87-11

THE USE OF SENSITIVITY ANALYSIS TO DESIGN AN EFFECTIVE MONITORING NETWORK AND ESTIMATE PARAMETERS FOR A TWO-DIMENSIONAL SOLUTE TRANSPORT MODEL

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ABSTRACT

In this paper, an analytical two-dimensional model of solute transport, including logitudinal and transverse dispersion along with advection, is considered. Additional considerations include an extended source of finite length, a retardation factor, exponential decay of the source production, and natural decay of the pollutant. A sensitivity coefficient can be defined and calculated for each parameter of interest. The sensitivity coefficients vary over space and time. In order to have an effective monitoring system, the wells must sample at times and space locations that have significant sensitivities to the parameters of interest. Spatial and temporal variations of the sensitivities for several parameters of the model will be illustrated. Sensitivity analysis allows one to make intelligent decisions regarding the spatial and temporal locations of physical measurements. Obviously, the network should evolve in space and time, depending on the parameter of interest. Some wells will become insensitive and may be dropped while new sensitive wells will need to be added. Sensitivity analysis provides a method to design an effective evolving monitoring network. Of course, initial estimates of the parameters must be assumed to get started; but the system can be self-correcting as it proceeds. Standard statistical techniques can be utilized to estimate the parameters and estimate the variance and confidence intervals. As the parameter estimates improve, the future design of the monitoring system and concentration prediction also improve.

INTRODUCTION

In this paper an analytical two-dimensional model of solute transport is considered. However, the formalism of sensitivity analysis and its use to design a monitoring network is very general and could be applied to most any model.

THE MODEL

This slide **(slide #1)** shows the two-dimensional model we will be working with. It includes longitudinal and transverse dispersion (D_L and D_T) along with advection (ν). Additional considerations include an extended source of finite length (2a), a retardation factor (R), exponential decay of the source production (α), and natural decay of the pollutant (λ). The next slide **(slide #2)** shows the analytical solution for this model. A modified version of the computer program published by Javandel et al. in Groundwater Transport was used to calculate the concentration over space and time.

SENSITIVITY FORMALISM

A sensitivity coefficient can be defined and calculated for each parameter of interest. The next slide **(slide #3)** shows the definition of a sensitivity coefficient (Z). Z_p will be the sensitivity of the concentration to a parameter p. The sensitivity coefficient represents the change in concentration that occurs when one parameter is changed by a small amount. In order to directly compare sensitivity coefficients for various parameters and to maximize computer accuracy, it is usually better to work with normalized sensitivity coefficients.

Sensitivity coefficients **(slide #4)** can be determined a number of ways. If an analytical solution for concentration is available, as in the model used for this paper, the sensitivity coefficients can be obtained by differentiating with respect to the parameter of interest. Sensitivity coefficients may also be obtained by solving the model twice with slightly different parameter values and forming a finite difference approximation, $\Delta C/\Delta P$. A partial differential equation for sensitivity coefficients may also be formulated and solved. It is very similar to the original model equation and usually requires little code modification.

The sensitivity coefficients vary over space and time. In order to have an effective monitoring system, the wells must sample at times and space locations that have significant sensitivities to the parameters of interest. The sensitivity matrix **(slide #5)** can be formed as shown. The columns are sensitivities with respect to a certain parameter. In this model, we have seven parameters, so we have seven columns. The rows are numbered from one to n and represent measurement points in space and time. In order to maximize parameter sensitivity, we should try to maximize the entries in the sensitivity matrix. In other words, perform the measurements at places and times that have large sensitivity coefficients.

The sensitivity matrix is pivotal to the rest of this paper. If two parameters are dependent, two columns of the sensitivity matrix will be identical except for a scaling factor. This will make parameter identification difficult or impossible. **(slide #6)** In ordinary least squares parameter estimation where the concentration errors are assumed to be additive, zero mean and uncorrelated, with constant variance, the parameter covariance matrix is given in this slide. The estimated standard error (e.s.e.) of parameter P_k is the square root of the k^{th} diagonal element. A good design for a monitoring well network will result in low values for the estimated standard error of all parameters. This translates into making measurements at space and time locations that have large sensitivity coefficients.

As mentioned earlier, if two sensitivity coefficients are dependent $\underset{\sim}{Z}^T\underset{\sim}{Z}$ is a singular matrix and the present formalism cannot be used. The sensitivity correlation matrix **(slide #7)** defined in this slide gives a way to look at the colinearity in the n-dimensional measurement space of the various sensitivity coefficients. The diagonal elements are all one. Any off-diagonal elements in the range of .9-1.0 indicate a high degree of colinearity and it may produce instability in parameter estimation. An off-diagonal element of 1.0 indicates complete dependence or colinearity. In this case, one of the parameters must be eliminated from consideration. From a practical standpoint, it may be that one would need to eliminate one of the parameters for each off-diagonal element which is greater than about .9.

MODEL RESULTS

The preceeding ideas will be illustrated by looking at results from the two-dimensional model defined earlier. The following physical parameters were used **(slide #8)**: ground-water pore velocity of .1 m/day, longitudinal dispersion coefficient of 1.0 m^2/day, transverse dispersion coefficient of .1 m^2/day, contamination source half-width of 50 m, natural decay constant of 0.0 $days^{-1}$, retardation factor of 1.0, and source decay constant of 0.0 $days^{-1}$. This slide shows the concentration contours after 4380 days or 12 years. The next slide (**slide #9**) shows a cross section of the concentration contour plot at y = 0 m. The next (**slide #10**) is a cross section at x = 260 m, and appears to be Gaussian in shape. The next slide (**slide #11**) shows the sensitivity with respect to ground-water pore velocity at 4380 days. The next two slides (**slides 12 and 13**) show cross sections at y = 0 m and x = 440 m. (**slide #14**) The sensitivity with respect to longitudinal dispersion coefficient is shown in this slide. It has a negative and positive peak. (**slides 15, 16, and 17**) Cross sections at y = 0 m, x = 340 m, and x = 540 m are shown in the next three slides. (**slide #18**) The sensitivity with respect to transverse dispersion coefficient is shown in this slide. Cross sections at y = 0 m and x = 200 m are shown in the next two slides (**slides 19 and 20**). Finally, the sensitivity with respect to source half-width is shown in this slide (**slide 21**). Cross sections at y = 50 m and x = 300 m are shown in the next two slides (**slides 22 and 23**).

We have not shown plots for the sensitivity with respect to the retardation factor, natural decay, and source decay. The sensitivity correlation matrix shows there is a high correlation between the sensitivity with respect velocity and retardation. This should probably be expected for R = 1.0. Therefore, we cannot estimate both velocity and retardation when R is close to one. Since the natural decay and source decay constants are zero, the corresponding sensitivities are also zero. Therefore, the rest of this paper will only deal with estimating four parameters and designing a network to measure them: ground-water velocity, longitudinal and transverse dispersion coefficients, and the source half-width.

At this point a comment is probably in order about the relative sensitivities of these four parameters. At 4380 days, the maximum sensitivity to source width is a little more than twice the maximum sensitivity to ground-water velocity. On the other hand, the maximum velocity sensitivity is a little more than an order of magnitude larger than the maximum sensitivities for the dispersion coefficients.

NETWORK DESIGN

It has been seen in the previous slides that the sensitivity coefficients for various parameters differ dramatically over space. They also evolve differently in time. Suppose we wish to design a network to measure the ground-water pore velocity accurately. The next slide (**slide #24**) shows the contour of 90% of the maximum value of the sensitivity with respect to velocity through time. If we locate observation wells within these contours at the specified times, we would expect to do a good job estimating the velocity.

The next slide (**slide #25**) shows the estimated standard error for the four parameters of interest through time. Wells have been located on a 20-m grid within the 90% contours; 89 measurements were used through space and time. A σ of .025 has been assumed. The error for velocity starts out at 6.3% at 730 days and decreases to .95% at 4380 days. However, the error for the transverse dispersion coefficient does not drop below about 33%. The error for source width and longitudinal dispersion coefficient is in the 5-8% range. By designing for a single parameter, we have a good estimate for velocity, acceptable accuracy for source width and longitudinal dispersion coefficient; but probably unacceptable accuracy for the transverse dispersion coefficient.

The next slide (**slide #26**) shows contours of 90% of the maximum value of the sensitivity with respect to the longitudinal dispersion coefficient. Locating wells on a 20-m grid inside these contours results in 78 measurements through space and time. If a σ .025 for the concentration measurements is assumed, the next slide (**slide #27**) shows the estimated standard error for the parameters. The error for the transverse dispersion coefficient is too large to show on this graph. It was 118% even at 4380 days. At 4380 days the error in veolcity is about 3%, the error in longitudinal dispersion coefficient is about 8%, and the error in source width is about 16%.

The preceeding two examples show that design on a single parameter will give acceptable results for that parameter but perhaps unacceptable results for others. Ideally, we would like to design a network to measure all parameters of interest simultaneously. The next series of slides (**slides 28-34**) show wells located on a 20-m grid at points which have at least 99% of the maximum sensitivity for any parameter. This series of slides show how the monitoring network evolves in space and time. Some wells will become insensitive and may be dropped while new sensitive wells will need to be added. This design resulted in 111 measurements through space and time.

Assuming a σ of .025 for the concentration measurements, the next slide (**slide #35**) shows the estimated standard error for the parameters. All parameters have been estimated to within about 4% at 4380 days. The dispersion coefficients are in the 3.5-4% range and source width and velocity are in the .1-.5% range. This example shows how sensitivity analysis can be used for simultaneous design of a monitoring network for several parameters.

CONCLUSIONS

This slide (**slide #36**) shows the basic ideas presented in this paper in using sensitivity analysis to design an effective monitoring-well system. Adopt a model of the dispersion process. Calculate and plot the sensitivity coefficients. Look for dependencies in parameters and sensitivity coefficients. Determine the number of parameters that can be estimated reliably. Design a monitoring-well system to sample at time and space locations that have the maximum sensitivity to the parameters of interest. Let the monitoring system evolve in time, dropping and adding wells as needed. Estimate parameters and standard errors as the system evolves. Make future predictions. Of course, initial estimates of the parameters must be assumed to get started; but the system can be self-correcting as it proceeds. As the parameter estimates improve, the future design of the monitoring system and concentration prediction also improve.

REFERENCES

Javandel, I., C. Doughty, and C.F. Tsang, 1984, Ground water transport: Handbook of mathematical models: American Geophysical Union, Washington, D.C.

Knopman, D.S. and C.I. Voss, 1987, Behavior of sensitivities in the one-dimensional advection-dispersion equation: Implications for parameter estimation and sampling design: Water Resources Research, 23(2): 253-272.

McElwee, C.D., 1985, Sensitivity analysis of ground-water models: Proceedings of the 1985 NATO Advanced Study Institute on fundamentals of transport phenomena in porous media: To be published by Martinus Nijhoff, edited by Jacob Bear and M. Yavuz Corapcioglu.

Wagner, B.J. and S.M. Gorelick, 1986, A statistical methodology for estimating transport parameters: Theory and application to one-dimensional advective-dispersive systems: Water Resources Research, 22(8): 1303-1315.

Slide #1

$$D_L \frac{\partial^2 c}{\partial x^2} + D_T \frac{\partial^2 c}{\partial y^2} - \nu \frac{\partial c}{\partial x} - \lambda RC = R \frac{\partial c}{\partial t}$$

$$C(0, y, t) = C_o e^{-\alpha t} \qquad -a \leqslant y \leqslant a$$

$$C(0, y, t) = 0 \quad \text{other values of } y$$

$$\lim_{y \to \pm\infty} \frac{\partial c}{\partial y} = 0$$

$$\lim_{x \to \infty} \frac{\partial c}{\partial x} = 0$$

Slide #2

$$C(x, y, t) = \frac{C_0 x}{4(\pi D_L)^{1/2}} \exp\left(\frac{\nu x}{2D_L} - \alpha t\right)$$

$$\cdot \int_0^{t/R} \exp\left[-\left(\lambda R - \alpha R + \frac{\nu^2}{4D_L}\right)\tau - \frac{x^2}{4D_L \tau}\right] \tau^{-3/2}$$

$$\cdot \left[\operatorname{erf}\left(\frac{a - y}{2(D_T \tau)^{1/2}}\right) + \operatorname{erf}\left(\frac{a + y}{2(D_T \tau)^{1/2}}\right)\right] d\tau$$

Slide #3

Definition of Sensitivity Coefficients

$$Z_P = \frac{\partial C}{\partial P}$$

Normalized Version

$$Z_P = \frac{P}{C_O} \frac{\partial C}{\partial P}$$

P = Any model parameter

Slide #4

Methods for Determining Sensitivity Coefficients.

1. Analytical expressions for the sensitivity coefficients.

2. Finite difference expression for sensitivity coefficients.

3. A partial differential equation for sensitivity coefficients.

Slide #5

Sensitivity Matrix

$$
\underset{\sim}{Z} = \begin{bmatrix}
Z_{\nu_1} & Z_{\alpha_1} & Z_{D_{L_1}} & Z_{R_1} & Z_{\lambda_1} & Z_{a_1} & Z_{D_{T_1}} \\
Z_{\nu_2} & & & & & & \cdot \\
Z_{\nu_3} & & & & & & \cdot \\
\cdot & & & & & & \cdot \\
\cdot & & & & & & \\
\cdot & & & & & & \\
Z_{\nu_n} & & \cdot & \cdot & \cdot & & Z_{D_{T_n}}
\end{bmatrix}
$$

n = number of measurements

Slide #6

Ordinary Least Squares

Parameter Covariance Matrix

$$\underset{\sim}{P} = (\underset{\sim}{Z}^T \underset{\sim}{Z})^{-1} \sigma^2$$

$\underset{\sim}{Z}$ = Sensitivity Matrix

σ^2 = Concentration Error Variance

$$\text{e.s.e. } P_k = \sqrt{P_{kk}}$$

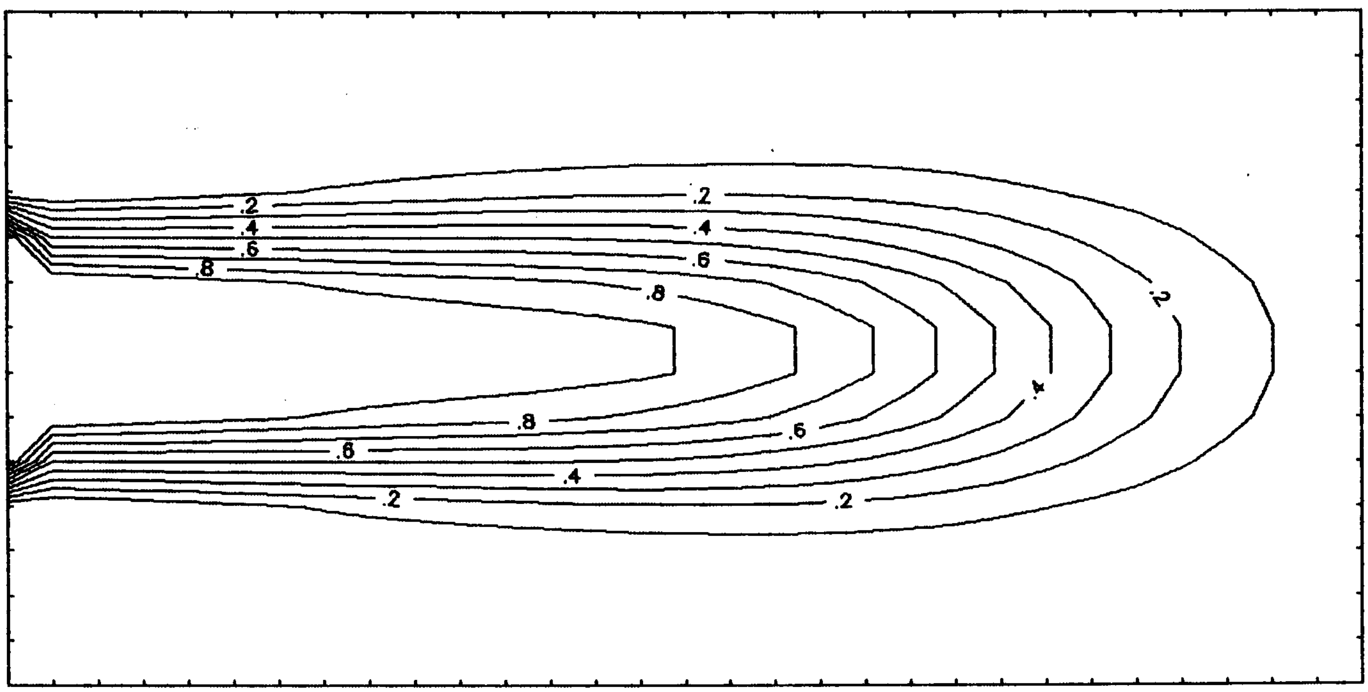
Slide # 7

Sensitivity Correlation Matrix

$$(SR)_{ik} = (\underset{\sim}{Z}^T \underset{\sim}{Z})_{ik} \Big/ \left[(\underset{\sim}{Z}^T \underset{\sim}{Z})_{ii} \quad (\underset{\sim}{Z}^T \underset{\sim}{Z})_{kk} \right]^{1/2}$$

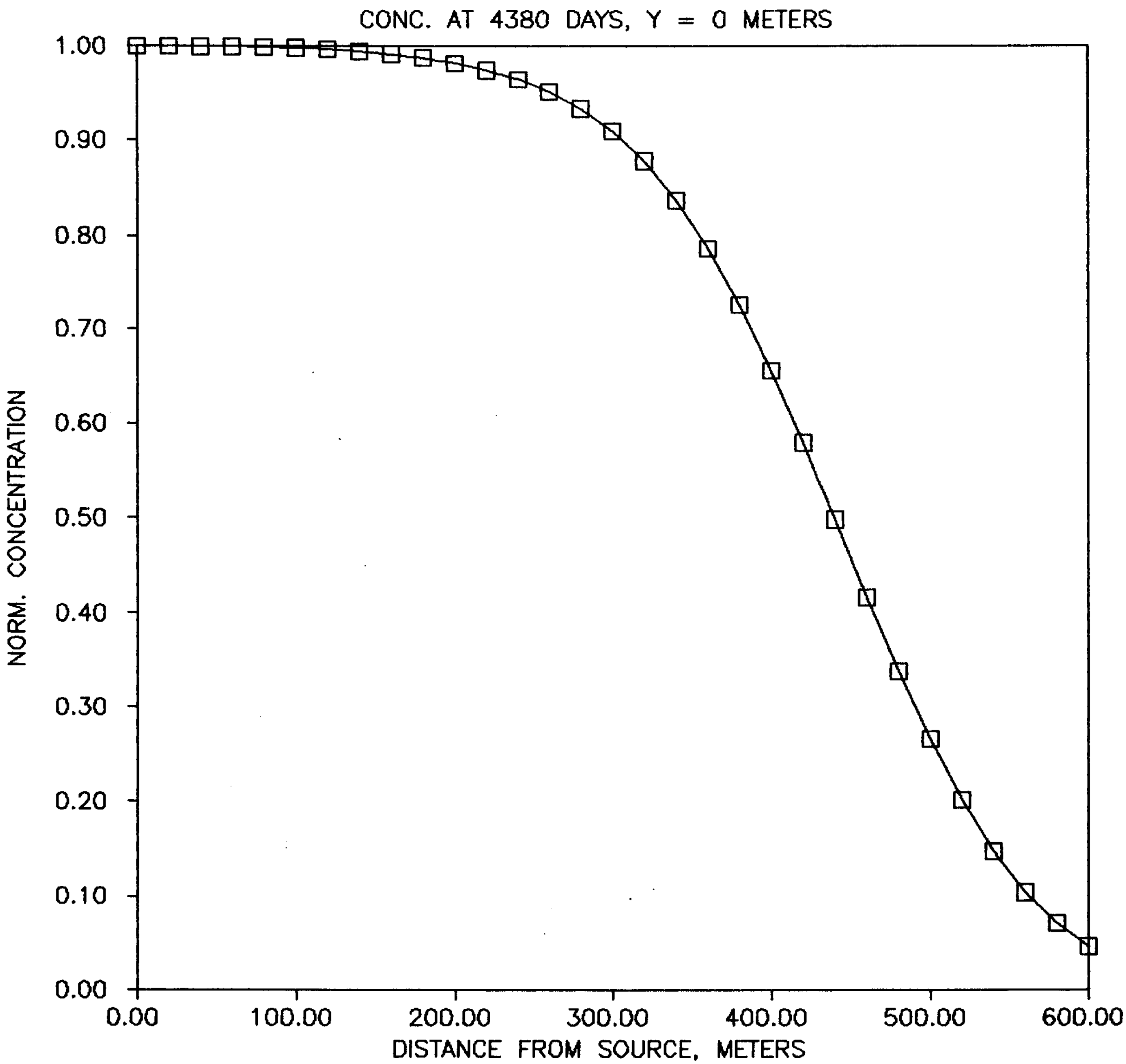
Problems if off-diagonal elements are about .9 or greater.

Slide #8

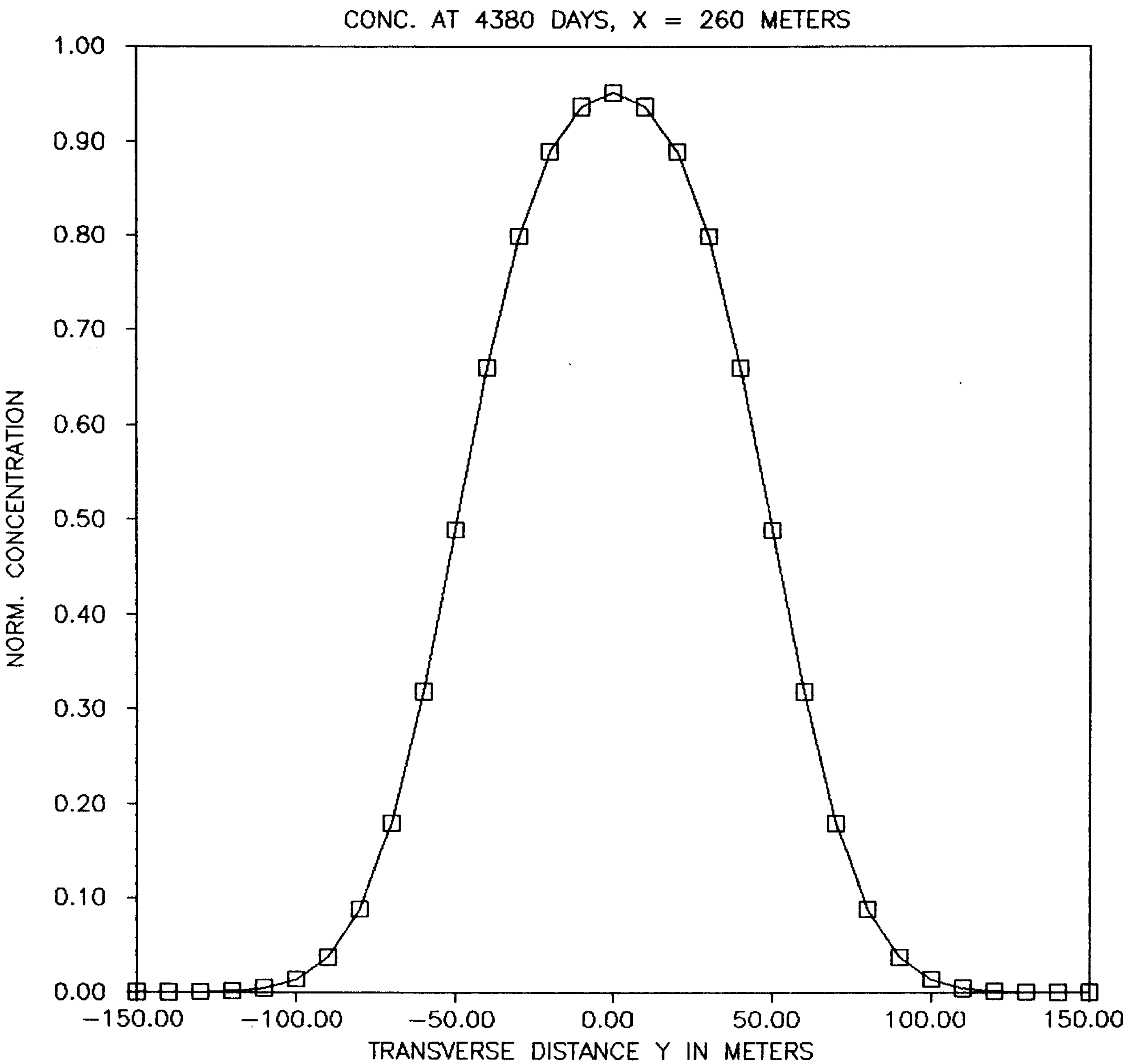


CONCENTRATION CONTOURS AT 4380 DAYS

Slide #9

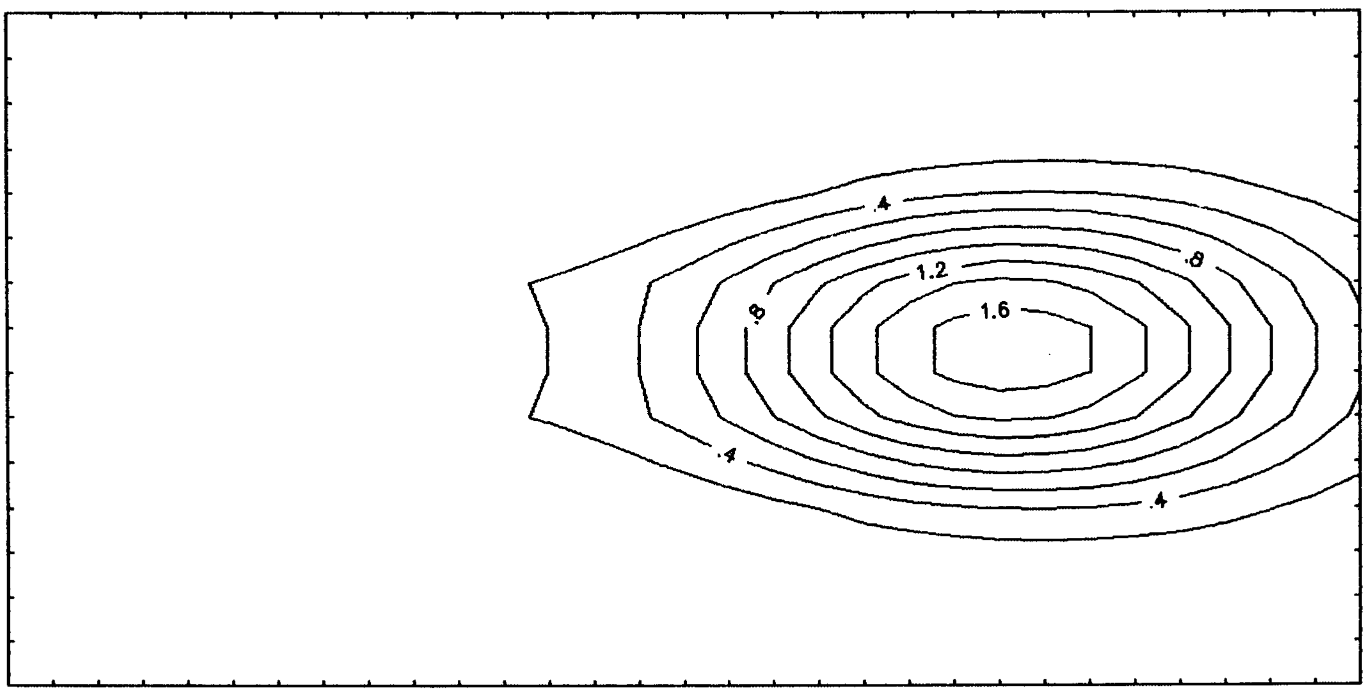

CONC. AT 4380 DAYS, Y = 0 METERS
NORM. CONCENTRATION
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
0.00
100.00
200.00
300.00
400.00
500.00
600.00
DISTANCE FROM SOURCE, METERS

Slide # 10



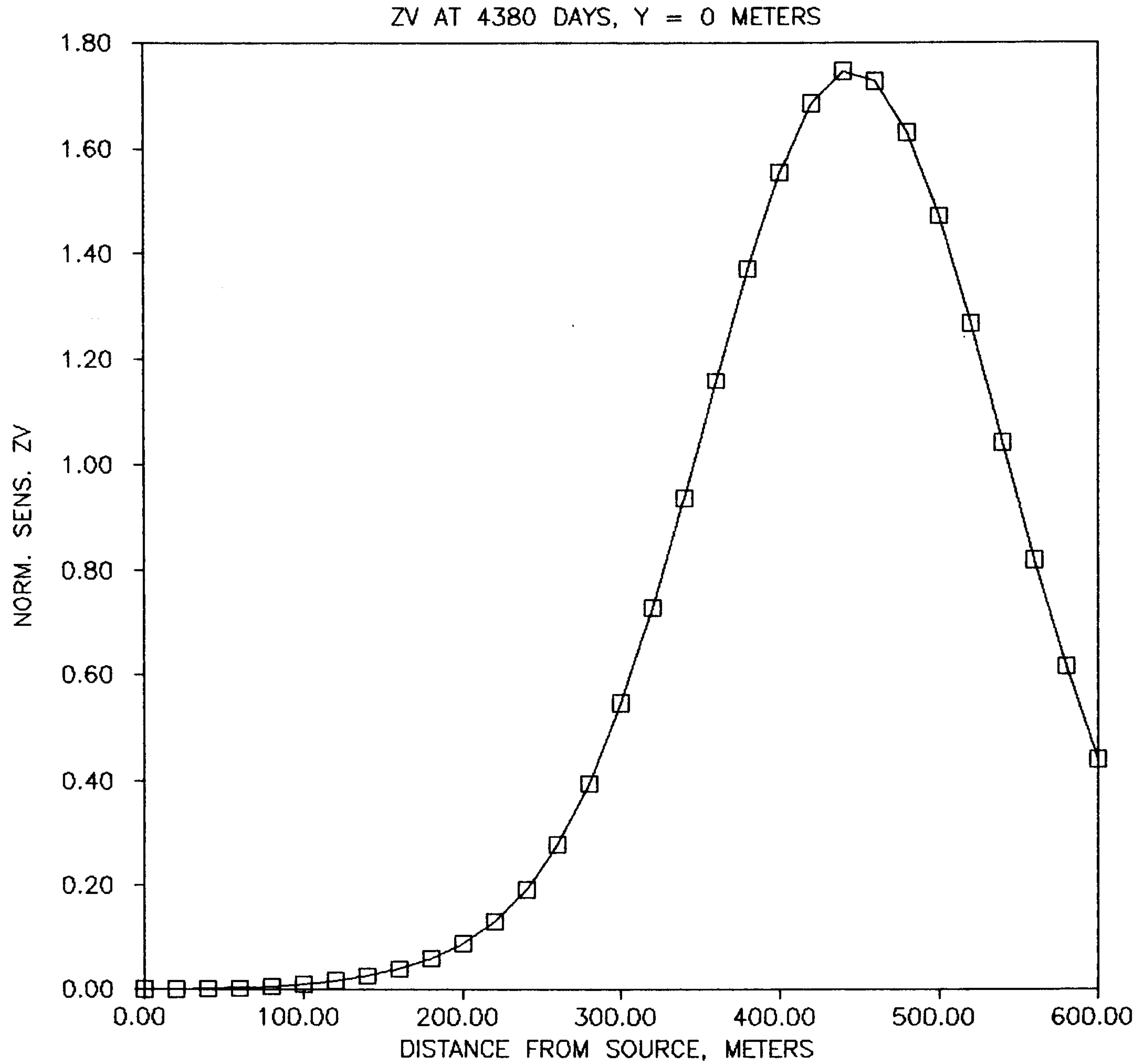
CONC. AT 4380 DAYS, X = 260 METERS
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
NORM. CONCENTRATION
−150.00
−100.00
−50.00
0.00
50.00
100.00
150.00
TRANSVERSE DISTANCE Y IN METERS

Slide #11

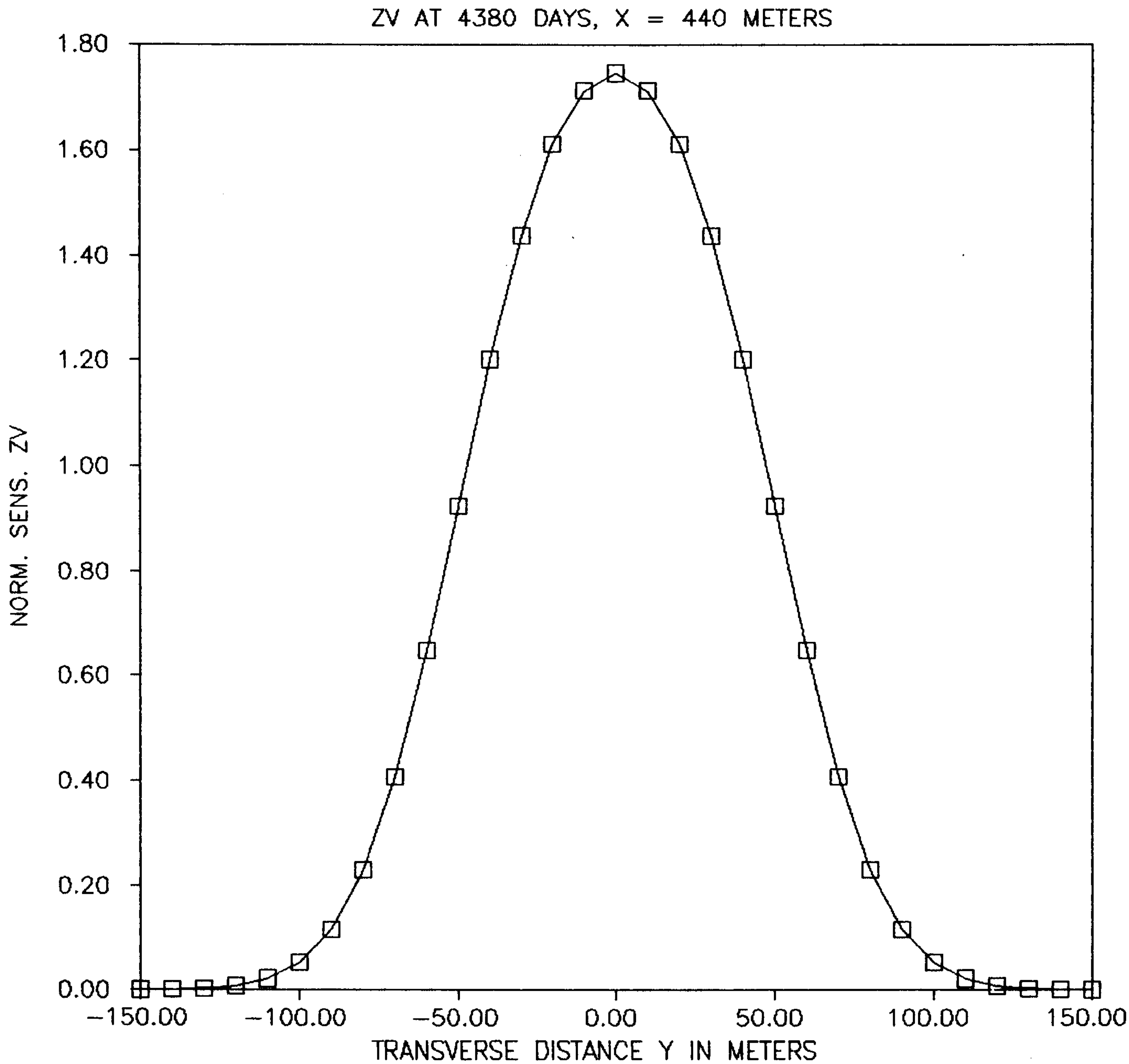


ZV CONTOURS AT 4380 DAYS

Slide # 12

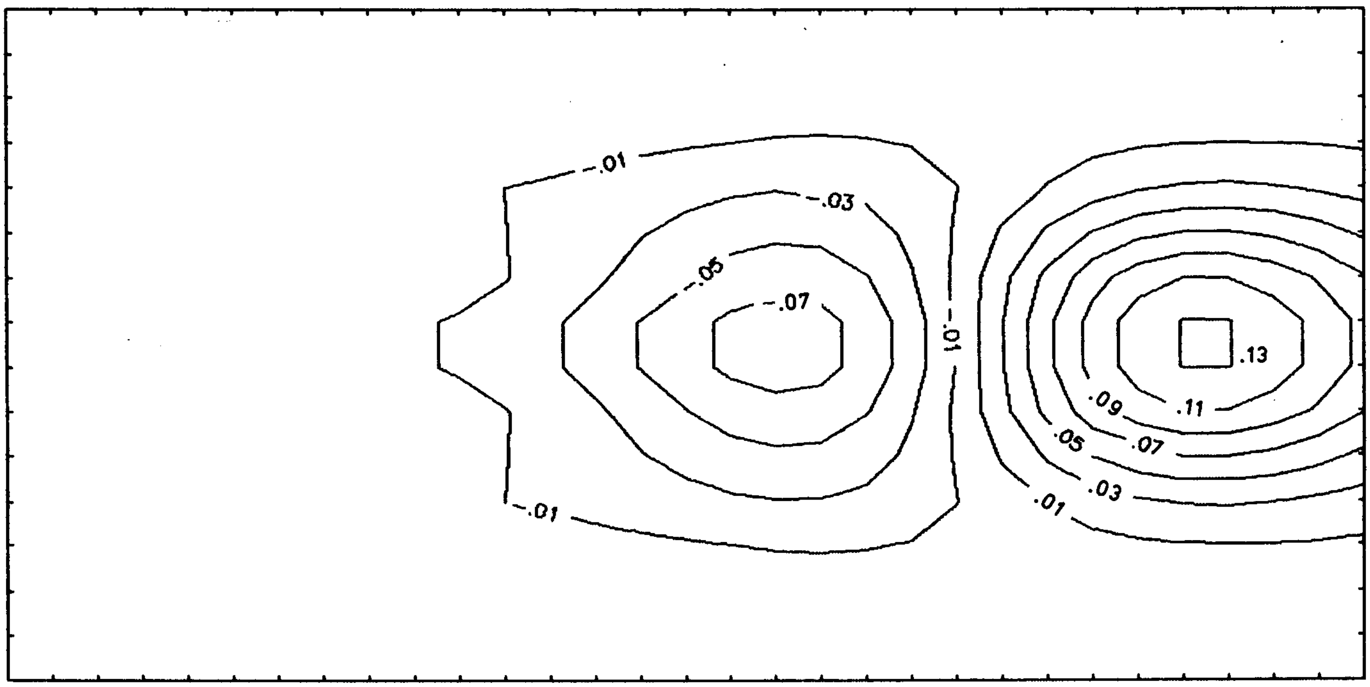

ZV AT 4380 DAYS, Y = 0 METERS
NORM. SENS. ZV
1.80
1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
0.00
100.00
200.00
300.00
400.00
500.00
600.00
DISTANCE FROM SOURCE, METERS

Slide # 13



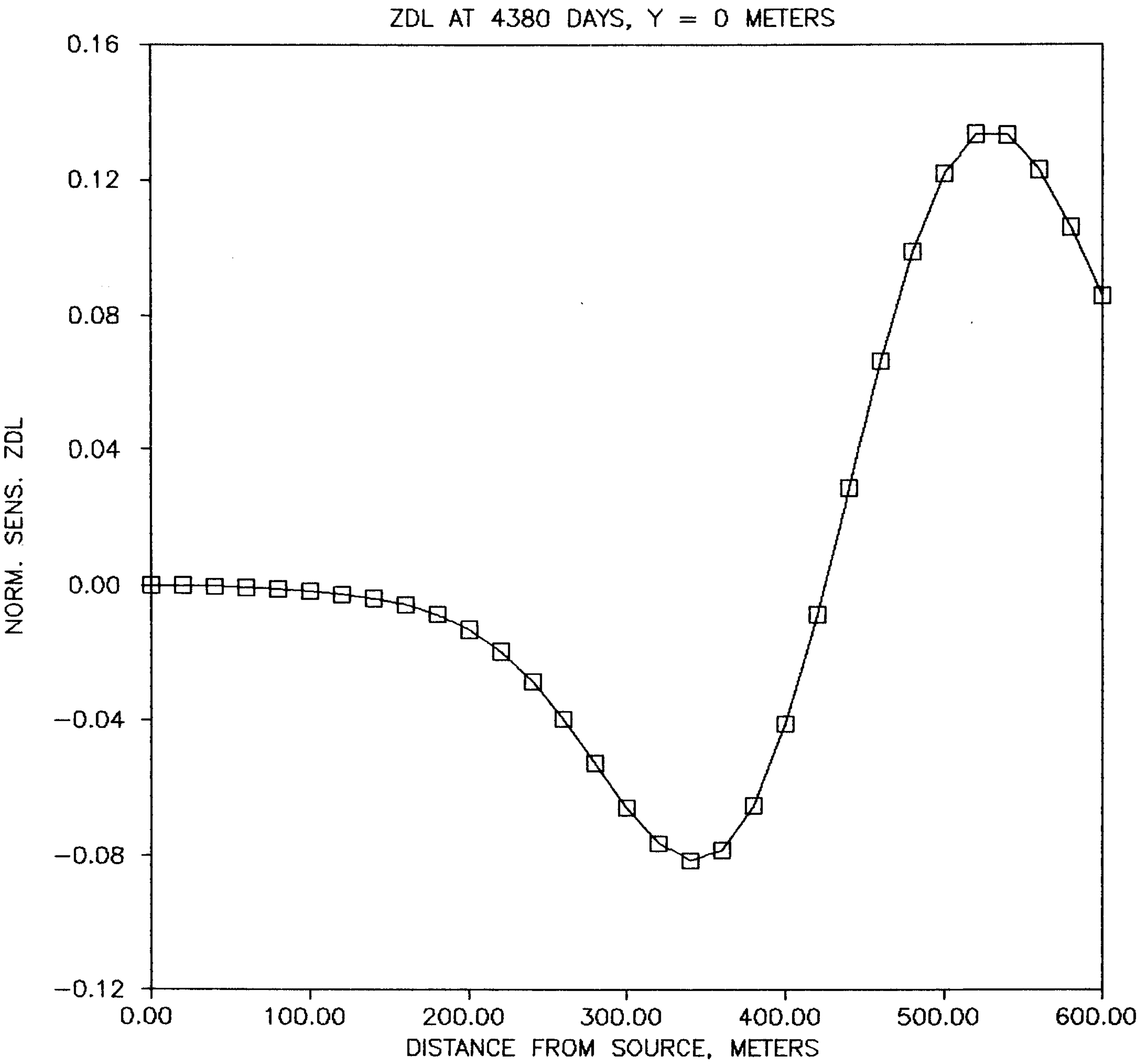
ZV AT 4380 DAYS, X = 440 METERS
NORM. SENS. ZV
1.80
1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
−150.00
−100.00
−50.00
0.00
50.00
100.00
150.00
TRANSVERSE DISTANCE Y IN METERS

Slide # 14

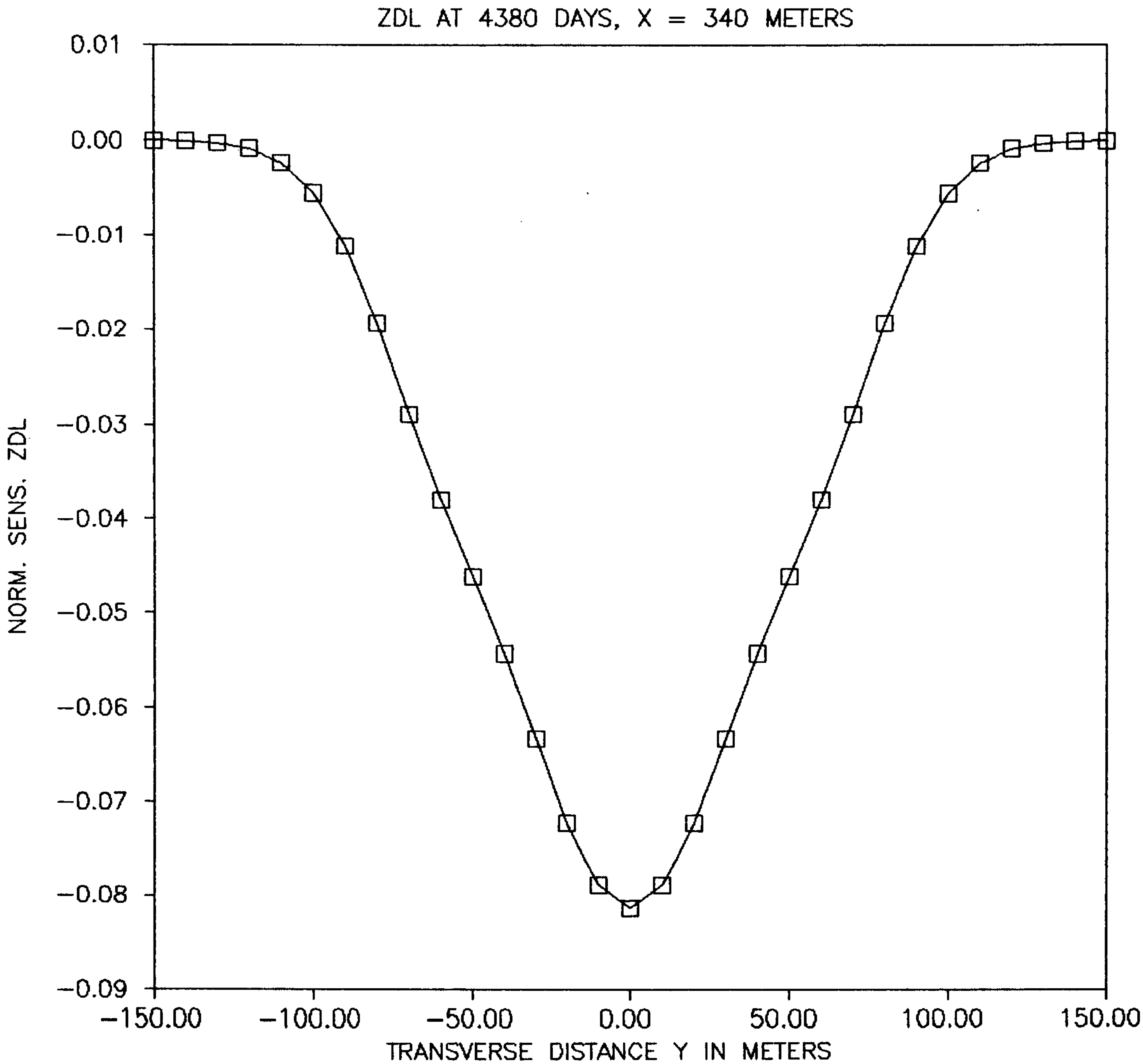


ZDL CONTOURS AT 4380 DAYS

Slide #15

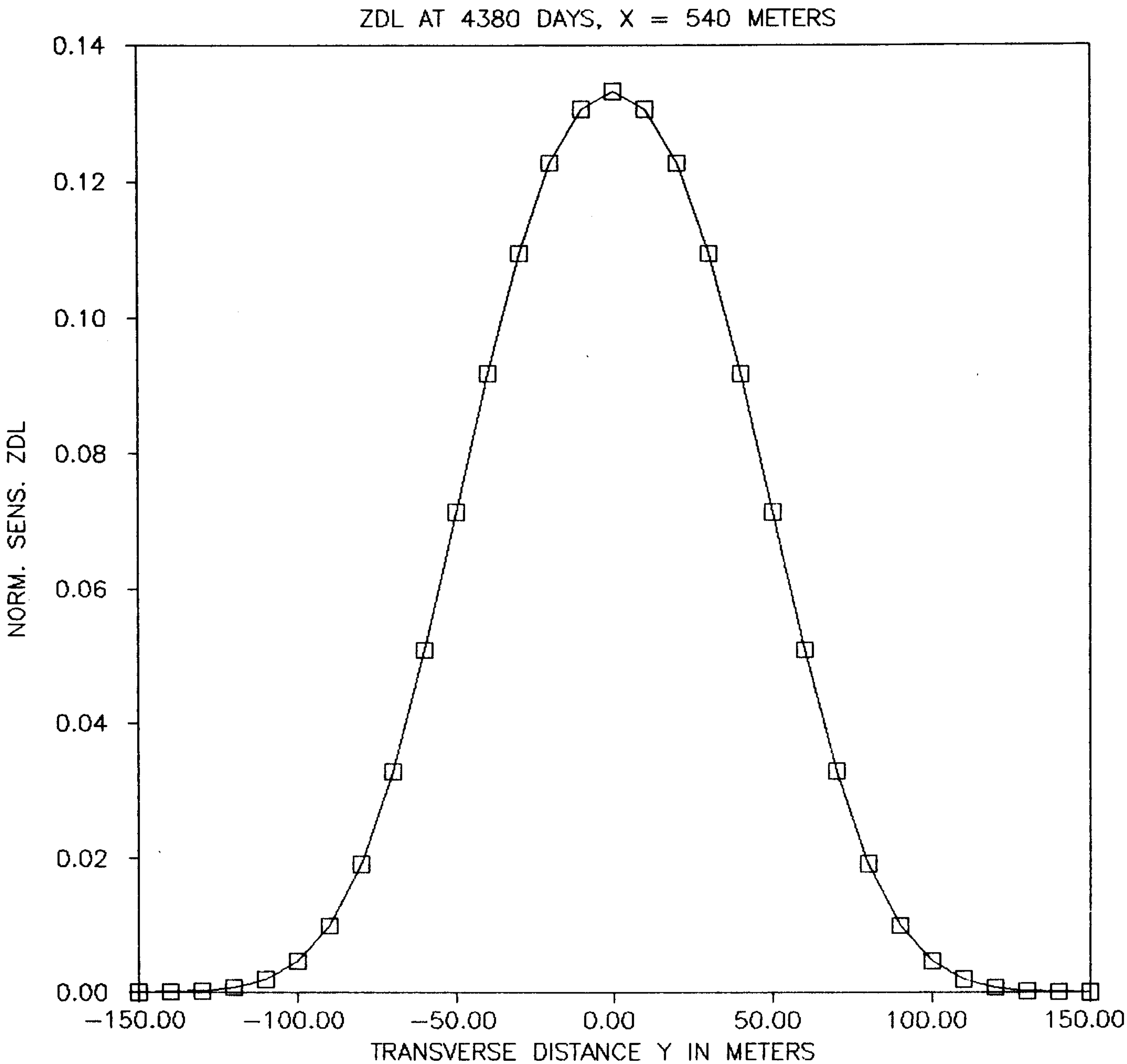

ZDL AT 4380 DAYS, Y = 0 METERS
0.16
0.12
0.08
0.04
0.00
-0.04
-0.08
-0.12
NORM. SENS. ZDL
0.00
100.00
200.00
300.00
400.00
500.00
600.00
DISTANCE FROM SOURCE, METERS

Slide # 16

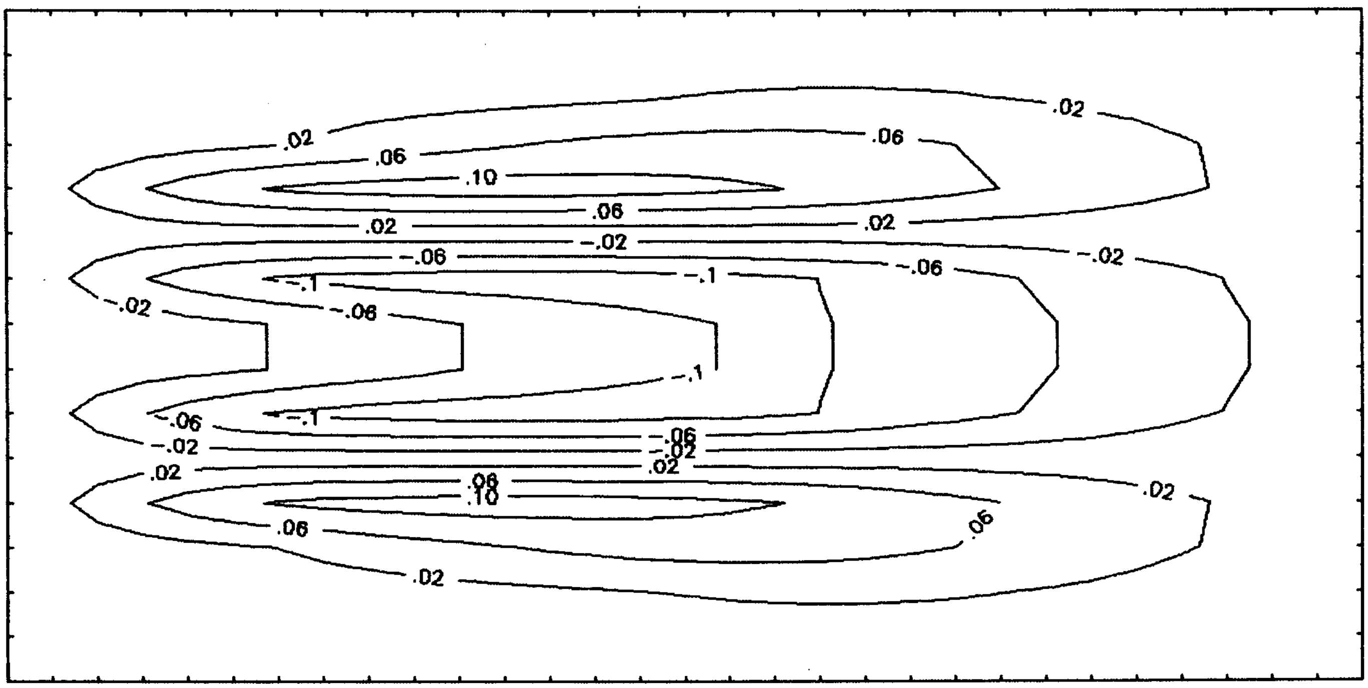


ZDL AT 4380 DAYS, X = 340 METERS
0.01
0.00
−0.01
−0.02
−0.03
−0.04
−0.05
−0.06
−0.07
−0.08
−0.09
NORM. SENS. ZDL
−150.00
−100.00
−50.00
0.00
50.00
100.00
150.00
TRANSVERSE DISTANCE Y IN METERS

Slide #17

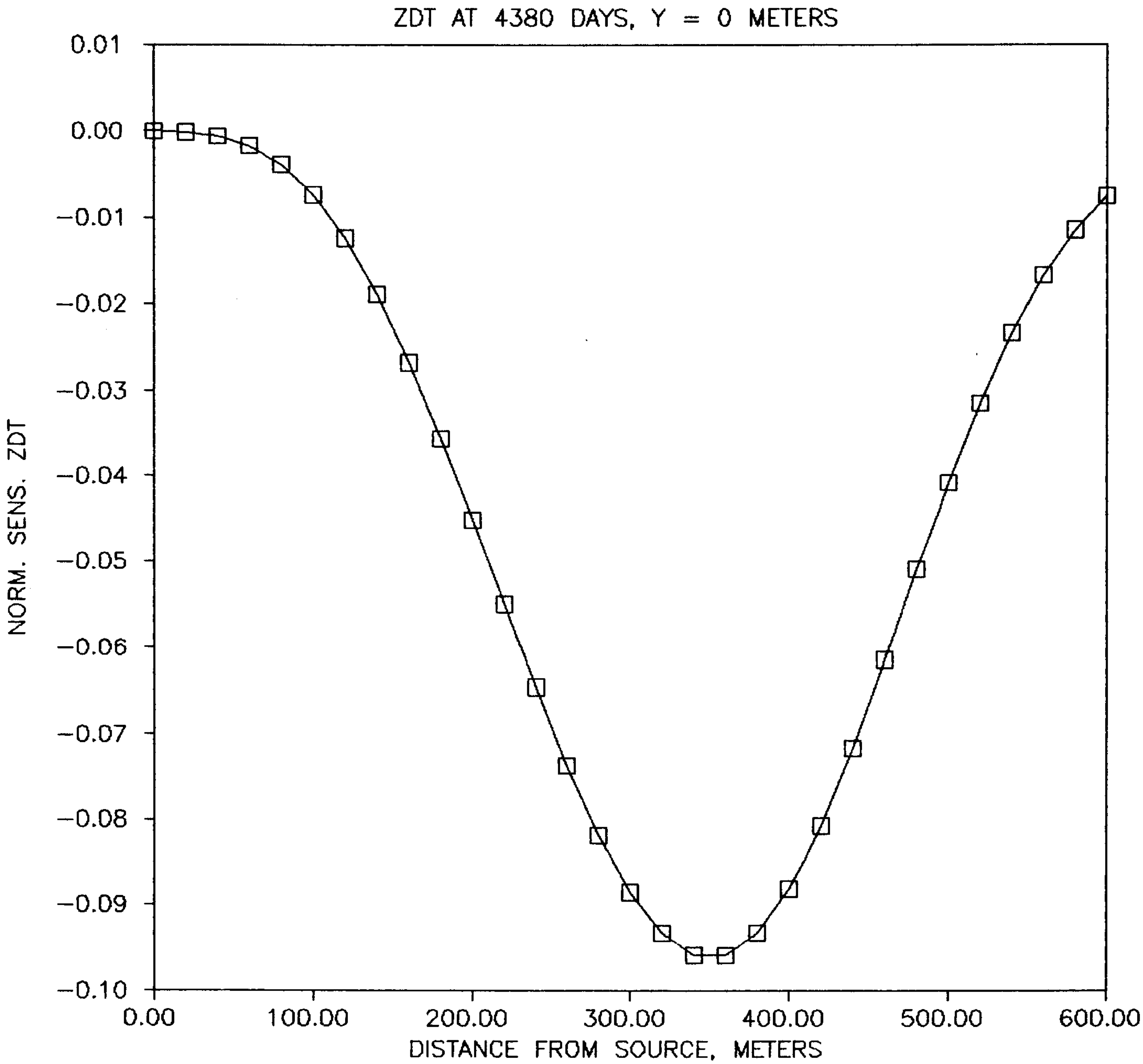

ZDL AT 4380 DAYS, X = 540 METERS
NORM. SENS. ZDL
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
-150.00
-100.00
-50.00
0.00
50.00
100.00
150.00
TRANSVERSE DISTANCE Y IN METERS

Slide # 18



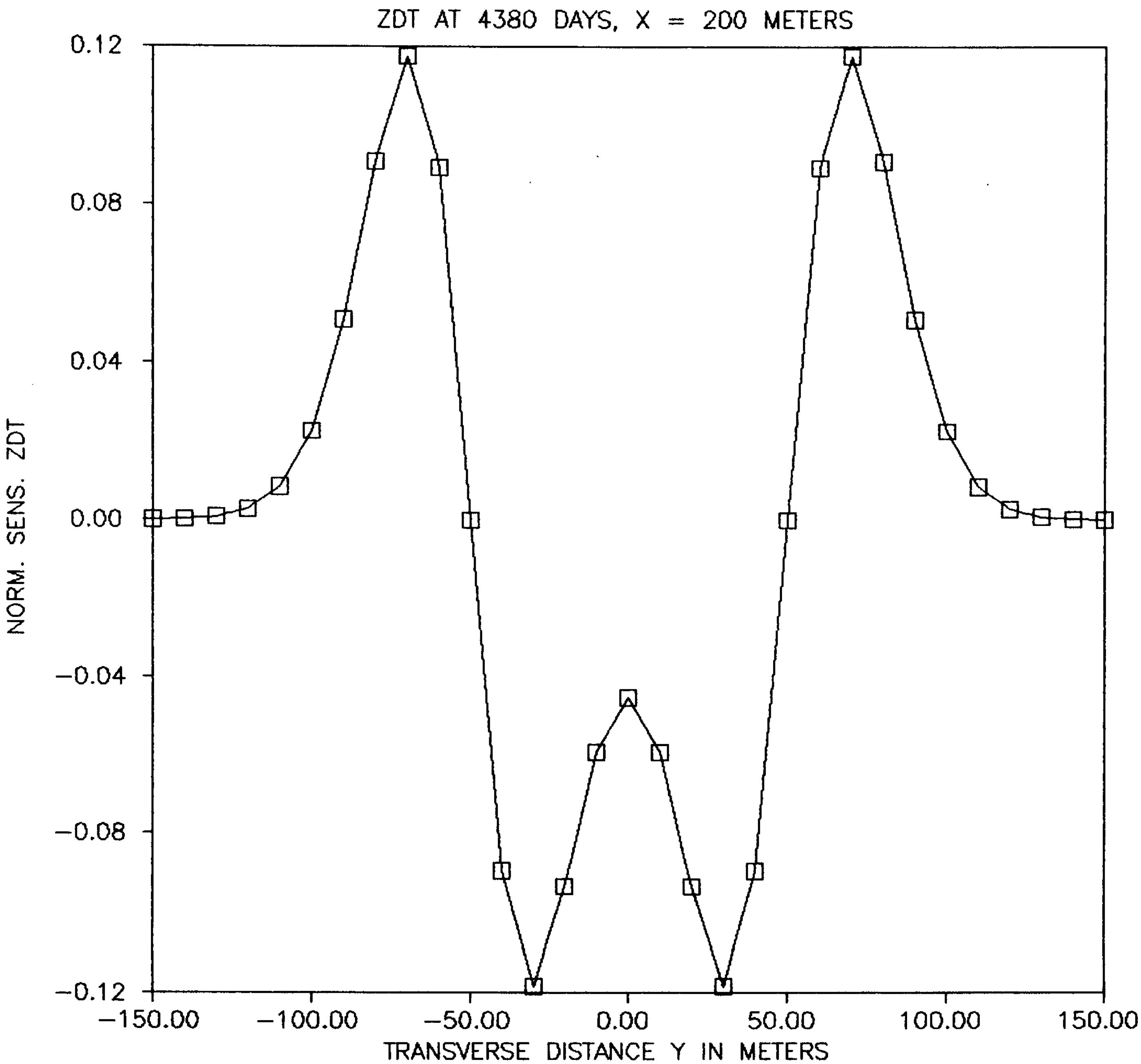
ZDT CONTOURS AT 4380 DAYS

Slide # 19

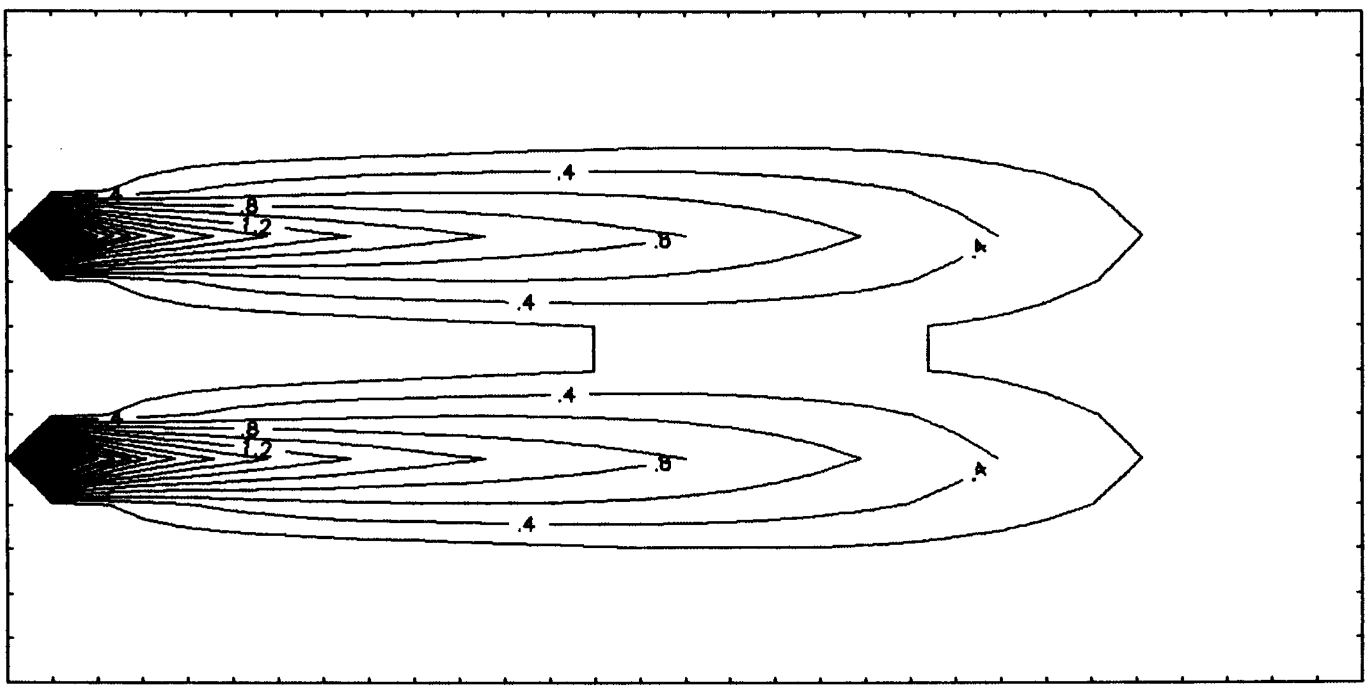


ZDT AT 4380 DAYS, Y = 0 METERS
0.01
0.00
−0.01
−0.02
−0.03
−0.04
−0.05
−0.06
−0.07
−0.08
−0.09
−0.10
NORM. SENS. ZDT
0.00
100.00
200.00
300.00
400.00
500.00
600.00
DISTANCE FROM SOURCE, METERS

Slide # 20

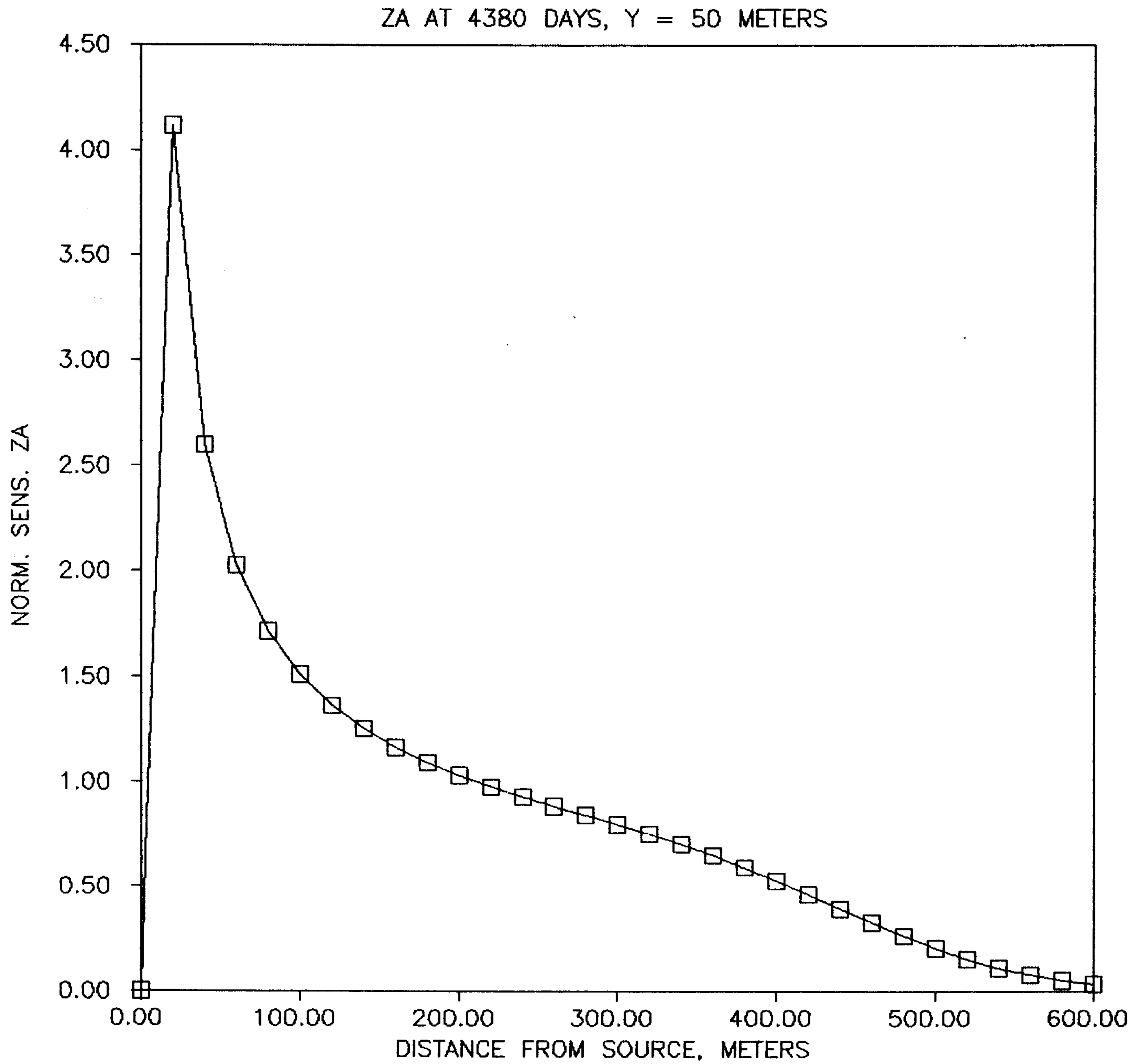

ZDT AT 4380 DAYS, X = 200 METERS
NORM. SENS. ZDT
TRANSVERSE DISTANCE Y IN METERS
0.12
0.08
0.04
0.00
−0.04
−0.08
−0.12
−150.00
−100.00
−50.00
0.00
50.00
100.00
150.00

Slide #21

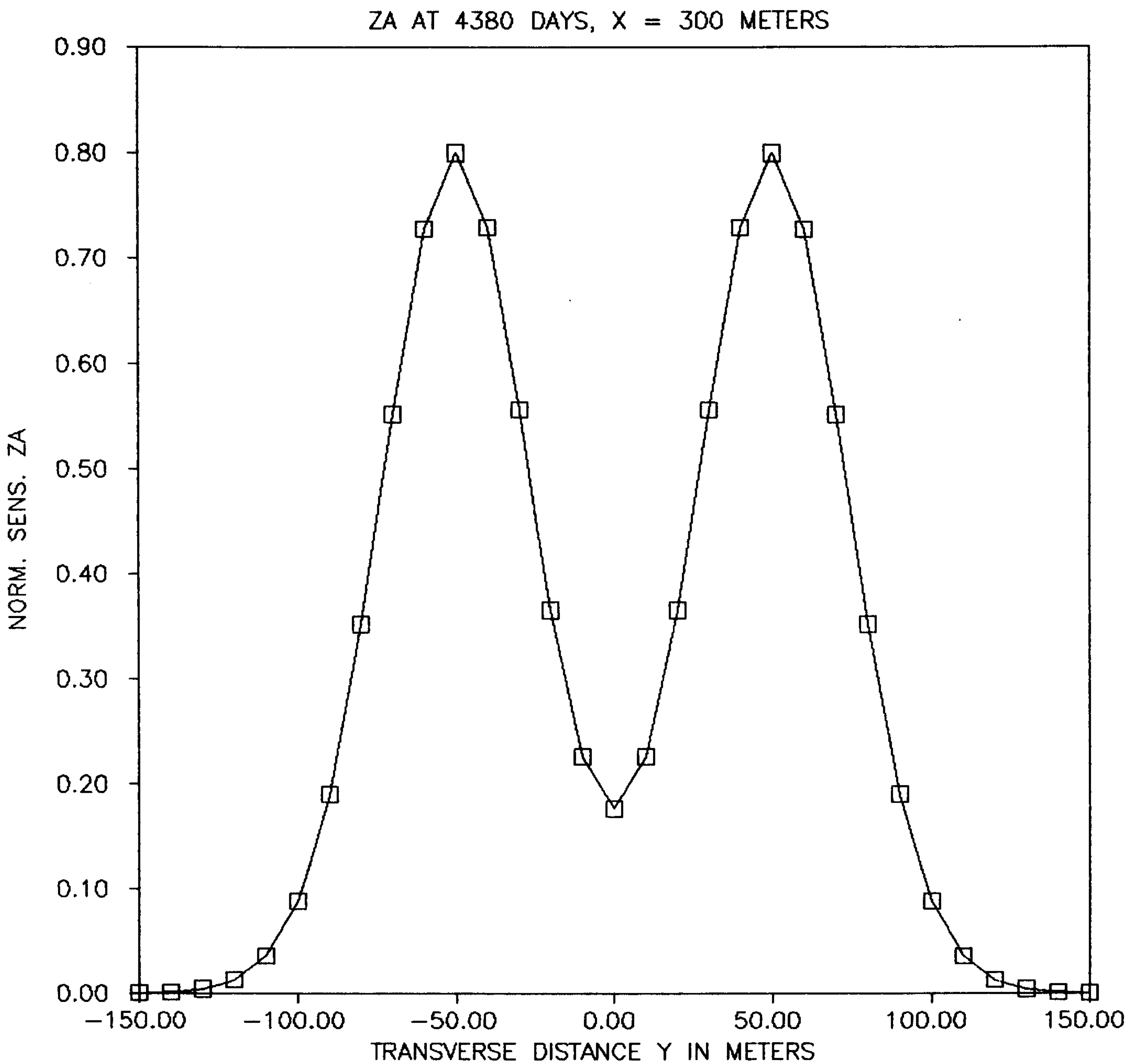


ZA CONTOURS AT 4380 DAYS

Slide # 22

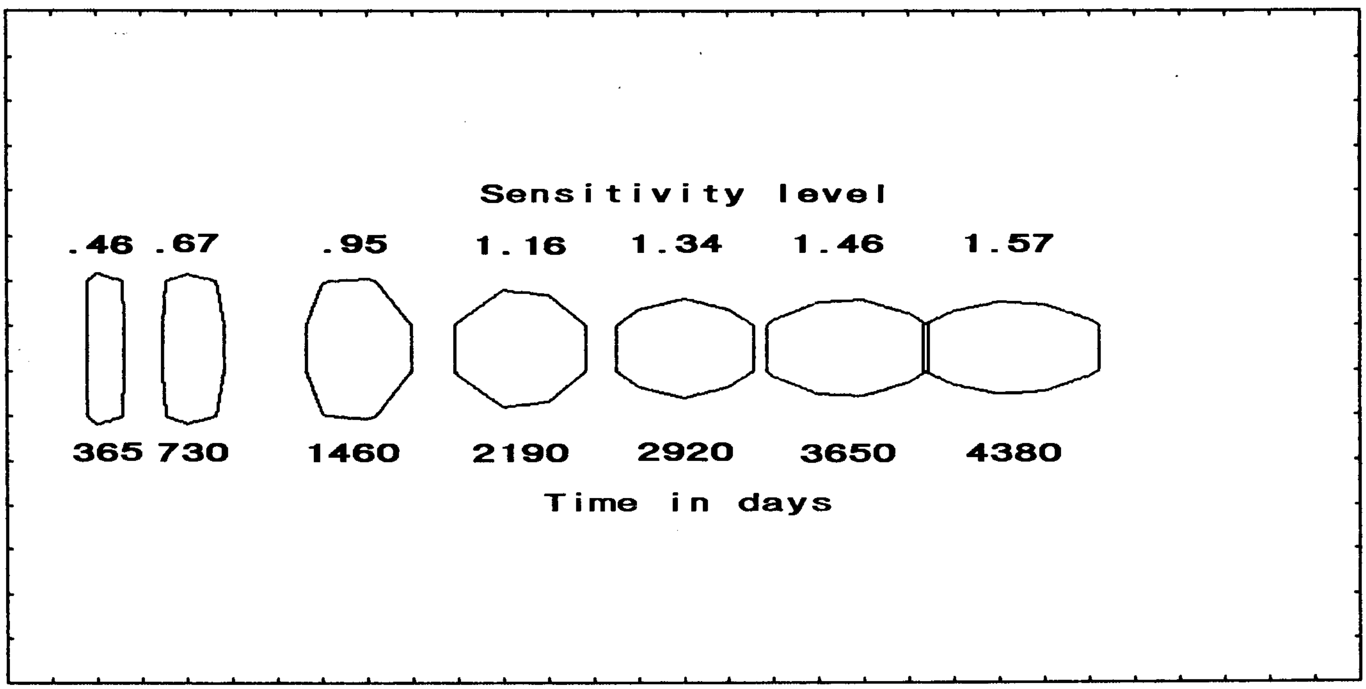

ZA AT 4380 DAYS, Y = 50 METERS
NORM. SENS. ZA
4.50
4.00
3.50
3.00
2.50
2.00
1.50
1.00
0.50
0.00
0.00
100.00
200.00
300.00
400.00
500.00
600.00
DISTANCE FROM SOURCE, METERS

Slide # 23



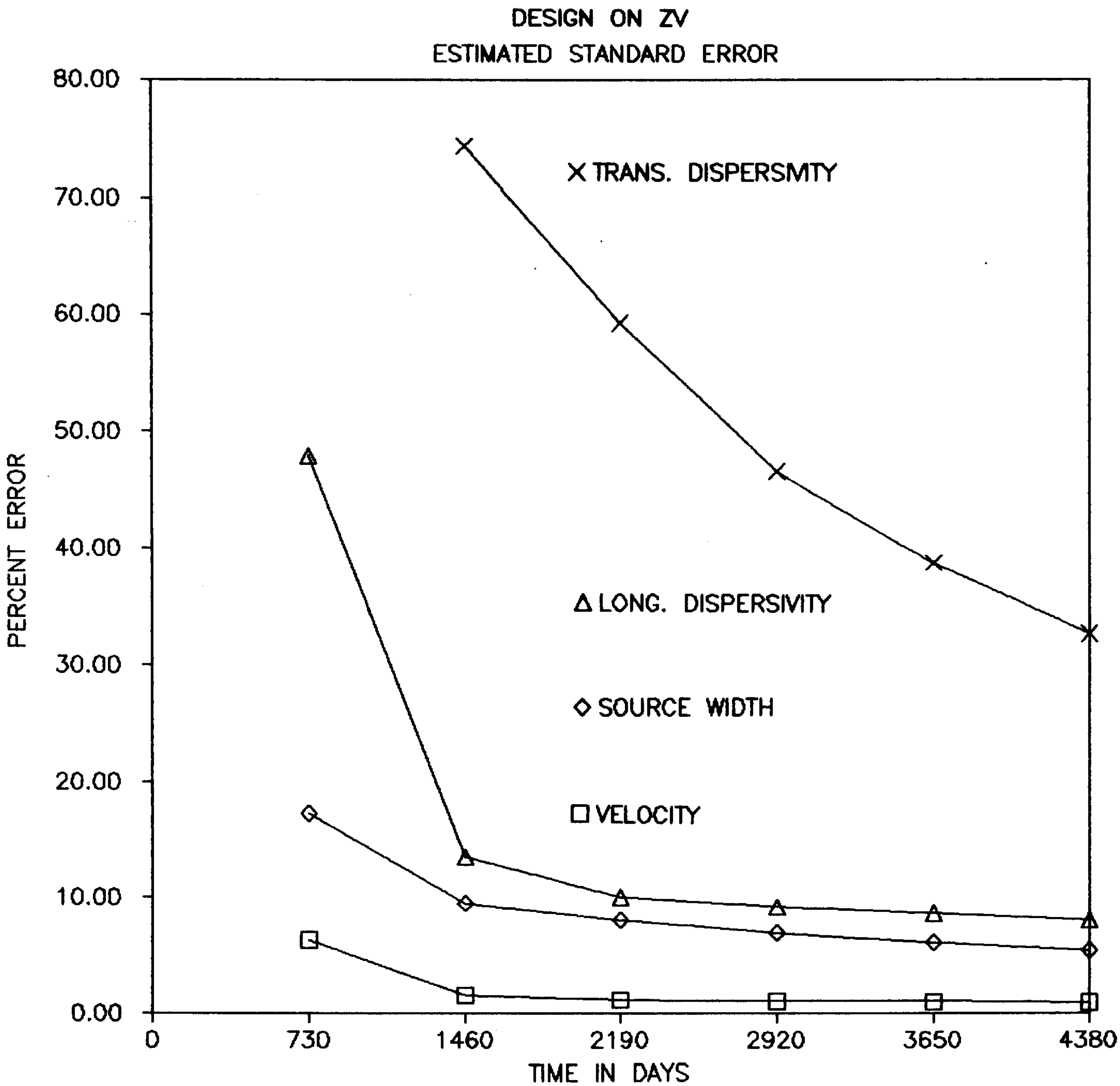
ZA AT 4380 DAYS, X = 300 METERS
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
NORM. SENS. ZA
-150.00
-100.00
-50.00
0.00
50.00
100.00
150.00
TRANSVERSE DISTANCE Y IN METERS

Slide # 24

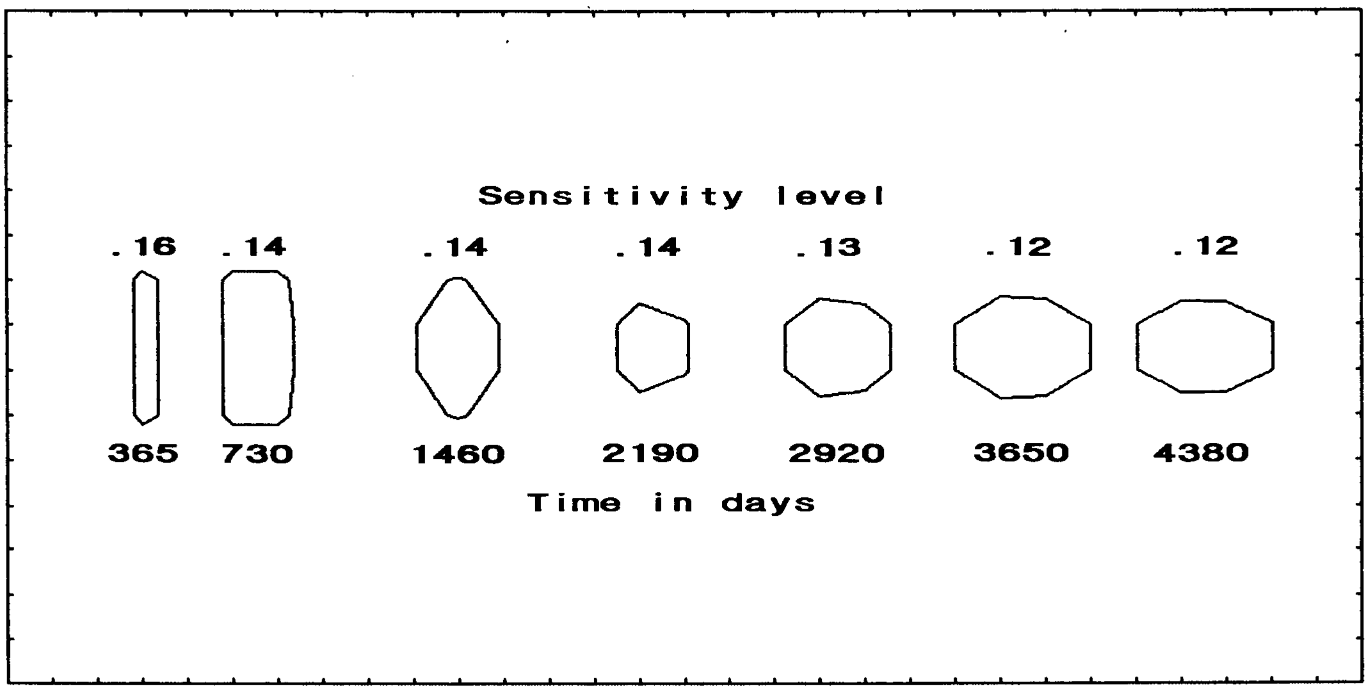


CONTOURS OF .9*ZVMAX

Slide #25

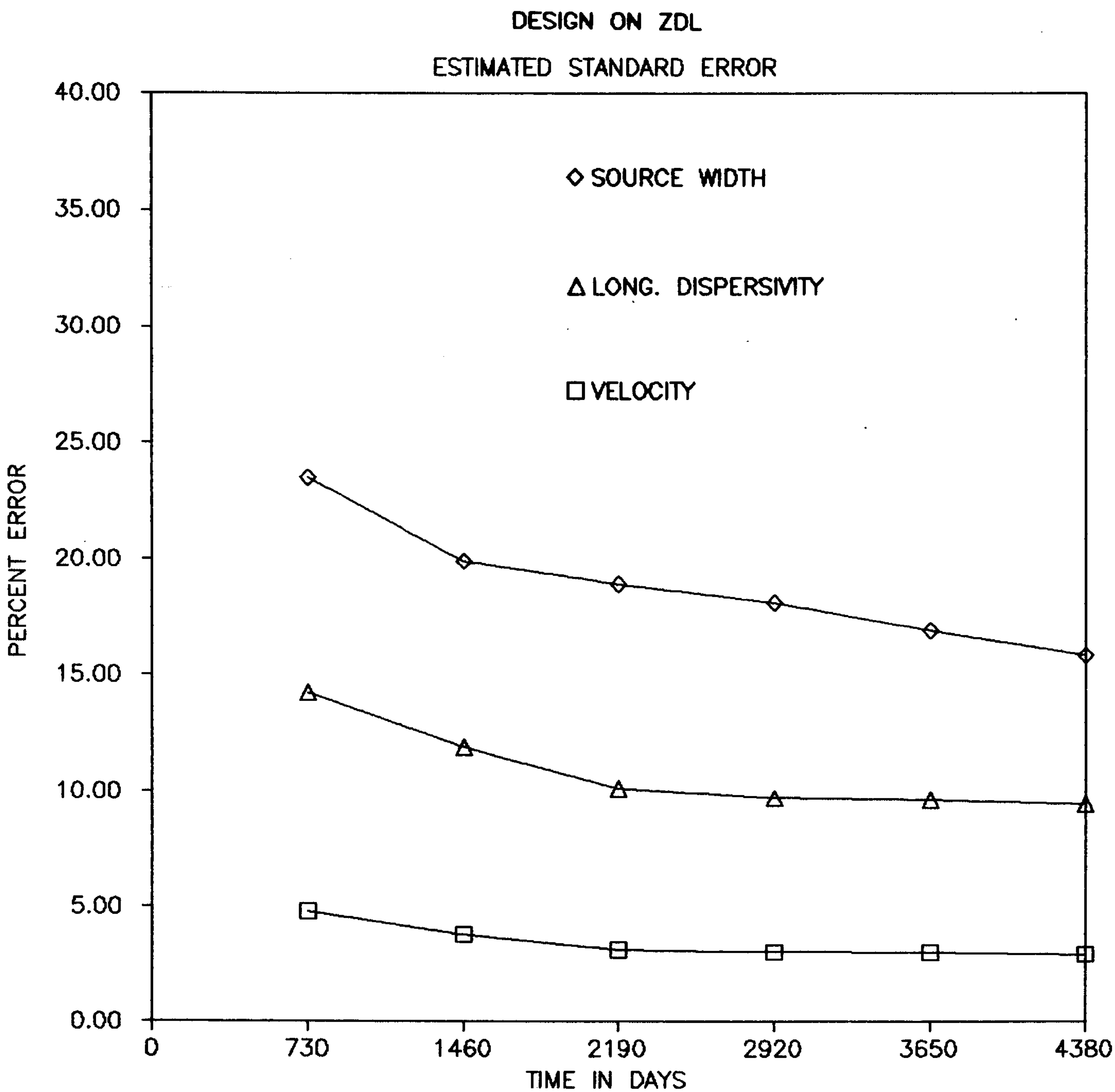

DESIGN ON ZV
ESTIMATED STANDARD ERROR
80.00
70.00
60.00
50.00
40.00
30.00
20.00
10.00
0.00
PERCENT ERROR
TRANS. DISPERSMTY
LONG. DISPERSIVITY
SOURCE WIDTH
VELOCITY
0
730
1460
2190
2920
3650
4380
TIME IN DAYS

Slide # 26

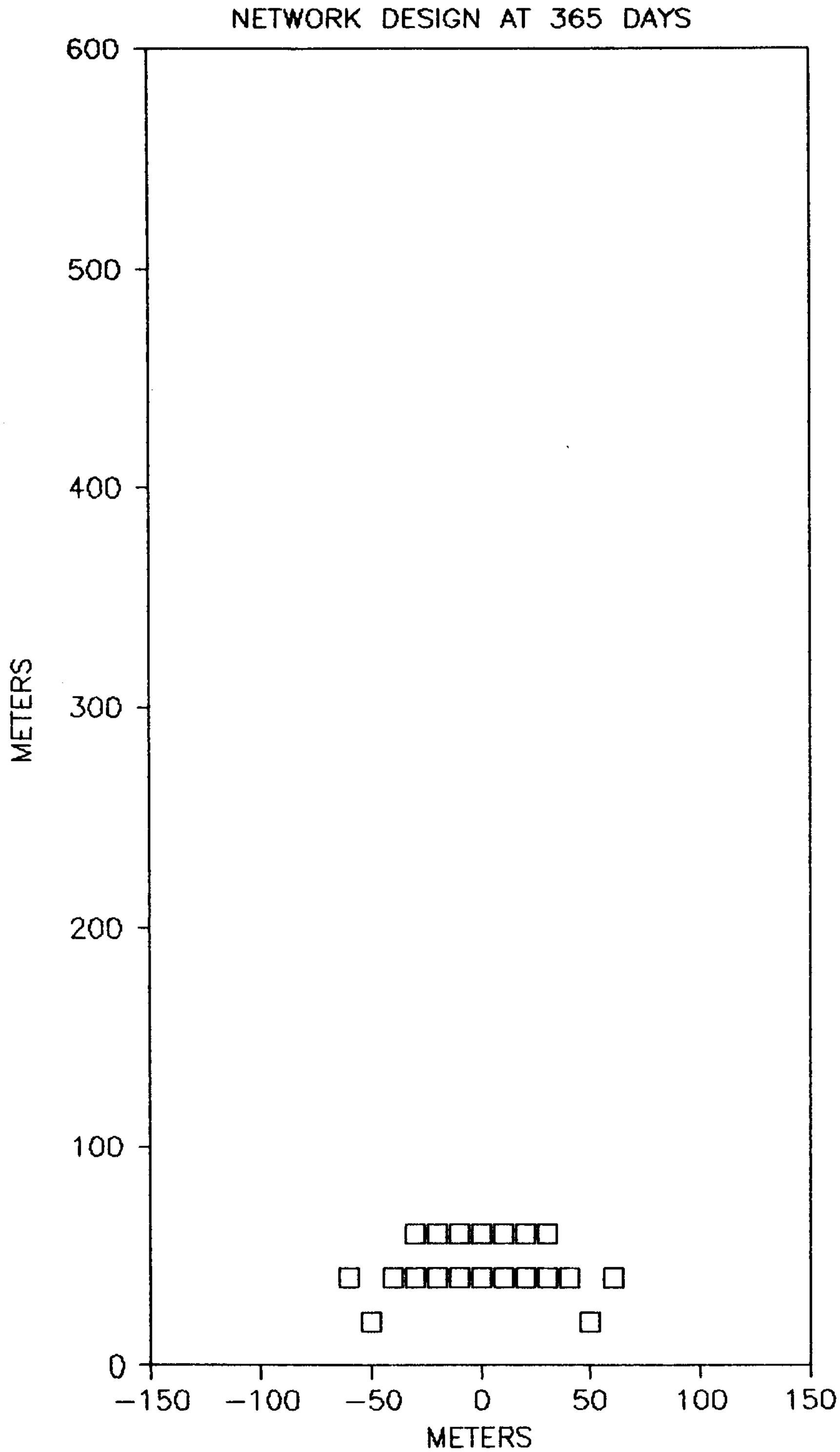


CONTOURS OF .9*ZDLMAX

Slide # 27

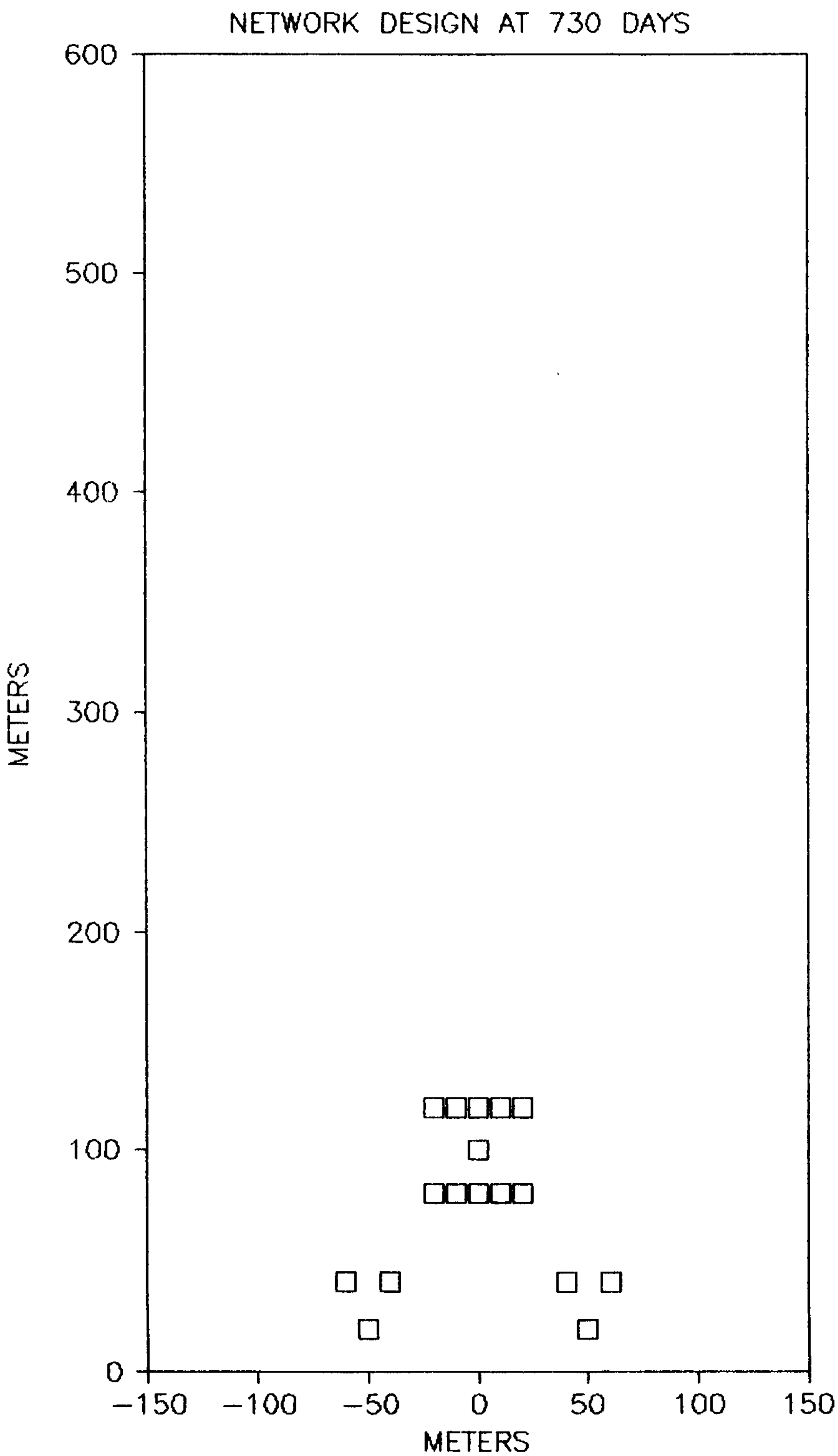

DESIGN ON ZDL
ESTIMATED STANDARD ERROR
SOURCE WIDTH
LONG. DISPERSIVITY
VELOCITY
PERCENT ERROR
40.00
35.00
30.00
25.00
20.00
15.00
10.00
5.00
0.00
0
730
1460
2190
2920
3650
4380
TIME IN DAYS

Slide # 28

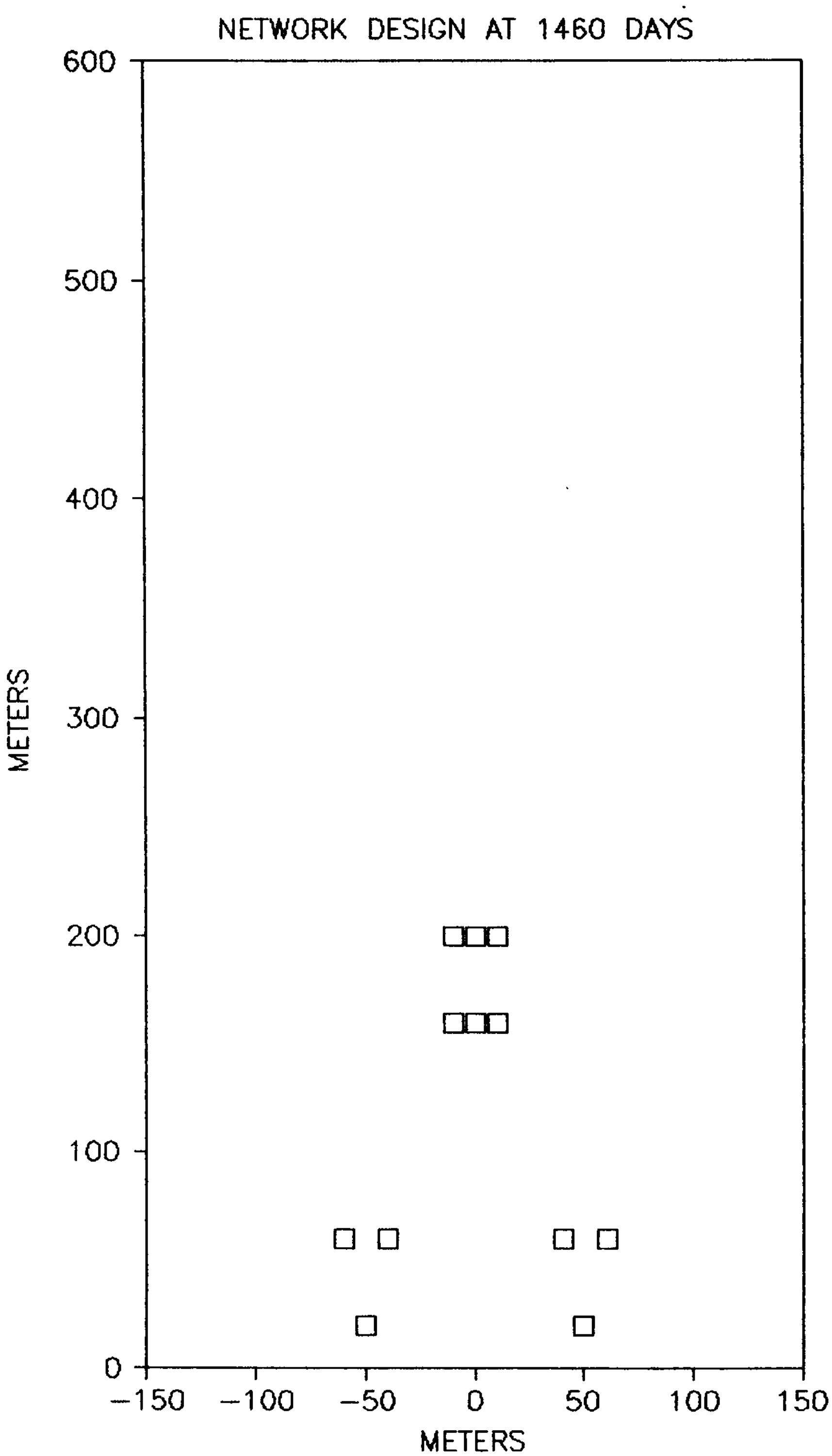


NETWORK DESIGN AT 365 DAYS
600
500
400
300
200
100
0
METERS
−150
−100
−50
0
50
100
150
METERS

Slide #29

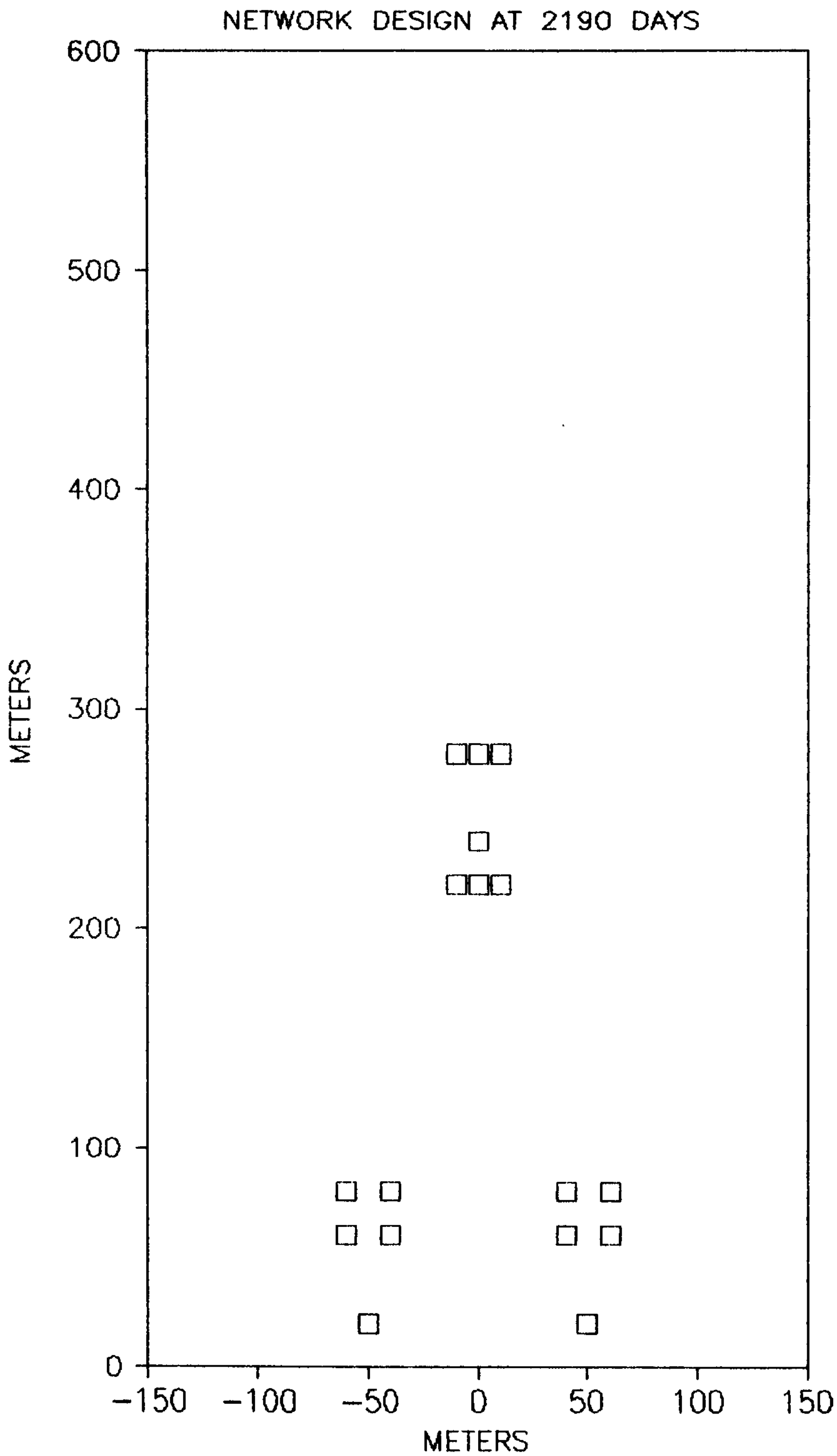

NETWORK DESIGN AT 730 DAYS
600
500
400
300
200
100
0
METERS
−150
−100
−50
0
50
100
150
METERS

Slide # 30

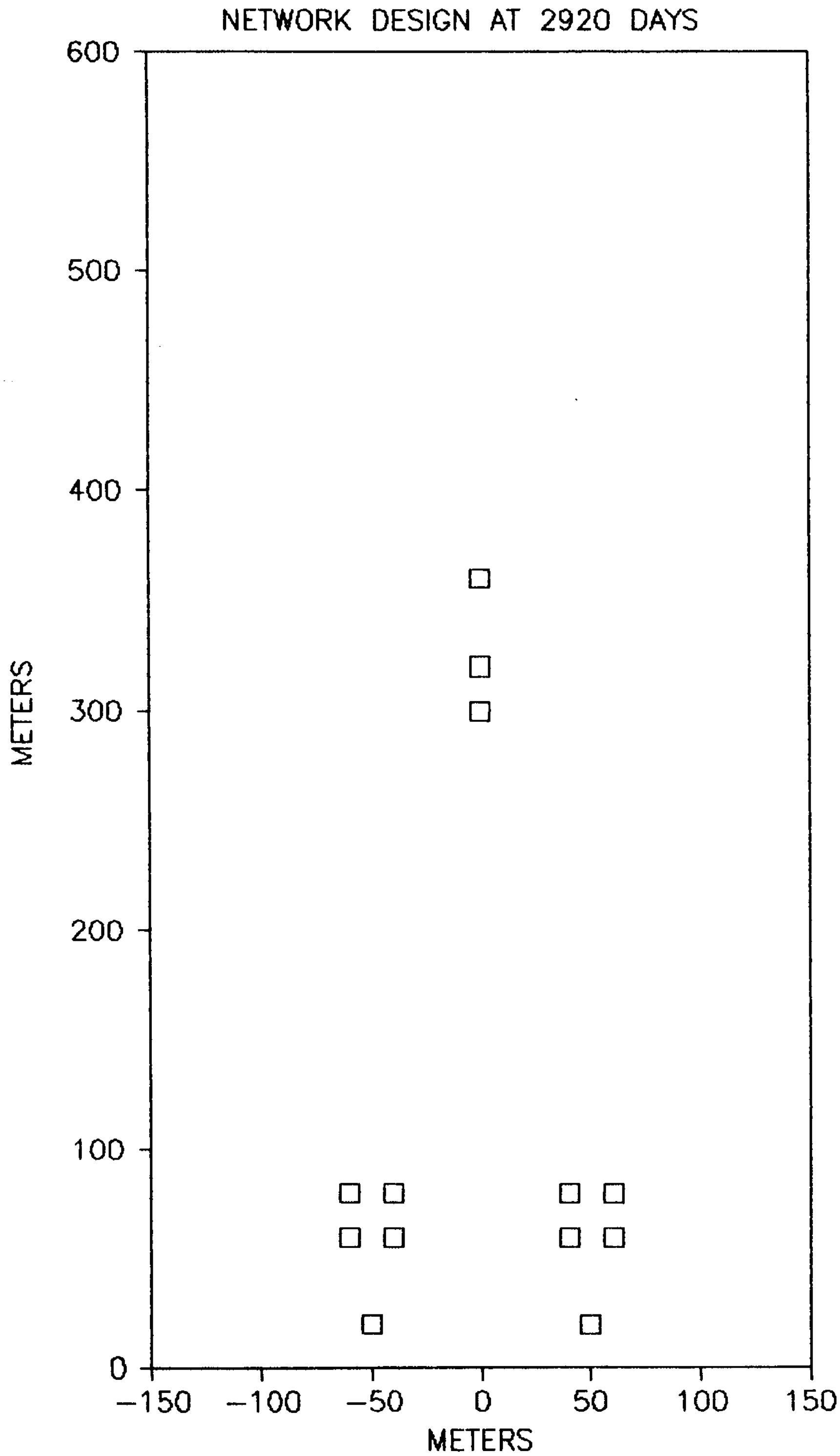


NETWORK DESIGN AT 1460 DAYS
600
500
400
300
200
100
0
METERS
-150
-100
-50
0
50
100
150
METERS

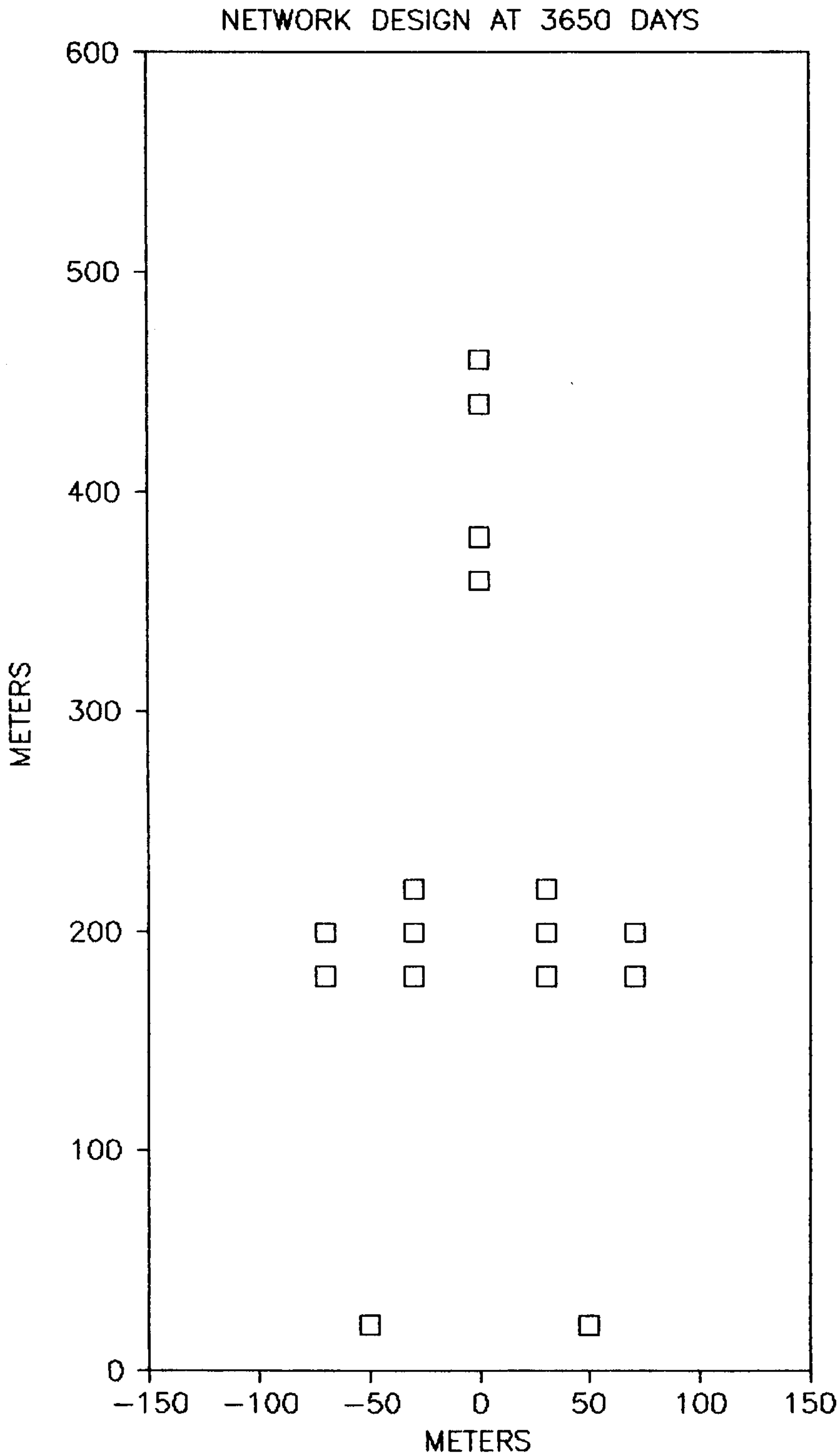
Slide # 31


NETWORK DESIGN AT 2190 DAYS
600
500
400
300
200
100
0
METERS
-150
-100
-50
0
50
100
150
METERS

Slide # 32

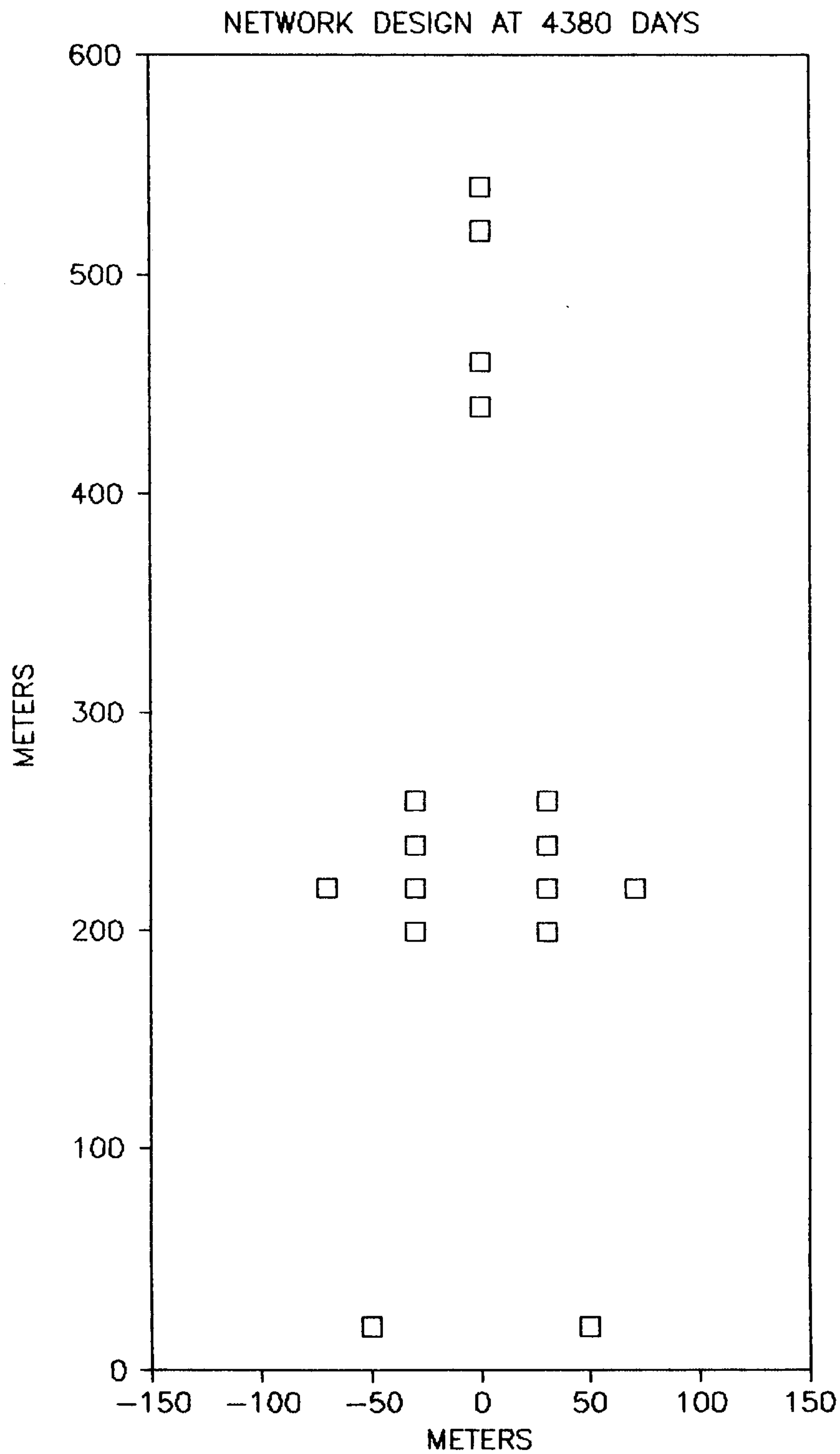

NETWORK DESIGN AT 2920 DAYS
600
500
400
300
200
100
0
METERS
−150
−100
−50
0
50
100
150
METERS

Slide # 33

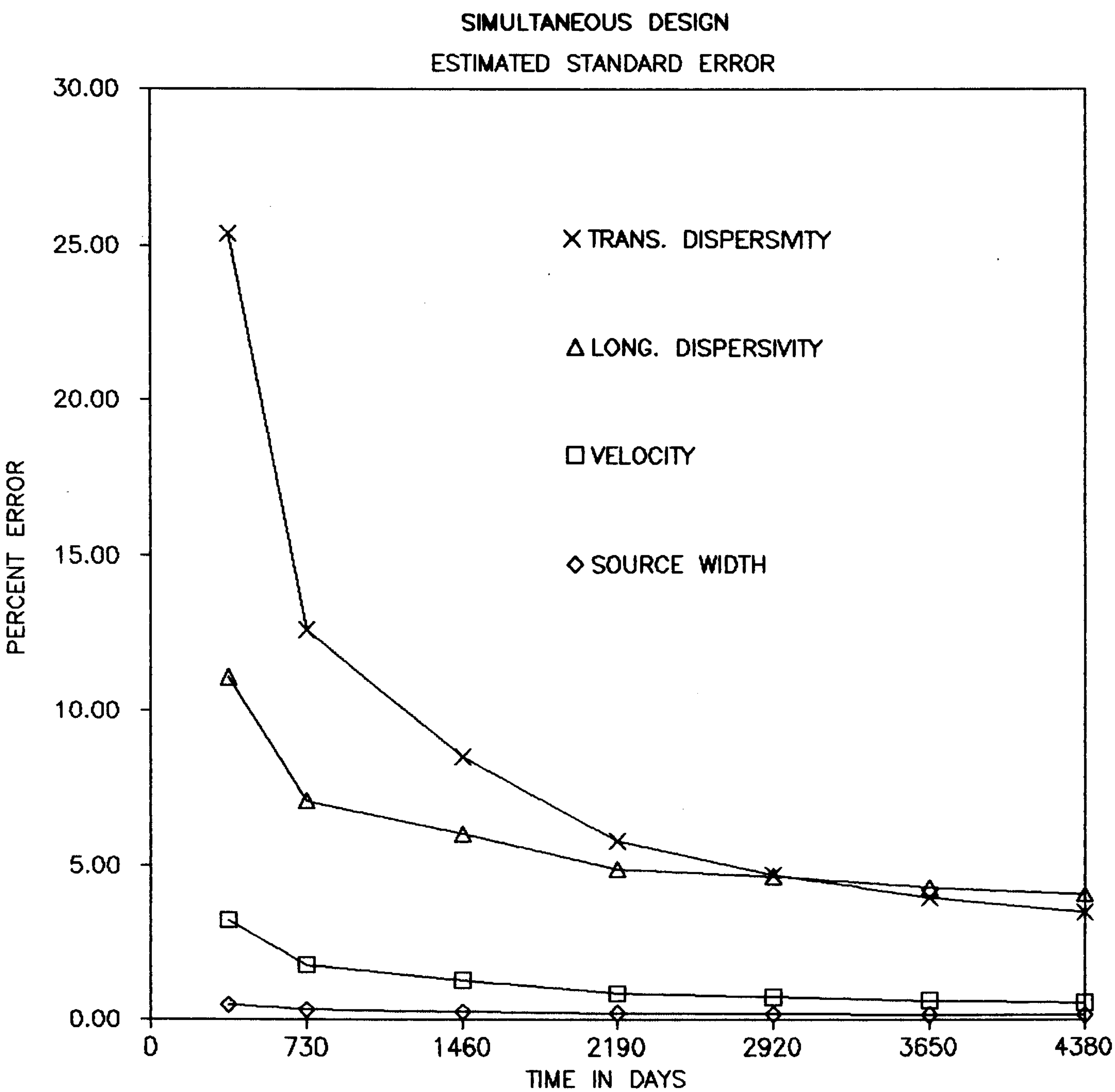


NETWORK DESIGN AT 3650 DAYS
600
500
400
300
200
100
0
METERS
−150
−100
−50
0
50
100
150
METERS

Slide # 34


NETWORK DESIGN AT 4380 DAYS
600
500
400
300
200
100
0
METERS
−150
−100
−50
0
50
100
150
METERS

Slide # 35


SIMULTANEOUS DESIGN
ESTIMATED STANDARD ERROR
PERCENT ERROR
30.00
25.00
20.00
15.00
10.00
5.00
0.00
0
730
1460
2190
2920
3650
4380
TIME IN DAYS
TRANS. DISPERSMTY
LONG. DISPERSIVITY
VELOCITY
SOURCE WIDTH

Slide # 36

CONCLUSIONS

For An Effective Monitoring System:

1. Plot sensitivity coefficients
2. Look for dependence in parameters
3. Sample at time and space locations that have the maximum sensitivity
4. Let the monitoring system evolve in time
5. Estimate parameters
6. Make future predictions