A Comparison of Sampling Design Criteria using a Lagrangian Particle Tracking Model for Transport in Porous Media

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Abstract

Sampling design algorithms are usually optimization problems posed in two ways: (1) Minimize the total cost of the sampling program without going below a prescribed minimum reliability measure, and (2) Maximize the reliability measure of the parameters without exceeding a prescribed maximum experimental budget. The variables that are optimized are the sampling locations and sampling times. The reliability measure is usually some measure of the parameter's variability or the prediction variability.

This research compares three reliability measures that operate on the estimated parameter's covariance matrix. A set of designs is selected and each reliability measure is used to select the best design of the set. The objective of this research is to determine if the A-optimal criterion, D-optimal criterion, and CR-optimal criterion choose the same design or different designs.

The particle tracking method is used to model the transport of mass in the porous medium. Particle tracking is difficult to implement because a large number of particles should be used to simulate continuum behavior. The large number of particles are simple to manage on a computer with a large memory, and the displacement calculations are simplified if the computer is fast. These reasons made the HARC NEC SX-2 a fine choice for this research.

Introduction

The need to predict and control the movement of pollutants carried by groundwater arises because of increased awareness of the environmental (and legal) consequences of contaminated groundwater. Models are used to predict the response of a groundwater system to various management policies. If the model is reasonably accurate, these predictions can be used to design remediation schemes and water supply protection policies. If the model is inaccurate, one can still make predictions and designs but will expect to be frequently disappointed by their designs. Estimating the parameters in these models, which is really the process of selecting a particular model from a family of models, is an important step in the design the remediation schemes and water supply protection policies.

Parameter estimation in groundwater has been studied by many, a state of the art review is given by Yeh (1986). The practice of parameter estimation in groundwater is complicated because the physical structure cannot be directly observed. The parameters must be inferred from observations at a few spatially and temporally distributed locations. The topic of sampling design covers the theory and practice of where, when, and how to sample so that the data obtained give the most information for a given budget. An important implied assumption in many sampling design problems is that the family of models is correct. For instance Darcy's law is seldom challenged as the model of flow in groundwater but the hydraulic conductivity value, which is the parameter that selects the particular model, is seldom accepted with complete confidence. Emerging stochastic theories of flow and transport are attempts to address the question of which model family is correct. The quantification of the "correctness" of a model is an area of emerging research that also relies on stochastic theories. The study of which model family is correct and how to quantify the "correctness" of a model is beyond the scope of this work.

An algorithm for sampling design that determines the observation locations and the sampling times should consider the trade-off between the economy of few locations and few samples with the increased information when many locations are sampled at many times. In transport problems a further challenge arises because a location becomes useless after the

contaminant mass has passed the location (Cleveland, 1989). Sampling design algorithms are usually optimization problems posed in two ways: (1) Minimize the total cost of the sampling program without going below a prescribed minimum reliability measure, and (2) Maximize the reliability measure of the parameters without exceeding a prescribed maximum experimental budget. These two approaches are probably equivalent (in optimization jargon (1) and (2) are duals) but this equivalence has not been proved. The variables that are optimized are the sampling locations and sampling times. The reliability measure is usually some measure of the parameter's variability or the prediction variability.

This research compares three reliability measures that operate on the estimated parameter's covariance matrix. A set of designs is selected and each reliability measure is used to select the best design of the set. The resulting designs are compared using a simulation sensitivity analysis to determine what features of the model sensitivites are selected for by the particular measures. The simulation model uses a Lagrangian particle tracking method to model transport because this method generates no numerical dispersion.

Background

Sampling design (experimental design) procedures developed in statistics are used in medicine, agriculture, automatic control, physics, geosciences, and other areas of research. Steinberg and Hunter (1984) reviewed experimental design and presented algorithm descriptions of the more successful schemes. Two popular measures of parameter reliability used in those schemes are the D-optimality measure and the A-optimality measure. A D-optimal design satisfies all constraints (cost, complexity, etc.) and minimizes the determinant of the parameter estimates' covariance matrix. The Wilk's generalized variance of a vector valued random variable is given by the determinant of the variable's covariance matrix, so this criterion can be viewed as a variance reducing approach. The A-optimality measure uses the trace of the estimate's covariance matrix.

Hsu and Yeh (1989) used A-optimailty considerations for minimizing pumping test costs subject to parameter reliability and institutional constraints. Nishikawa and Yeh (1989) used D-optimality considerations for a similar problem. The combinatorial problem was solved using exhaustive search. The problem was tractable by this method because the unknown parameter set was kept small enough so that the matrix determinants could be performed analytically. For larger parameter sets the D-optimal or A-optimal criterion could be determined by co-factor expansion or singular value decomposition, but the computational burden becomes large because of the combinatorial nature of the problems.

Cleveland and Yeh (1990) used a simplified measure that used the trace of the estimates' information matrix for maximizing the information in a tracer test experiment subject to a fixed experimental budget. This measure, which they called CR-optimality, has computational advantages because the inversion of a matrix is avoided and the combinatorial problem can be solved using zero-one dynamic programming.

Statistical implications for transport parameter identification were studied by Wagner and Gorelick (1987). They found that parameters are more reliably estimated if sampling is distributed in both space and time. Knopman and Voss (1987) studied the behavior of sensitivities in one-

dimensional solute transport equations and found that parameters are most accurately estimated at points with high sensitivity to the parameters but designs that minimize the variance of one estimate do not necessarily minimize the variance of other estimates.

Cleveland (1989) suggested that D-optimal designs, A-optimal designs, and CR-optimal designs all tend to choose designs that sample at points in space and time where some "joint" sensitivity to all the estimated parameters is high. McKinney and Loucks (1991) used an independent uncertainty approach with Monte-Carlo analysis and generated designs with this tendency. One interesting observation is that Cleveland (1989), Nishikawa (1989), and McKinney (1991) have noted that the designs generated are counter intuitive. An explanation is that the parameter sensitivity is a function contaminant mass. As the mass becomes more diffuse in space the ability to detect concentration contrasts as a result of subtle parameter changes is decreased. Design algorithms that tend to choose designs where "joint" sensitivity is high, will always choose designs near source areas and steep concentration gradients. This work presents an example where the A-optimal criterion, D-optimal criterion, and CR-optimal criterion all tend to choose designs with this property. This fact indicates that another design criterion should be sought that selects designs based on a different property.

Objectives

The objective of this research is to determine if the A-optimal criterion, D- optimal criterion, and CR-optimal criterion choose the same design or different designs. Simulation is used to generate covariance structures for four designs and then determine the value of each of the evaluator functions. This investigation requires a simulation model that describes the flow and transport of a contaminant in a porous medium, a method of computing the partial derivatives of the model with respect to the transport parameters, and the calculation of the performance criteria for each design.

Flow and Transport Modeling

The transport equation of a conservative solute is (Dagan,1987),

$$n_e \frac{\partial C}{\partial t} + = div\,(\,\boldsymbol{D}\ \boldsymbol{grad}(C) - C\,\boldsymbol{q}) \qquad (1)$$

where C is the concentration, $\boldsymbol{q}$ is the fluid seepage velocity, n_e is the effective porosity, and $\boldsymbol{D}$ is the hydrodynamic dispersion tensor.

The potentiometric head field is obtained by solving the following equation that describes the hydraulic head in a confined isotropic aquifer (Bear, 1972),

$$\frac{\partial h}{\partial t} + N = div\,(\boldsymbol{K}\ \boldsymbol{grad}\,(h)) \qquad (2)$$

where h is the hydraulic head, $\boldsymbol{K}$ is the hydraulic conductivity tensor, and N is a source term.

The seepage velocity field is obtained from the potentiometric head distribution by Darcy's law (Bear, 1972)

$$\boldsymbol{q} = -\,\boldsymbol{K}\ \boldsymbol{grad}(h). \qquad (3)$$

The numerical solution of Equation (1) poses problems because solution schemes often introduce purely numerical dispersion. This research uses the Discrete Particle Random Walk (DPRW) method that models the effects of convective transport using a Lagrangian approach, and the effects of kinematic dispersion using a random walk model (Ahlstrom et al. 1977; Prickett et al. 1981). The DPRW method is one of several Lagrangian type methods for solving differential equations that involve the convective transport of mass. Lagrangian methods de-couple the

convective transport, which is a hyperbolic type differential equation, and the dispersive transport, which is a parabolic type differential equation. The convective part is solved using the method of characteristics and the dispersive part by any parabolic method.

The DPRW method has the advantage in that it does not introduce numerical dispersion, it conserves mass, and it can take into account reactions during transport. The DPRW method has an additional advantage because it can be easily adapted test emerging transport theories that are based on particle position probabilities. The method is difficult to implement because a large number of particles should be used to simulate continuous behavior. The large number of particles are easily handled using any computer with a large memory, but the determination of displacement is simplified if that computer is also fast. These reasons made the HARC NEC SX-2 a good choice for this method.

The DPRW method models particle transport with step equations of the form,

$$x(t + \Delta t) = x(t) + \frac{q(t)}{n_e} * \Delta t + z \qquad (4)$$

where $x(t)$ is the position vector of a particle at time t , $q(t)$ is the seepage velocity vector at $x(t)$ and time t, Δt is the time step, and z is a random deviate from a multivariate normal distribution with a covariance matrix given by $(2*\Delta t * D)$. The second term in (4) represents the convective transport and the third term represents the dispersive transport. Typically the velocity field is augmented with a dispersion gradient to account for stagnation zones in a variable velocity field. This procedure was replaced in this study by including molecular diffusion in the dispersion tensor. This approach simplifies the modelling and still produces the desired behavior of some spreading even at zero velocity points.

The relationship between Equation (1) and (4) is be illustrated by coupling a hyperbolic convective transport equation, and a parabolic dispersion equation. If the concentration is defined as the number of particles of the same mass in a small volume Equation (4) without the random displacement closely approximates the behavior of the a hyperbolic convective transport equation,

$$n_e \frac{\partial C}{\partial t} = -div\,(C\,q) \qquad (5)$$

The random displacement term closely approximates the behavior of a parabolic dispersion equation along a characteristic curve,

$$n_e \frac{\partial C}{\partial t} = div(D\ grad(C)) \qquad (6)$$

Coupling Equations (5) and (6) in an Eulerian sense produces Equation (1). Other methods such as the U.S.G.S. MOC (method of characteristics) code (Konikow and Bredehoeft, 1978) actually solve (5) and (6) then recombine the results. The DPRW method, which has full analogy to the Fokker-Plank equation (Thompson et al.,1989), closely approximates (5) and (6) when a large number of particles are used. When the random step is taken from the Normal distribution, Fickian type dispersion is reproduced.

The seepage velocity used in Equation (4) is obtained from Equations (2) and (3). Equation (2) is solved using an alternating direction implicit scheme on a rectangular grid. The scheme is unconditionally stable, and is economical in its use of computer memory(Marsily, 1986). The gradient of the head distribution is determined by numerical differentiation using a centered difference scheme. This gradient is then used in Equation (3) to produce the seepage velocity field.

Model Sensitivities

The partial derivative field of modeled concentration with respect to the transport parameters (dispersivities, conductivities, porosities, etc.) is called the sensitivity field. These sensitivities are used to construct performance measures for selecting competing designs. The method used to compute the sensitivity field for a particular design in this work is the influence coefficient method (Yeh, 1986). The sensitivities at a design location are computed by divided differences and assembled into the Jacobian matrix for the particular design. For instance, suppose two sample locations at three times are used. The Jacobian would have the form

$$
\mathbf{J} = \begin{bmatrix}
\frac{\partial C}{\partial \theta_1}(x_1,t_1) & \frac{\partial C}{\partial \theta_2}(x_1,t_1) & \frac{\partial C}{\partial \theta_3}(x_1,t_1) \cdots & \frac{\partial C}{\partial \theta_k}(x_1,t_1) \\
\frac{\partial C}{\partial \theta_1}(x_2,t_1) & \frac{\partial C}{\partial \theta_2}(x_2,t_1) & \frac{\partial C}{\partial \theta_3}(x_2,t_1) \cdots & \frac{\partial C}{\partial \theta_k}(x_2,t_1) \\
\frac{\partial C}{\partial \theta_1}(x_1,t_2) & \frac{\partial C}{\partial \theta_2}(x_1,t_2) & \frac{\partial C}{\partial \theta_3}(x_1,t_2) \cdots & \frac{\partial C}{\partial \theta_k}(x_1,t_2) \\
\frac{\partial C}{\partial \theta_1}(x_2,t_2) & \frac{\partial C}{\partial \theta_2}(x_2,t_2) & \frac{\partial C}{\partial \theta_3}(x_2,t_2) \cdots & \frac{\partial C}{\partial \theta_k}(x_2,t_2) \\
\frac{\partial C}{\partial \theta_1}(x_1,t_3) & \frac{\partial C}{\partial \theta_2}(x_1,t_3) & \frac{\partial C}{\partial \theta_3}(x_1,t_3) \cdots & \frac{\partial C}{\partial \theta_k}(x_1,t_3) \\
\frac{\partial C}{\partial \theta_1}(x_2,t_3) & \frac{\partial C}{\partial \theta_2}(x_2,t_3) & \frac{\partial C}{\partial \theta_3}(x_2,t_3) \cdots & \frac{\partial C}{\partial \theta_k}(x_2,t_3)
\end{bmatrix}
$$

where θ_i is the i-th parameter of interest.

Design Performance Criteria

An optimal design algorithm typically uses an optimization model to locate as well as schedule sampling sites. A performance criterion is used to evaluate a design's relative performance. This criterion can be based on a measure of the estimates' covariance matrix, information matrix, or on some output error criterion. This research tests performance criterion based on the estimate's covariance and information matrix.

The performance measure is constructed from sensitivity information. For an additive-error model

$$\mathbf{C}_{Obs} = \mathbf{C}_{Model}(\theta) + \mathbf{Error}$$

where

$\mathbf{C}_{Obs}$ = vector of observed concentrations in space and time

$\mathbf{C}_{Model}$ = vector of simulated concentrations in space and time

$E(\mathbf{Error}) = 0$

$V(\mathbf{Error}) = \Sigma$

in which Σ is the common covariance matrix of the error. The symbols E and V denote expectation and covariance operators. Assuming a least-squares-parameter estimation scheme is used, a linear

approximation to the estimate's covariance matrix is (Yeh and Yoon, 1981):

$$V(\theta) = M\Sigma M^T$$

where

$$M = (J^T J)^{-1} J^T$$

For this work the special case is considered where the error structure is

$$\Sigma = \sigma^2 I$$

where σ^2 is the variance and **I** is the identity matrix. The approximation of the estimate's covariance matrix is

$$V(\theta) = \sigma^2 (J^T J)^{-1}$$

The information matrix is the inverse of the covariance matrix.

Optimal designs are those which optimize some measure of the covariance structure of the estimates. When the estimates have small variance they are said to be reliable. To achieve reliable estimates minimizing the "size" of the covariance matrix or maximizing the "size" of the information matrix is required. The measures of size investigated in this work are: (1) The determinant of the covariance matrix (D-optimality). (2) The trace of the covariance matrix (A-optimality). (3) The trace of the information matrix (CR-optimality with weight matrix **I**).

Different designs only generate different Jacobians, therefore the σ^2 is ignored. Cleveland and Yeh (1990) proposed CR-optimality as a computationally simple alternative to D and A optimal design criteria. It avoids having to invert the Jacobian and reduces the computational effort in evaluating different designs in a combinatorial optimization algorithm.

This research computes these criterion in the following manner. The model is operated and the Jacobian for a particular design is constructed using the influence coefficient method. The Jacobian is multiplied by its transpose to construct the information matrix. The eigenvalues for this matrix are computed using Jacobi rotations. Because the matrix is real symmetric, the eigenvalues are real. The running product of the eigenvalues is used to compute the determinant of the information matrix. The running sum gives the trace of the matrix. This value is the CR-optimality criterion. The determinant is saved as a check. The matrix is inverted using repeated

Gauss-Sidell iteration with varying right hand side vectors that span the parameter space. This inverse is the linear approximation of the estimates' covariance matrix. The determinant is computed using Jacobi rotations to compute the eigenvalues of the matrix. This determinant is the D-optimality criterion. The running sum of these eigenvalues gives the A-optimality criterion.

Experimental Design

The next step after a performance criterion is selected is to construct an optimization algorithm to construct and select optimal designs according to the problem constraints. Such design problems tend to be nonlinear integer programming problems. In this work an optimization algorithm was not used because the number of designs was small and the designs were pre-specified. The selection criteria are calculated for each design and the best design evaluated by inspection. The evaluation is different for each criterion: CR-optimality maximizes its measure, A-optimality minimizes its measure, and D-optimality minimizes its measure.

Example Problem

A hypothetical tracer test is modeled in the hypothetical inhomogeneous aquifer shown on Figure 1. Two known tracer slugs are injected over a finite time near well W-1. The first mass slug is assumed to be "injected" without disturbing the flow, the second mass slug is introduced on the up-gradient side of well W-1. Water is continuously injected at well W-1 and extracted at well W-2. The underlying hydraulic and transport parameters are listed in Table 1.

The four designs to be tested are listed in Table 2. Designs 1 and 2 are images of each other (symmetric about the injection well). Designs 3 and 4 are also mirror images of each other (symmetric about x=8.00 meters).

Figures 2 through 4 show the mass envelope at different times during the simulated tracer test. The tracer masses were split (using the injection schedule above) to bias the selection criterion. Previous experience with optimal design algorithms indicated that the algorithms tend to select designs near a concentration source (Cleveland and Yeh, 1991; McKinney, 1991) and the split masses were thought to be more challenging for the selection criteria.

Table 3 lists the performance criteria for each design. The CR-optimal, A-optimal, and D-

optimal criterion behave similarly when testing image designs. From these criteria one can conclude that design 1 is better than design 2 and design 4 is better that design 3. The CR-optimal, A-optimal, and the D-optimal criterion select design 4 as the best. By construction, CR-optimal designs and D-optimal designs should select sample locations that have a high (in magnitude) parameter sensitivity over time.

Figures 5 through 7 show contour maps of the concentration sensitivity to hydraulic conductivity in Zone 1 at different times. Figures 8 through 10 show the concentration sensitivity to hydraulic conductivity in Zone 2 at different times. Figures 11 through 16 show the sensitivity to longitudinal dispersivity in each zone at different times. The high sensitivity regions in the maps are at locations where the contour lines indicate steep topography.

Figures 5 and 8 show the high sensitivity locations to conductivity for a simulation time of one month at locations where the mass envelope map indicates relatively steep concentration gradients. The sensitivity maps of longitudinal dispersion (Figures 11 through 16) are more difficult to interpret but show slightly "out of phase" behavior as compared to the hydraulic conductivity sensitivity. At later simulation times, the mass envelope spreads (Figure 3). The sensitivity to hydraulic conductivity is still high at locations with high concentration gradients. The dispersivity maps exhibit a more pronounced "out of phase" high sensitivity behavior. This behavior was observed by Knoppman and Voss (1987). In their work with one-dimensional advection-dispersion models, they showed that the maximum sensitivity to dispersion occurs at locations with maximum concentration profile curvature. The locations maximum curvature in the particle tracking model occurs slightly out of phase with the locations of steep concentration gradients. In this example, many of these locations occur at the periphery of the mass envelope.

These contour maps indicate the locations of the candidate design points as small dots on the maps. For the three sampling times times shown, design 4 has at least one sample location in or near a high sensitivity region at all times. Because all the selection criterion are constructed to select locations with high sensitivity the design that has sample locations frequently in regions of high sensitivity should be selected.

In this study using these designs the CR-optimal and D-optimal criterion selected designs that included sampling locations in both zones. This behavior was not observed in earlier studies by Cleveland (1989) and Cleveland and Yeh (1990). The fundamental difference in this study is the use of a particle tracking approach rather than classical density (concentration) tracking. An explanation for the "improved" behavior is that a particle tracking approach preserves concentration contrasts even at very low concentrations. Further research should extend this work into three dimensions, and include a non-linear integer programming routine to construct the best cost constrained designs for various hypothetical aquifers.

Conclusion

This research compared three reliability measures that operate on the estimated parameter's covariance matrix. A set of designs was selected and each reliability measure is used to select the best design of the set. The resulting designs were compared using a simulation sensitivity analysis to determine what features of the model sensitivites are selected for by the particular measures. The design selection criterion select designs that sample at locations with steep sensitivity topography. CR-optimality, A-optimality, and D-optimality all select the same optimal design for the four design problem presented here. Further work is needed to determine the generality of this behavior. Such work could be used to determine whether CR-optimality, which is computationally easier, can be substituted for A-optimality or D-optimality.

Improved behavior over earlier work was observed. The improved behavior is attributed to the simulation method that can preserve concentration contrasts even at low modeled concentrations. The simulation model used a Lagrangian particle tracking method to model transport because this method generates no numerical dispersion. Although not emphasized, the particle tracking method used here requires considerable memory and computer speed, and the HARC NEC SX-2 supercomputer was critical to the success of this study.

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Table1. Aquifer Parameters

Parameter	Zone 1	Zone 2
K(meters/year)	100.00	50.00
n_e	0.30	0.20
b(meters)	10.00	10.00
α_L	10.00	10.00
α_T	1.00	1.00
Injection Rate (meters/year)	1000.00	
Extraction Rate (meters/year)		1000.00

Table 2. Candidate Designs

Design	Sampling Locations
1	A,C,E
2	B,F,D
3	D,F,H
4	E,I,G

Table 3. Performance Criteria for Four Designs

Design	CR-optimality	A-optimality	D-optimality
1	$6.944 \cdot 10^{2}$	$1.885 \cdot 10^{0}$	5.308^{-10}
2	$6.578 \cdot 10^{2}$	$9.383 \cdot 10^{0}$	2.911^{-6}
3	$5.001 \cdot 10^{2}$	$4.216 \cdot 10^{0}$	3.854^{-7}
4	$8.750 \cdot 10^{2}$	$2.791 \cdot 10^{-1}$	9.537^{-15}

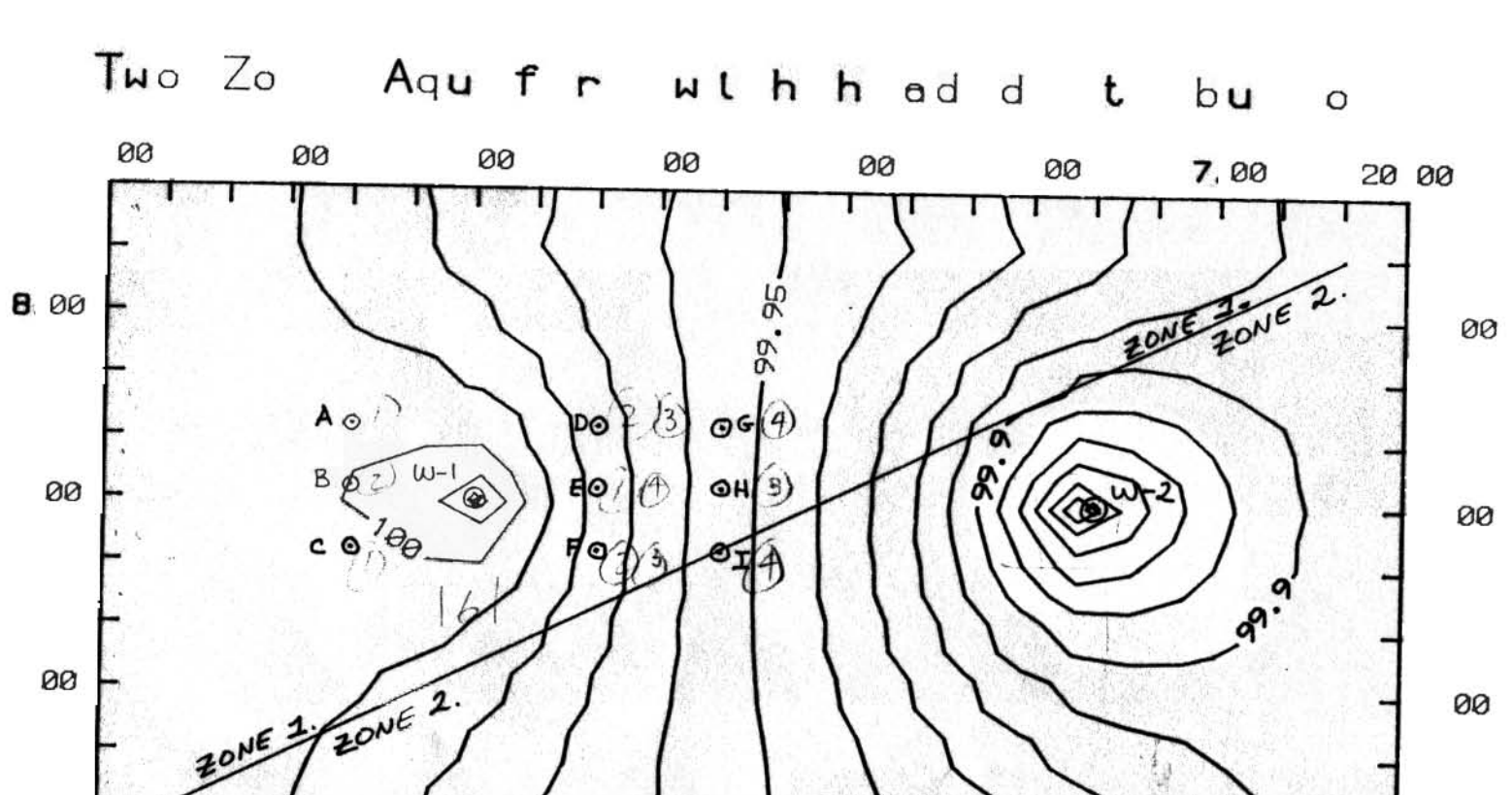

Figure **H**ypothetical Aquifer for lamplin Design.

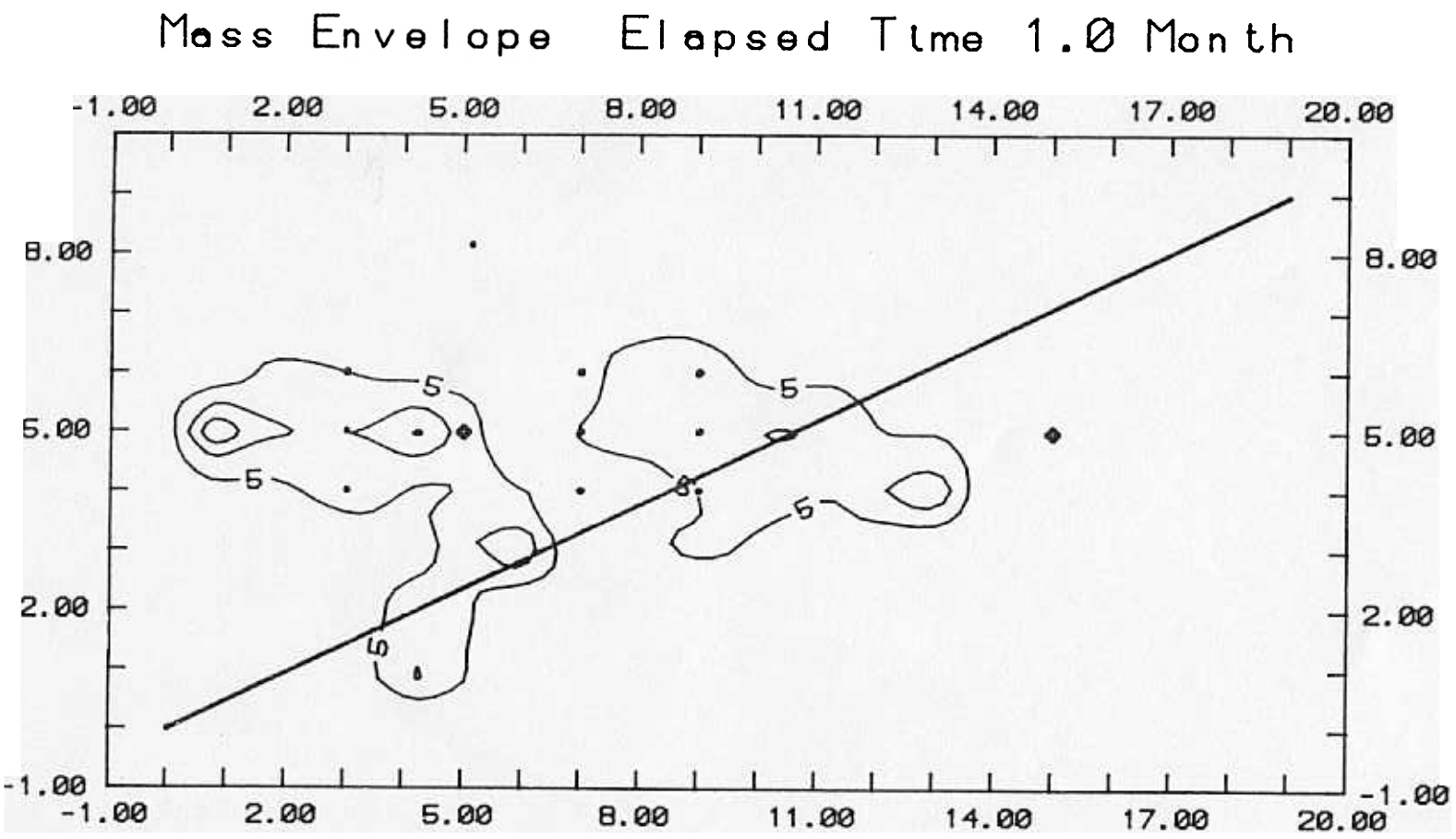

Figure 2. Mass Envelope for Parameters in Table 1.

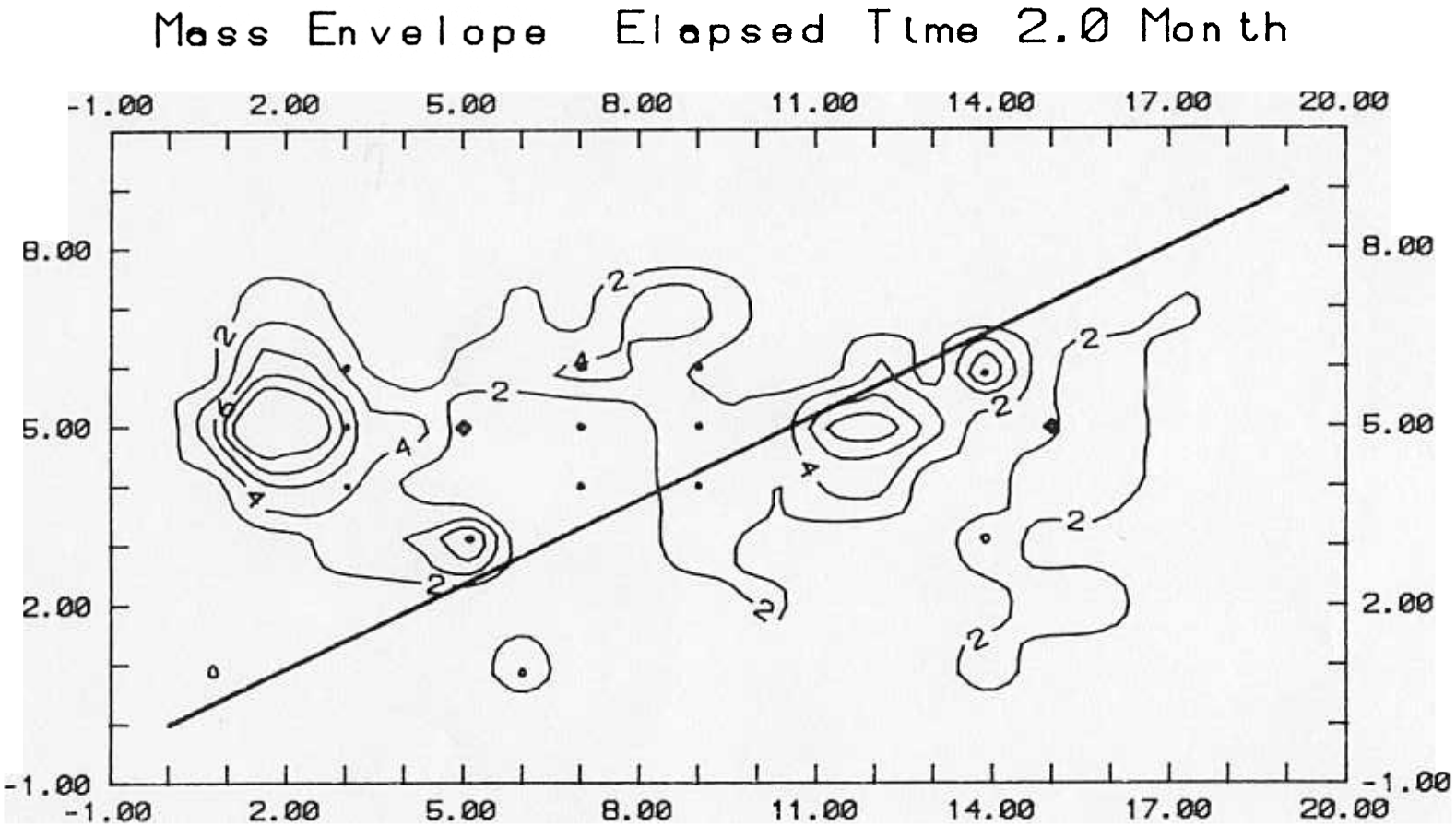

Figure 3. Mass Envelope for Parameters in Table 1.

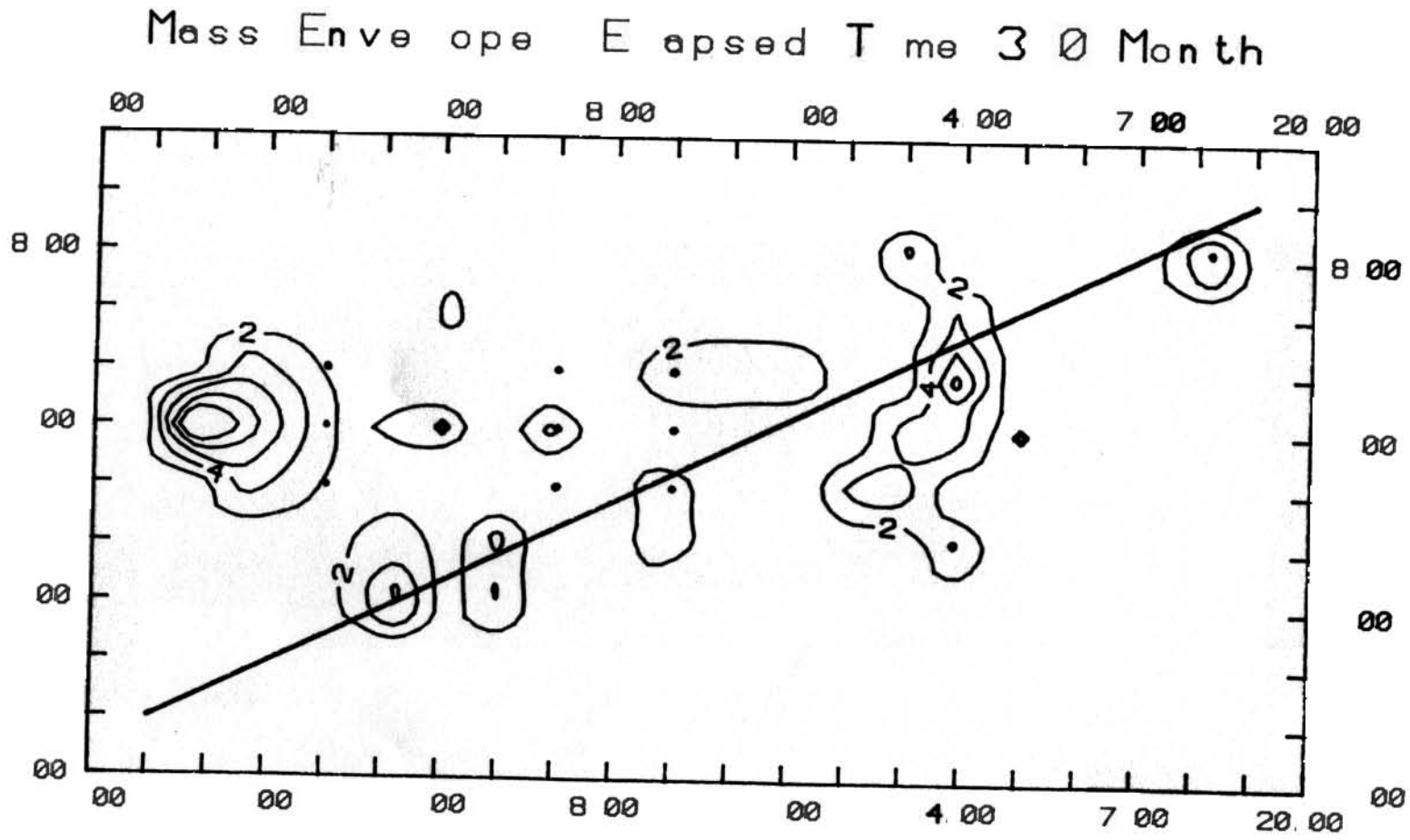

Figure Mass Envelope for Parameters in Table

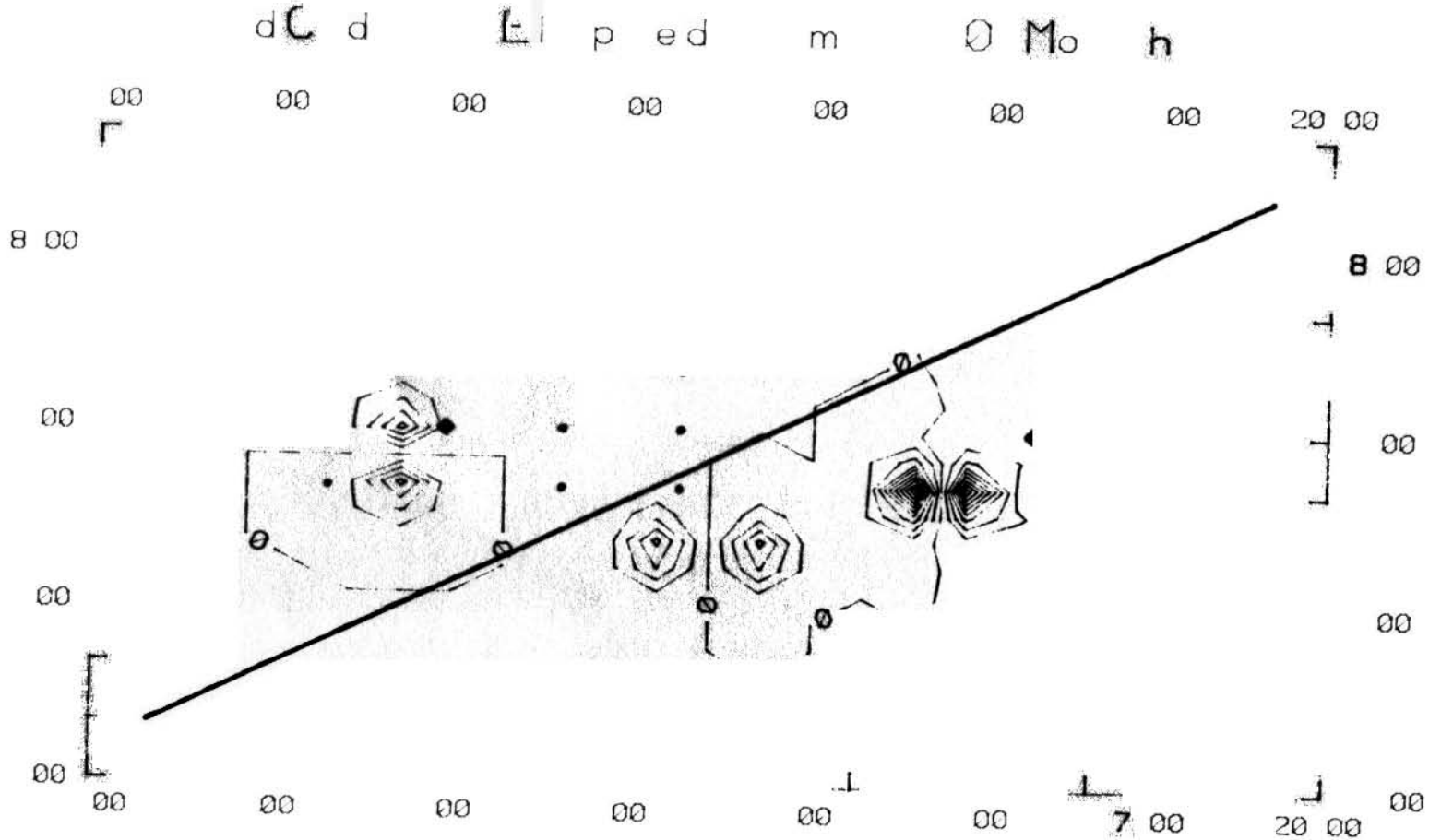

Figure Sensitivity to Hydraulic Conductivity in Zone

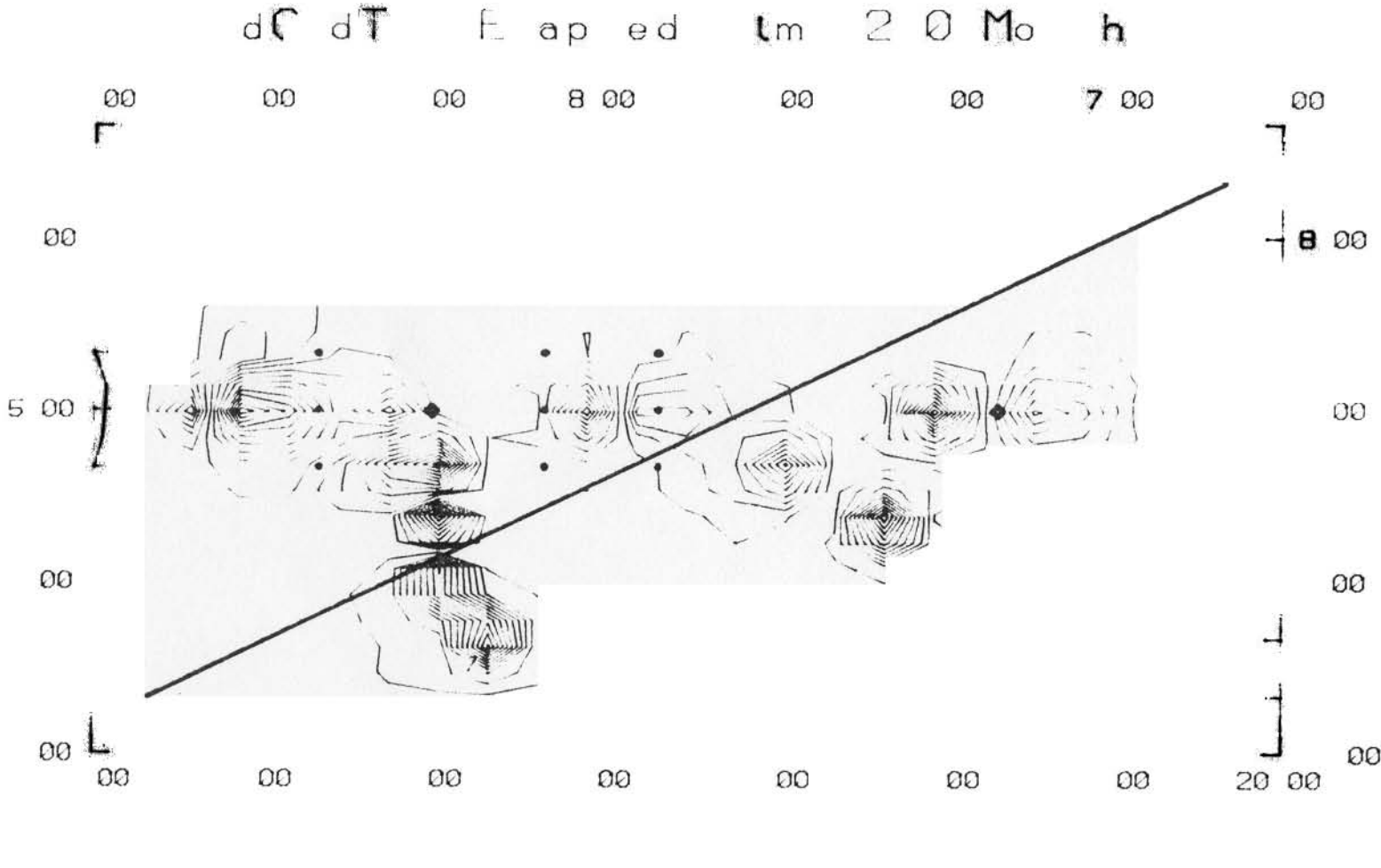

Figure **6.** Sensitivity to Hydraulic Conductivity in Zone

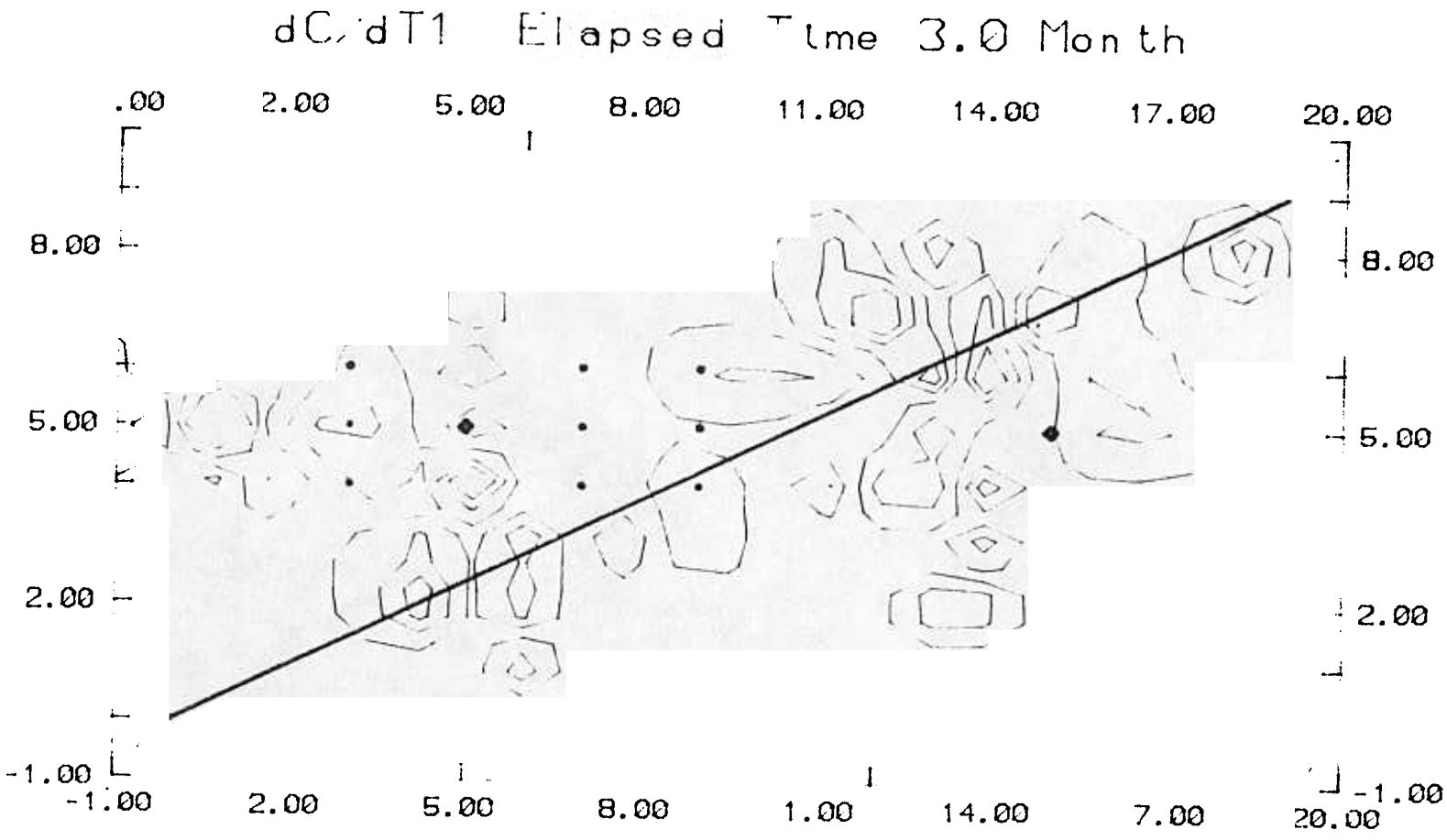

Figure 7. Sensitivity to Hydraulic Conductivity in Zone 1.

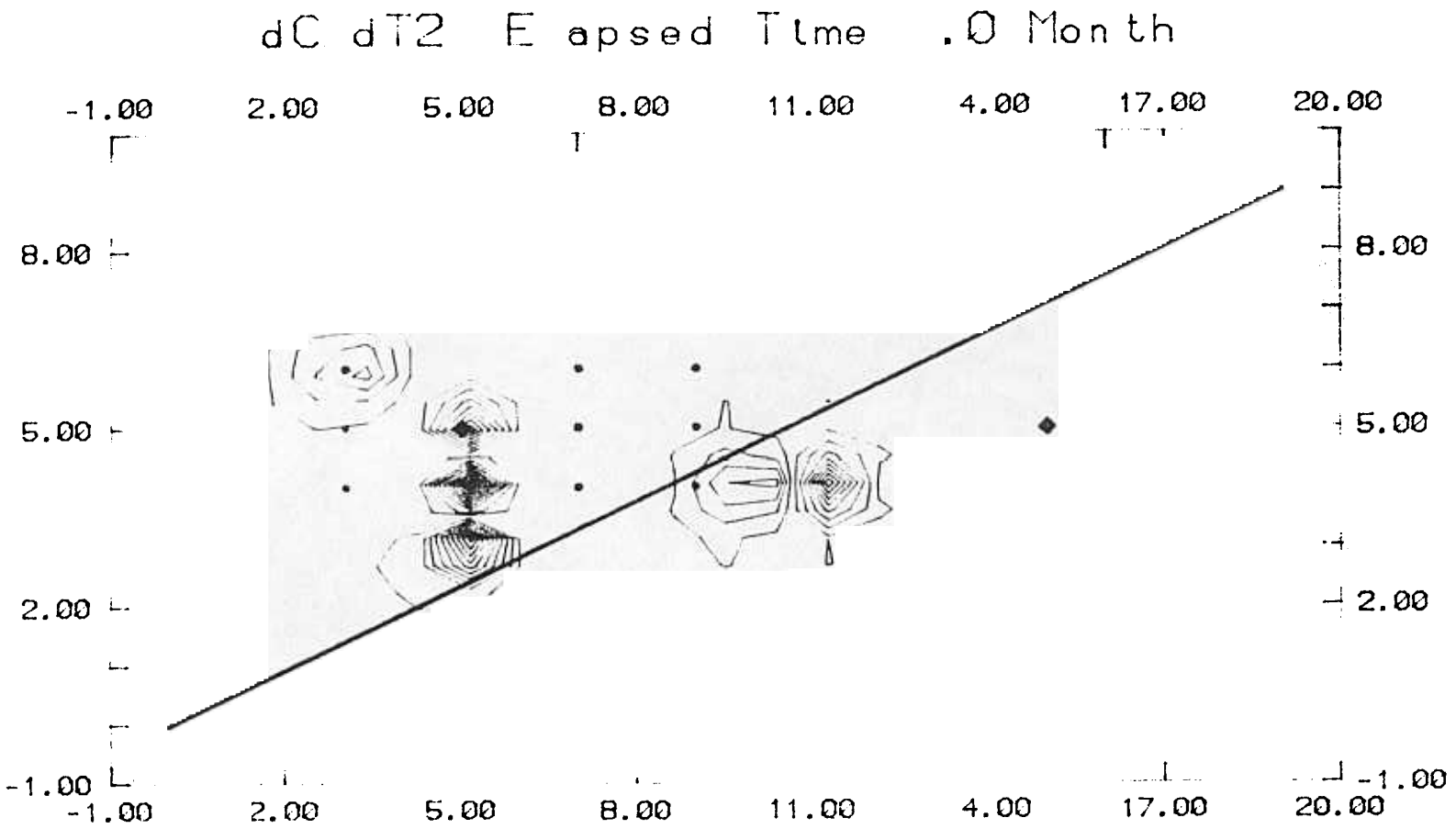

Figure 8. Sensitivity to Hydraulic Conductivity in Zone 2.

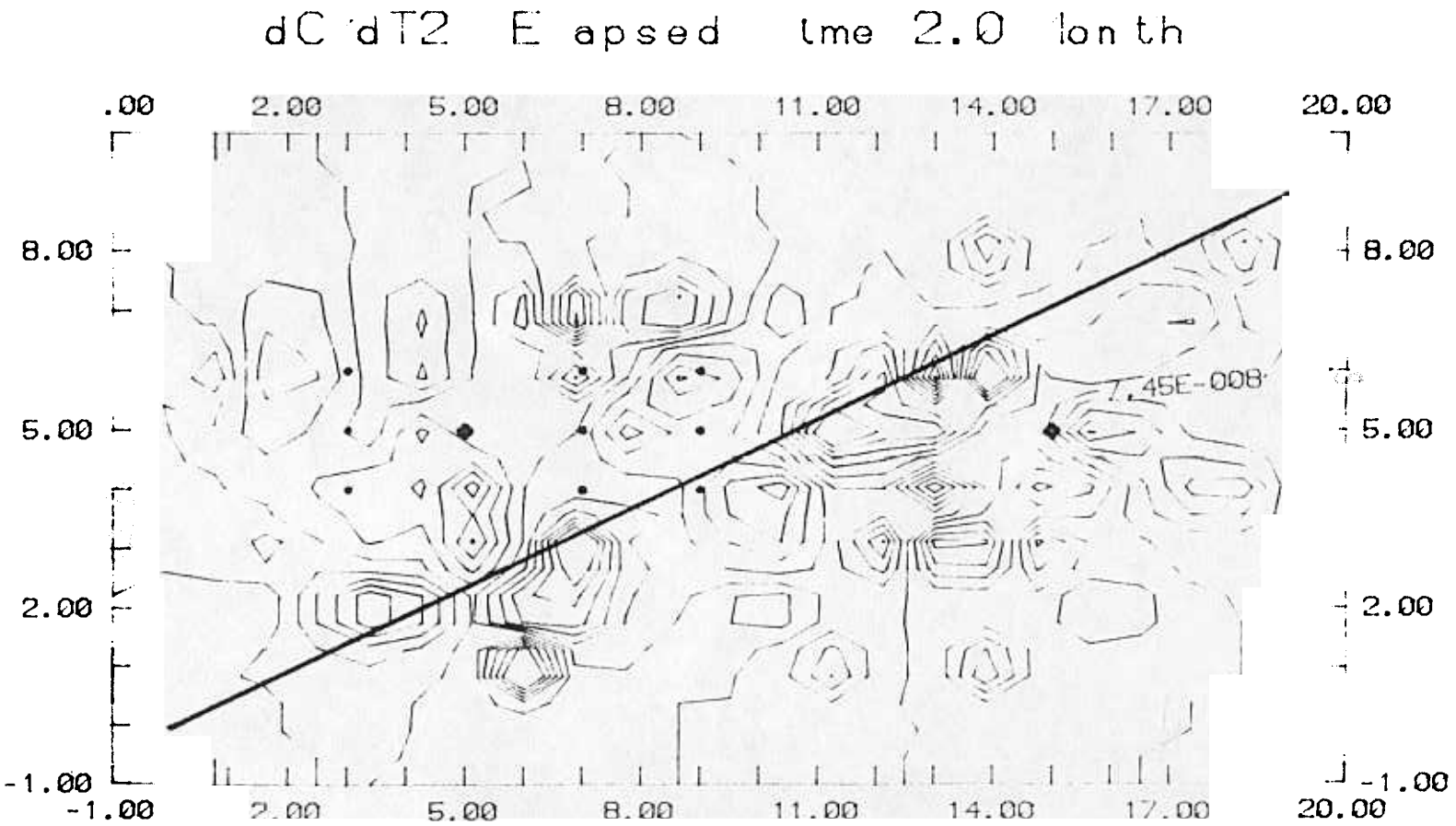

Figure 9. Sensitivity to Hydraulic Conductivity in Zone 2.

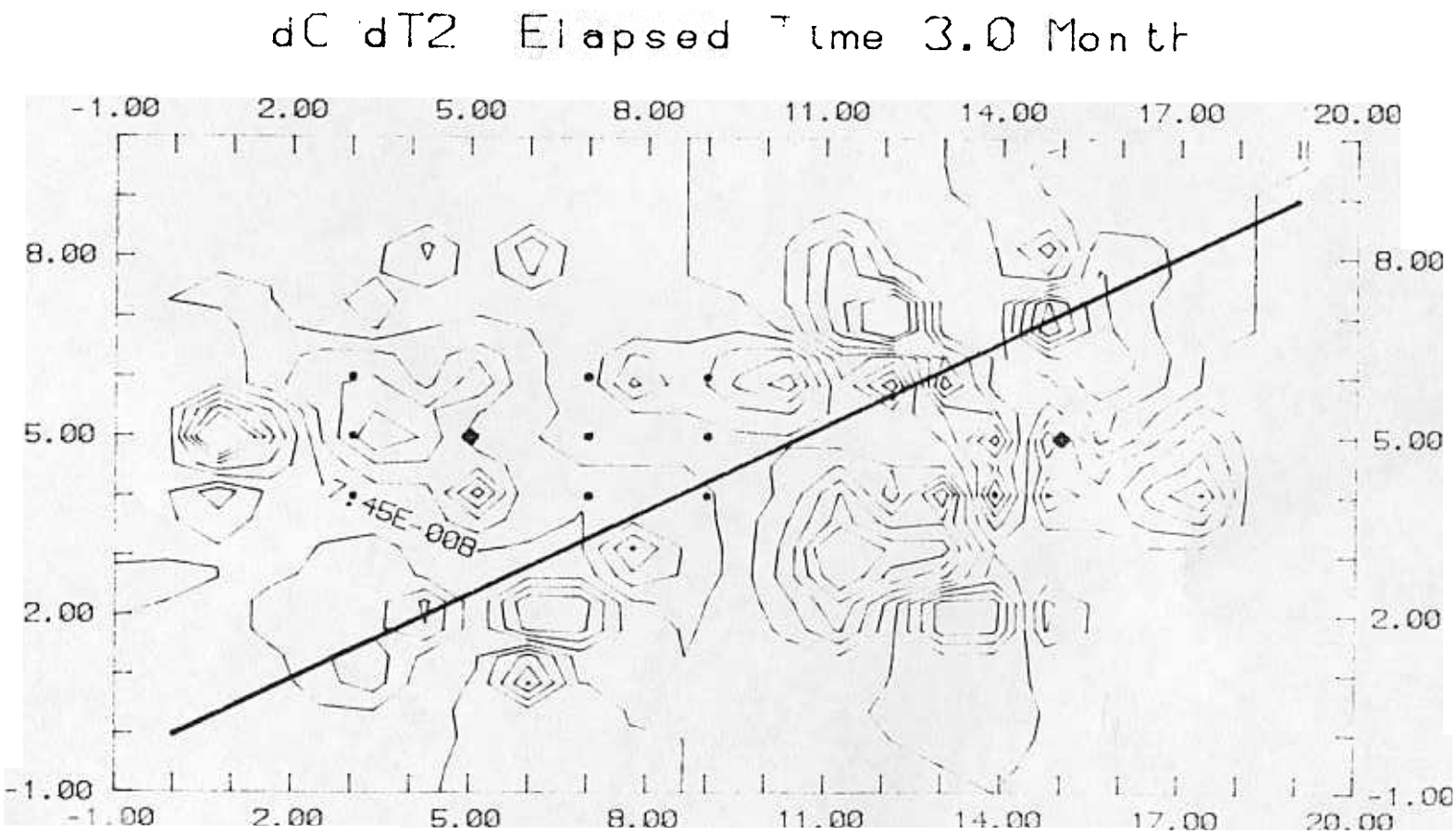

Figure 10. Sensitivity to Hydraulic Conductivity in Zone 2.

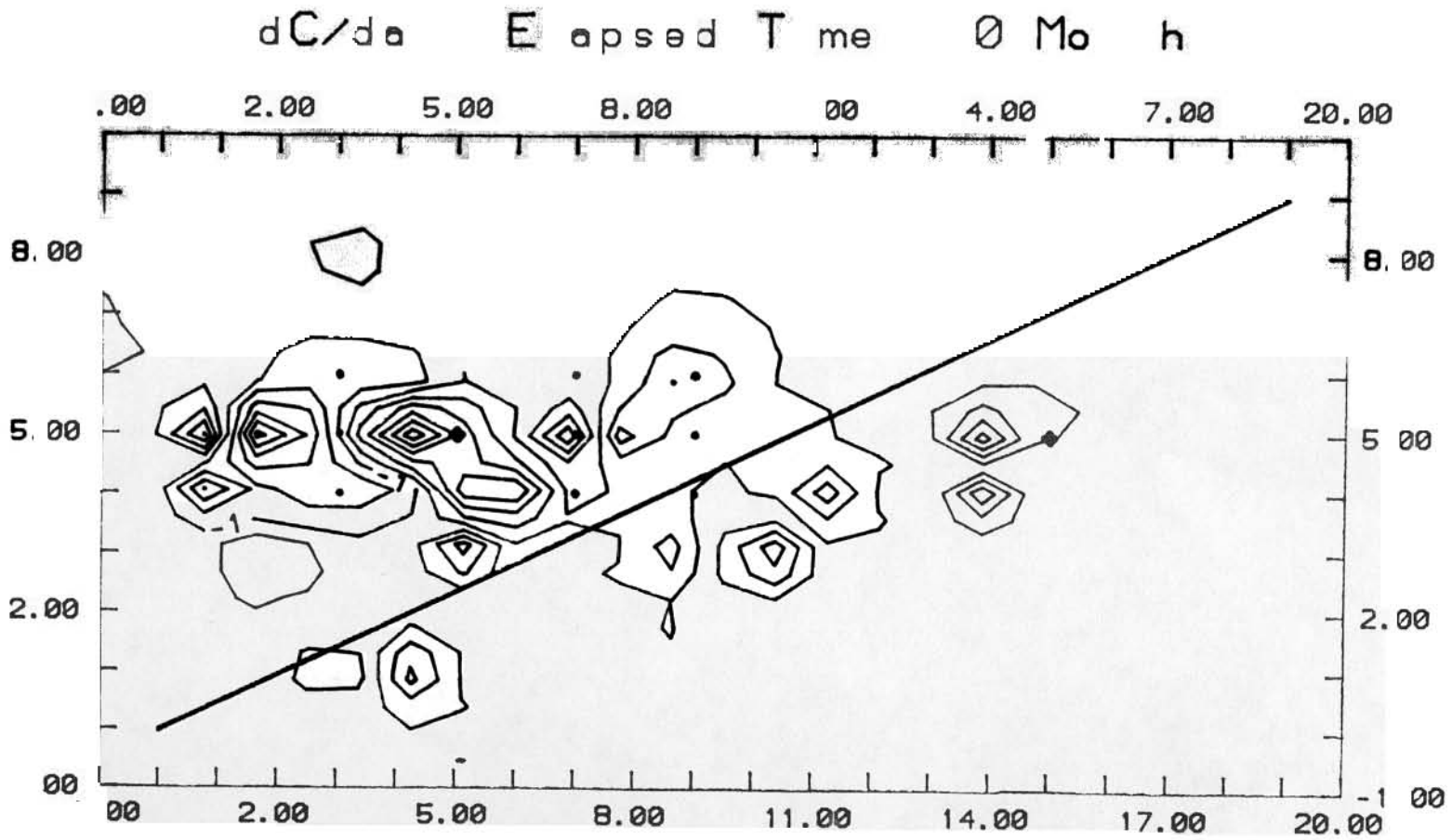

Figure Sensitivity to Dispersivity Zone

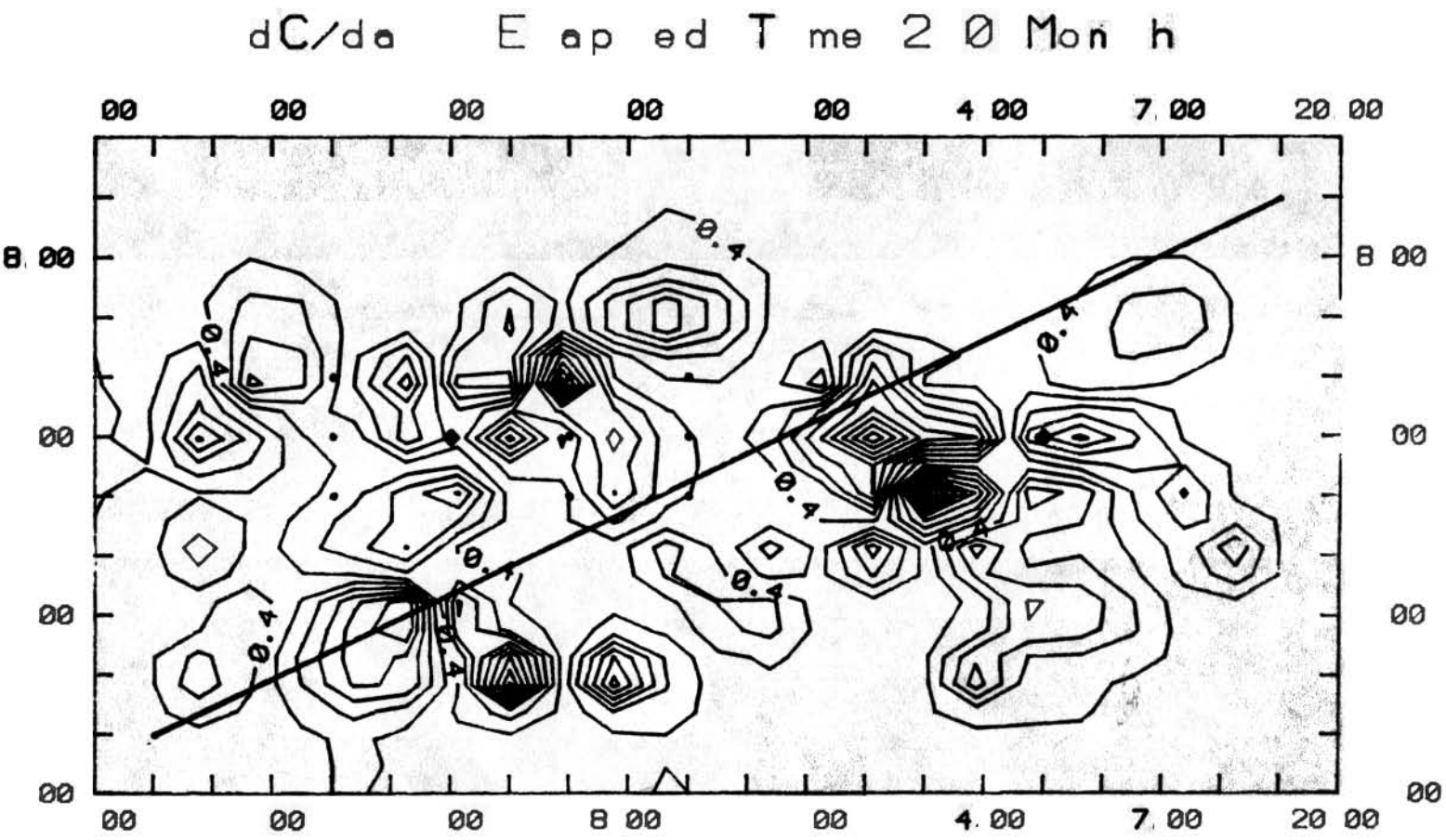

Fig Sen vity to Di persivi Zo

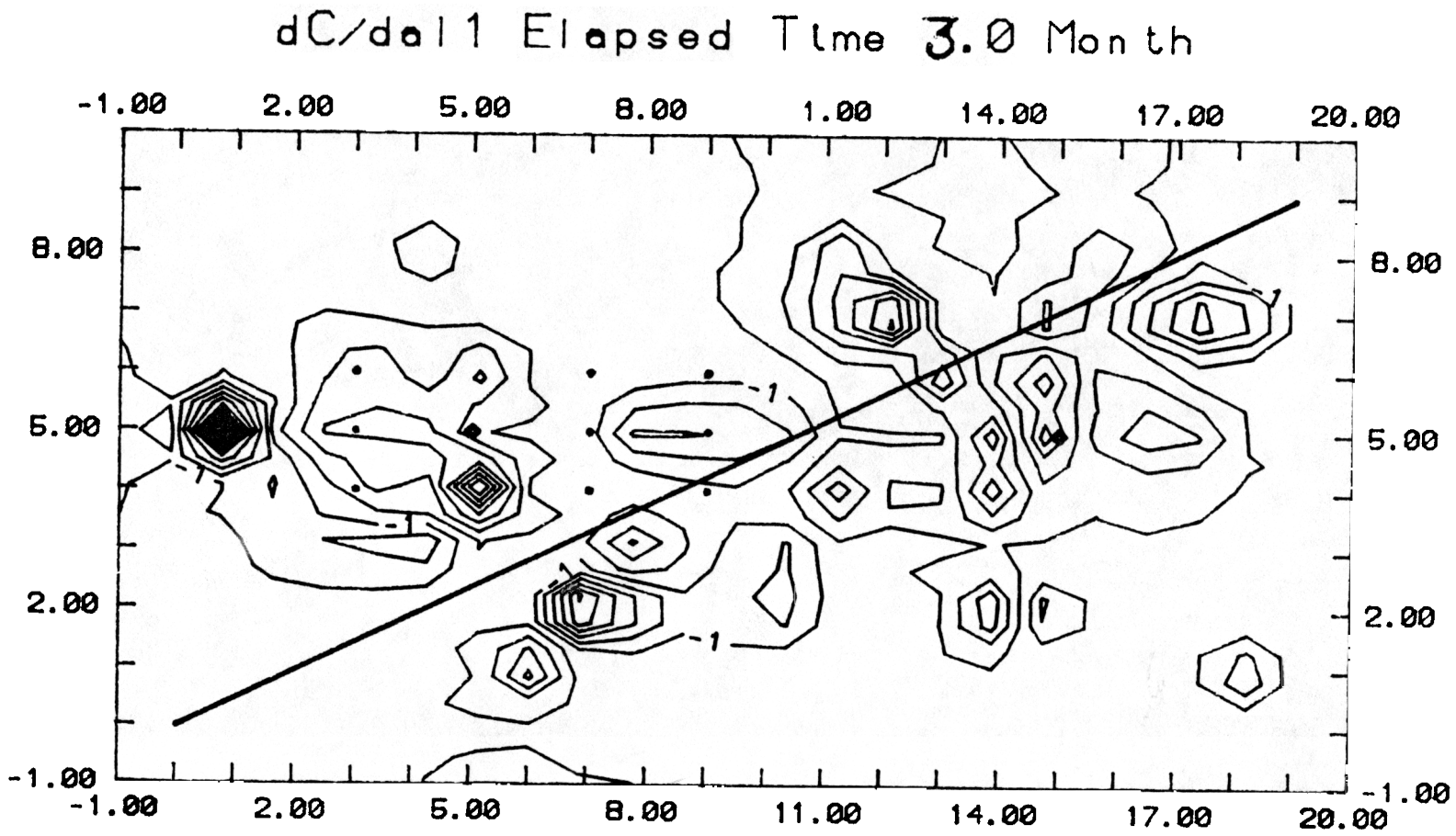

Figure 13. Sensitivity to Dispersivity in Zone 1.

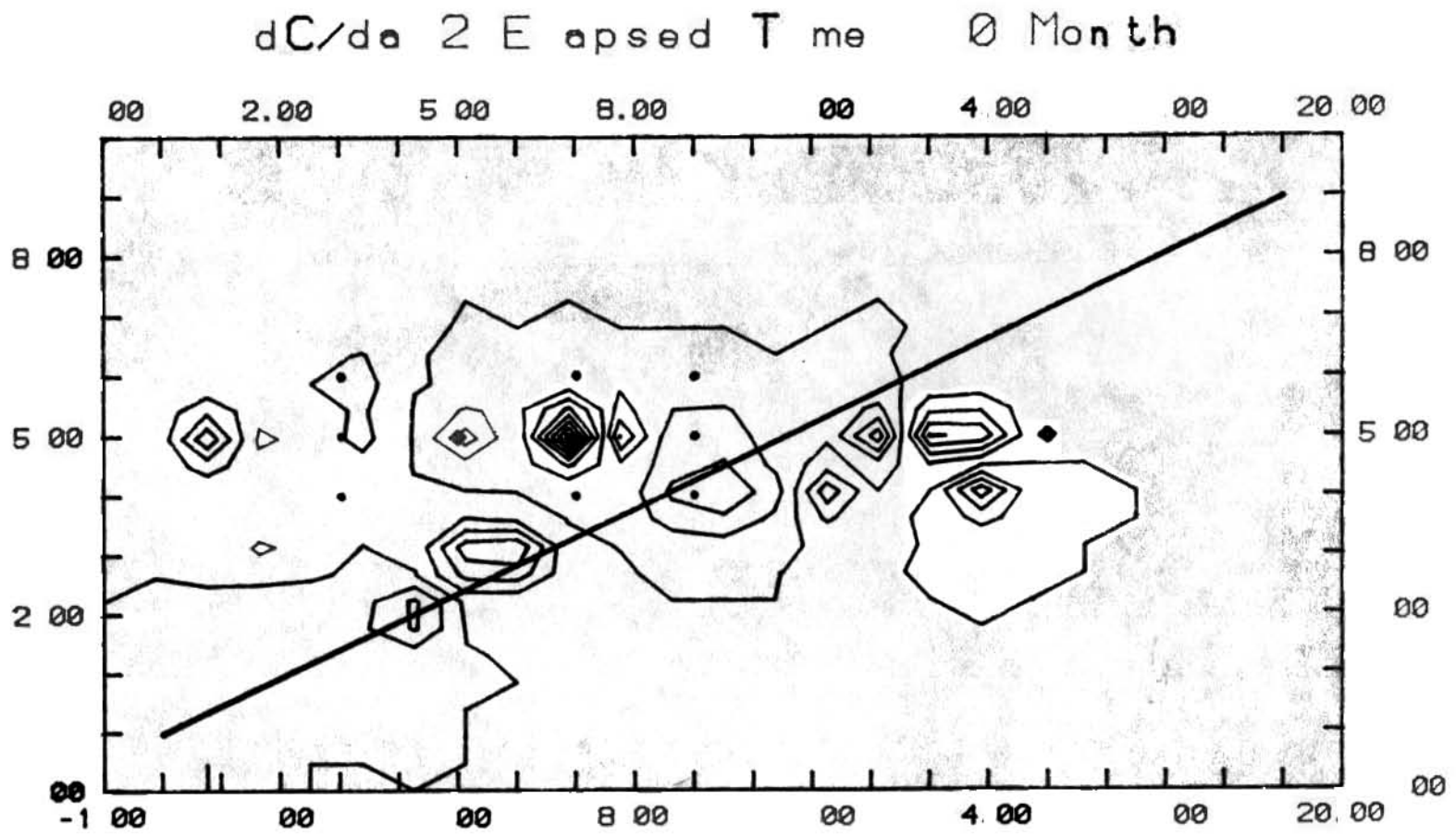

Figure 4. Sensitivity to Dispersivity in Zone 2.

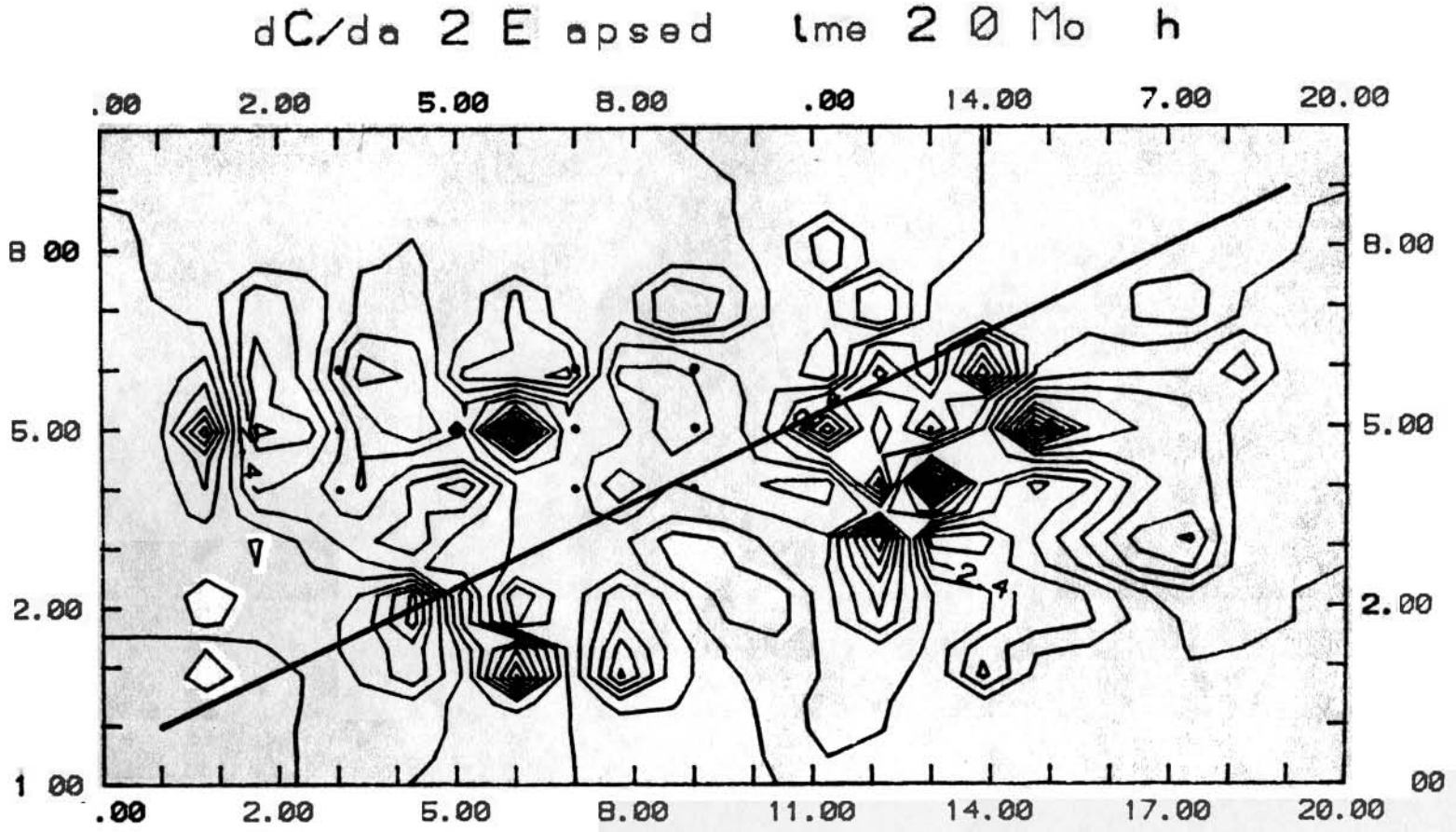

Figure 15. Sensitivity to Dispersivity in Zone 2.

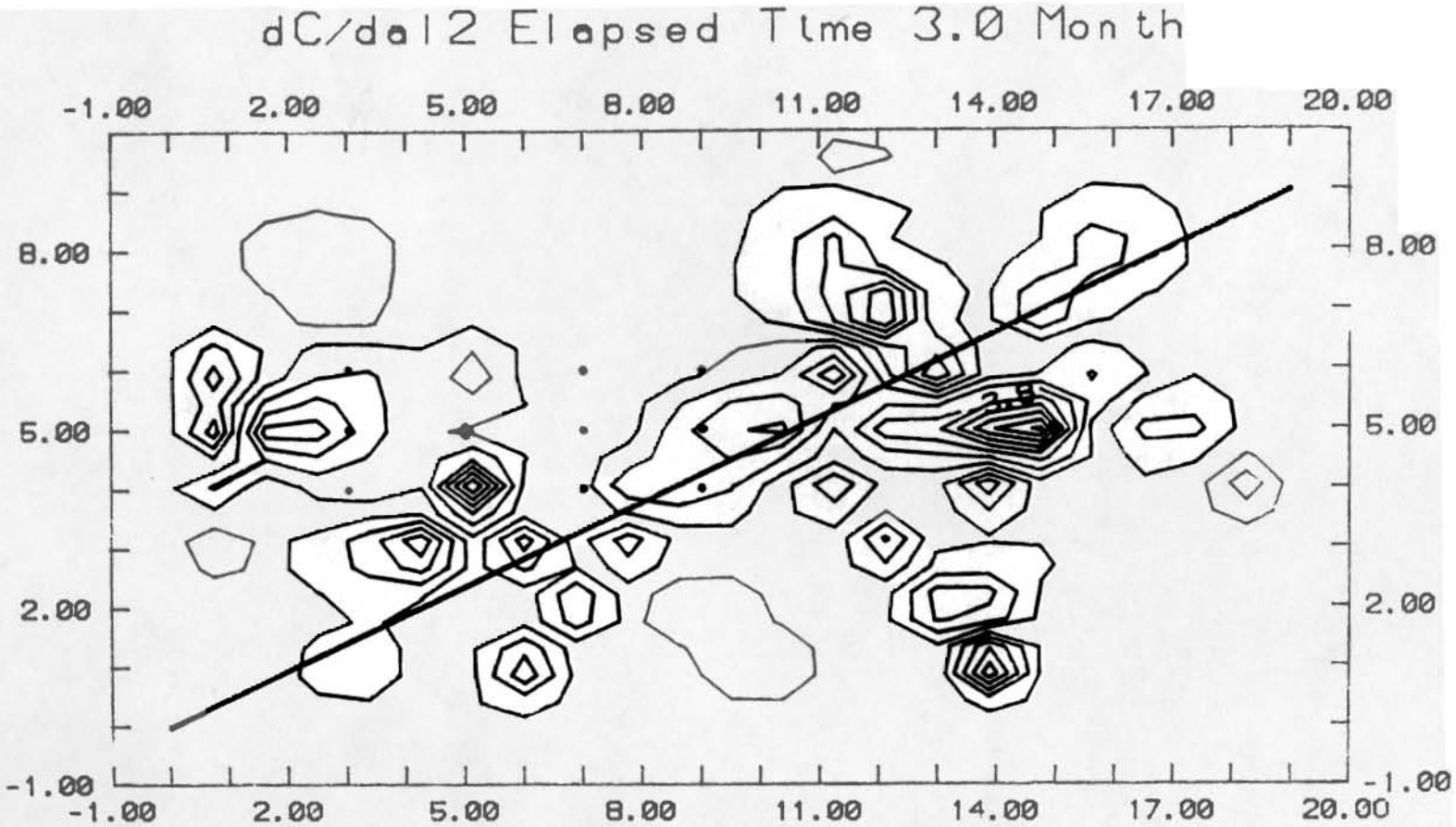

Figure 16. Sensitivity to Dispersivity in Zone 2.