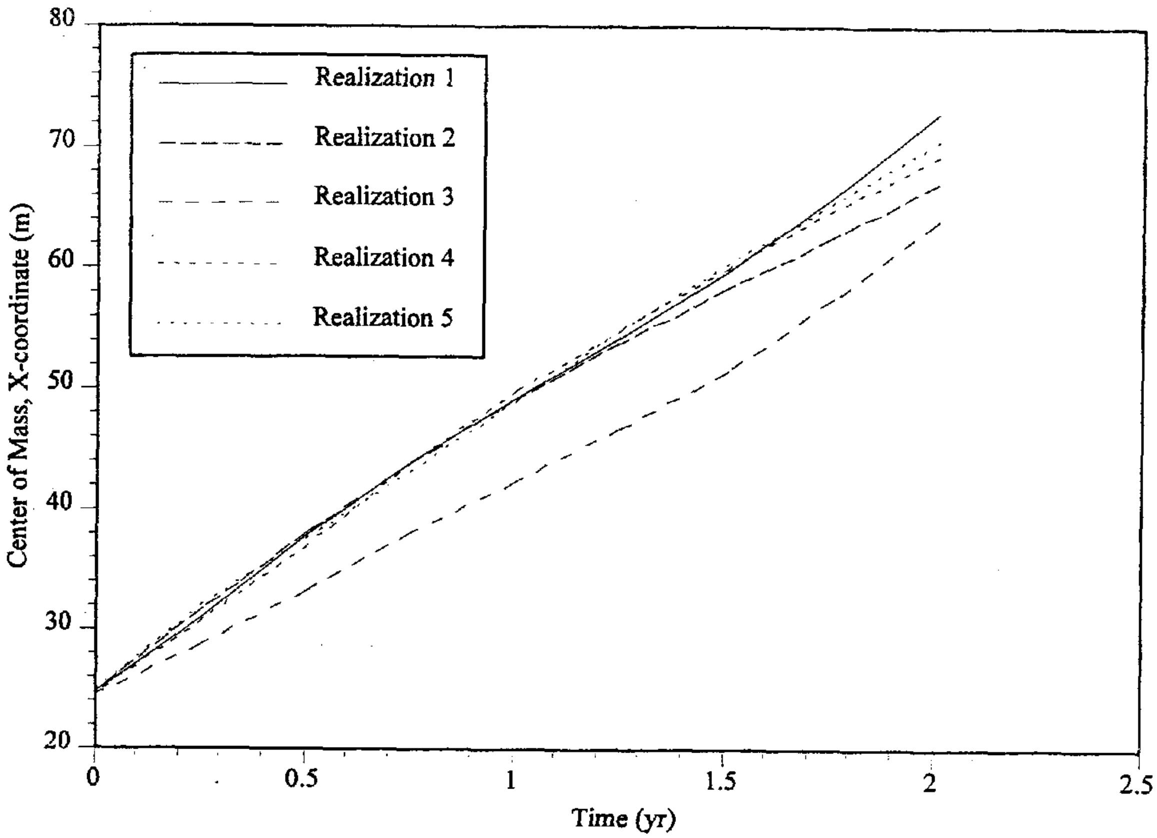
# GRAPHS



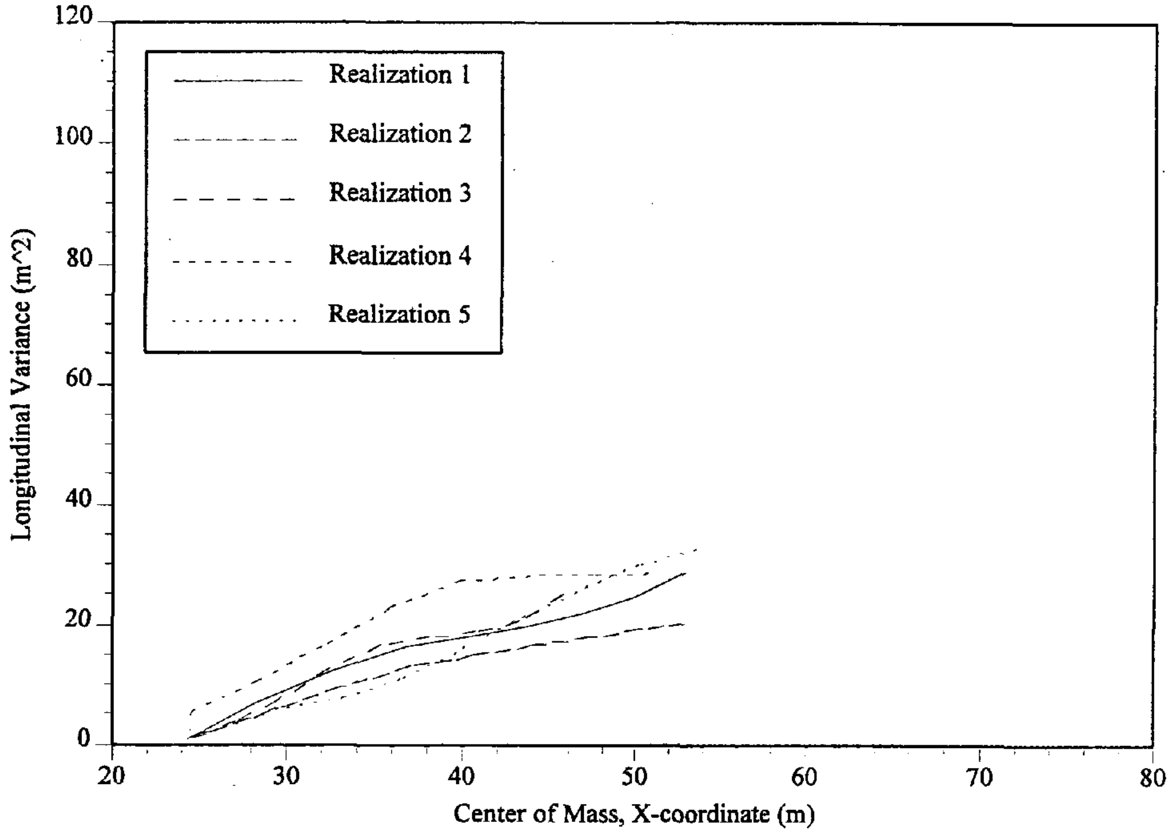
Conservative simulations in a weakly heterogeneous flow field with 1 kg of bromide. All concentrations used in calculations.



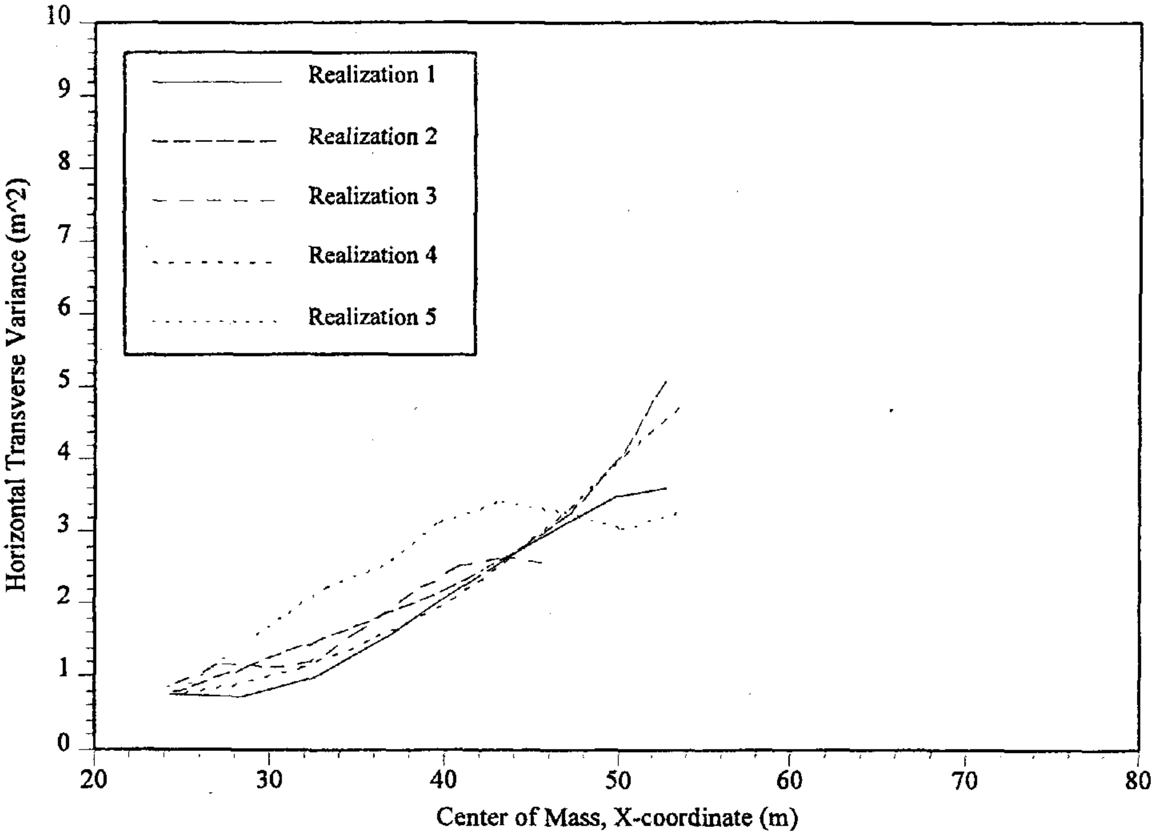
Conservative simulations in a weakly heterogeneous flow field with 1 kg of bromide. All concentrations used in calculations.



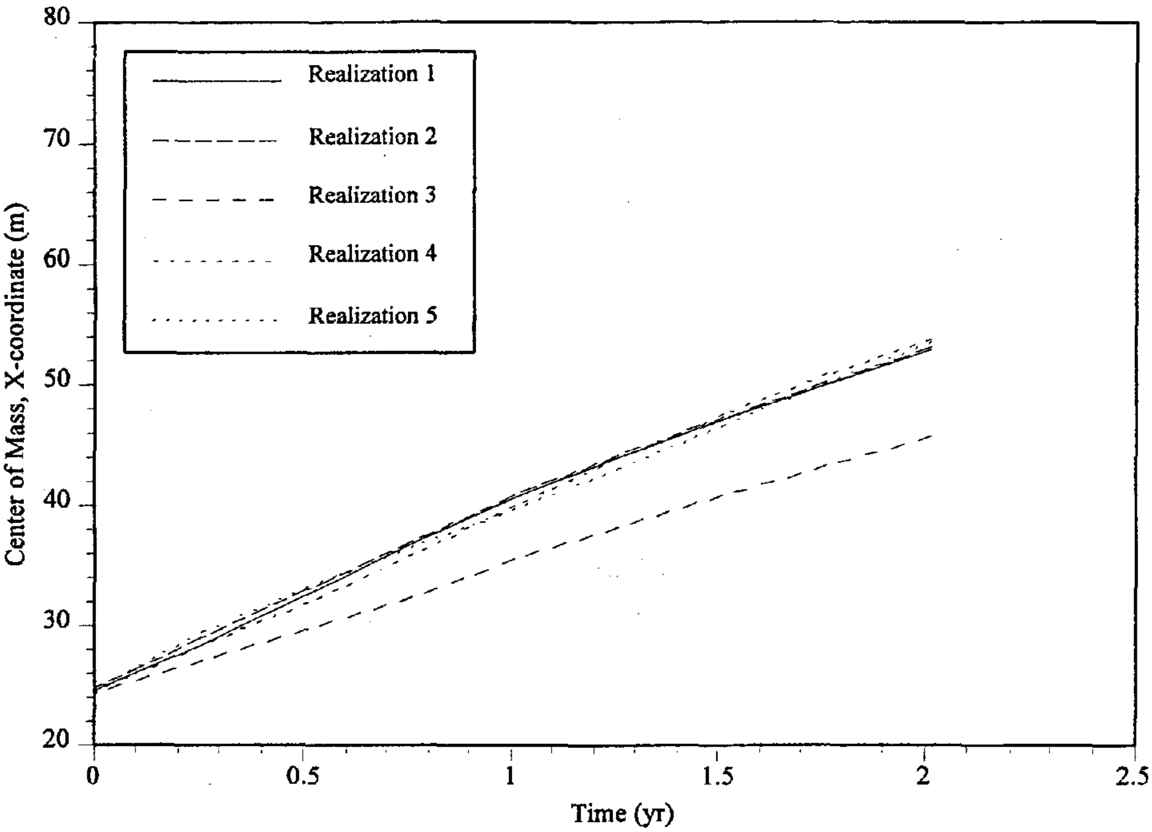
Conservative simulations in a weakly heterogeneous flow field with 1 kg of bromide. All concentrations used in calculations.



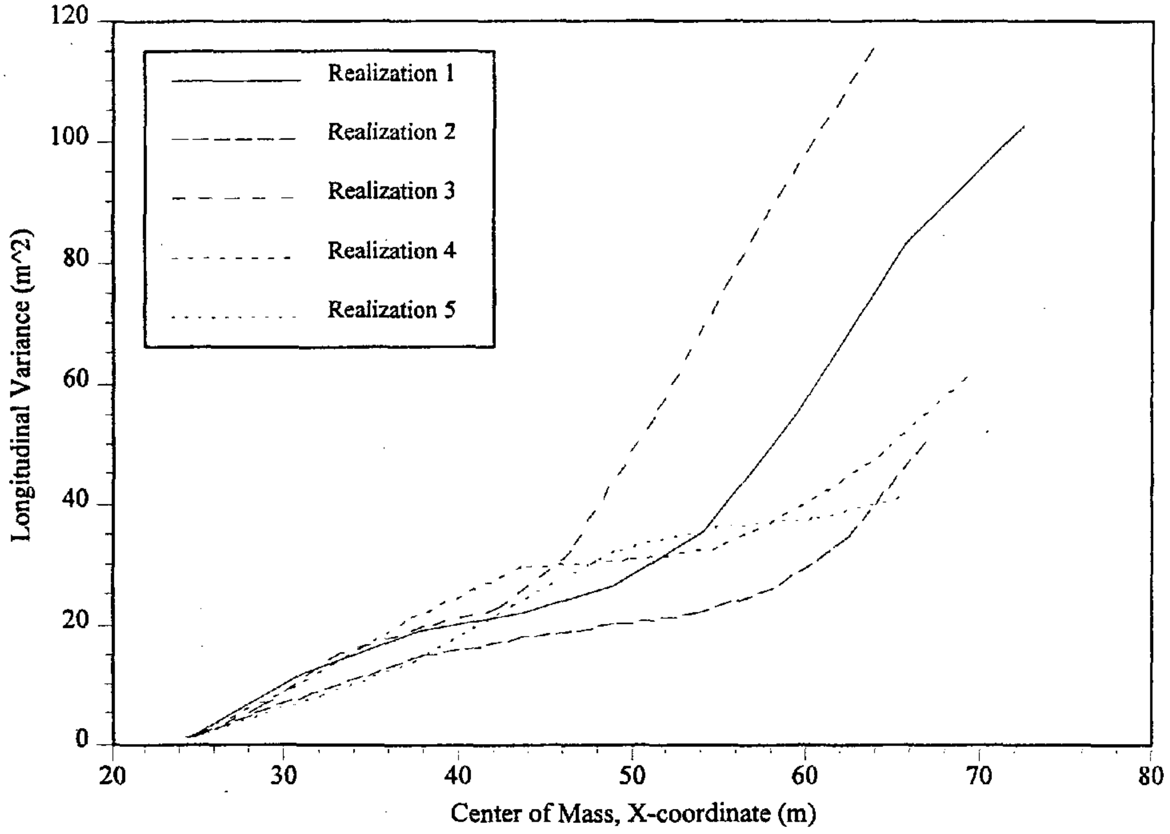
Reactive simulations in a weakly heterogeneous flow field with 1 kg of bromide. All concentrations used in calculations.



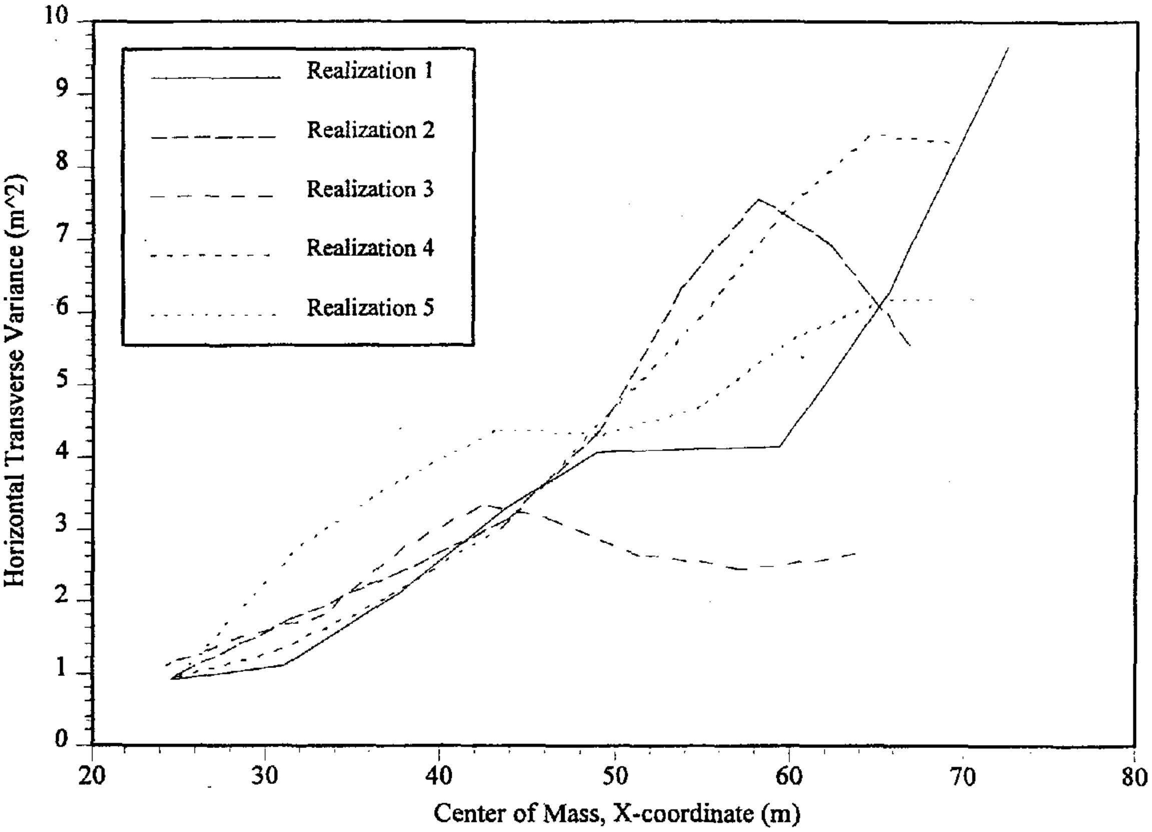
Reactive simulations in a weakly heterogeneous flow field with 1 kg of bromide. All concentrations used in calculations.



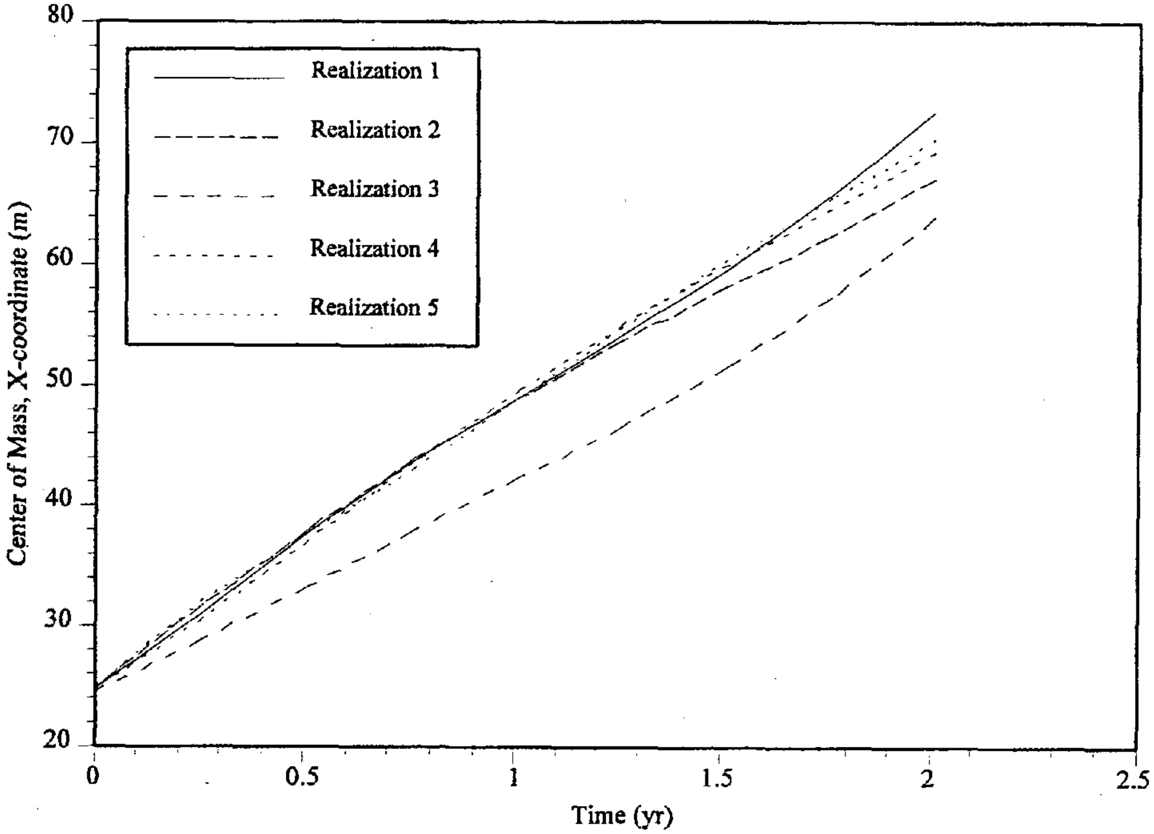
Reactive simulations in a weakly heterogeneous flow field with 1 kg of bromide. All concentrations used in calculations.



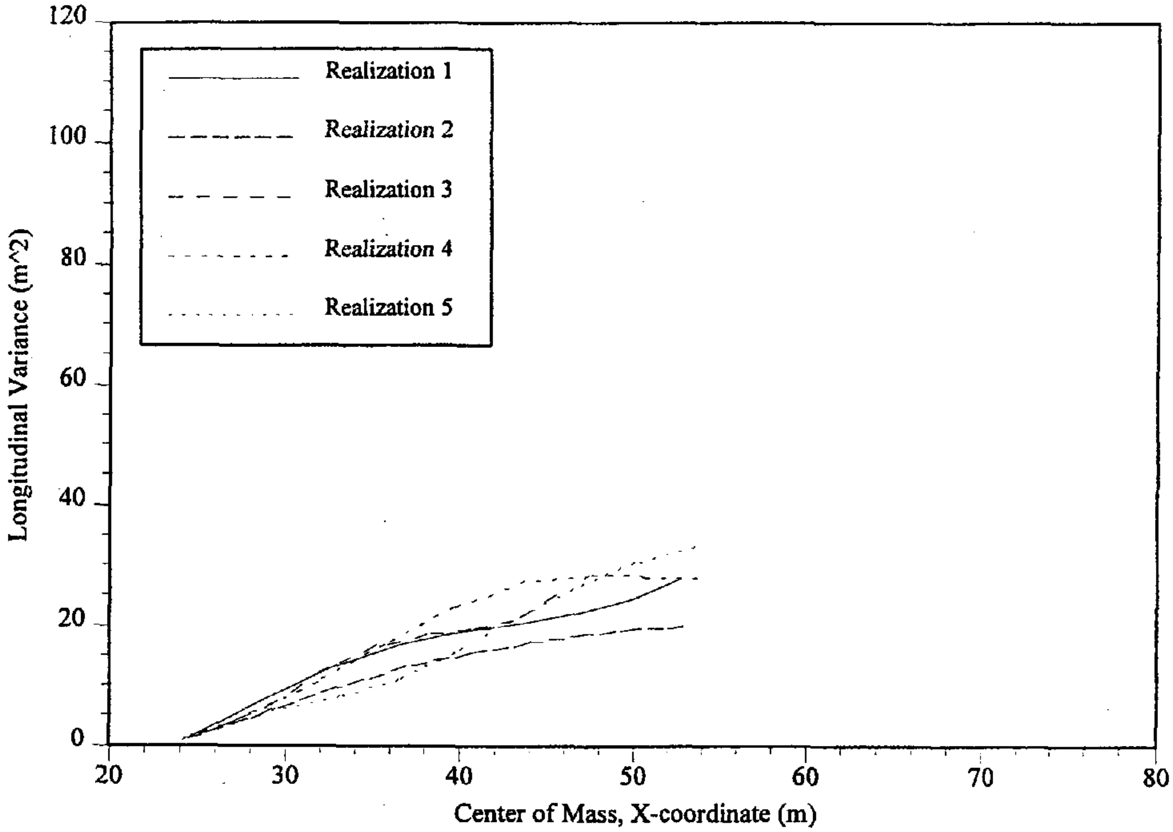
Conservative simulations in a weakly heterogeneous flow field with 1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



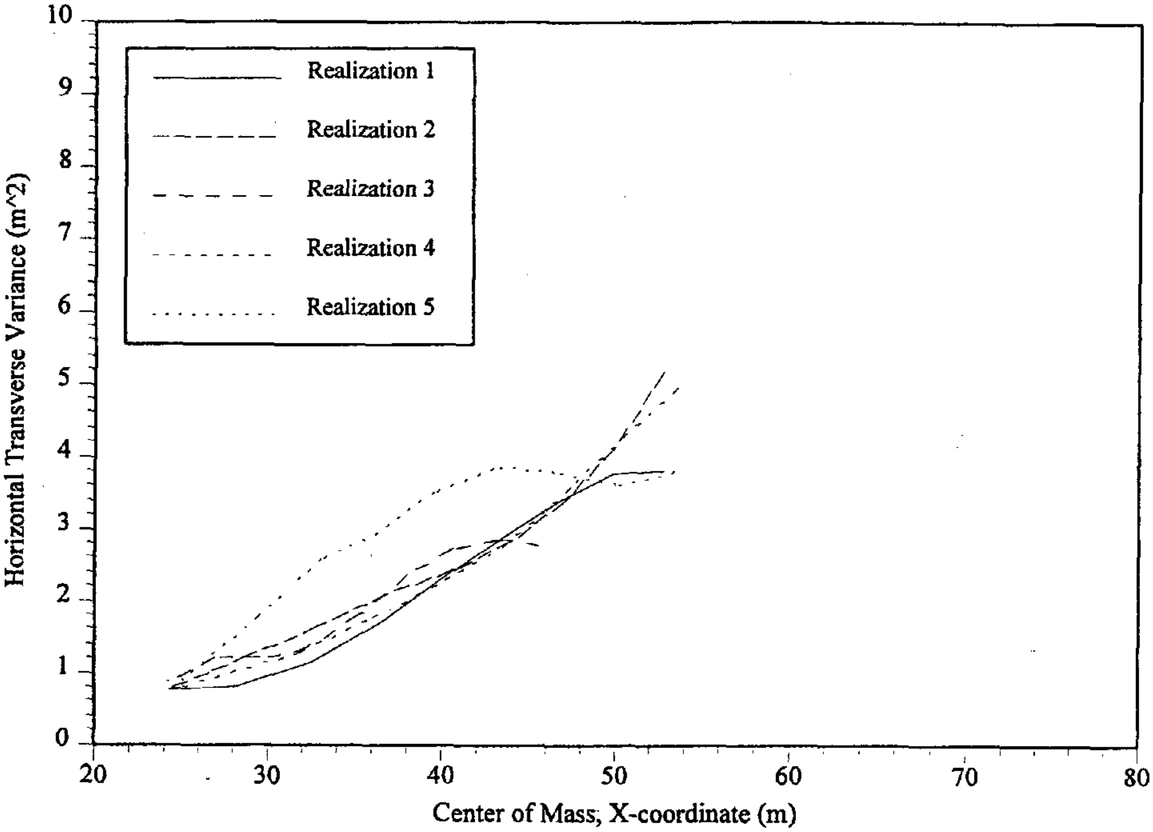
Conservative simulations in a weakly heterogeneous flow field with 1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



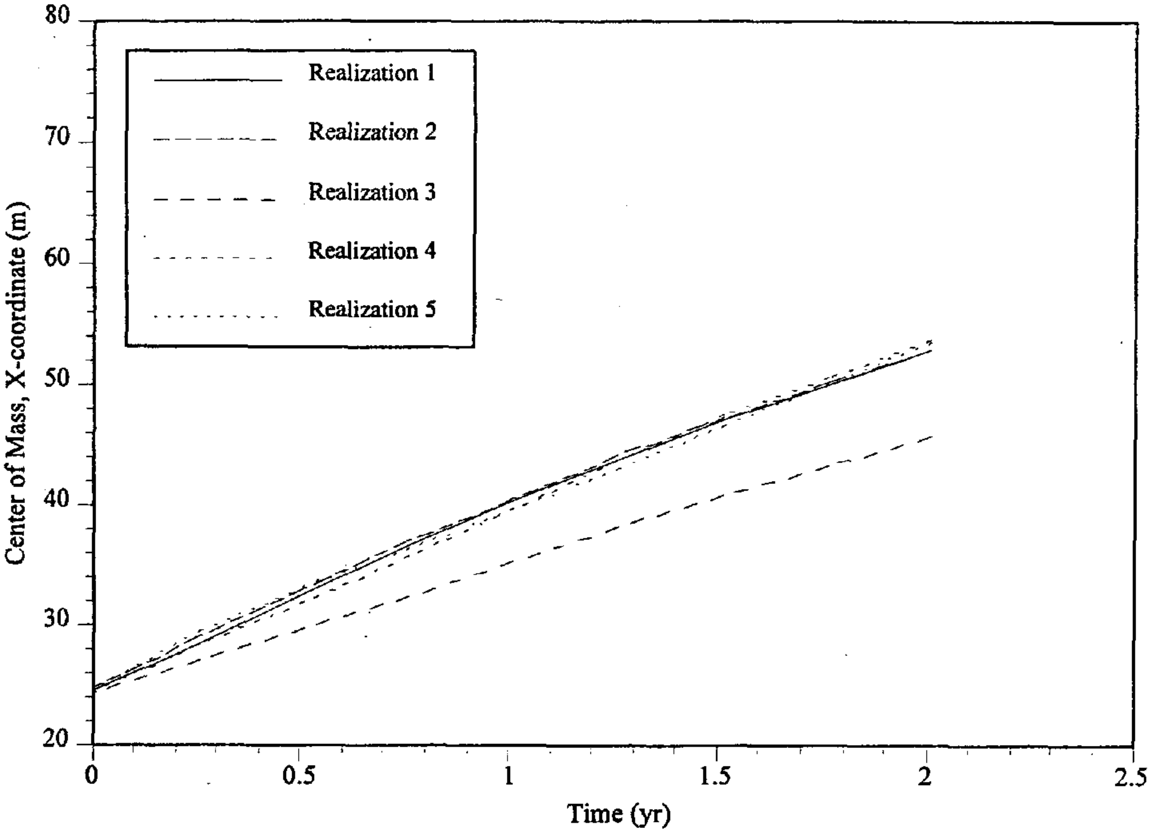
Conservative simulations in a weakly heterogeneous flow field with 1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



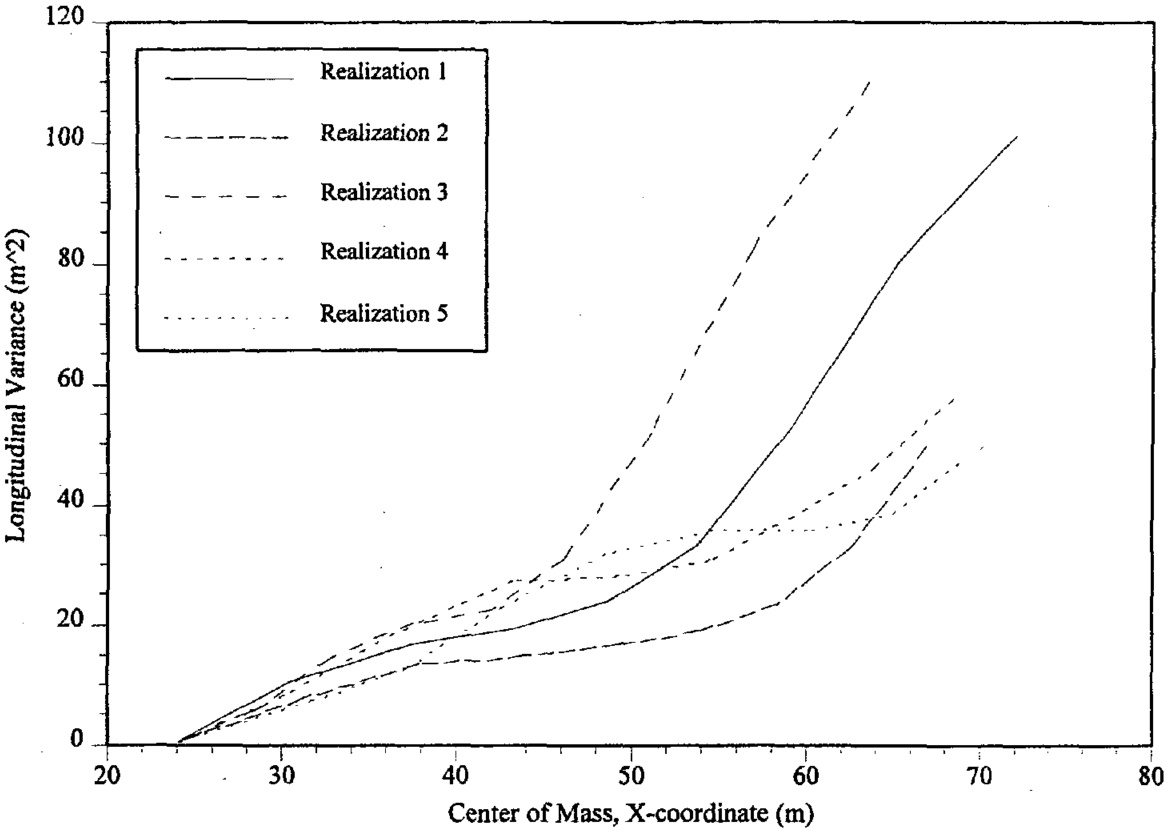
Reactive simulations in a weakly heterogeneous flow field with 1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



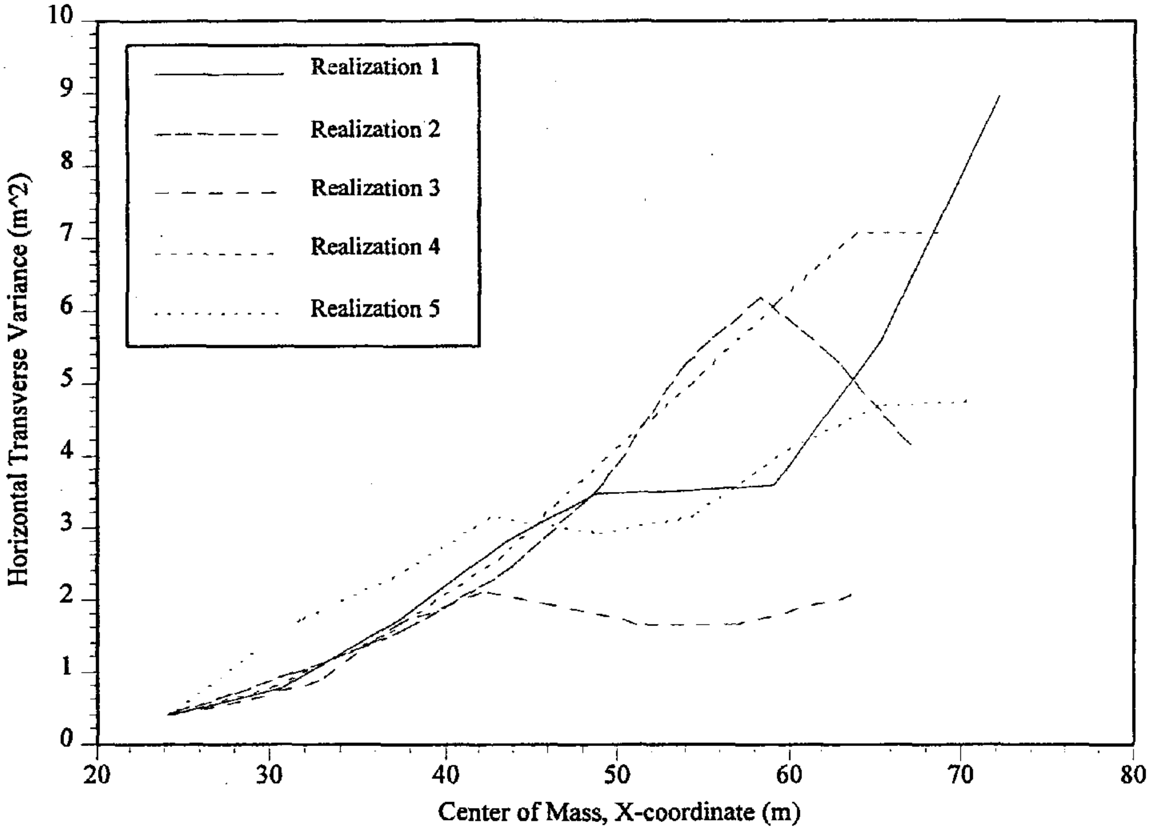
Reactive simulations in a weakly heterogeneous flow field with 1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



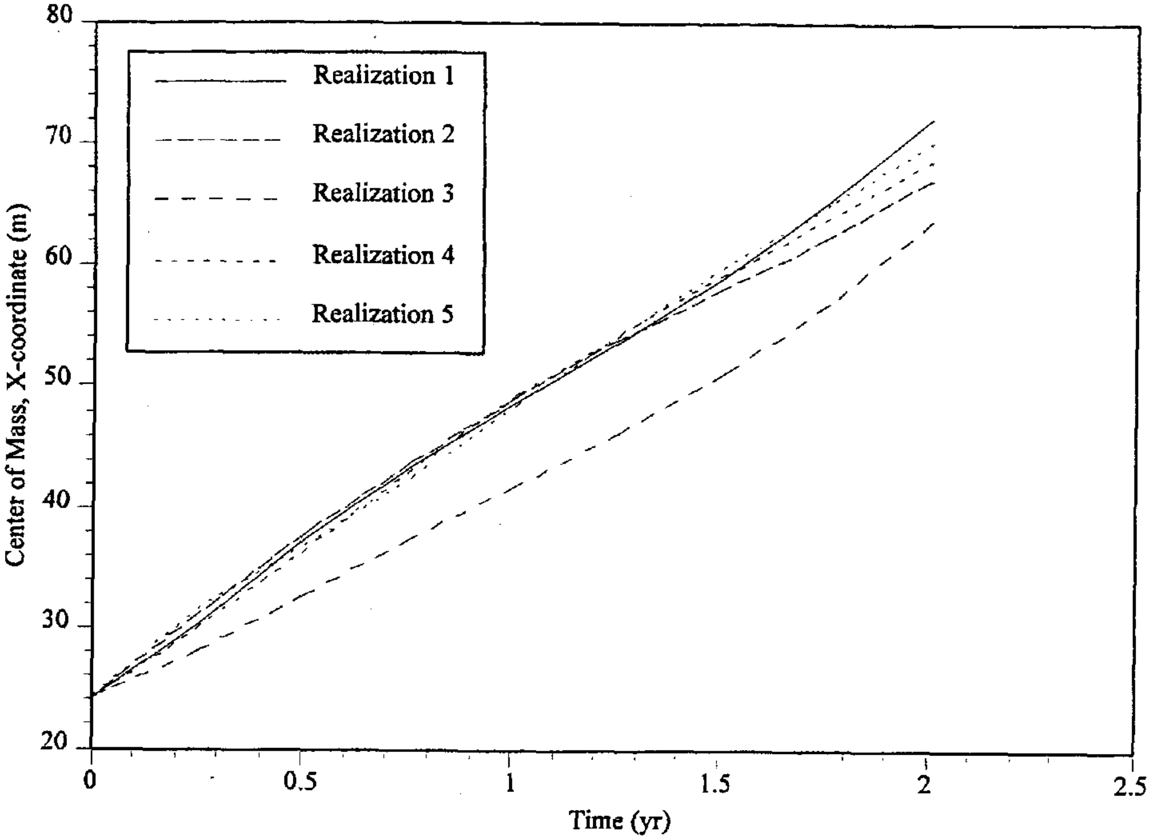
Reactive simulations in a weakly heterogeneous flow field with 1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



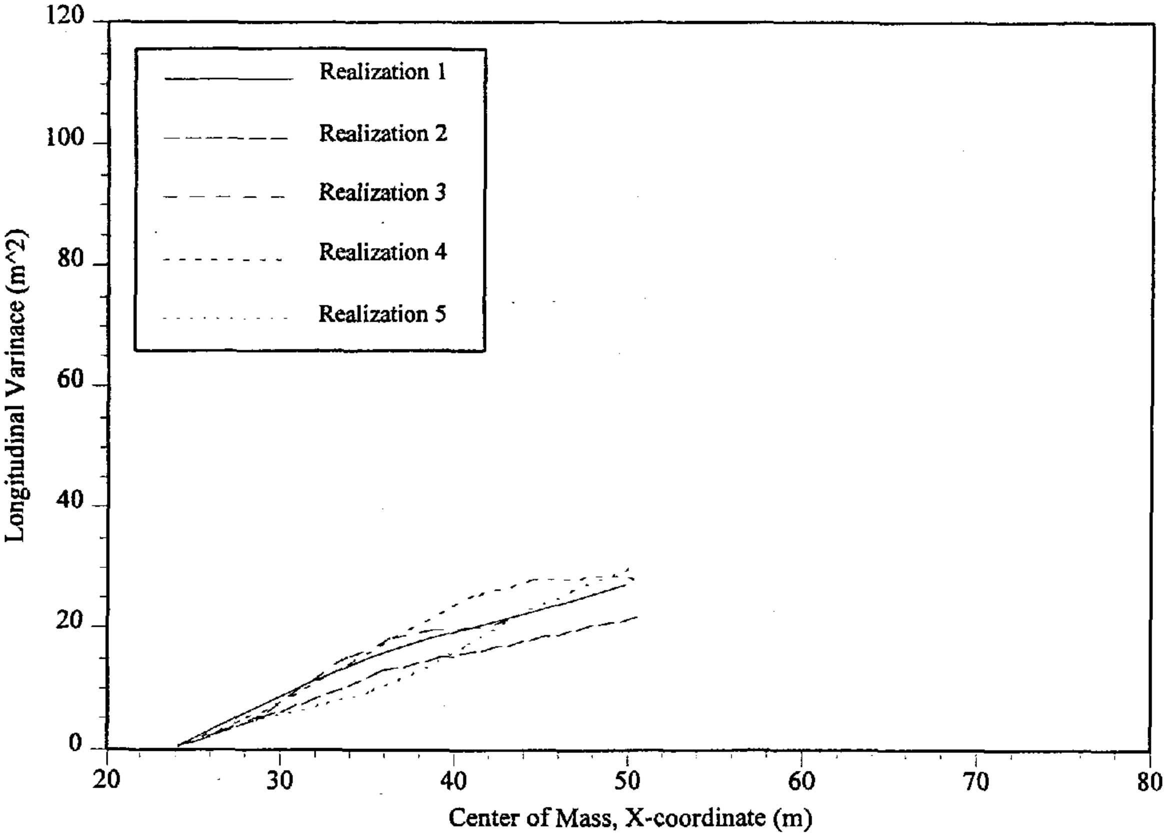
Conservative simulations in a weakly heterogeneous flow field with 0.1 kg of bromide. All Concentrations used in calculations.



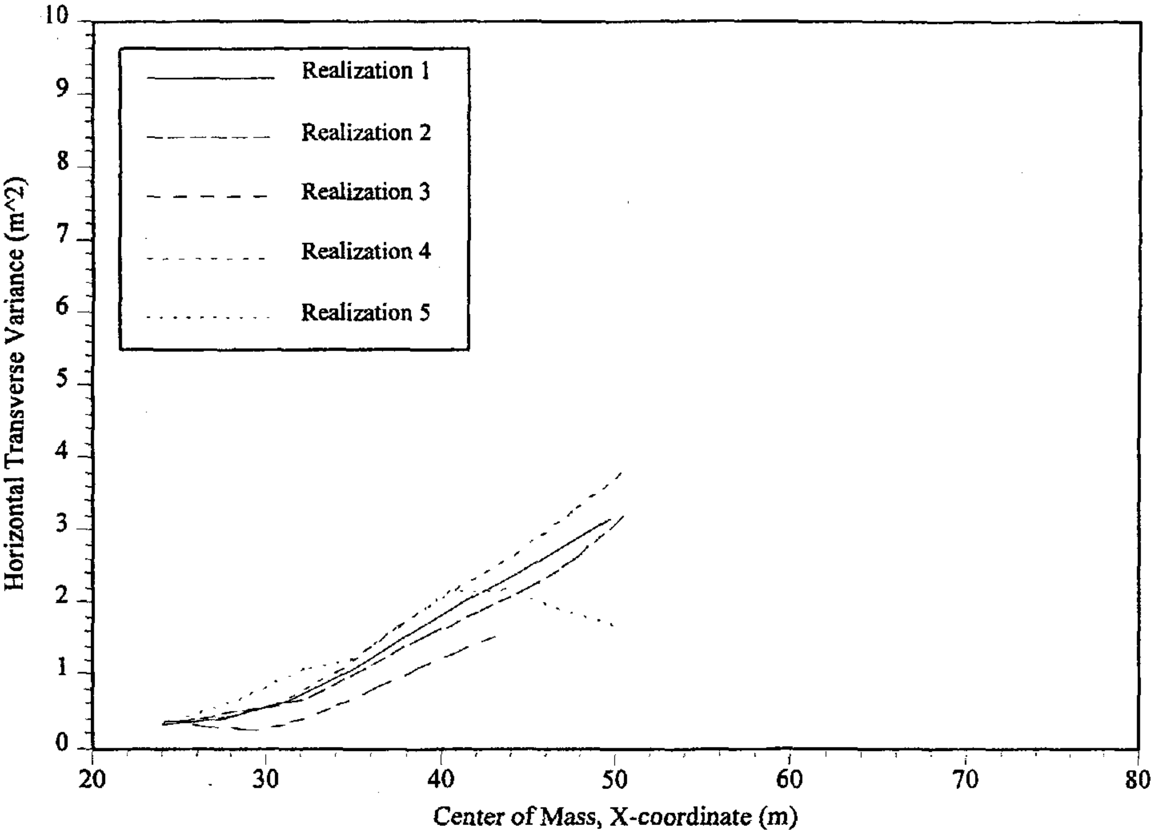
Conservative simulations in a weakly heterogeneous flow field with 0.1 kg of bromide. All concentrations used in calculations.



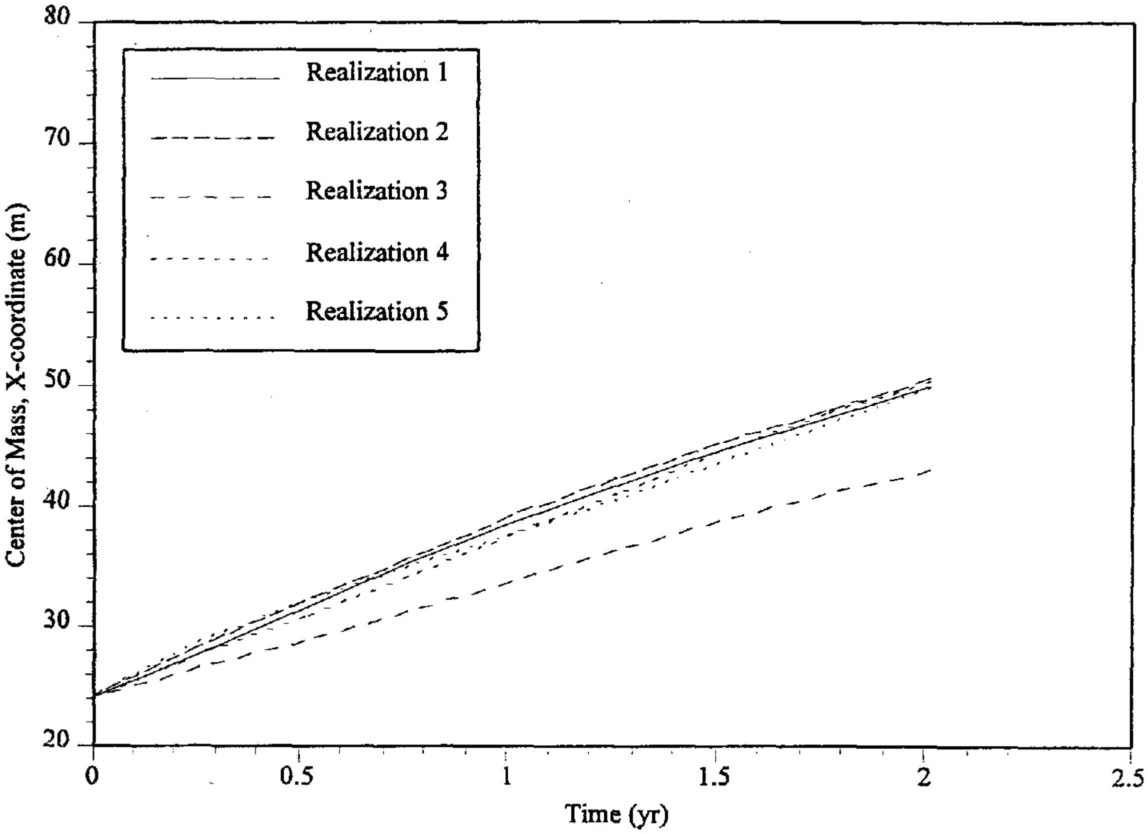
Conservative simulations in a weakly heterogeneous flow field with 0.1 kg of bromide. All concentrations used in calculations.



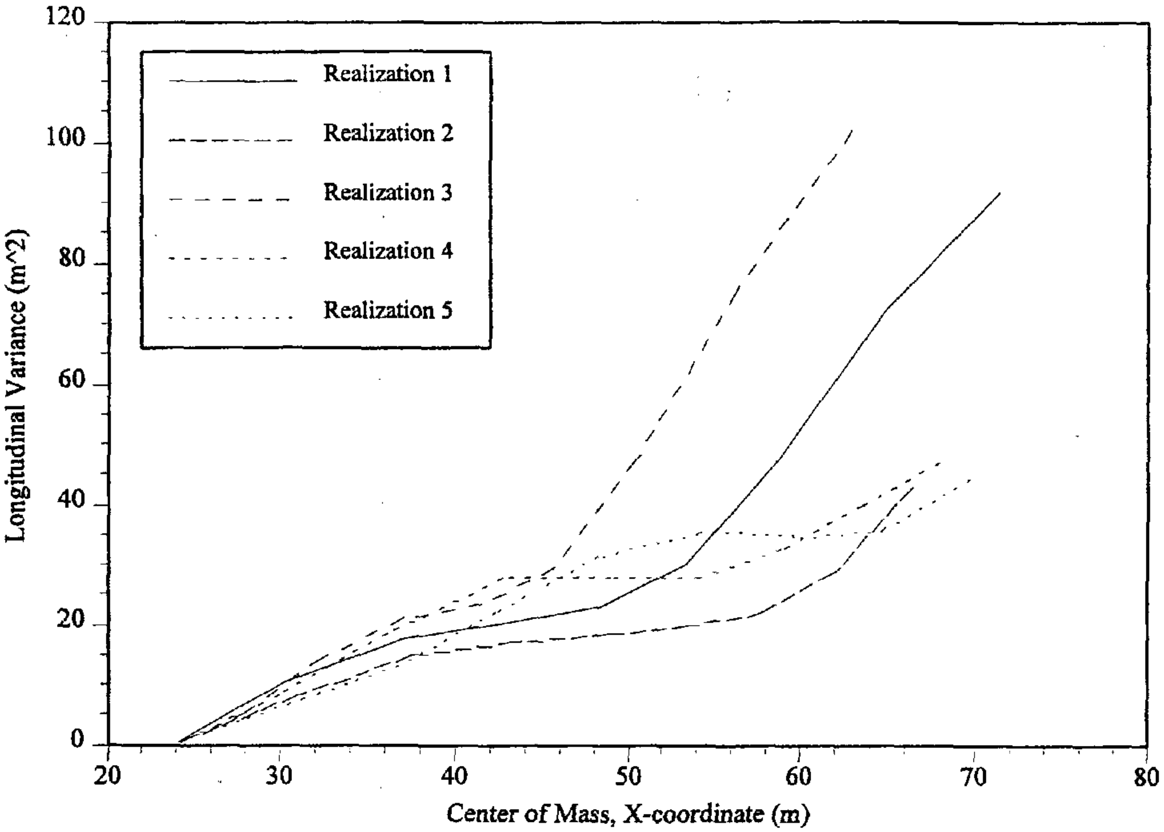
Reactive simulations in a weakly heterogeneous flow field with 0.1 kg of bromide. All concentrations used in calculations.



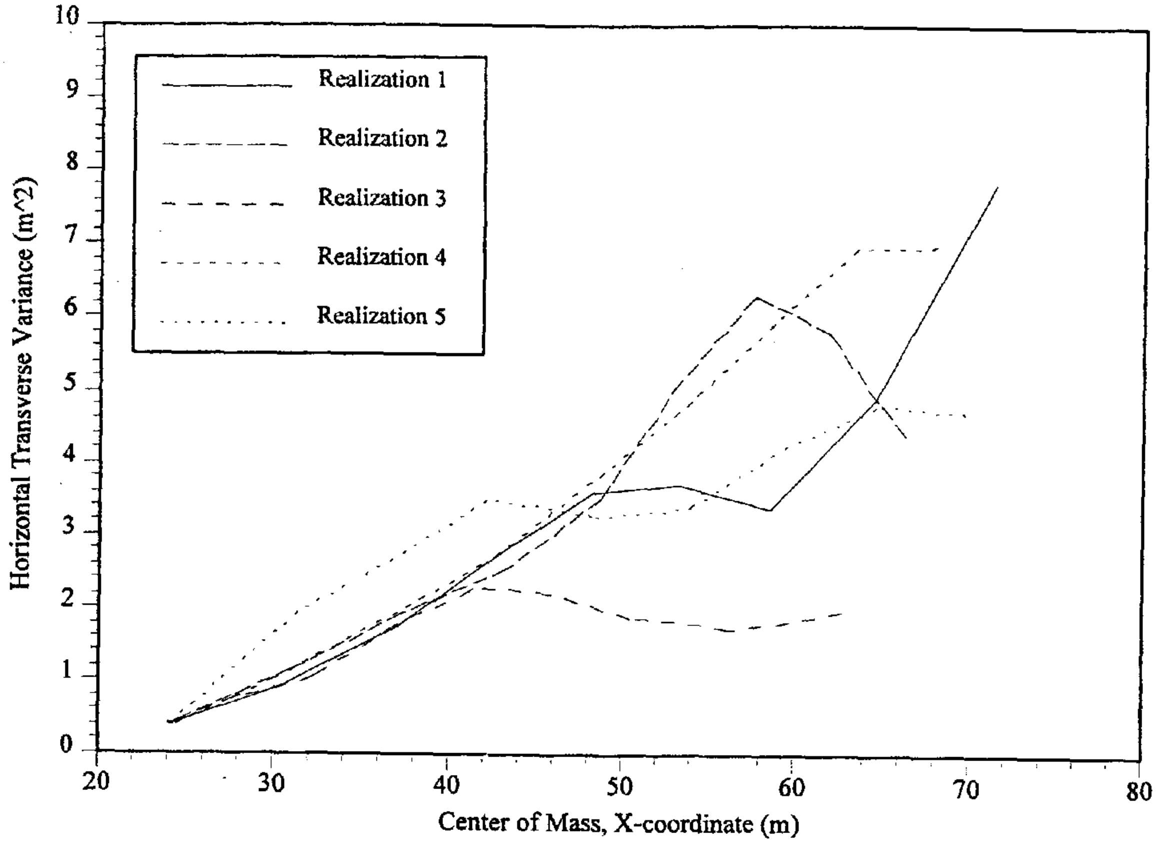
Reactive simulations in a weakly heterogeneous flow field with 0.1 kg of bromide. All concentrations used in calculations.



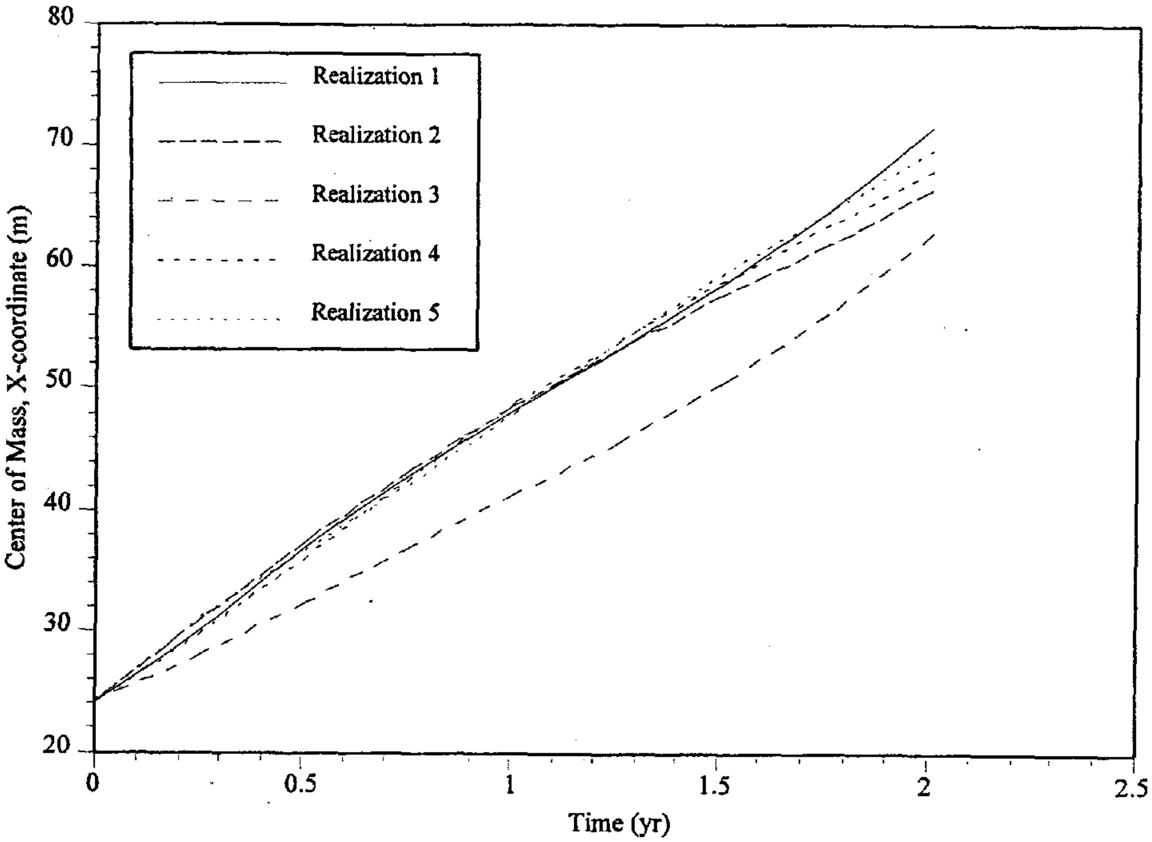
Reactive simulations in a weakly heterogeneous flow field with 0.1 kg of bromide. All concentrations used in calculations.



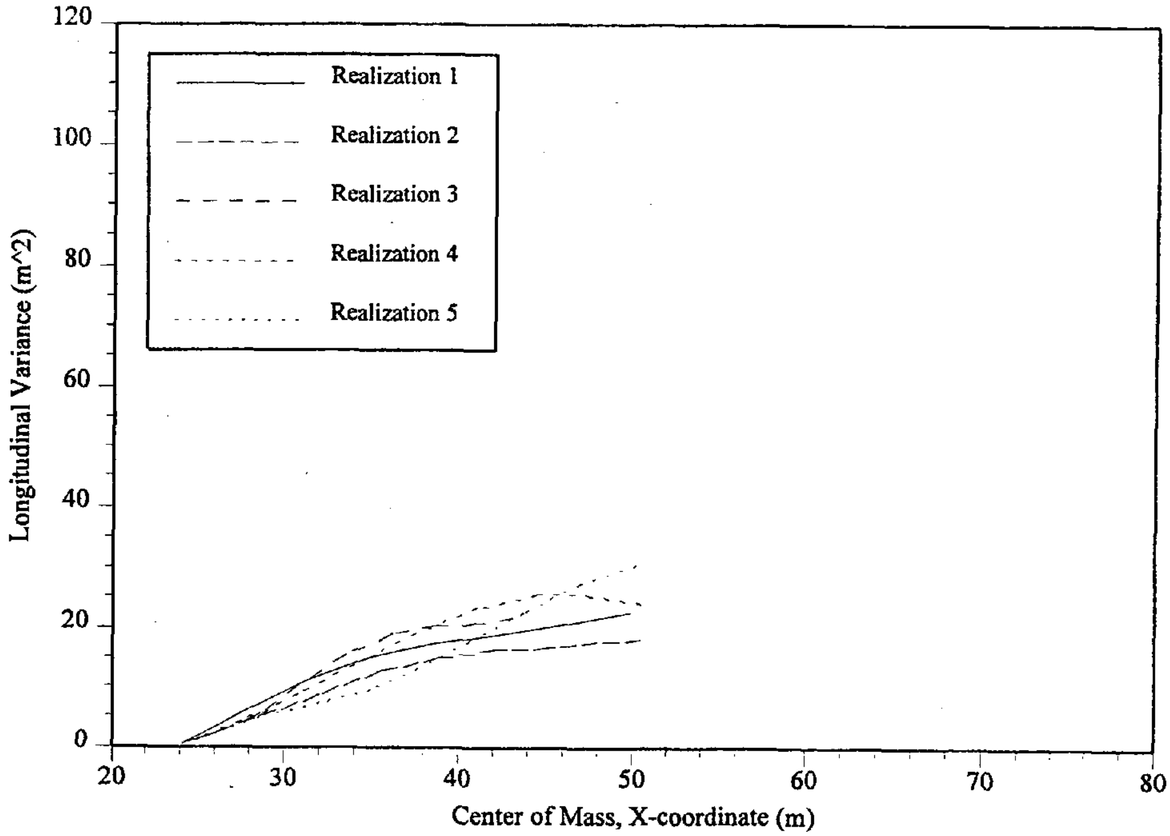
Conservative simulations in a weakly heterogeneous flow field with 0.1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



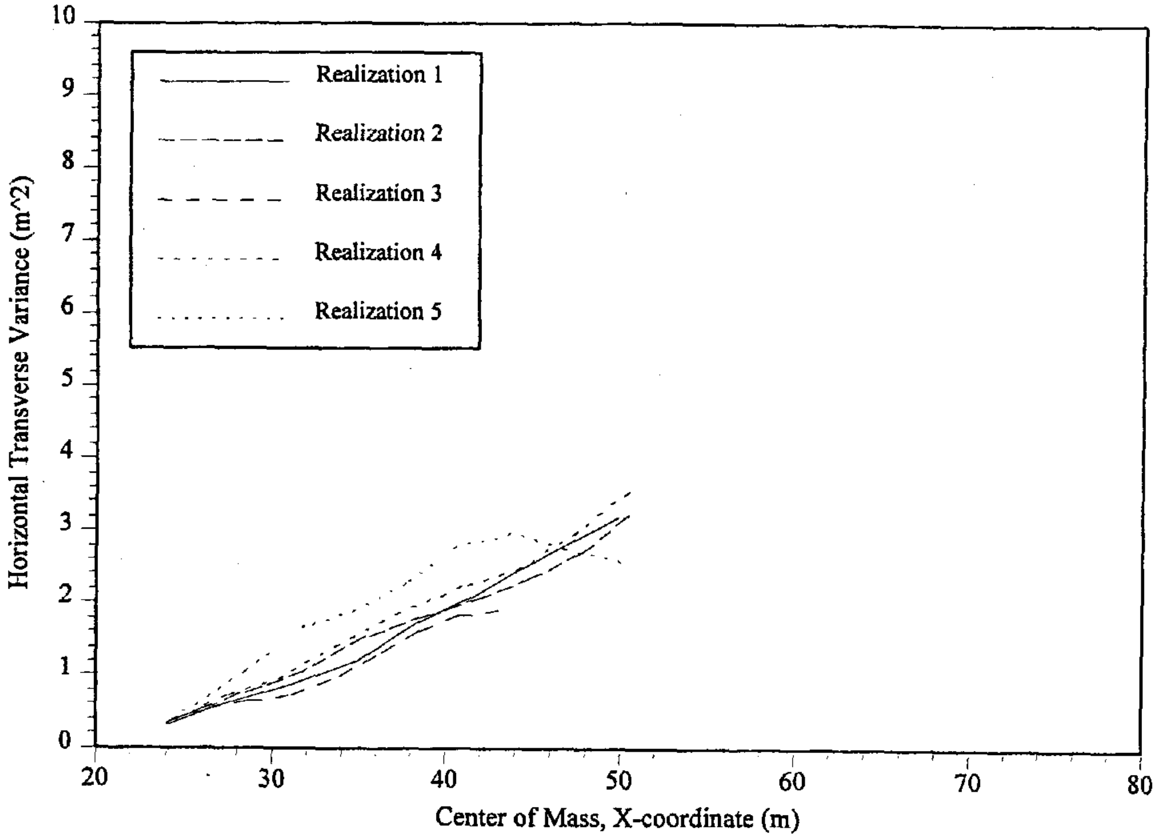
Conservative simulations in a weakly heterogeneous flow field with 0.1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



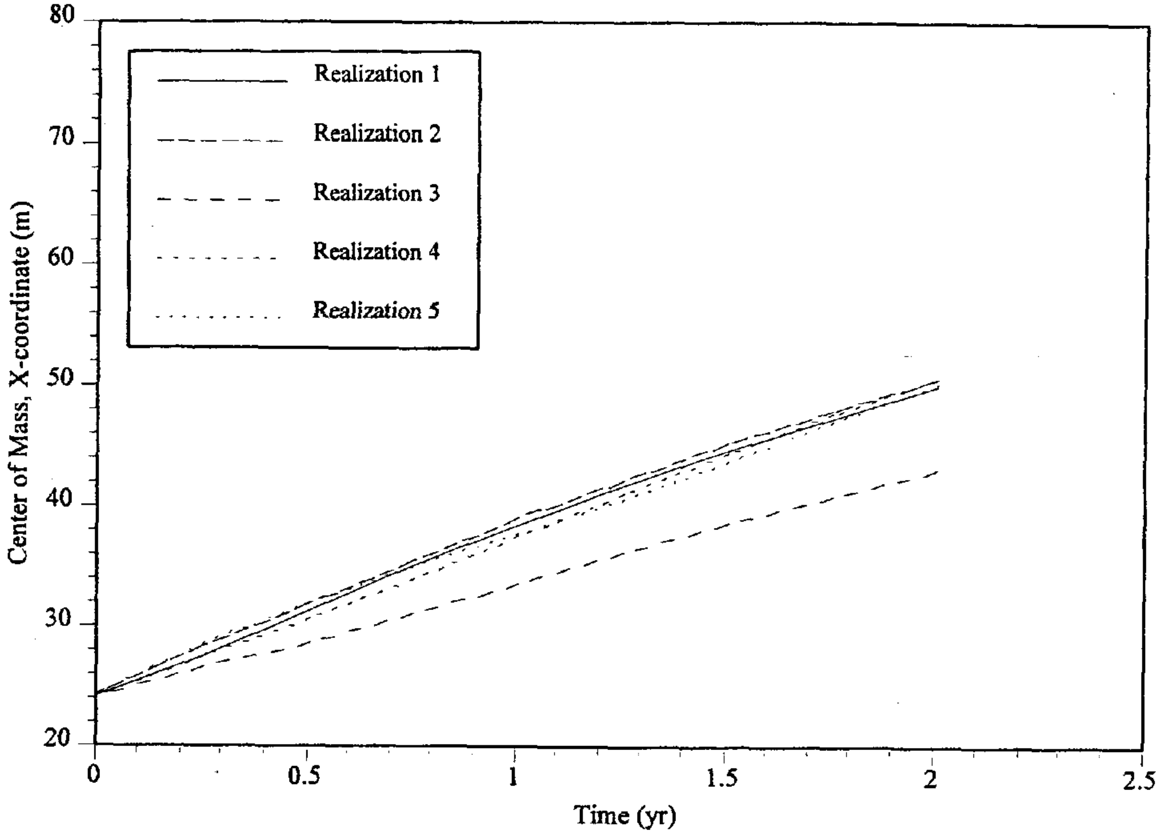
Conservative simulations in a weakly heterogeneous flow field with 0.1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



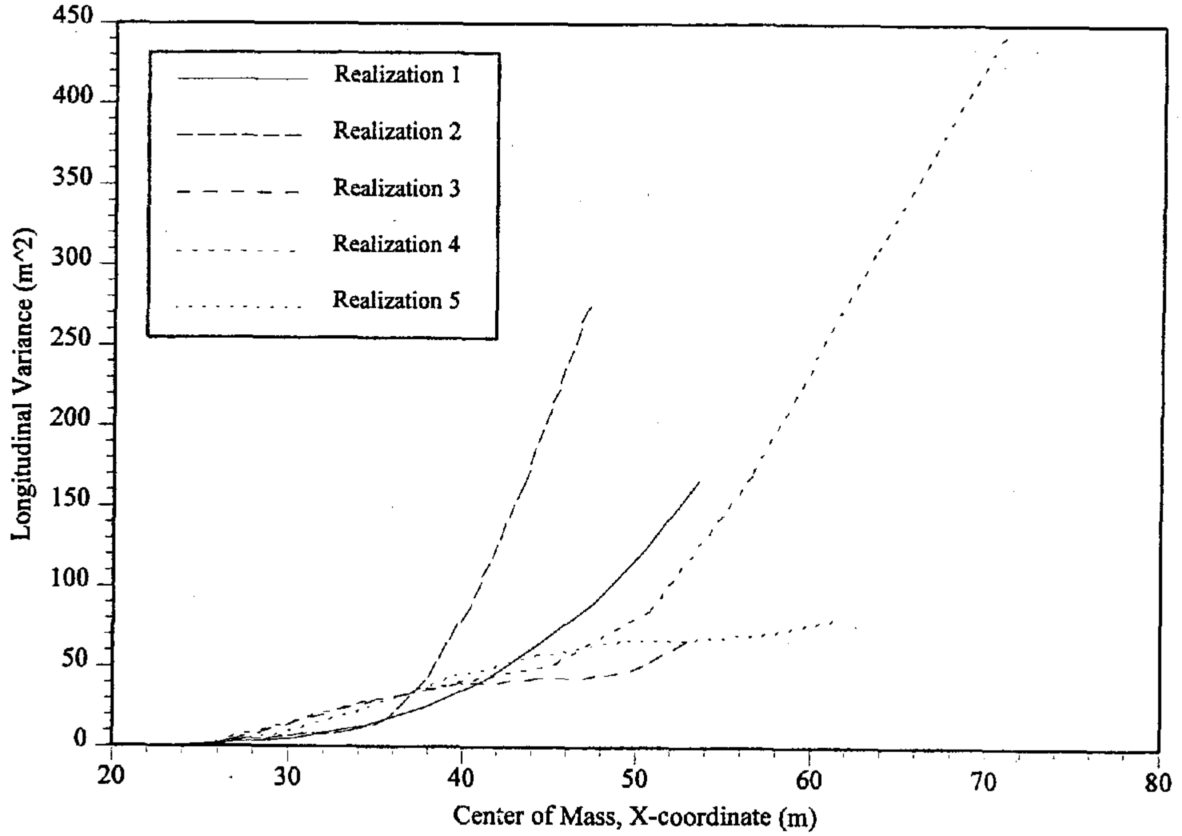
Reactive simulations in a weakly heterogeneous flow field with 0.1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



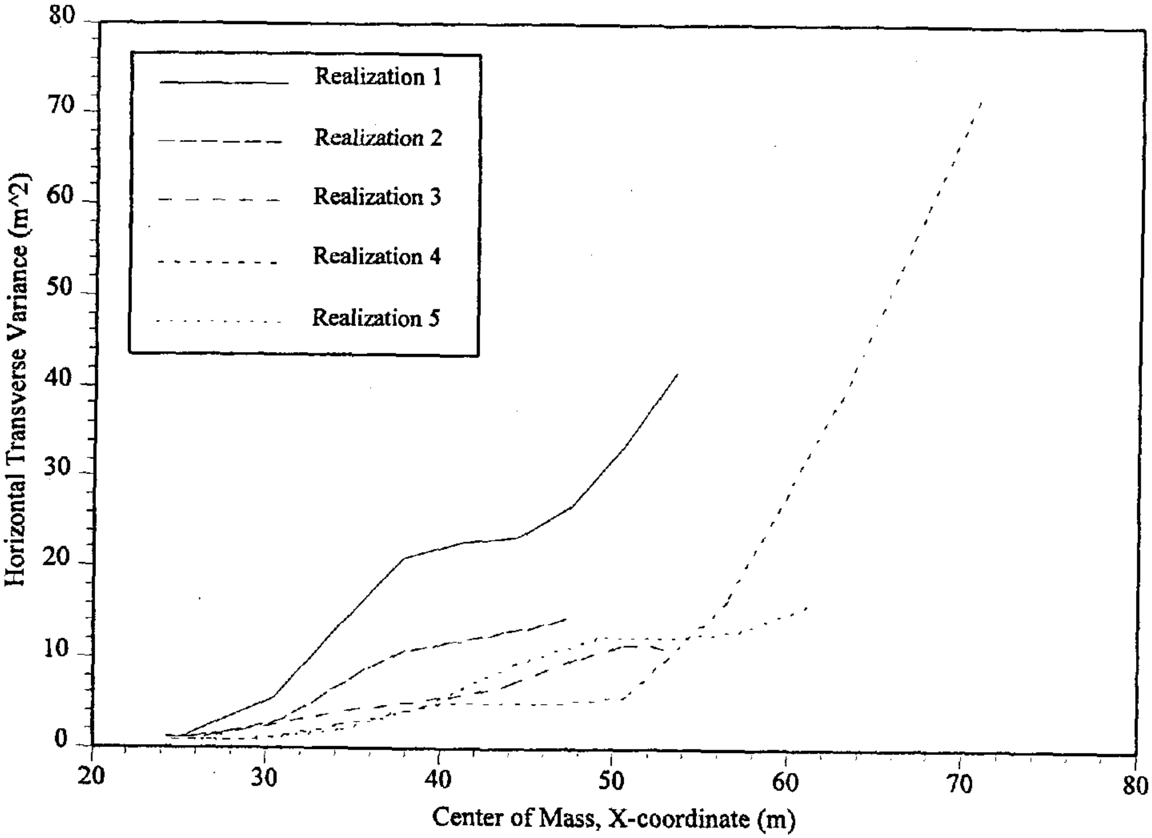
Reactive simulations in a weakly heterogeneous flow field with 0.1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



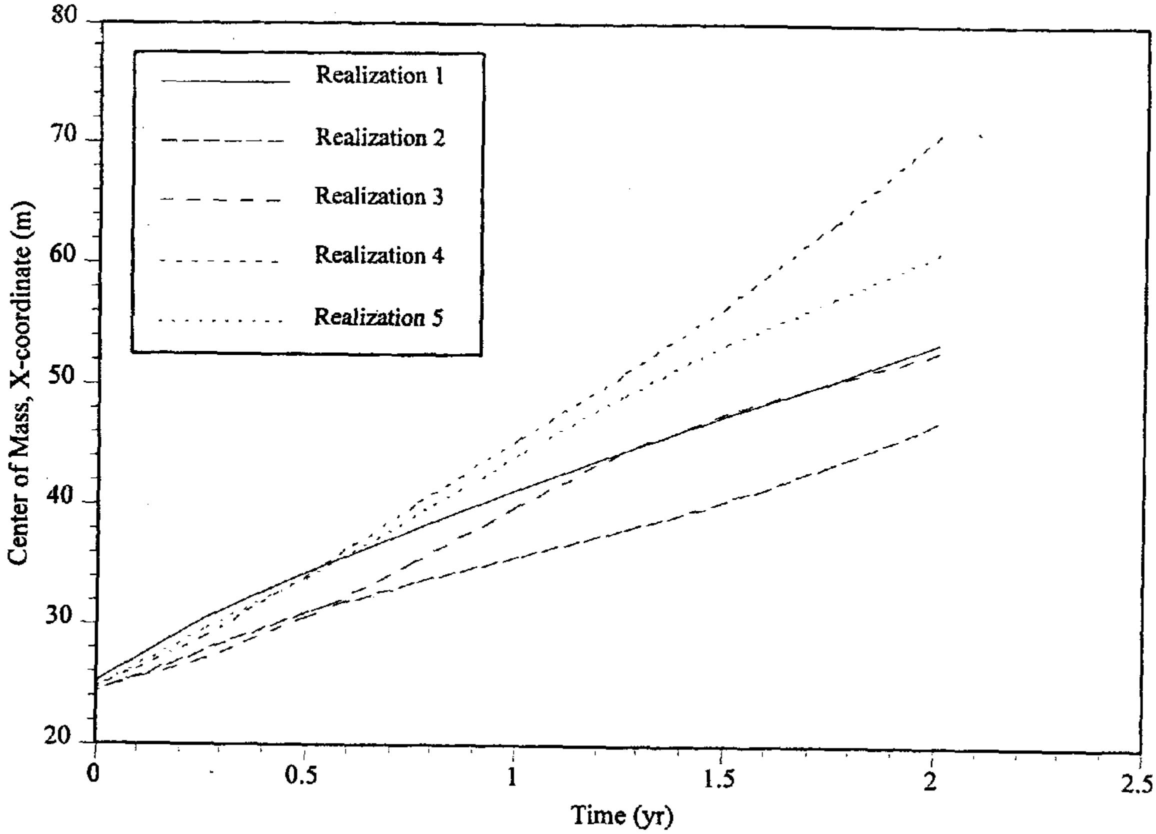
Reactive simulations in a weakly heterogeneous flow field with 0.1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



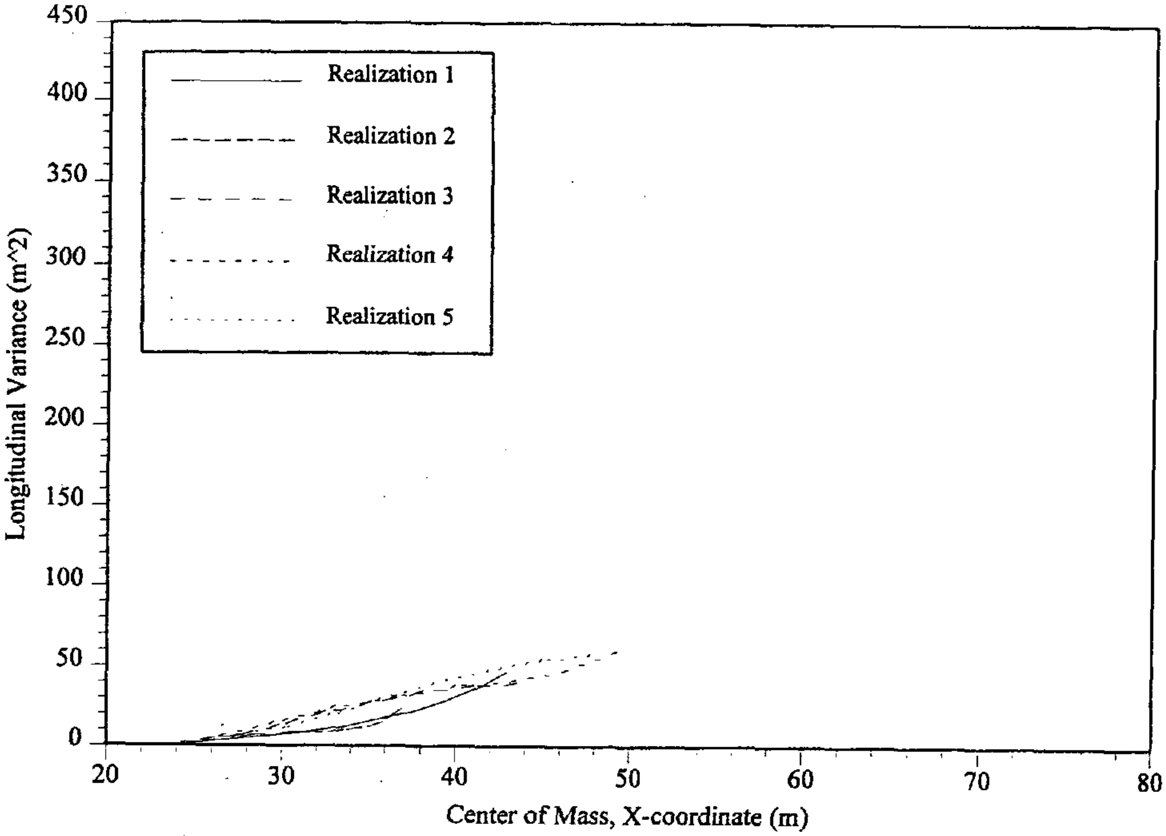
Conservative simulations in a strongly heterogeneous flow field with 1 kg of bromide. All concentrations used in calculations.



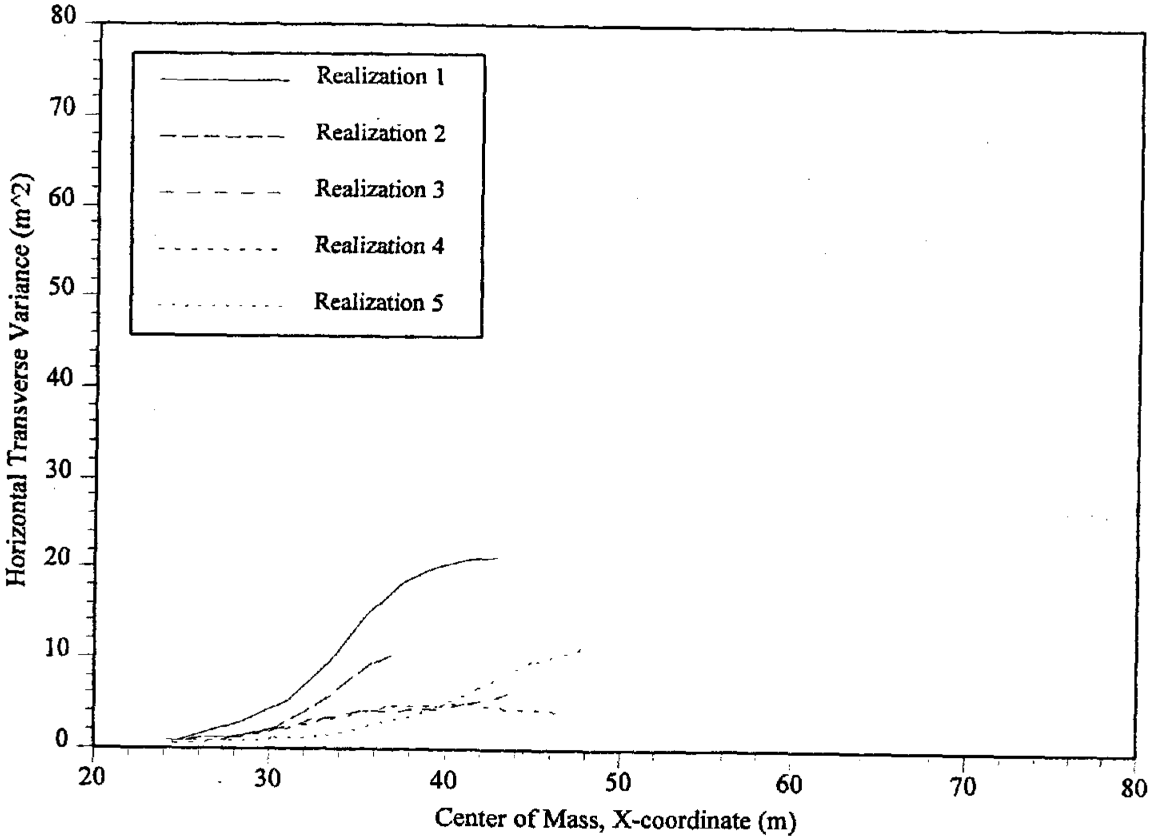
Conservative simulations in a strongly heterogeneous flow field with 1 kg of bromide. All concentrations used in calculations.



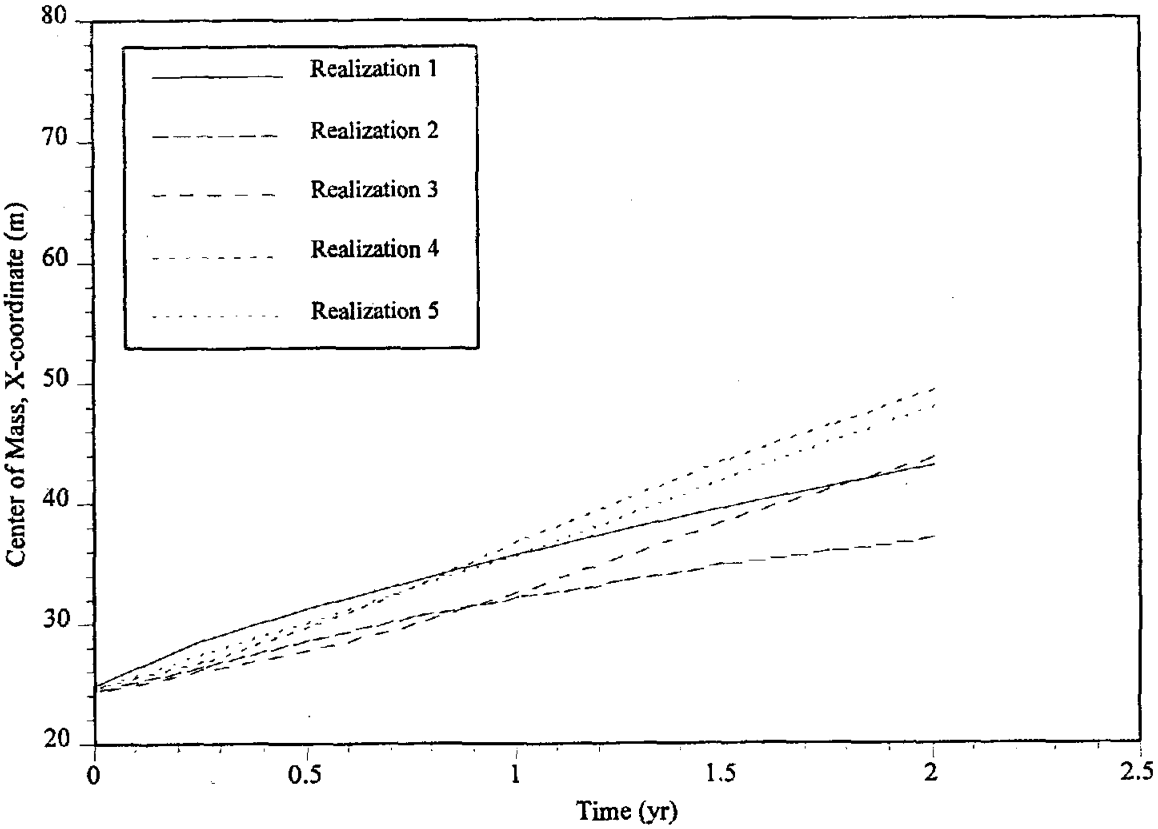
Conservative simulations in a strongly heterogeneous flow field with 1 kg of bromide. All concentrations used in caluclations.



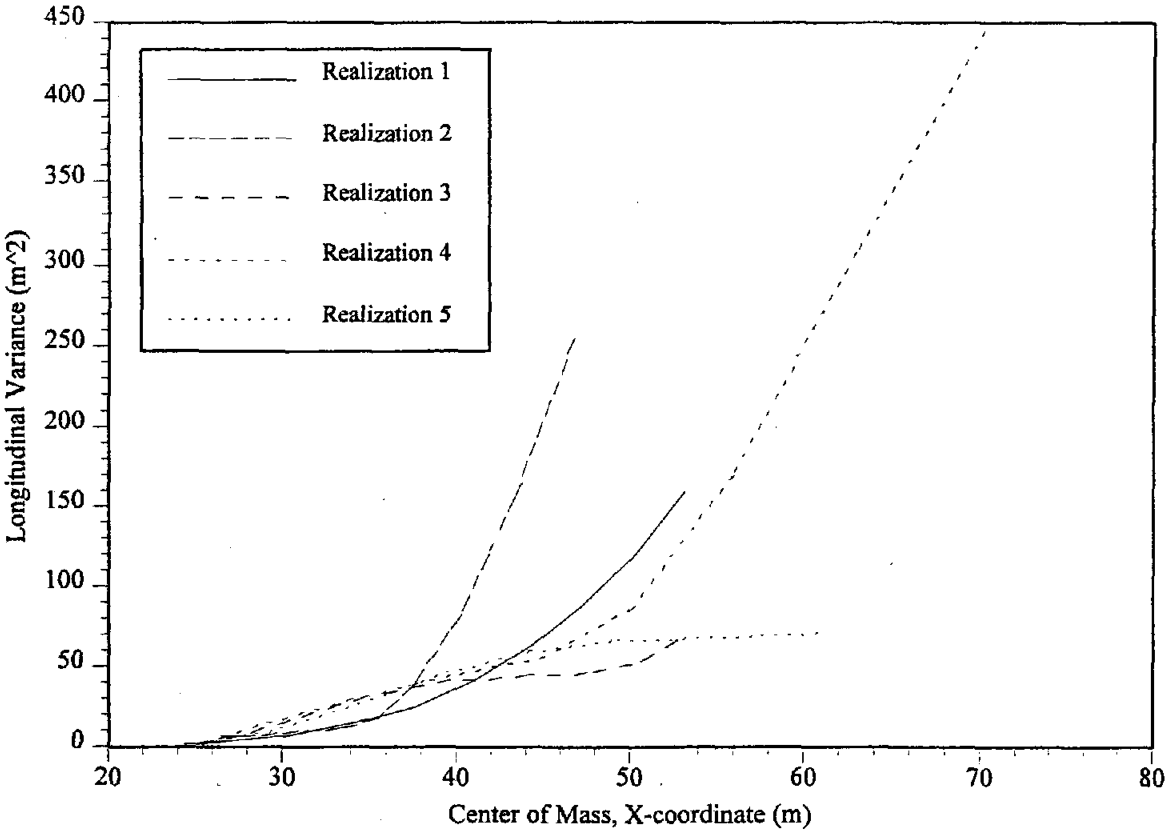
Reactive simulations in a strongly heterogeneous flow field with 1 kg of bromide. All concentrations used in calculations.



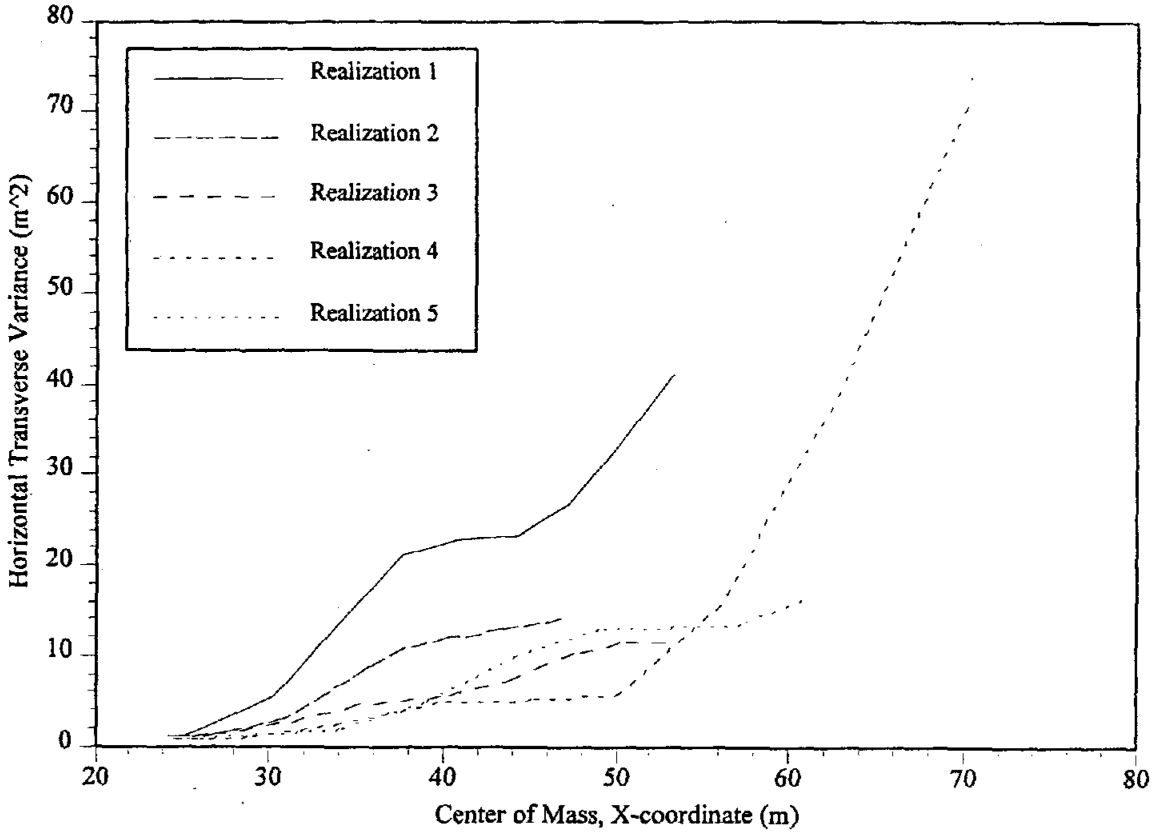
Reactive simulations in a strongly heterogeneous flow field with 1 kg of bromide. All concentrations used in calculations.



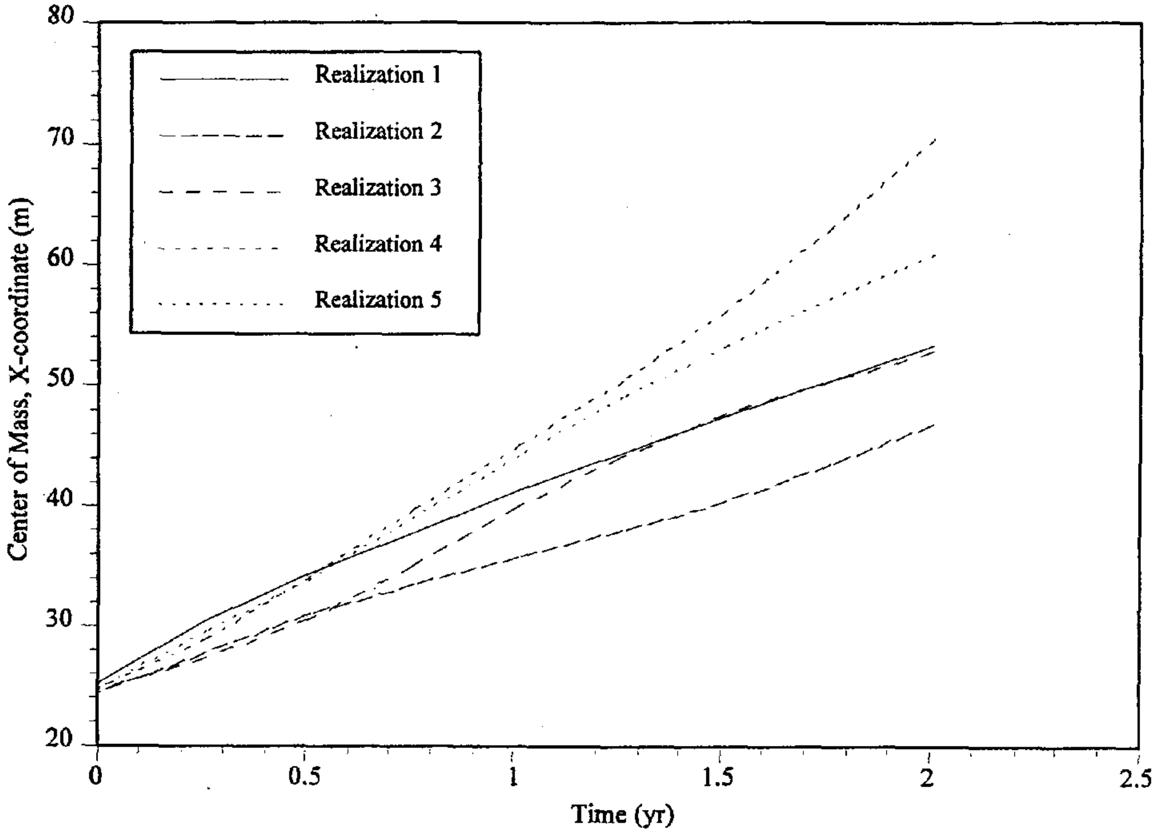
Reactive simulations in a strongly heterogeneous flow field with 1 kg of bromide. All concentrations used in calculations.



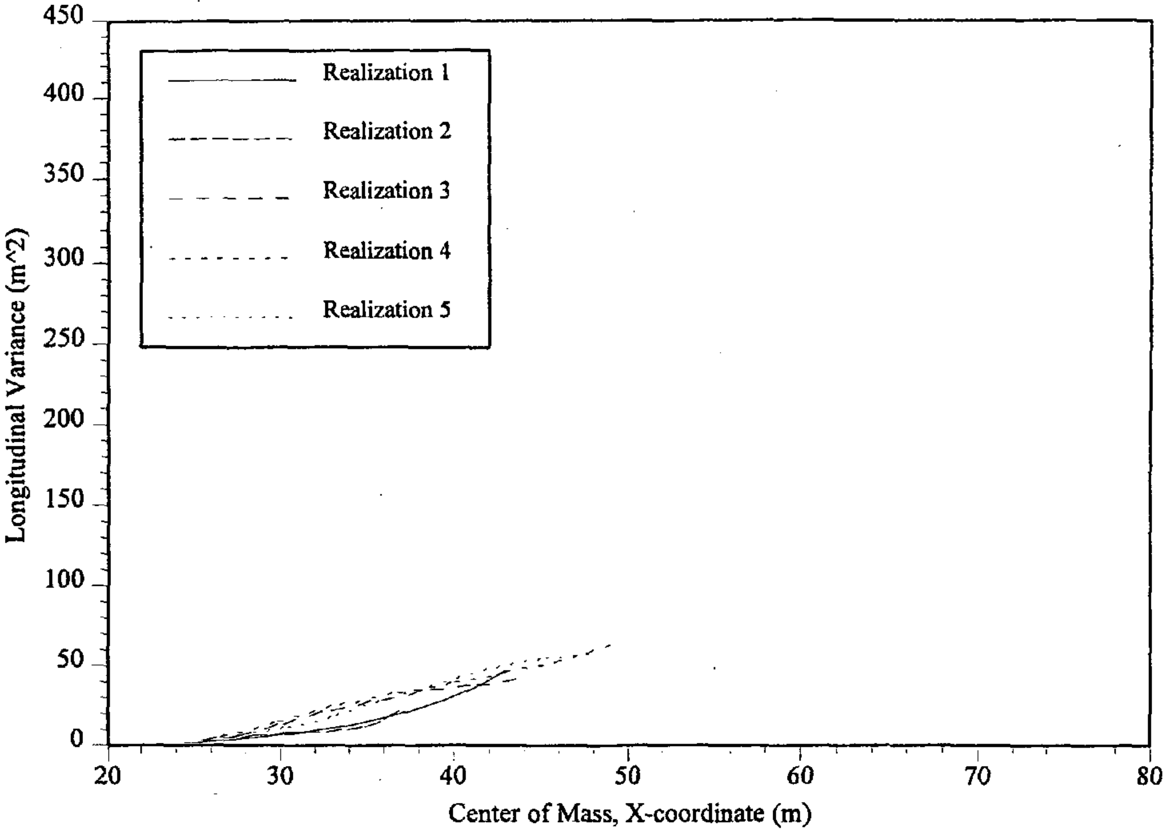
Conservative simulations in a strongly heterogeneous flow field with 1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



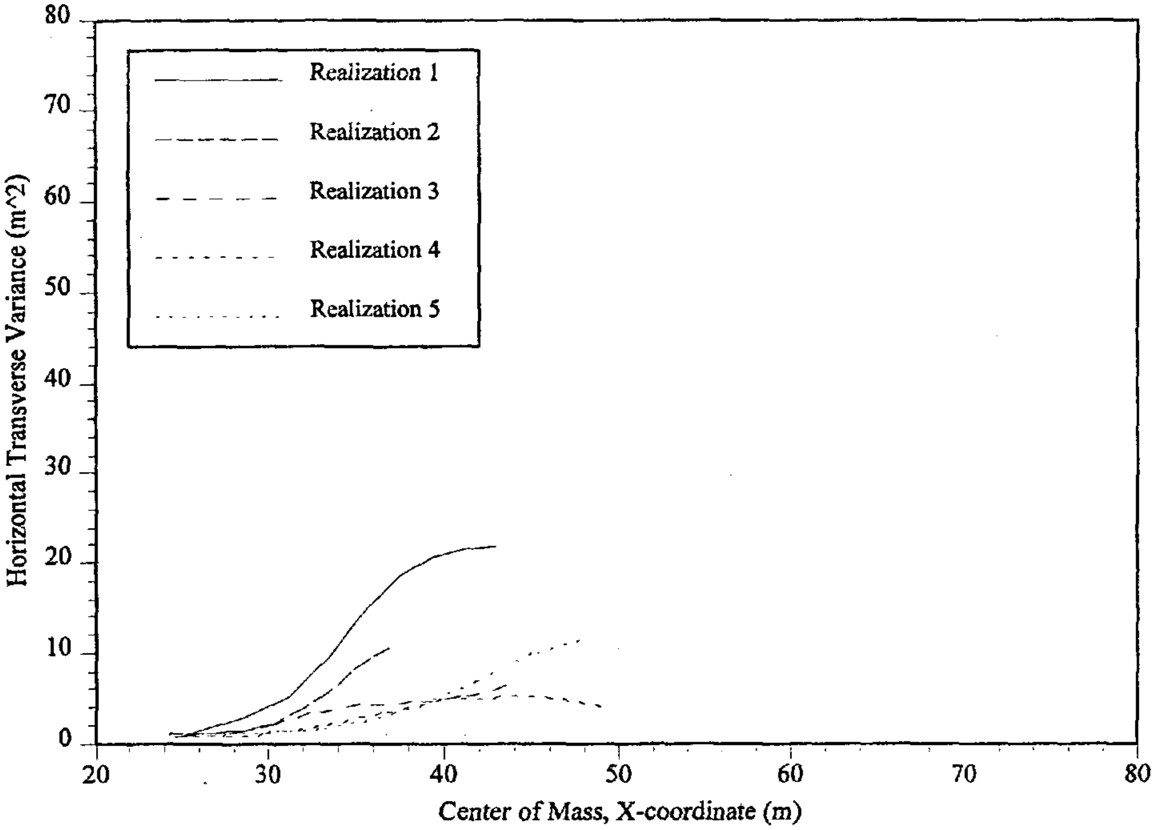
Conservative simulations in a strongly heterogeneous flow field with 1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



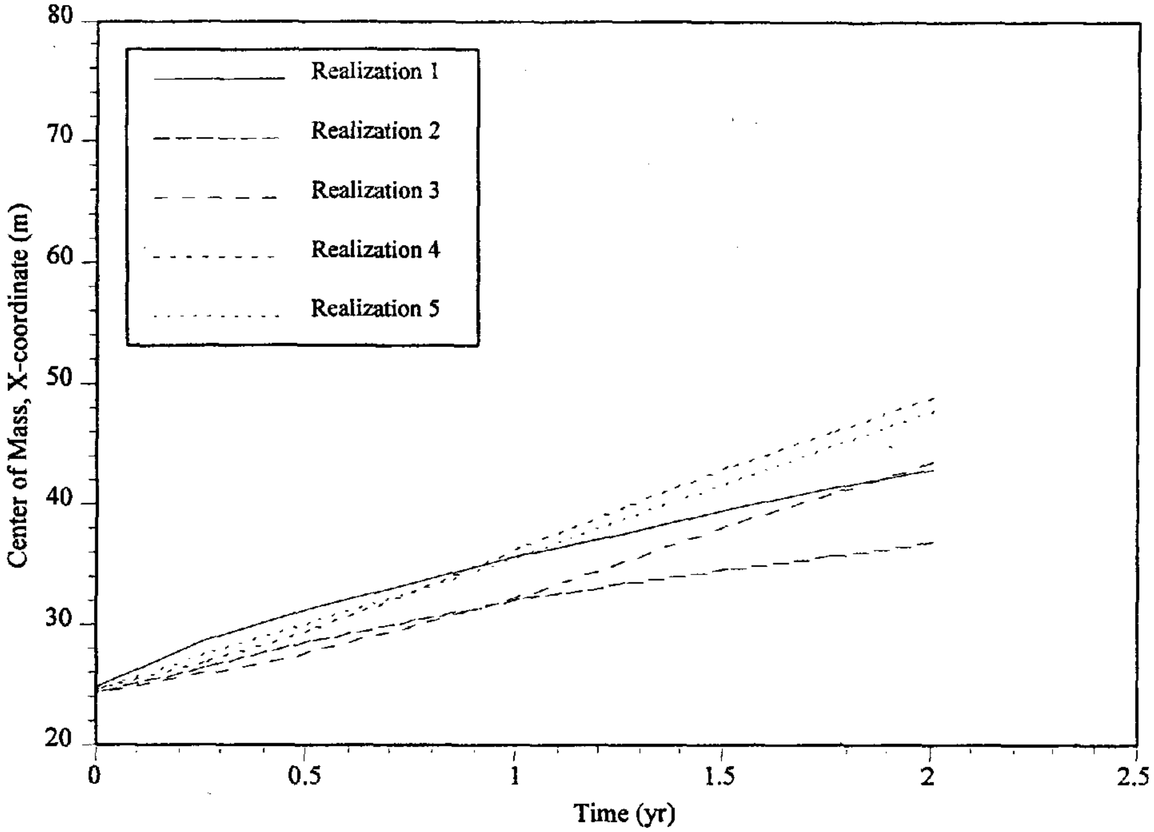
Conservative simulations in a strongly heterogeneous flow field with 1kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



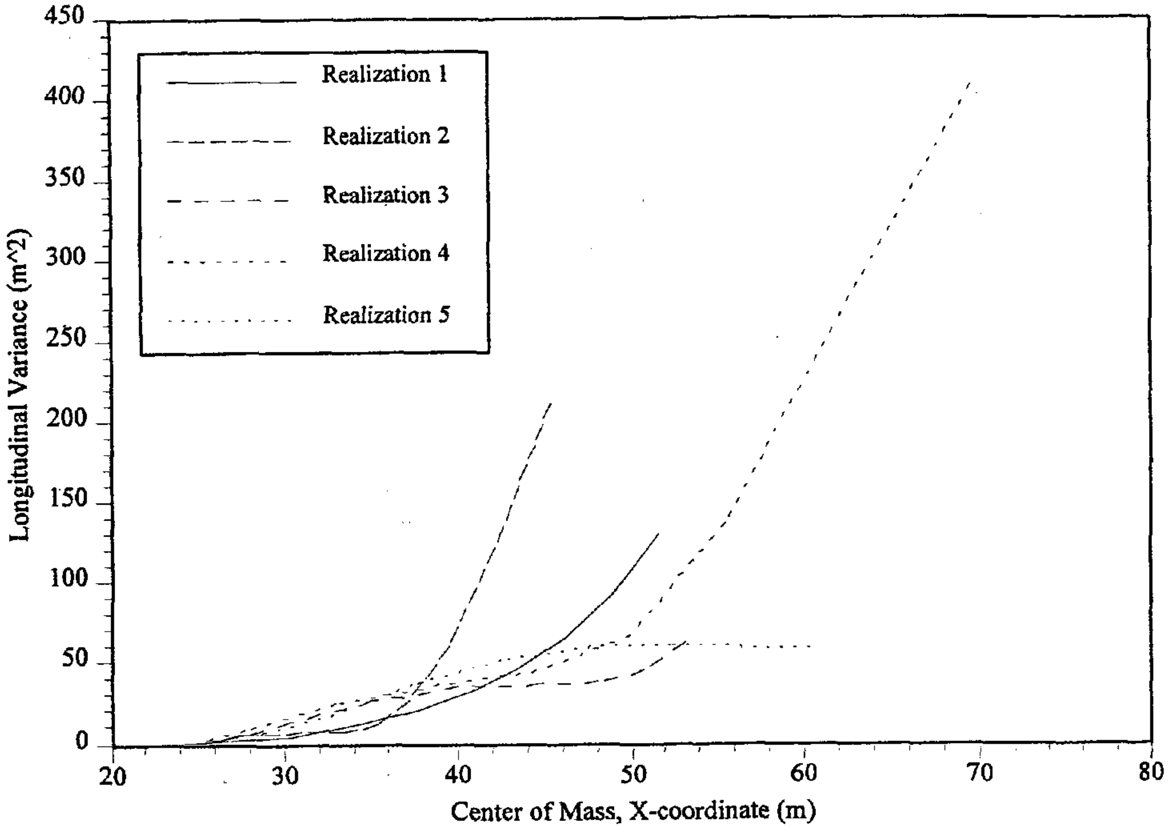
Reactive simulations in a strongly heterogeneous flow field with 1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



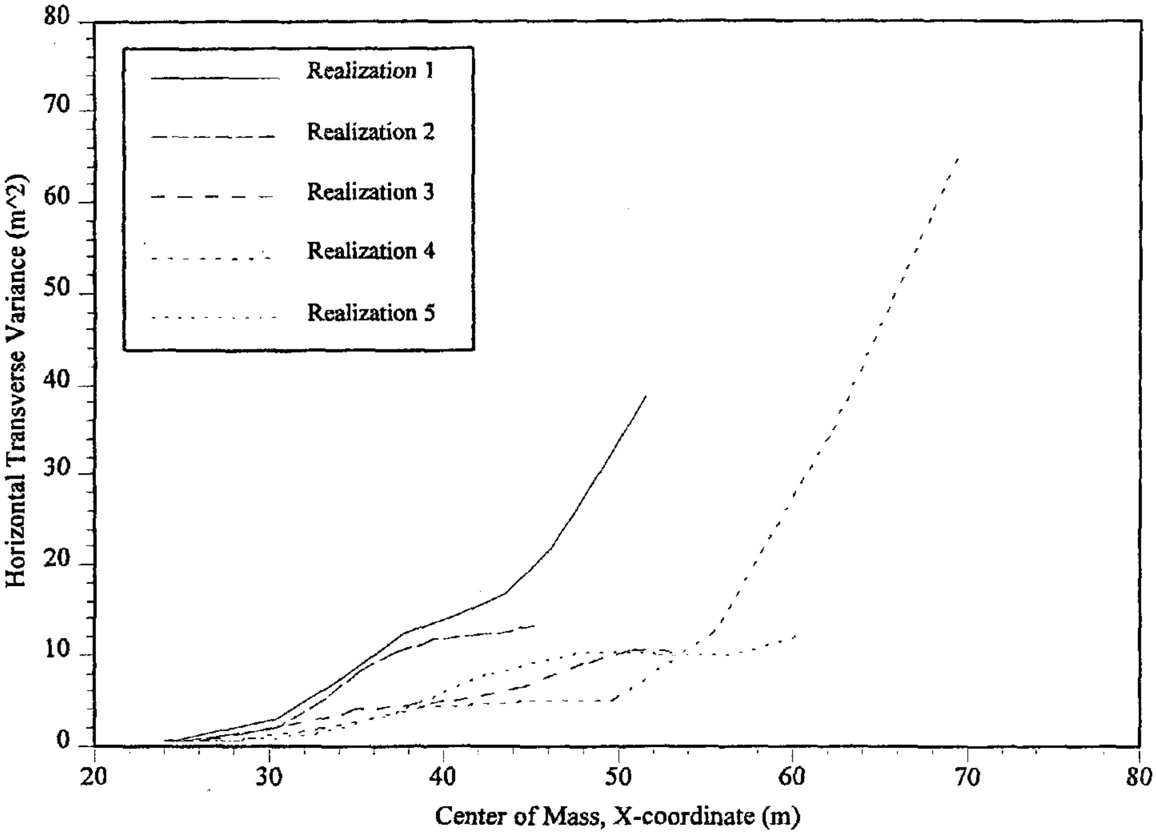
Reactive simulations in a strongly heterogeneous flow field with 1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



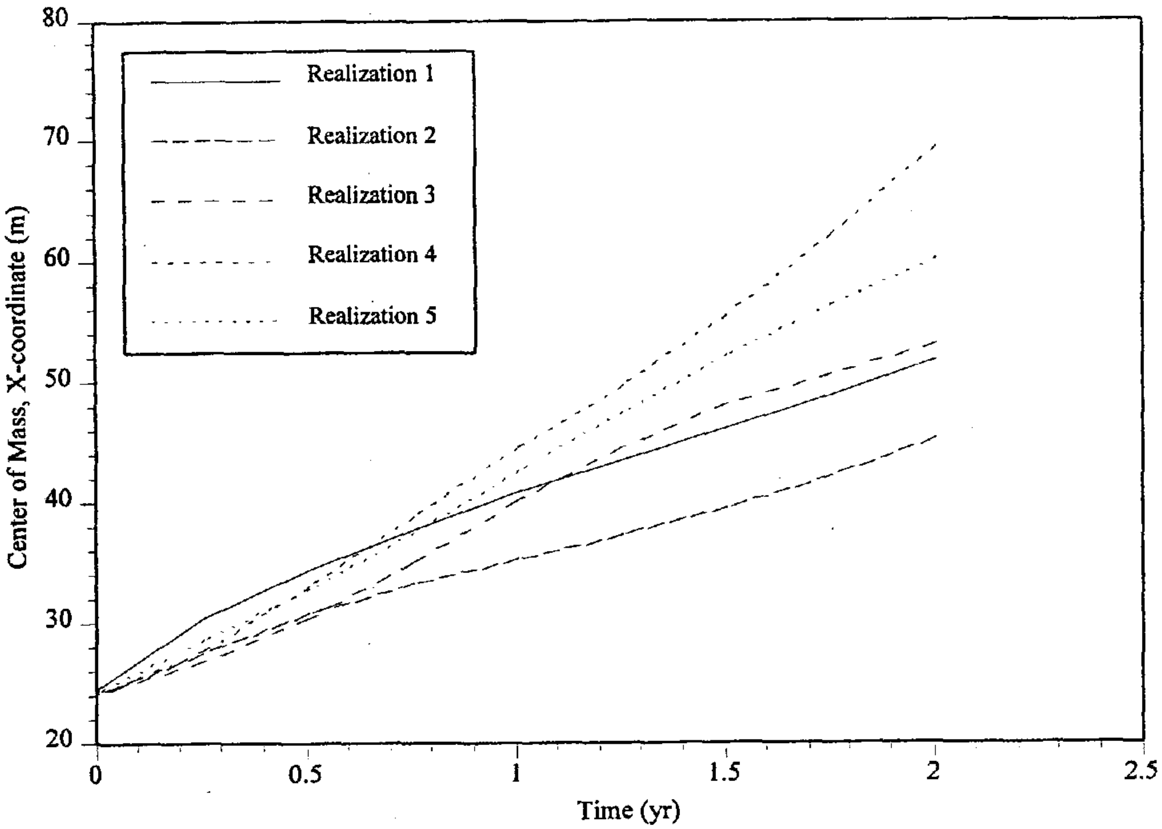
Reactive simulations in a strongly heterogeneous flow field with 1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



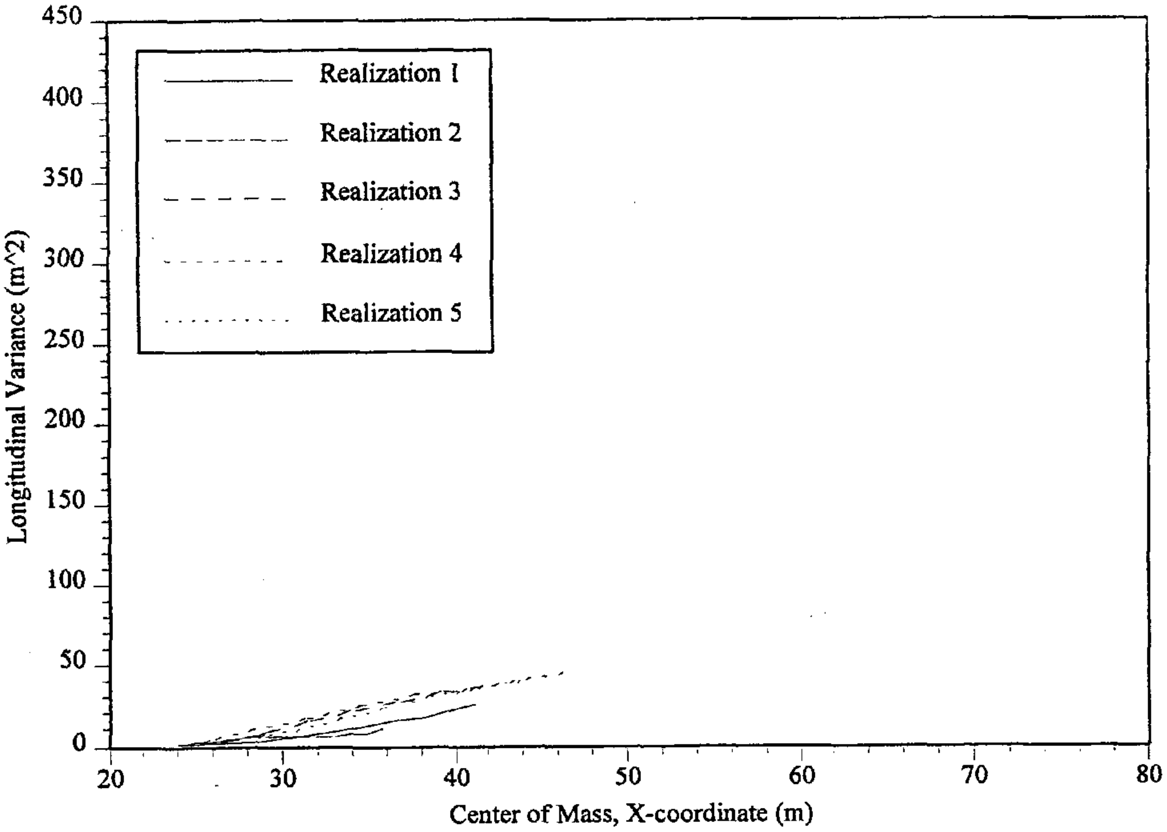
Conservative simulations in a strongly heterogeneous flow field with 0.1 kg of bromide. All concentrations used in calculations.



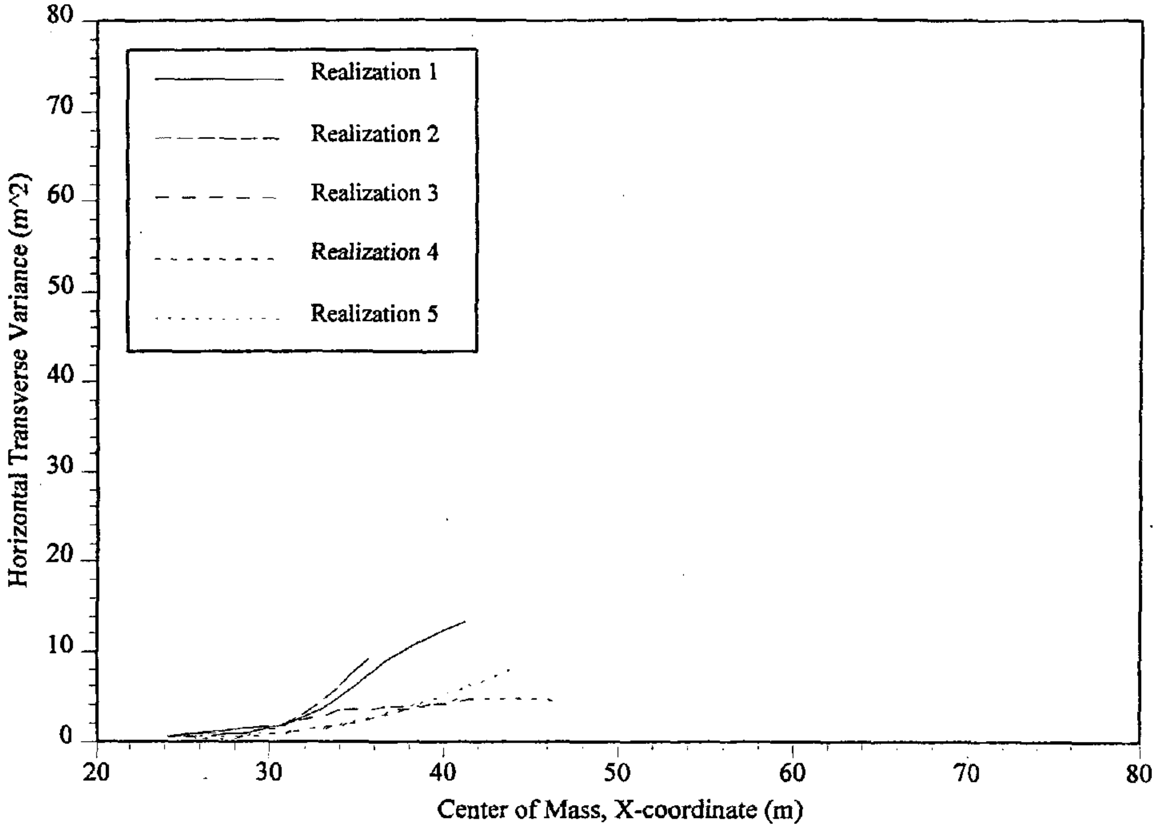
Conservative simulations in a strongly heterogeneous flow field with 0.1 kg of bromide. All concentrations used in calculations.



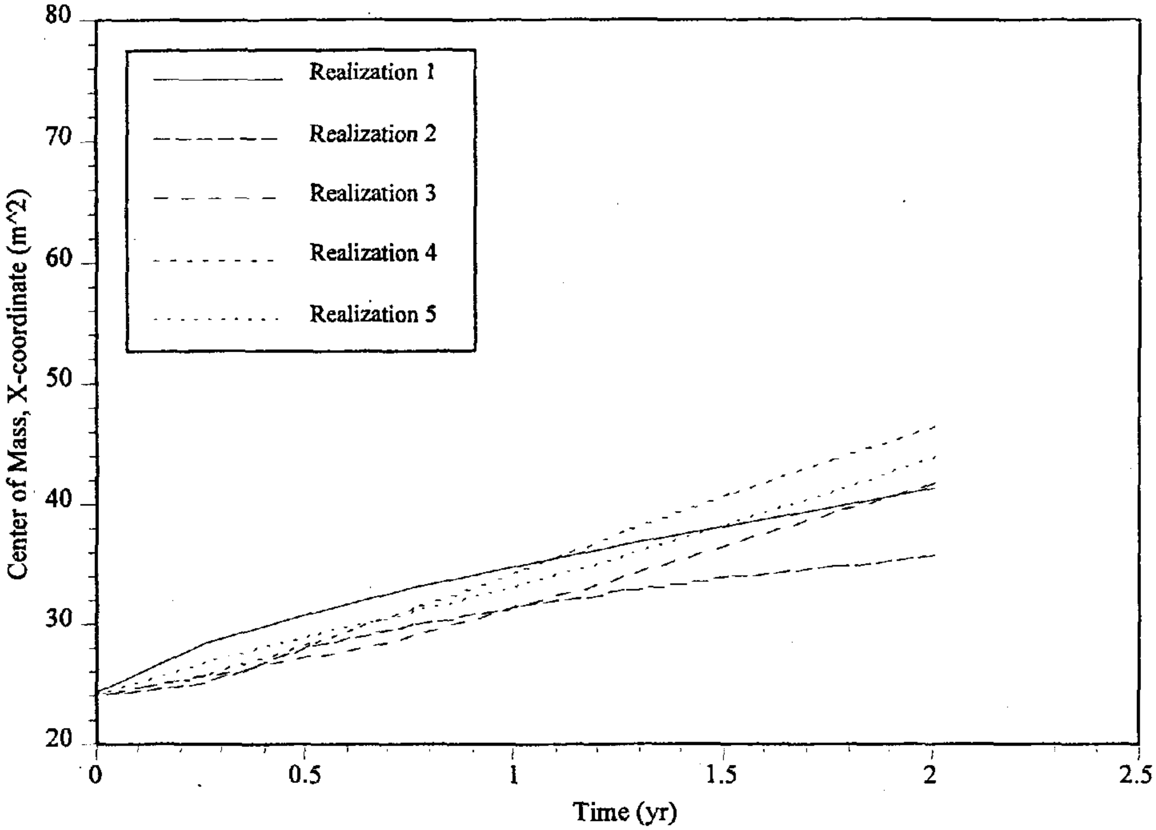
Conservative simulations in a strongly heterogeneous flow field with 0.1 kg of bromide. All concentrations used in calculations.



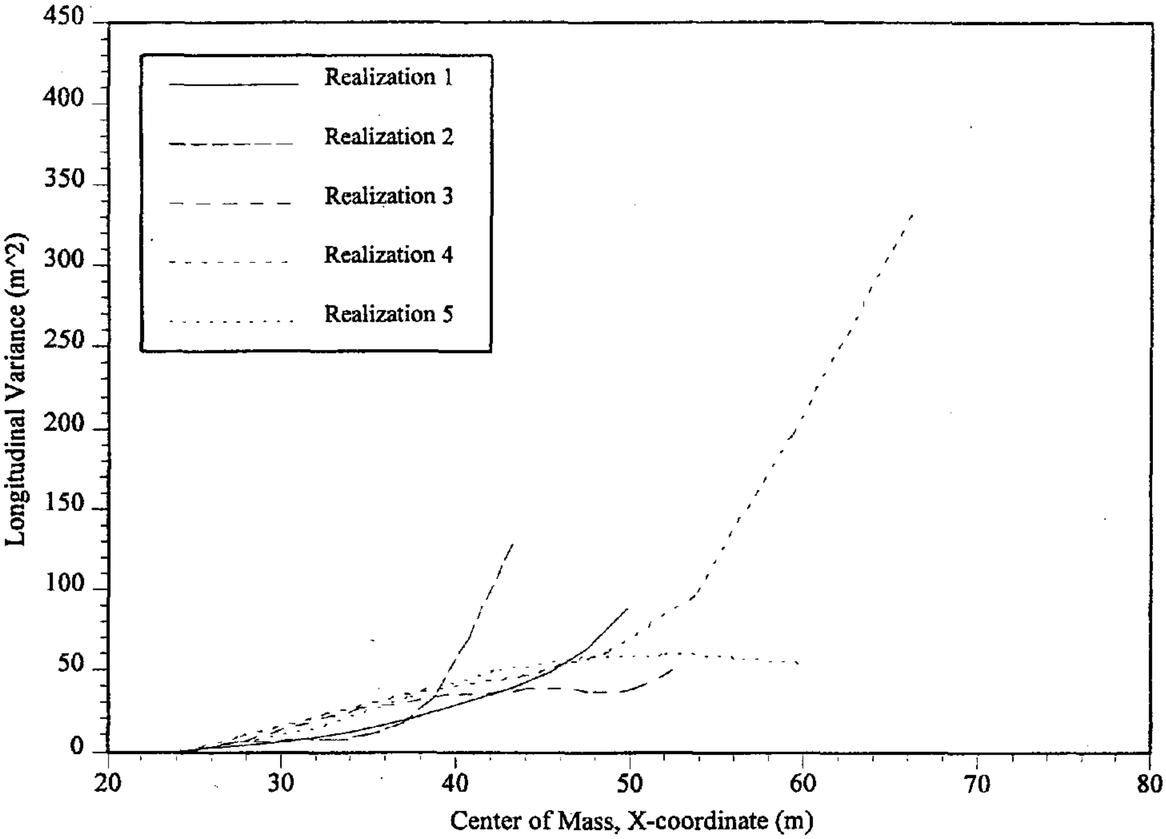
Reactive simulations in a strongly heterogeneous flow field with 0.1 kg of bromide. All concentrations used in calculations.



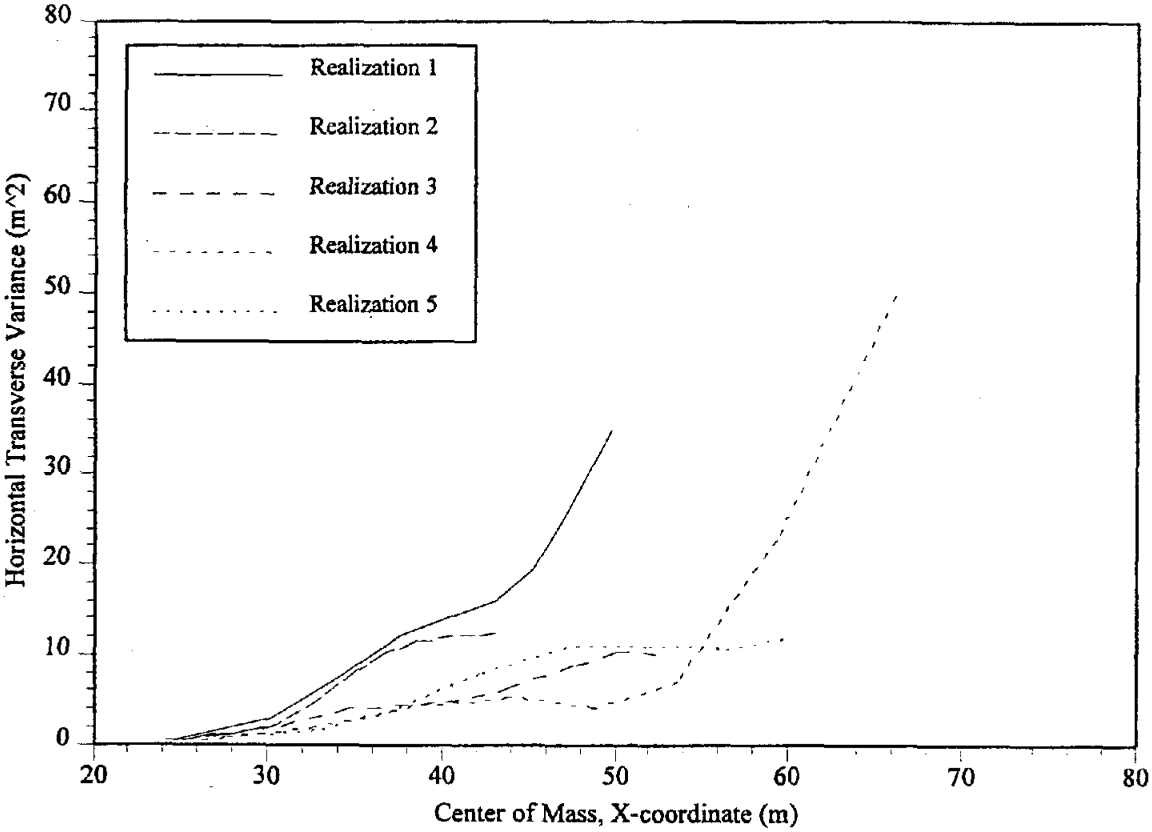
Reactive simulations in a strongly heterogeneous flow field with 0.1 kg of bromide. All concentrations used in calculations.



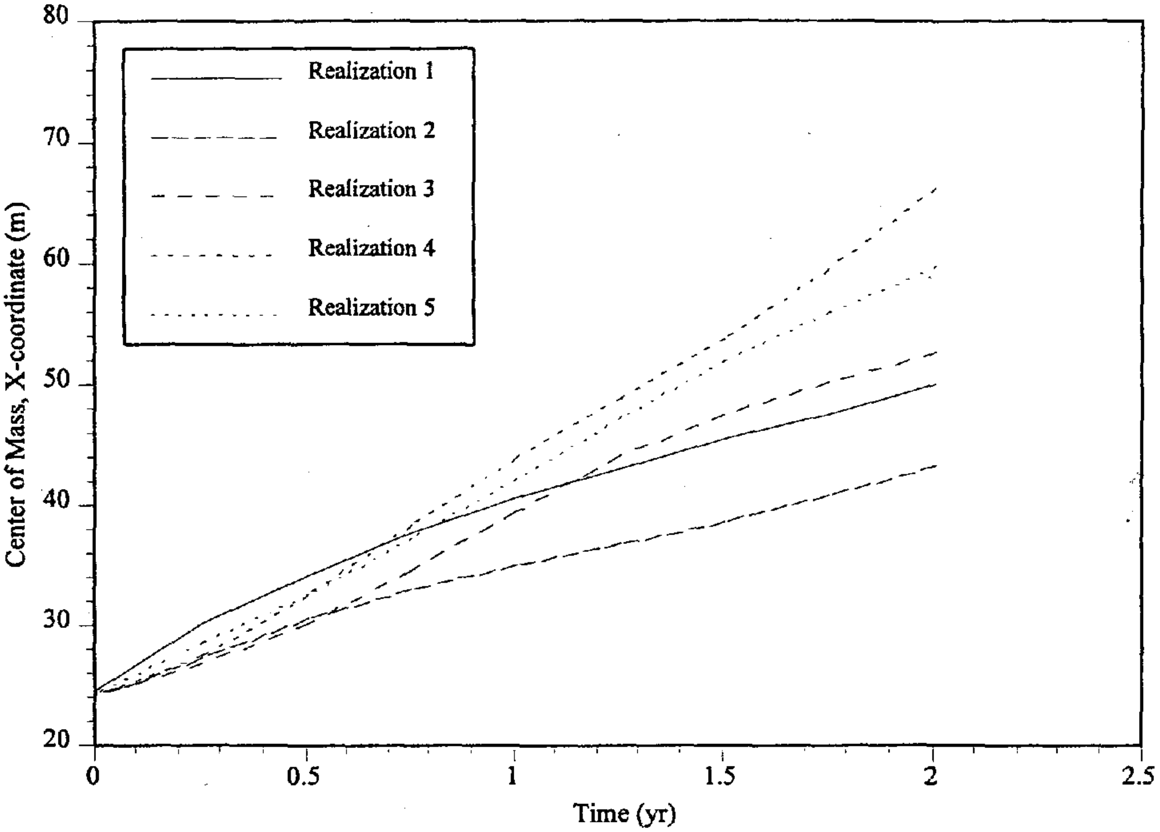
Reactive simulations in a strongly heterogeneous flow field with 0.1 kg of bromide. All concentrations used in calculations.



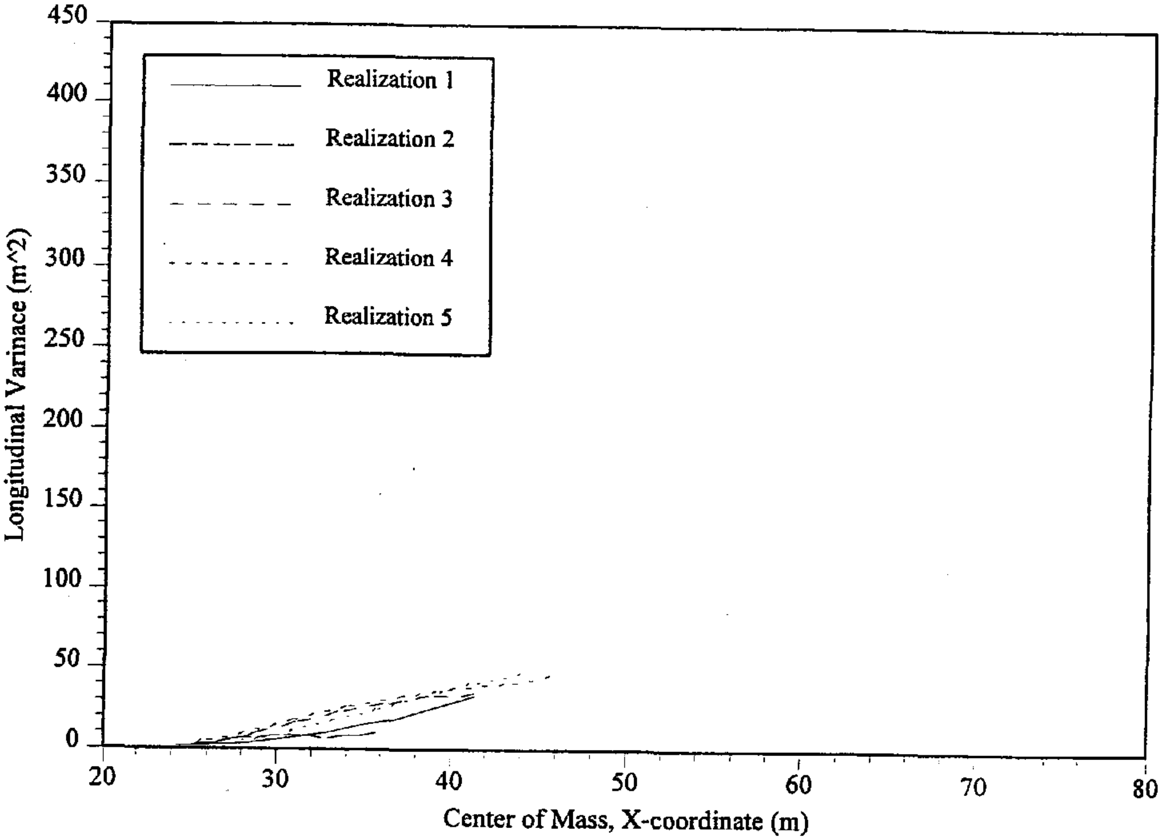
Conservative simulations in a strongly heterogeneous flow field with 0.1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



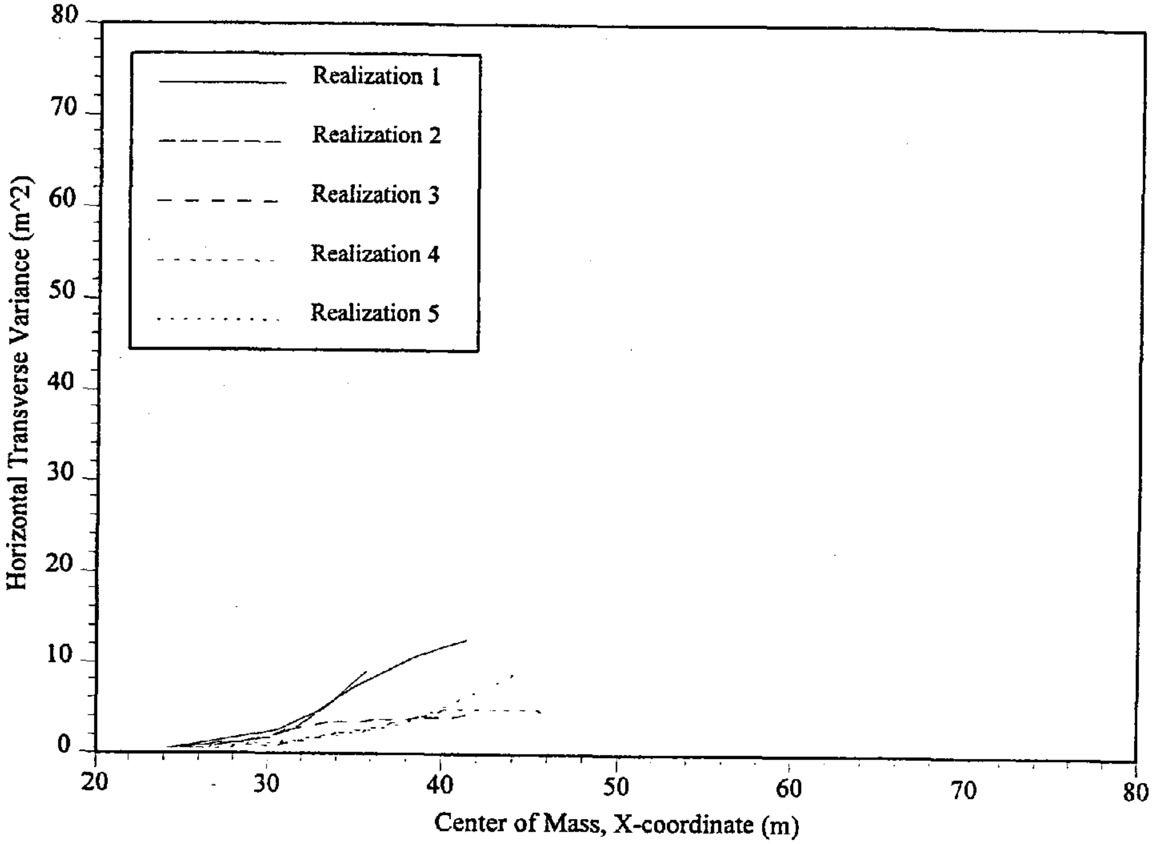
Conservative simulations in a strongly heterogeneous flow field with 0.1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



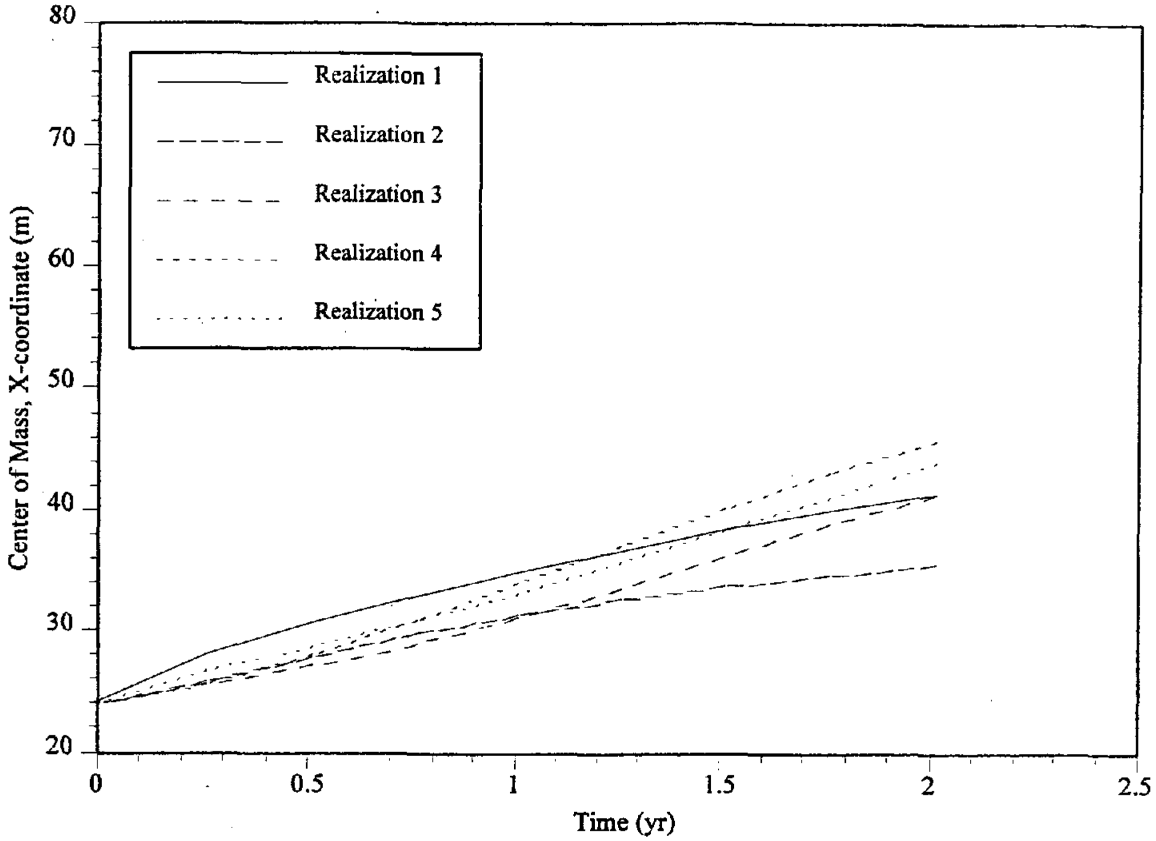
Conservative simulations in a strongly heterogeneous flow field with 0.1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



Reactive simulations in a strongly heterogeneous flow field with 0.1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



Reactive simulations in a strongly heterogeneous flow field with 0.1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.



Reactive simulations in a strongly heterogeneous flow field with 0.1 kg of bromide. Only concentrations greater than 0.1 ppm used in calculations.

# APPENDIX E

# FORTRAN PROGRAMS

```
* THIS PROGRAM TAKES THE RAW NODE CONCENTRATION OUTPUT FROM SUTRA AND
* CALCULATES THE SPATIAL MOMENTS, ZEROTH THROUGH FOURTH.
* A GRID FILE IS ALSO CREATED FOR CONTOURING THE RESULTS IN SURFER.
* ONLY CONCENTRATIONS GREATER THAN 0.1 PPM ARE USED IN THE CALCULATIONS.
* THIS PROGRAM IS DIMENSIONED FOR 9216 ELEMENTS (COLUMBUS & BORDEN AQUIFERS)
* REVISED JULY 8, 1996
*
      PROGRAM SURFHET
      REAL M000,M100,M010,M110,M200,M020,M300,M030,M400,M040,
     + XC,YC,SIGMAXX,SIGMAYY,SIGMAXY,SKX,SKY,KRX,KRY
      DIMENSION C(9500),N(9500),CIJ(9500),XIJ(9500),YIJ(9500)
      OPEN (UNIT=7,FILE='CONC.IN',STATUS='OLD')
      OPEN (UNIT=8,FILE='CONC.TXT',STATUS='UNKNOWN')
      OPEN (UNIT=9,FILE='MOMENTS',STATUS='UNKNOWN')
      P=0.35
      V=1
      D=998.2
C
C  REDUCE THE RAW SUTRA NODE CONCENTRATION OUTPUT FROM 6 COLUMNS TO 1
C
      DO 10 K=1,9420,6
        READ (7,200)N(K),C(K),N(K+1),C(K+1),N(K+2),C(K+2),N(K+3),
     +          C(K+3),N(K+4),C(K+4),N(K+5),C(K+5)
200     FORMAT (7X,I5,G16.8,I5,G16.8,I5,G16.8,I5,G16.8,I5,G16.8,I5,
     +        G16.8)
10    CONTINUE
      READ (7,300)N(9421),C(9421),N(9422),C(9422),N(9423),C(9423),
     +          N(9424),C(9424),N(9425),C(9425)
300   FORMAT (7X,I5,G16.8,I5,G16.8,I5,G16.8,I5,G16.8,I5,G16.8)
C
C  AVERAGE THE 4 NODE CONCENTRATIONS AROUND EACH ELEMENT TO PERFORM
C  THE MOMENT CALCULATIONS ON THE ELEMENTS (RATHER THAN THE NODES) AND
C  CALCULATE THE X AND Y-COORDINATES OF EACH ELEMENT
C
      DO 20 I=1,144,1
      DO 30 J=1,64,1
        C1=((I-1)*65+J)
        C2=(I*65+J)
        C3=(I*65+1+J)
        C4=((I-1)*65+1+J)
        CIJ(K)=(C(C1)+C(C2)+C(C3)+C(C4))/4
        IF (CIJ(K).LT.1.0E-7) THEN
          CIJ(K)=0.0
        ENDIF
        XIJ(K)=(I-0.5)
        YIJ(K)=(J-0.5)
        WRITE (8,400)XIJ(K),YIJ(K),CIJ(K)
400     FORMAT (E16.8,E16.8,E16.8)
30    CONTINUE
20    CONTINUE
C
C  READ IN THE ELEMENT CONCENTRATIONS AND COORDINATES CALCULATED ABOVE
C
      CLOSE (8)
      OPEN (UNIT=8,FILE='CONC.TXT',STATUS='UNKNOWN')
      DO 35 K=1,9216,1
```

Program SURFHET (continued)

```
      READ (8,400)XIJ(K),YIJ(K),CIJ(K)
35    CONTINUE
C
C  ZEROTH MOMENT (TOTAL MASS)
C
     SUM=0.0
     DO 40 K=1,9216,1
      SUM=SUM+CIJ(K)*P*V*D
40    CONTINUE
     M000=SUM
C
C  FIRST MOMENT, X (CENTER OF MASS IN THE X DIRECTION)
C
     SUM=0.0
     DO 50 K=1,9216,1
      SUM=SUM+CIJ(K)*P*V*D*XIJ(K)
50    CONTINUE
     M100=SUM
     XC=M100/M000
C
C  FIRST MOMENT, Y (CENTER OF MASS IN THE Y DIRECTION)
C
     SUM=0.0
     DO 55 K=1,9216,1
      SUM=SUM+CIJ(K)*P*V*D*YIJ(K)
55    CONTINUE
     M010=SUM
     YC=M010/M000
C
C  SECOND MOMENT, XX (SPATIAL VARIANCE IN THE X DIRECTION)
C
     SUM=0.0
     DO 60 K=1,9216,1
      SUM=SUM+CIJ(K)*P*V*D*(XIJ(K)**2)
60    CONTINUE
     M200=SUM
     SIGMAXX=(M200/M000)-(XC**2)
C
C  SECOND MOMENT, YY (SPATIAL VARIANCE IN THE Y DIRECTION)
C
     SUM=0.0
     DO 70 K=1,9216,1
      SUM=SUM+CIJ(K)*P*V*D*(YIJ(K)**2)
70    CONTINUE
     M020=SUM
     SIGMAYY=(M020/M000)-YC**2
C
C  SECOND MOMENT, XY (SPATIAL COVARIANCE)
C
     SUM=0.0
     DO 80 K=1,9216,1
      SUM=SUM+CIJ(K)*P*V*D*XIJ(K)*YIJ(K)
80    CONTINUE
     M110=SUM
     SIGMAXY=(M110/M000)-(XC*YC)
```

Program SURFHET (continued)

```
C  THIRD MOMENT, X (SKEWNESS OF THE PLUME IN THE X DIRECTION)
C
      SUM=0.0
      DO 90 K=1,9216,1
        SUM=SUM+CIJ(K)*P*V*D*((XIJ(K)-XC)**3)
90    CONTINUE
      M300=SUM
      SKX=M300/(M000*(SIGMAXX**(3/2)))
C
C  THIRD MOMENT, Y (SKEWNESS OF THE PLUME IN THE Y DIRECTION)
C
      SUM=0.0
      DO 100 K=1,9216,1
        SUM=SUM+CIJ(K)*P*V*D*((YIJ(K)-YC)**3)
100   CONTINUE
      M030=SUM
      SKY=M030/(M000*(SIGMAYY**(3/2)))
C
C  FOURTH MOMENT, X (KURTOSIS OF THE PLUME IN THE X DIRECTION)
C
      SUM=0.0
      DO 110 K=1,9216,1
        SUM=SUM+CIJ(K)*P*V*D*((XIJ(K)-XC)**4)
110   CONTINUE
      M400=SUM
      KRX=M400/(M000*(SIGMAXX**2))
C  FOURTH MOMENT, Y (KURTOSIS OF THE PLUME IN THE Y DIRECTION)
      SUM=0.0
      DO 120 K=1,9216,1
        SUM=SUM+CIJ(K)*P*V*D*((YIJ(K)-YC)**4)
120   CONTINUE
      M040=SUM
      KRY=M040/(M000*(SIGMAYY**2))
      WRITE (9,500)M000,XC,YC,SIGMAXX,SIGMAYY,SIGMAXY,SKX,SKY,KRX,KRY
500   FORMAT (//,'****S P A T I A L   M O M E N T   C A L C U',
     A 'L A T I O N S****',//,
     B '####################################',/,
     C '# CONCENTRATIONS < 0.1 PPM OMITTED #',/,
     D '####################################',////,
     E 'MASS OF BROMIDE (KG)',/2X,'M000=',G14.7,//,
     F 'CENTER OF MASS, X-COORDINATE (M)',/2X,'XC=',G14.7,//,
     G 'CENTER OF MASS, Y-COORDINATE (M)',/2X,'YC=',G14.7,//,
     H 'SPATIAL VARIANCE, XX',/2X,'SIGMAXX=',G14.7,//,
     I 'SPATIAL VARIANCE, YY',/2X,'SIGMAYY=',G14.7,//,
     J 'SPATIAL COVARIANCE, XY',/2X,'SIGMAXY=',G14.7,//,
     K 'SKEWNESS OF THE PLUME, X',/2X,'SKX=',G14.7,//,
     L 'SKEWNESS OF THE PLUME, Y',/2X,'SKY=',G14.7,//,
     M 'KURTOSIS OF THE PLUME, X',/2X,'KRX=',G14.7,//,
     N 'KURTOSIS OF THE PLUME, Y',/2X,'KRY=',G14.7)
      CLOSE (7)
      CLOSE (8)
      CLOSE (9)
      STOP
      END
```

```
* THIS PROGRAM TAKES THE RAW NODE CONCENTRATION OUTPUT FROM SUTRA AND
* CALCULATES THE SPATIAL MOMENTS, ZEROTH THROUGH FOURTH.  A GRID FILE IS
* ALSO CREATED FOR CONTOURING THE RESULTS IN SURFER.  ALL CONCENTRATIONS
* ARE USED IN THE CALCULATIONS.  THIS PROGRAM IS DIMENSIONED FOR 9216
* ELEMENTS (COLUMBUS AND BORDEN AQUIFERS).  REVISED JULY 8, 1996
*
      PROGRAM SURFHET2
      REAL M000,M100,M010,M110,M200,M020,M300,M030,M400,M040,
     +  XC,YC,SIGMAXX,SIGMAYY,SIGMAXY,SKX,SKY,KRX,KRY
      DIMENSION C(9500),N(9500),CIJ(9500),XIJ(9500),YIJ(9500)
      OPEN (UNIT=7,FILE='CONC.IN',STATUS='OLD')
      OPEN (UNIT=8,FILE='CONC.TXT',STATUS='UNKNOWN')
      OPEN (UNIT=9,FILE='MOMENTS',STATUS='UNKNOWN')
      P=0.35
      V=1
      D=998.2
C
C  REDUCE THE RAW SUTRA NODE CONCENTRATION OUTPUT FROM 6 COLUMNS TO 1
C
      DO 10 K=1,9420,6
       READ (7,200)N(K),C(K),N(K+1),C(K+1),N(K+2),C(K+2),N(K+3),
     +           C(K+3),N(K+4),C(K+4),N(K+5),C(K+5)
200    FORMAT (7X,I5,G16.8,I5,G16.8,I5,G16.8,I5,G16.8,I5,G16.8,I5,
     +        G16.8)
10    CONTINUE
      READ (7,300)N(9421),C(9421),N(9422),C(9422),N(9423),C(9423),
     +          N(9424),C(9424),N(9425),C(9425)
300   FORMAT (7X,I5,G16.8,I5,G16.8,I5,G16.8,I5,G16.8,I5,G16.8)
C
C  AVERAGE THE 4 NODE CONCENTRATIONS AROUND EACH ELEMENT TO PERFORM
C  THE MOMENT CALCULATIONS ON THE ELEMENTS (RATHER THAN THE NODES) AND
C  CALCULATE THE X AND Y-COORDINATES OF EACH ELEMENT
C
      DO 20 I=1,144,1
      DO 30 J=1,64,1
       C1=((I-1)*65+J)
       C2=(I*65+J)
       C3=(I*65+1+J)
       C4=((I-1)*65+1+J)
       CIJ(K)=(C(C1)+C(C2)+C(C3)+C(C4))/4
       XIJ(K)=(I-0.5)
       YIJ(K)=(J-0.5)
       WRITE (8,400)XIJ(K),YIJ(K),CIJ(K)
400    FORMAT (E16.8,E16.8,E16.8)
30    CONTINUE
20    CONTINUE
C
C  READ IN THE ELEMENT CONCENTRATIONS AND COORDINATES CALCULATED ABOVE
C
      CLOSE (8)
      OPEN (UNIT=8,FILE='CONC.TXT',STATUS='UNKNOWN')
      DO 35 K=1,9216,1
       READ (8,400)XIJ(K),YIJ(K),CIJ(K)
35    CONTINUE
C
C  ZEROTH MOMENT (TOTAL MASS)
```

Program SURFHET2 (continued)

```
      SUM=0.0
      DO 40 K=1,9216,1
        SUM=SUM+CIJ(K)*P*V*D
40    CONTINUE
      M000=SUM
C
C  FIRST MOMENT, X (CENTER OF MASS IN THE X DIRECTION)
C
      SUM=0.0
      DO 50 K=1,9216,1
        SUM=SUM+CIJ(K)*P*V*D*XIJ(K)
50    CONTINUE
      M100=SUM
      XC=M100/M000
C
C  FIRST MOMENT, Y (CENTER OF MASS IN THE Y DIRECTION)
C
      SUM=0.0
      DO 55 K=1,9216,1
        SUM=SUM+CIJ(K)*P*V*D*YIJ(K)
55    CONTINUE
      M010=SUM
      YC=M010/M000
C
C  SECOND MOMENT, XX (SPATIAL VARIANCE IN THE X DIRECTION)
C
      SUM=0.0
      DO 60 K=1,9216,1
        SUM=SUM+CIJ(K)*P*V*D*(XIJ(K)**2)
60    CONTINUE
      M200=SUM
      SIGMAXX=(M200/M000)-(XC**2)
C
C  SECOND MOMENT, YY (SPATIAL VARIANCE IN THE Y DIRECTION)
C
      SUM=0.0
      DO 70 K=1,9216,1
        SUM=SUM+CIJ(K)*P*V*D*(YIJ(K)**2)
70    CONTINUE
      M020=SUM
      SIGMAYY=(M020/M000)-YC**2
C
C  SECOND MOMENT, XY (SPATIAL COVARIANCE)
C
      SUM=0.0
      DO 80 K=1,9216,1
        SUM=SUM+CIJ(K)*P*V*D*XIJ(K)*YIJ(K)
80    CONTINUE
      M110=SUM
      SIGMAXY=(M110/M000)-(XC*YC)
C
C  THIRD MOMENT, X (SKEWNESS OF THE PLUME IN THE X DIRECTION)
C
      SUM=0.0
      DO 90 K=1,9216,1
```

Program SURFHET2 (continued)

```
       SUM=SUM+CIJ(K)*P*V*D*((XIJ(K)-XC)**3)
90     CONTINUE
      M300=SUM
      SKX=M300/(M000*(SIGMAXX**(3/2)))
C
C  THIRD MOMENT, Y (SKEWNESS OF THE PLUME IN THE Y DIRECTION)
C
      SUM=0.0
      DO 100 K=1,9216,1
       SUM=SUM+CIJ(K)*P*V*D*((YIJ(K)-YC)**3)
100    CONTINUE
      M030=SUM
      SKY=M030/(M000*(SIGMAYY**(3/2)))
C
C  FOURTH MOMENT, X (KURTOSIS OF THE PLUME IN THE X DIRECTION)
C
      SUM=0.0
      DO 110 K=1,9216,1
       SUM=SUM+CIJ(K)*P*V*D*((XIJ(K)-XC)**4)
110    CONTINUE
      M400=SUM
      KRX=M400/(M000*(SIGMAXX**2))
C
C  FOURTH MOMENT, Y (KURTOSIS OF THE PLUME IN THE Y DIRECTION)
C
      SUM=0.0
      DO 120 K=1,9216,1
       SUM=SUM+CIJ(K)*P*V*D*((YIJ(K)-YC)**4)
120    CONTINUE
      M040=SUM
      KRY=M040/(M000*(SIGMAYY**2))
      WRITE (9,500)M000,XC,YC,SIGMAXX,SIGMAYY,SIGMAXY;SKX,SKY,KRX,KRY
500    FORMAT (//,'****S P A T I A L  M O M E N T  C A L C U L',
     A 'A T I O N S****',//,
     B '###########################################',/,
     C '# ALL CONCENTRATIONS USED IN CALCULATIONS #',/,
     D '###########################################',////,
     E 'MASS OF BROMIDE (KG)',/2X,'M000=',G14.7,//,
     F 'CENTER OF MASS, X-COORDINATE (M)',/2X,'XC=',G14.7,//,
     G 'CENTER OF MASS, Y-COORDINATE (M)',/2X,'YC=',G14.7,//,
     H 'SPATIAL VARIANCE, XX',/2X,'SIGMAXX=',G14.7,//,
     I 'SPATIAL VARIANCE, YY',/2X,'SIGMAYY=', G14.7,//,
     J 'SPATIAL COVARIANCE, XY',/2X,'SIGMAXY=',G14.7,//,
     K 'SKEWNESS OF THE PLUME, X',/2X,'SKX=',G14.7,//,
     L 'SKEWNESS OF THE PLUME, Y',/2X,'SKY=',G14.7,//,
     M 'KURTOSIS OF THE PLUME, X',/2X,'KRX=',G14.7,//,
     N 'KURTOSIS OF THE PLUME, Y',/2X,'KRY=',G14.7)
      CLOSE (7)
      CLOSE (8)
      CLOSE (9)
      STOP
      END
```

```
* THIS PROGRAM TAKES THE OUTPUT FROM GUTJAHR'S RANDOM
* FIELD GENERATOR AND PUTS IT IN THE FORMAT REQUIRED
* TO GRID IN SURFER
*
   DIMENSION OUT(9500),XIJ(9500),YIJ(9500),SURF(9500)
   OPEN (UNIT=8,FILE='FIELD',STATUS='OLD')
   OPEN (UNIT=9,FILE='COND.TXT',STATUS='UNKNOWN')
*
* READ THE VALUES GENERATED BY GUTJAHR'S PROGRAM
*
   DO 10 K=1,9216,1
    READ (8,15) OUT(K)
15   FORMAT (E21.14)
10  CONTINUE
*
* CALCULATE THE X AND Y COORDINATES FOR EACH ELEMENT, SHIFT THE
* MEAN TO -5.0 AND PRINT IT OUT
*
   DO 30 I=1,144,1
   DO 40 J=1,64,1
    SURF(K)=OUT((I-1)*64+J)-5.0
    XIJ(K)=(I-0.5)
    YIJ(K)=(J-0.5)
    WRITE (9,100)XIJ(K),YIJ(K),SURF(K)
100    FORMAT (E16.8,E16.8,E16.8)
40  CONTINUE
30  CONTINUE
   CLOSE (8)
   CLOSE (9)
   STOP
   END
```

```
* This program calculates the mean and variance of the random hydraulic
* conductivity fields used in SUTRA.    August 6, 1996
*
      PROGRAM MEANVAR
      DOUBLE PRECISION MEAN,VARIANCE,SUM,MEANF,VARF
      DIMENSION COND(20000)
      OPEN (UNIT=8,FILE='FIELD',STATUS='OLD')
      OPEN (UNIT=9,FILE='MEAN',STATUS='UNKNOWN')
      DO 10 I=1,16384,1
       READ (8,100) COND(I)
100   FORMAT (D21.14)
10    CONTINUE
      SUM=0.0
      DO 20 I=1,16384,1   ! Calculate mean of entire field
       SUM=SUM+COND(I)
20    CONTINUE
      MEANF=(SUM/16384)
      SUM=0.0
      DO 30 I=1,16384,1   ! Calculate variance of entire field
       SUM=SUM+((COND(I))-MEANF)**2
30    CONTINUE
      VARF=(SUM/16383)
      SUM=0.0
      DO 40 I=1,9216,1    ! Calculate mean of field used in SUTRA
       SUM=SUM+COND(I)
40    CONTINUE
      MEAN=(SUM/9216)
      SUM=0.0
      DO 50 I=1,9216,1    ! Calculate variance of field used in SUTRA
       SUM=SUM+((COND(I))-MEAN)**2
50    CONTINUE
      VARIANCE=(SUM/9215)
      WRITE (9,200) MEANF,VARF,MEAN,VARIANCE
200   FORMAT (//,2X,'MEAN OF ENTIRE FIELD........= ',D14.8,
     +         /,2X,'VARIANCE OF ENTIRE FIELD....= ',D14.8,
     +       ///,2X,'MEAN OF TRUNCATED FIELD.....= ',D14.8,
     +         /,2X,'VARIANCE OF TRUNCATED FIELD.= ',D14.8)
      CLOSE (8)
      CLOSE (9)
      STOP
      END
```

```
* This program puts the *.d6 output file of pressures and concentrations
* in the proper format for the *.d55 file to use as initial conditions for
* simulation restart.
*
    PROGRAM PRESCONC
    DOUBLE PRECISION CONC(9500),PRES(9500)
    DIMENSION NODE(9500),NOD(9500)    ! CAN'T DECLARE INTEGERS AS DP
    OPEN (UNIT=7,FILE='CONCPRES.IN',STATUS='OLD')
    OPEN (UNIT=8,FILE='RESTART.D55',STATUS='UNKNOWN')
    TIME=6.34752D+07   ! SIMULATION ET
*
* READ PRESSURES FOR EACH NODE
*
    DO 10 I=1,9415,6
     READ (7,100)NOD(I),PRES(I),NOD(I+1),PRES(I+1),NOD(I+2),
   +         PRES(I+2),NOD(I+3),PRES(I+3),NOD(I+4),PRES(I+4),
   +         NOD(I+5),PRES(I+5)
100   FORMAT (7X,I5,D16.10,I5,D16.10,I5,D16.10,I5,D16.10,I5,D16.10,
   +       I5,D16.10)
10   CONTINUE
    READ (7,200)NOD(9421),PRES(9421),NOD(9422),PRES(9422),NOD(9423),
   +        PRES(9423),NOD(9424),PRES(9424),NOD(9425),PRES(9425)
200  FORMAT (7X,I5,D16.10,I5,D16.10,I5,D16.10,I5,D16.10,I5,D16.10)
*
* READ CONCENTRATIONS FOR EACH NODE
*
    DO 20 I=1,9415,6
     READ (7,100)NODE(I),CONC(I),NODE(I+1),CONC(I+1),NODE(I+2),
   +         CONC(I+2),NODE(I+3),CONC(I+3),NODE(I+4),CONC(I+4),
   +         NODE(I+5),CONC(I+5)
20   CONTINUE
    READ (7,200)NODE(9421),CONC(9421),NODE(9422),CONC(9422),
   +        NODE(9423),CONC(9423),NODE(9424),CONC(9424),
   +        NODE(9425),CONC(9425)
*
* WRITE THE ET AND PRESSURES / CONCENTRATIONS FOR EACH NODE
*
    WRITE (8,350)TIME
350   FORMAT (D20.10)
    DO 30 I=1,9421,4
     WRITE (8,300)PRES(I),PRES(I+1),PRES(I+2),PRES(I+3)
300  FORMAT (4D20.10)
30   CONTINUE
    WRITE (8,400)PRES(9425)
400  FORMAT (D20.10)
    DO 40 I=1,9421,4
     WRITE (8,300)CONC(I),CONC(I+1),CONC(I+2),CONC(I+3)
40   CONTINUE
    WRITE (8,400)CONC(9425)
    CLOSE (7)
    CLOSE (8)
    STOP
    END
```

```
* THIS PROGRAM TAKES THE OUTPUT FROM GUTJAHR'S RANDOM FIELD
* GENERATOR AND PUTS IT IN THE FORMAT REQUIRED FOR DATASET
* # 15B IN SUTRA'S D5 FILE
*
      DIMENSION OUT(9500),COND(9500),PERM(9500)
      OPEN (UNIT=8,FILE='FIELD',STATUS='OLD')
      OPEN (UNIT=9,FILE='15B',STATUS='UNKNOWN')
*
* READ THE VALUES GENERATED BY GUTJAHR'S PROGRAM
*
      DO 10 I=1,9216,1
       READ (8,15) OUT(I)
15      FORMAT (E21.14)
10     CONTINUE
*
* CONVERT FROM ln HYDRAULIC CONDUTIVITY TO HYDRAULIC CONDUCTIVITY AND
* CHANGE THE MEAN FROM 0.0 TO -5.0
*
      DO 30 I=1,9216,1
       COND(I)=2.7182818**(OUT(I)-5.0)
30     CONTINUE
*
* CONVERT FROM HYDRAULIC CONDUCTIVITY TO INTRINSIC PERMEABILITY,
* CENTIMETERS TO METERS (K) AND PRINT OUT THE RESULTS IN THE PROPER
* FORMAT FOR DATASET 15B IN SUTRA
*
      DO 40 I=1,9216,1
       PERM(I)=((COND(I))*(1.024687595E-7))/100
       WRITE (9,45) I,PERM(I),PERM(I),1.0,1.0,1.0,1.0,1.0
45      FORMAT (I5,5X,D10.4,D10.4,F10.3,F10.3,F10.3,F10.3,F10.3)
40     CONTINUE
      CLOSE (8)
      CLOSE (9)
      STOP
      END
```

```
* THIS PROGRAM TAKES THE OUTPUT FROM GUTJAHR'S RANDOM FIELD
* GENERATOR AND PUTS IT IN THE FORMAT REQUIRED FOR DATASET
* # 15B IN SUTRA'S D5 FILE #### 36,864 ELEMENTS ####
      INTEGER A,B,C,D,E
      DIMENSION OUT(9500),COND(9500),PERM(9500),PERME(40000)
      OPEN (UNIT=8,FILE='FIELD',STATUS='OLD')
      OPEN (UNIT=9,FILE='15B',STATUS='UNKNOWN')
*
*  READ THE VALUES GENERATED BY GUTJAHR'S PROGRAM
*
      DO 10 I=1,9216,1
       READ (8,15) OUT(I)
15      FORMAT (E21.14)
10     CONTINUE
*
*  CONVERT FROM ln HYDRAULIC CONDUTIVITY TO HYDRAULIC CONDUCTIVITY AND
*  CHANGE THE MEAN FROM 0.0 TO -5.0
*
      DO 30 I=1,9216,1
       COND(I)=2.7182818**(OUT(I)-5.0)
30     CONTINUE
*
*  CONVERT FROM HYDRAULIC CONDUCTIVITY TO INTRINSIC PERMEABILITY,
*  CENTIMETERS TO METERS (K) AND PRINT OUT THE RESULTS IN THE PROPER
*  FORMAT FOR DATASET 15B IN SUTRA
*
      DO 40 I=1,9216,1
       PERM(I)=((COND(I))*(1.024687595E-7))/100
40     CONTINUE
*  BREAK EACH OF THE 9216 ELEMENTS INTO 4 ELEMENTS OF THE SAME
*  PERMEABILITY FOR A TOTAL OF 36,864 ELEMENTS
      E=1
      DO 50 K=1,287,2
      DO 60 J=1,127,2
       I=E
       A=(J+(K-1)*128)
       B=(J+1+(K-1)*128)
       C=(J+(K)*128)
       D=(J+1+(K)*128)
       PERME(A)=PERM(I)
       PERME(B)=PERM(I)
       PERME(C)=PERM(I)
       PERME(D)=PERM(I)
        WRITE (9,45) A,PERME(A),PERME(A),1.0,1.0,1.0,1.0,1.0
45          FORMAT (I5,5X,D10.4,D10.4,F10.3,F10.3,F10.3,F10.3,F10.3)
        WRITE (9,45) B,PERME(B),PERME(B),1.0,1.0,1.0,1.0,1.0
        WRITE (9,45) C,PERME(C),PERME(C),1.0,1.0,1.0,1.0,1.0
        WRITE (9,45) D,PERME(D),PERME(D),1.0,1.0,1.0,1.0,1.0
       WRITE (*,*) E
       E=E+1
60     CONTINUE
50     CONTINUE
      CLOSE (8)
      CLOSE (9)
      STOP
      END
```

```
* THIS PROGRAM SETS UP ALL NO-FLOW BOUNDARIES IN THE PROPER FORMAT
* FOR SUTRA'S DATASET 19.  MODEL DISCRETIZATION TEST, DIMENSIONED
* FOR 289 X 129 NODES (TOTAL CONSTANT HEAD NODES = 832)
*
      PROGRAM DDATA19
      INTEGER NODE
      REAL PRES,CONC
      OPEN (UNIT=8,FILE='19',STATUS='UNKNOWN')
      DO 10 J=1,289,1
      DO 20 I=1,129,128
       NODE=129*(J-1)+I
       PRES=103524.7-((39.15486111)/2)*(J-1)
       CONC=0.0
       WRITE (8,100)NODE,PRES,CONC
100       FORMAT (I5,F20.2,F20.1)
20   CONTINUE
10   CONTINUE
      DO 30 I=2,128,1
       NODE=I
       PRES=103524.7
       CONC=0.0
       WRITE (8,100)NODE,PRES,CONC
30   CONTINUE
      DO 40 I=37154,37280,1
       NODE=I
       PRES=97886.4
       CONC=0.0
       WRITE (8,100)NODE,PRES,CONC
40   CONTINUE
      CLOSE (8)
      STOP
      END
```

```
* THIS PROGRAM SETS UP ALL NO-FLOW BOUNDARIES IN THE PROPER FORMAT
* FOR SUTRA'S DATASET 19 (DIMENSIONED FOR 145 X 65 NODES)
*
      PROGRAM DATA19
      INTEGER NODE
      REAL PRES,CONC
      OPEN (UNIT=8,FILE='19',STATUS='UNKNOWN')
      DO 10 J=1,145,1
      DO 20 I=1,65,64
        NODE=65*(J-1)+I
        PRES=103524.7-(39.15486111)*(J-1)
        CONC=0.0
        WRITE (8,100)NODE,PRES,CONC
100       FORMAT (I5,F20.2,F20.1)
20      CONTINUE
10      CONTINUE
      DO 30 I=2,64,1
        NODE=I
        PRES=103524.7
        CONC=0.0
        WRITE (8,100)NODE,PRES,CONC
30      CONTINUE
      DO 40 I=9362,9424,1
        NODE=I
        PRES=97886.4
        CONC=0.0
        WRITE (8,100)NODE,PRES,CONC
40      CONTINUE
      CLOSE (8)
      STOP
      END
```

```
* THIS PROGRAM TAKES THE RAW NODE CONCENTRATION OUTPUT FROM SUTRA AND
* CALCULATES THE SPATIAL MOMENTS, ZEROTH THROUGH FOURTH.
* A GRID FILE IS ALSO CREATED FOR CONTOURING THE RESULTS IN SURFER.
* ONLY CONCENTRATIONS GREATER THAN 0.1 PPM ARE USED IN THE CALCULATIONS.
* THIS PROGRAM IS DIMENSIONED FOR 36,864 ELEMENTS (DISCRETIZATION TEST)
* THE NODE INTEGER FIELD WAS INCREASED TO 6 TO ACCOMODATE 37,281 NODES
* REVISED JULY 8, 1996
*
      PROGRAM DSURFHET
      REAL M000,M100,M010,M110,M200,M020,M300,M030,M400,M040,
     +  XC,YC,SIGMAXX,SIGMAYY,SIGMAXY,SKX,SKY,KRX,KRY
      DIMENSION C(38000),N(38000),CIJ(38000),XIJ(38000),YIJ(38000)
      OPEN (UNIT=7,FILE='CONC.IN',STATUS='OLD')
      OPEN (UNIT=8,FILE='CONC.TXT',STATUS='UNKNOWN')
      OPEN (UNIT=9,FILE='MOMENTS',STATUS='UNKNOWN')
      P=0.35
      V=0.25
      D=998.2
C
C  REDUCE THE RAW SUTRA NODE CONCENTRATION OUTPUT FROM 6 COLUMNS TO 1
C
      DO 10 K=1,37278,6
        READ (7,200)N(K),C(K),N(K+1),C(K+1),N(K+2),C(K+2),N(K+3),
     +          C(K+3),N(K+4),C(K+4),N(K+5),C(K+5)
200     FORMAT (7X,I6,G16.8,I6,G16.8,I6,G16.8,I6,G16.8,I6,G16.8,I6,
     +       G16.8)
10      CONTINUE
      READ (7,300)N(37279),C(37279),N(37280),C(37280),N(37281),
     +         C(37281)
300    FORMAT (7X,I6,G16.8,I6,G16.8,I6,G16.8)
C
C  AVERAGE THE 4 NODE CONCENTRATIONS AROUND EACH ELEMENT TO PERFORM
C  THE MOMENT CALCULATIONS ON THE ELEMENTS (RATHER THAN THE NODES) AND
C  CALCULATE THE X AND Y-COORDINATES OF EACH ELEMENT
C
      DO 20 I=1,288,1
      DO 30 J=1,128,1
        C1=((I-1)*129+J)
        C2=(I*129+J)
        C3=(I*129+1+J)
        C4=((I-1)*129+1+J)
        CIJ(K)=(C(C1)+C(C2)+C(C3)+C(C4))/4
        IF (CIJ(K).LT.1.0E-7) THEN
          CIJ(K)=0.0
        ENDIF
        XIJ(K)=(I*0.5)-0.25
        YIJ(K)=(J*0.5)-0.25
        WRITE (8,400)XIJ(K),YIJ(K),CIJ(K)
400     FORMAT (E16.8,E16.8,E16.8)
30      CONTINUE
20      CONTINUE
C
C  READ IN THE ELEMENT CONCENTRATIONS AND COORDINATES CALCULATED ABOVE
C
      CLOSE (8)
      OPEN (UNIT=8,FILE='CONC.TXT',STATUS='UNKNOWN')
```

Program DSURFHET (continued)

```
      DO 35 K=1,36864,1
        READ (8,400)XIJ(K),YIJ(K),CIJ(K)
35      CONTINUE
C
C  ZEROTH MOMENT (TOTAL MASS)
C
      SUM=0.0
      DO 40 K=1,36864,1
        SUM=SUM+CIJ(K)*P*V*D
40      CONTINUE
      M000=SUM
C
C  FIRST MOMENT, X (CENTER OF MASS IN THE X DIRECTION)
C
      SUM=0.0
      DO 50 K=1,36864,1
        SUM=SUM+CIJ(K)*P*V*D*XIJ(K)
50      CONTINUE
      M100=SUM
      XC=M100/M000
C
C  FIRST MOMENT, Y (CENTER OF MASS IN THE Y DIRECTION)
C
      SUM=0.0
      DO 55 K=1,36864,1
        SUM=SUM+CIJ(K)*P*V*D*YIJ(K)
55      CONTINUE
      M010=SUM
      YC=M010/M000
C
C  SECOND MOMENT, XX (SPATIAL VARIANCE IN THE X DIRECTION)
C
      SUM=0.0
      DO 60 K=1,36864,1
        SUM=SUM+CIJ(K)*P*V*D*(XIJ(K)**2)
60      CONTINUE
      M200=SUM
      SIGMAXX=(M200/M000)-(XC**2)
C
C  SECOND MOMENT, YY (SPATIAL VARIANCE IN THE Y DIRECTION)
C
      SUM=0.0
      DO 70 K=1,36864,1
        SUM=SUM+CIJ(K)*P*V*D*(YIJ(K)**2)
70      CONTINUE
      M020=SUM
      SIGMAYY=(M020/M000)-YC**2
C
C  SECOND MOMENT, XY (SPATIAL COVARIANCE)
C
      SUM=0.0
      DO 80 K=1,36864,1
        SUM=SUM+CIJ(K)*P*V*D*XIJ(K)*YIJ(K)
80      CONTINUE
      M110=SUM
```

Program DSURFHET (continued)

```
      SIGMAXY=(M110/M000)-(XC*YC)
C
C  THIRD MOMENT, X (SKEWNESS OF THE PLUME IN THE X DIRECTION)
C
      SUM=0.0
      DO 90 K=1,36864,1
       SUM=SUM+CIJ(K)*P*V*D*((XIJ(K)-XC)**3)
90     CONTINUE
      M300=SUM
      SKX=M300/(M000*(SIGMAXX**(3/2)))
C
C  THIRD MOMENT, Y (SKEWNESS OF THE PLUME IN THE Y DIRECTION)
C
      SUM=0.0
      DO 100 K=1,36864,1
       SUM=SUM+CIJ(K)*P*V*D*((YIJ(K)-YC)**3)
100    CONTINUE
      M030=SUM
      SKY=M030/(M000*(SIGMAYY**(3/2)))
C  FOURTH MOMENT, X (KURTOSIS OF THE PLUME IN THE X DIRECTION)
      SUM=0.0
      DO 110 K=1,36864,1
       SUM=SUM+CIJ(K)*P*V*D*((XIJ(K)-XC)**4)
110    CONTINUE
      M400=SUM
      KRX=M400/(M000*(SIGMAXX**2))
C  FOURTH MOMENT, Y (KURTOSIS OF THE PLUME IN THE Y DIRECTION)
      SUM=0.0
      DO 120 K=1,36864,1
       SUM=SUM+CIJ(K)*P*V*D*((YIJ(K)-YC)**4)
120    CONTINUE
      M040=SUM
      KRY=M040/(M000*(SIGMAYY**2))
      WRITE (9,500)M000,XC,YC,SIGMAXX,SIGMAYY,SIGMAXY,SKX,SKY,KRX,KRY
500    FORMAT (//,'***S P A T I A L   M O M E N T   C A L C U L A T I O'
     A  ' N S***',/,'      36,864 ELEMENTS (Discretization test)',//,
     B  '####################################',/,
     C  '# CONCENTRATIONS < 0.1 PPM OMITTED #',/,
     D  '####################################',////,
     E  'MASS OF BROMIDE (KG)',/2X,'M000=',G14.7,//,
     F  'CENTER OF MASS, X-COORDINATE (M)',/2X,'XC=',G14.7,//,
     G  'CENTER OF MASS, Y-COORDINATE (M)',/2X,'YC=',G14.7,//,
     H  'SPATIAL VARIANCE, XX',/2X,'SIGMAXX=',G14.7,//,
     I  'SPATIAL VARIANCE, YY',/2X,'SIGMAYY=',G14.7,//,
     J  'SPATIAL COVARIANCE, XY',/2X,'SIGMAXY=',G14.7,//,
     K  'SKEWNESS OF THE PLUME, X',/2X,'SKX=',G14.7,//,
     L  'SKEWNESS OF THE PLUME, Y',/2X,'SKY=',G14.7,//,
     M  'KURTOSIS OF THE PLUME, X',/2X,'KRX=',G14.7,//,
     N  'KURTOSIS OF THE PLUME, Y',/2X,'KRY=',G14.7)
      CLOSE (7)
      CLOSE (8)
      CLOSE (9)
      STOP
      END
```

```
* THIS PROGRAM TAKES THE RAW NODE CONCENTRATION OUTPUT FROM SUTRA AND
* CALCULATES THE SPATIAL MOMENTS, ZEROTH THROUGH FOURTH.
* A GRID FILE IS ALSO CREATED FOR CONTOURING THE RESULTS IN SURFER.
* ALL CONCENTRATIONS ARE USED IN THE CALCULATIONS.
* THIS PROGRAM IS DIMENSIONED FOR 36,864 ELEMENTS (DISCRETIZATION TEST)
* THE NODE INTEGER FIELD WAS INCREASED TO 6 TO ACCOMODATE 37,281 NODES
* REVISED JULY 8, 1996
*
      PROGRAM DSURFHE2
      REAL M000,M100,M010,M110,M200,M020,M300,M030,M400,M040,
     +  XC,YC,SIGMAXX,SIGMAYY,SIGMAXY,SKX,SKY,KRX,KRY
      DIMENSION C(38000),N(38000),CIJ(38000),XIJ(38000),YIJ(38000)
      OPEN (UNIT=7,FILE='CONC.IN',STATUS='OLD')
      OPEN (UNIT=8,FILE='CONC.TXT',STATUS='UNKNOWN')
      OPEN (UNIT=9,FILE='MOMENTS',STATUS='UNKNOWN')
      P=0.35
      V=0.25
      D=998.2
C
C  REDUCE THE RAW SUTRA NODE CONCENTRATION OUTPUT FROM 6 COLUMNS TO 1
C
      DO 10 K=1,37278,6
       READ (7,200)N(K),C(K),N(K+1),C(K+1),N(K+2),C(K+2),N(K+3),
     +          C(K+3),N(K+4),C(K+4),N(K+5),C(K+5)
200     FORMAT (7X,I6,G16.8,I6,G16.8,I6,G16.8,I6,G16.8,I6,G16.8,I6,
     +       G16.8)
10     CONTINUE
      READ (7,300)N(37279),C(37279),N(37280),C(37280),N(37281),
     +        C(37281)
300    FORMAT (7X,I6,G16.8,I6,G16.8,I6,G16.8)
C
C  AVERAGE THE 4 NODE CONCENTRATIONS AROUND EACH ELEMENT TO PERFORM
C  THE MOMENT CALCULATIONS ON THE ELEMENTS (RATHER THAN THE NODES) AND
C  CALCULATE THE X AND Y-COORDINATES OF EACH ELEMENT
C
      DO 20 I=1,288,1
      DO 30 J=1,128,1
       C1=((I-1)*129+J)
       C2=(I*129+J)
       C3=(I*129+1+J)
       C4=((I-1)*129+1+J)
       CIJ(K)=(C(C1)+C(C2)+C(C3)+C(C4))/4
       XIJ(K)=(I*0.5)-0.25
       YIJ(K)=(J*0.5)-0.25
       WRITE (8,400)XIJ(K),YIJ(K),CIJ(K)
400     FORMAT (E16.8,E16.8,E16.8)
30     CONTINUE
20     CONTINUE
C
C  READ IN THE ELEMENT CONCENTRATIONS AND COORDINATES CALCULATED ABOVE
C
      CLOSE (8)
      OPEN (UNIT=8,FILE='CONC.TXT',STATUS='UNKNOWN')
      DO 35 K=1,36864,1
       READ (8,400)XIJ(K),YIJ(K),CIJ(K)
35     CONTINUE
```

Program DSURFHET2 (continued)

```
C
C  ZEROTH MOMENT (TOTAL MASS)
C
      SUM=0.0
      DO 40 K=1,36864,1
        SUM=SUM+CIJ(K)*P*V*D
40    CONTINUE
      M000=SUM
C
C  FIRST MOMENT, X (CENTER OF MASS IN THE X DIRECTION)
C
      SUM=0.0
      DO 50 K=1,36864,1
        SUM=SUM+CIJ(K)*P*V*D*XIJ(K)
50    CONTINUE
      M100=SUM
      XC=M100/M000
C
C  FIRST MOMENT, Y (CENTER OF MASS IN THE Y DIRECTION)
C
      SUM=0.0
      DO 55 K=1,36864,1
        SUM=SUM+CIJ(K)*P*V*D*YIJ(K)
55    CONTINUE
      M010=SUM
      YC=M010/M000
C
C  SECOND MOMENT, XX (SPATIAL VARIANCE IN THE X DIRECTION)
C
      SUM=0.0
      DO 60 K=1,36864,1
        SUM=SUM+CIJ(K)*P*V*D*(XIJ(K)**2)
60    CONTINUE
      M200=SUM
      SIGMAXX=(M200/M000)-(XC**2)
C
C  SECOND MOMENT, YY (SPATIAL VARIANCE IN THE Y DIRECTION)
C
      SUM=0.0
      DO 70 K=1,36864,1
        SUM=SUM+CIJ(K)*P*V*D*(YIJ(K)**2)
70    CONTINUE
      M020=SUM
      SIGMAYY=(M020/M000)-YC**2
C
C  SECOND MOMENT, XY (SPATIAL COVARIANCE)
C
      SUM=0.0
      DO 80 K=1,36864,1
        SUM=SUM+CIJ(K)*P*V*D*XIJ(K)*YIJ(K)
80    CONTINUE
      M110=SUM
      SIGMAXY=(M110/M000)-(XC*YC)
C
C  THIRD MOMENT, X (SKEWNESS OF THE PLUME IN THE X DIRECTION)
```

Program DSURFHET2 (continued)

```
      SUM=0.0
      DO 90 K=1,36864,1
       SUM=SUM+CIJ(K)*P*V*D*((XIJ(K)-XC)**3)
90     CONTINUE
      M300=SUM
      SKX=M300/(M000*(SIGMAXX**(3/2)))
C
C  THIRD MOMENT, Y (SKEWNESS OF THE PLUME IN THE Y DIRECTION)
C
      SUM=0.0
      DO 100 K=1,36864,1
       SUM=SUM+CIJ(K)*P*V*D*((YIJ(K)-YC)**3)
100    CONTINUE
      M030=SUM
      SKY=M030/(M000*(SIGMAYY**(3/2)))
C
C  FOURTH MOMENT, X (KURTOSIS OF THE PLUME IN THE X DIRECTION)
C
      SUM=0.0
      DO 110 K=1,36864,1
       SUM=SUM+CIJ(K)*P*V*D*((XIJ(K)-XC)**4)
110    CONTINUE
      M400=SUM
      KRX=M400/(M000*(SIGMAXX**2))
C
C  FOURTH MOMENT, Y (KURTOSIS OF THE PLUME IN THE Y DIRECTION)
C
      SUM=0.0
      DO 120 K=1,36864,1
       SUM=SUM+CIJ(K)*P*V*D*((YIJ(K)-YC)**4)
120    CONTINUE
      M040=SUM
      KRY=M040/(M000*(SIGMAYY**2))
     WRITE (9,500)M000,XC,YC,SIGMAXX,SIGMAYY,SIGMAXY,SKX,SKY,KRX,KRY
500  FORMAT(//,'***S P A T I A L   M O M E N T',
     a  '  C A L C U L A T I O N S***',
     A  /,'        36,864 ELEMENTS (Discretization test)',//,
     B  '###########################################',/,
     C  '# ALL CONCENTRATIONS USED IN CALCULATIONS #',/,
     D  '###########################################',////,
     E  'MASS OF BROMIDE (KG)',/2X,'M000=',G14.7,//,
     F  'CENTER OF MASS, X-COORDINATE (M)',/2X,'XC=',G14.7,//,
     G  'CENTER OF MASS, Y-COORDINATE (M)',/2X,'YC=',G14.7,//,
     H  'SPATIAL VARIANCE, XX',/2X,'SIGMAXX=',G14.7,//,
     I  'SPATIAL VARIANCE, YY',/2X,'SIGMAYY=',G14.7,//,
     J  'SPATIAL COVARIANCE, XY',/2X,'SIGMAXY=',G14.7,//,
     K  'SKEWNESS OF THE PLUME, X',/2X,'SKX=',G14.7,//,
     L  'SKEWNESS OF THE PLUME, Y',/2X,'SKY=',G14.7,//,
     M  'KURTOSIS OF THE PLUME, X',/2X,'KRX=',G14.7,//,
     N  'KURTOSIS OF THE PLUME, Y',/2X,'KRY=',G14.7)
      CLOSE (7)
      CLOSE (8)
      CLOSE (9)
      STOP
      END
```

# APPENDIX F

# MODEL TESTING DATA

WATSUTRA was tested by running a reactive simulation and comparing the solute solution with that of SUTRA. It was found that a nearly identical solution was obtained. The method of moment calculations was the same as SUTRA's to the third or fourth significant figure. The longitudinal and horizontal transverse apparent dispersivities were identical to those calculated using SUTRA. WATSUTRA was run with both transient flow and solute transport because the routine for steady-state flow was not working properly. The model is actually steady-state flow; it was found that running transient flow did not change the pressure distribution (the pressure distribution at the start of the simulation was identical to the distribution at 2 years). The only difference in running transient flow rather than steady-state flow is more calculations since there are no stresses on the system (e.g. no pumping periods).

WatSutra Varification Test

Weakly Heterogeneous

Realization 1

1 Kilogram of Bromide

**************************************************************************************

Reactive Run

All Concentrations Used in Calculations

**************************************************************************************

| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) |  | (Unitless values) |  |  |
| 0 | 0.6574 | 24.3978 | 32.0631 | 0.9055 | 0.7668 | 0.3537 | 0.0658 | 3.2124 | 2.8273 |
| 0.0114 | 0.6545 | 24.5454 | 32.0823 | 1.1002 | 0.7572 | 0.4525 | 0.0763 | 3.3010 | 2.7850 |
| 0.2614 | 0.6229 | 28.3377 | 32.3356 | 6.8112 | 0.7072 | 0.4469 | 0.1631 | 2.8130 | 2.1765 |
| 0.5113 | 0.6059 | 32.5868 | 32.3748 | 12.3621 | 0.9783 | -0.1720 | 0.1393 | 2.9527 | 2.9817 |
| 0.7613 | 0.5971 | 36.7364 | 32.3462 | 16.1052 | 1.5368 | -0.8912 | 0.0274 | 3.0662 | 3.4211 |
| 1.0113 | 0.5916 | 40.4959 | 32.2255 | 18.1346 | 2.1779 | -1.3121 | -0.1099 | 3.2946 | 3.5137 |
| 1.2612 | 0.5885 | 43.8592 | 32.0111 | 19.9495 | 2.6995 | -1.3642 | -0.4867 | 3.3862 | 3.3644 |
| 1.5112 | 0.5858 | 46.9701 | 31.7508 | 22.1861 | 3.1452 | -1.3491 | -0.9202 | 3.4109 | 3.0674 |
| 1.7612 | 0.5836 | 49.9294 | 31.4872 | 24.7928 | 3.5175 | -1.2188 | -0.9692 | 3.5039 | 2.8887 |
| 2.0114 | 0.5816 | 52.8136 | 31.2133 | 28.5865 | 3.6093 | -0.4644 | -0.6897 | 3.6699 | 2.7628 |

**************************************************************************************

Reactive Run

Only Concentrations Greater Than 0.1 ppm Used in Calculations

**************************************************************************************

| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) |  | (Unitless values) |  |  |
| 0 | 0.6574 | 24.3967 | 32.0628 | 0.9041 | 0.7661 | 0.3409 | 0.0624 | 3.1742 | 2.8118 |
| 0.0114 | 0.6545 | 24.5444 | 32.0815 | 1.0967 | 0.7563 | 0.4419 | 0.0696 | 3.2558 | 2.7817 |
| 0.2614 | 0.6321 | 28.3023 | 32.3279 | 6.7853 | 0.8072 | 0.4518 | 0.0404 | 2.7623 | 3.1102 |
| 0.5113 | 0.6233 | 32.4651 | 32.3653 | 12.5884 | 1.1373 | -0.1506 | 0.1078 | 2.8448 | 3.4194 |
| 0.7613 | 0.6127 | 36.5847 | 32.3423 | 16.6705 | 1.6960 | -0.9823 | 0.0998 | 2.9645 | 3.5130 |
| 1.0113 | 0.6047 | 40.3534 | 32.2287 | 18.7524 | 2.3447 | -1.4814 | -0.0051 | 3.2169 | 3.5795 |
| 1.2612 | 0.5987 | 43.7431 | 32.0168 | 20.4053 | 2.8909 | -1.5347 | -0.3754 | 3.3158 | 3.6951 |
| 1.5112 | 0.5936 | 46.8980 | 31.7559 | 22.2077 | 3.4018 | -1.3627 | -0.7972 | 3.2369 | 3.6646 |
| 1.7612 | 0.5892 | 49.8910 | 31.4891 | 24.4428 | 3.7719 | -1.1571 | -0.8993 | 3.2785 | 3.3664 |
| 2.0114 | 0.5850 | 52.7969 | 31.2068 | 27.9335 | 3.7796 | -0.2921 | -0.7255 | 3.4070 | 3.0171 |

**************************************************************************************

Discretization Test (37,281 nodes)

Weakly Heterogeneous

Realization 1

1 Kilogram of Bromide

*************************************************************************************

Reactive Run

All Concentrations Used in Calculations

*************************************************************************************

| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.6626 | 24.4528 | 32.0746 | 0.6328 | 0.4726 | 0.3619 | 0.0746 | 3.1293 | 2.7652 |
| 0.0114 | 0.6585 | 24.6080 | 32.0946 | 0.8333 | 0.4698 | 0.3735 | 0.0632 | 3.1358 | 2.7742 |
| 0.2614 | 0.6288 | 28.5530 | 32.3284 | 7.0723 | 0.5193 | -0.0146 | -0.0203 | 2.6402 | 2.8937 |
| 0.5113 | 0.6154 | 32.7883 | 32.3655 | 12.9947 | 0.7736 | -0.7983 | 0.0277 | 2.8893 | 2.9650 |
| 0.7613 | 0.6063 | 36.8552 | 32.3226 | 16.8916 | 1.2237 | -1.7196 | 0.0563 | 3.1530 | 3.0763 |
| 1.0113 | 0.5998 | 40.5552 | 32.1997 | 18.9012 | 1.7363 | -2.1290 | 0.0364 | 3.5276 | 3.1717 |
| 1.2612 | 0.5949 | 43.9463 | 31.9981 | 20.6747 | 2.2371 | -2.0411 | -0.1244 | 3.6290 | 3.4296 |
| 1.5112 | 0.5909 | 47.1158 | 31.7575 | 22.4982 | 2.7544 | -1.9239 | -0.3378 | 3.5673 | 3.5350 |
| 1.7612 | 0.5875 | 50.1001 | 31.4895 | 24.3352 | 3.2037 | -1.6949 | -0.4141 | 3.5794 | 3.3992 |
| 2.0114 | 0.5847 | 52.9873 | 31.1914 | 27.6487 | 3.4042 | -0.6702 | -0.2797 | 3.6872 | 3.2259 |

*************************************************************************************

Reactive Run

Only Concentrations Greater Than 0.1 ppm Used in Calculations

*************************************************************************************

| Time | Mass | XC | YC | Var X | Var Y | SKX | SKY | KRX | KRY |
|---|---|---|---|---|---|---|---|---|---|
| (yr) | (kg) | (m) | (m) | (m^2) | (m^2) | | (Unitless values) | | |
| 0 | 0.6626 | 24.4525 | 32.0745 | 0.6314 | 0.4725 | 0.3581 | 0.0738 | 3.1134 | 2.7575 |
| 0.0114 | 0.6584 | 24.6078 | 32.0945 | 0.8312 | 0.4688 | 0.3694 | 0.0628 | 3.1165 | 2.7677 |
| 0.2614 | 0.6285 | 28.5520 | 32.3281 | 7.0529 | 0.5179 | -0.0223 | -0.0239 | 2.6206 | 2.8740 |
| 0.5113 | 0.6150 | 32.7878 | 32.3652 | 12.9339 | 0.7696 | -0.7993 | 0.0247 | 2.8660 | 2.9234 |
| 0.7613 | 0.6056 | 36.8544 | 32.3224 | 16.7716 | 1.2135 | -1.7072 | 0.0535 | 3.1153 | 3.0130 |
| 1.0113 | 0.5989 | 40.5572 | 32.1998 | 18.7050 | 1.7197 | -2.0732 | 0.0389 | 3.4518 | 3.0975 |
| 1.2612 | 0.5938 | 43.9510 | 31.9980 | 20.3895 | 2.2153 | -1.9216 | -0.1200 | 3.4935 | 3.3547 |
| 1.5112 | 0.5895 | 47.1238 | 31.7571 | 22.0718 | 2.7276 | -1.7416 | -0.3379 | 3.3614 | 3.4813 |
| 1.7612 | 0.5859 | 50.1092 | 31.4885 | 23.7692 | 3.1712 | -1.4772 | -0.4194 | 3.3097 | 3.3576 |
| 2.0114 | 0.5828 | 52.9988 | 31.1884 | 26.9363 | 3.3632 | -0.4288 | -0.2957 | 3.4217 | 3.1741 |

*************************************************************************************

```
Homogeneous Simulation
0.5 Kilogram of Bromide
All Concentrations Used in Calculations
**********************************************
Conservative Run
**********************************************
Time        Mass       XC         Var X       Var Y
(yr)        (kg)       (m)        (m^2)       (m^2)
**********************************************
   0.0000    0.4973    15.8751      2.2226     1.4826
   0.5006    0.4973    33.8704    143.6283     5.1080
   1.0011    0.4973    51.8464    285.3527     8.7318
   1.5016    0.4973    69.8028    428.4481    12.3541
   2.0022    0.4973    87.7548    572.0367    15.9757
   2.5000    0.4973   105.6075    714.9858    19.5768
   3.0005    0.4973   123.5578    858.8140    23.1948
   3.5011    0.4973   141.5085   1002.5800    26.8059
   4.0016    0.4973   159.4587   1146.3390    30.4030
   4.5022    0.4973   177.4012   1289.0420    33.9765
   5.0000    0.4970   195.1709   1421.9960    37.4934
**********************************************
```

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