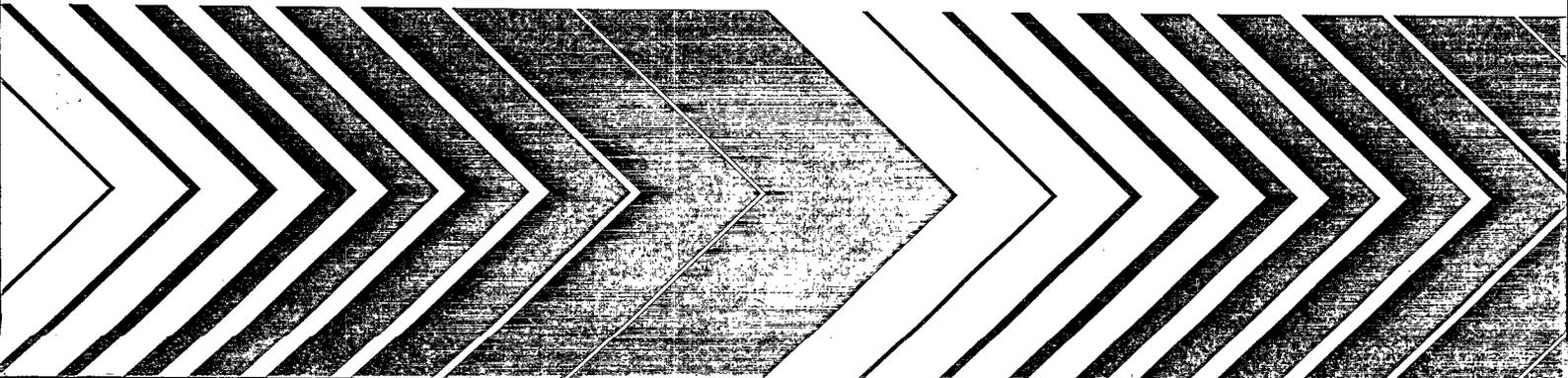
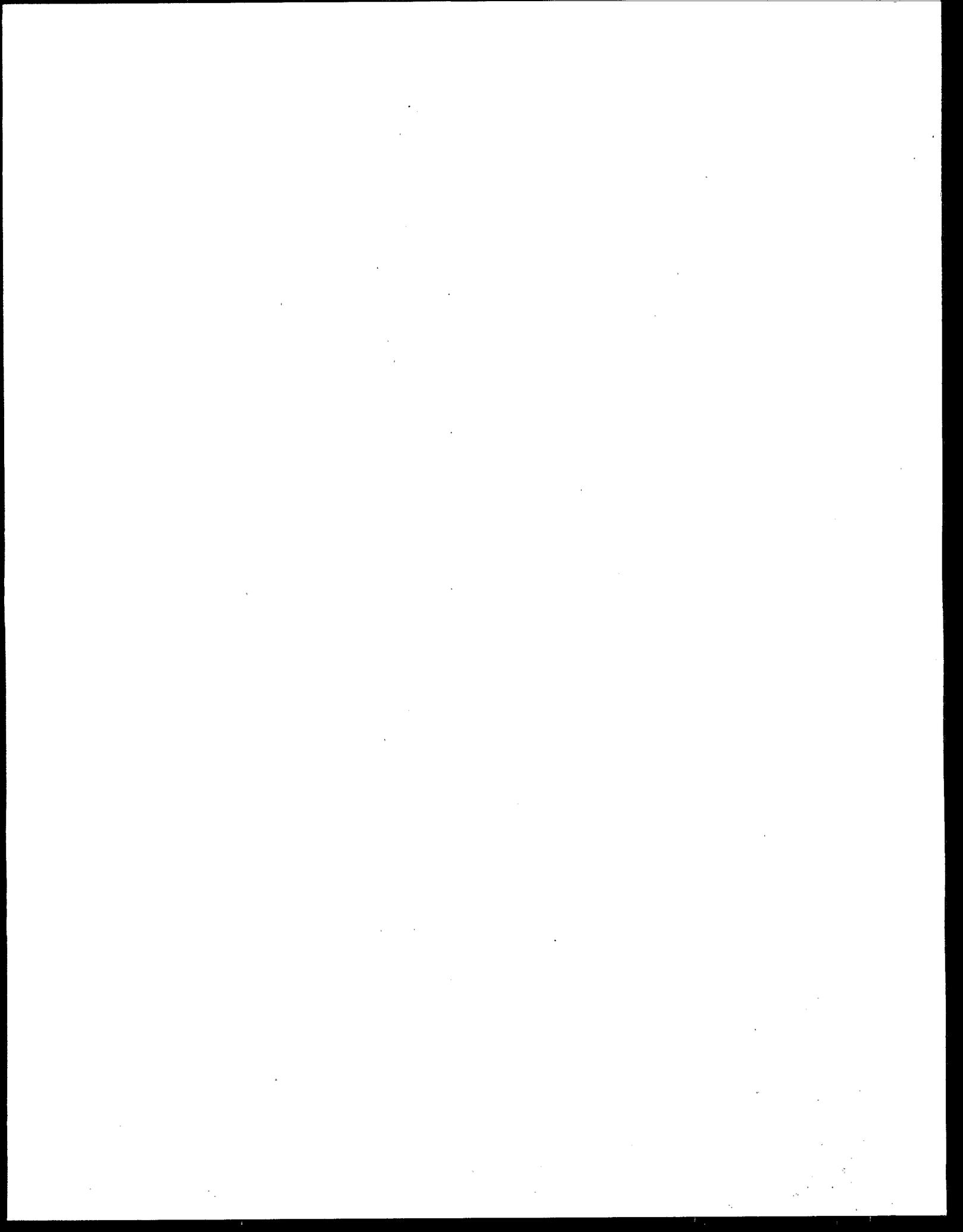




Statistical Estimation and Visualization of Ground-Water Contamination Data





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Notice

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All research projects making conclusions or recommendations based on environmentally related measurements and funded by the Environmental Protection Agency are required to participate in the Agency Quality Assurance Program. This project was conducted under an approved Quality Assurance Project Plan. The procedures specified in this plan were used without exception. Information on the plan and documentation of the quality assurance activities and results are available from the Principal Investigator.

Foreword

The U.S. Environmental Protection Agency is charged by Congress with protecting the Nation's land, air, and water resources. Under a mandate of national environmental laws, the Agency strives to formulate and implement actions leading to a compatible balance between human activities and the ability of natural systems to support and nurture life. To meet these mandates, EPA's research program is providing data and technical support for solving environmental problems today and building a science knowledge base necessary to manage our ecological resources wisely, understand how pollutants affect our health, and prevent or reduce environmental risks in the future.

The National Risk Management Research Laboratory is the Agency's center for investigation of technological and management approaches for reducing risks from threats to human health and the environment. The focus of the Laboratory's research program is on methods for the prevention and control of pollution to air, land, water, and subsurface resources; protection of water quality in public water systems; remediation of contaminated sites and ground water; and prevention and control of indoor air pollution. The goal of this research effort is to catalyze the development and implementation of innovative, cost-effective environmental technologies; develop scientific and engineering information needed by EPA to support regulatory and policy decisions; and provide technical support and information transfer to ensure effective implementation of environmental regulations and strategies.

This work presents methods of visualizing and animating statistical estimates of ground water and/or soil contamination over a region from observations of the contaminant for that region. The primary statistical methods used to produce the regional estimates are nonparametric regression and geostatistical modeling (kriging). Nonparametric regression can be used as a more "rough and ready" method to produce surface estimates with little outside intervention, whereas geostatistical modeling produces prediction errors. Finally, a method is proposed for estimating the total amount of contaminant present in a region. This report is published and made available by EPA's Office of Research and Development to assist the user community.



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Abstract

This work presents methods of visualizing and animating statistical estimates of ground water and/or soil contamination over a region from observations of the contaminant for that region. The primary statistical methods used to produce the regional estimates are nonparametric regression and geostatistical modeling (kriging). Nonparametric regression can be used as a more "rough and ready" method to produce surface estimates with little outside intervention, whereas geostatistical modeling produces prediction errors.

Animation of changes in the estimated level of contaminant or chemical as observations are removed illustrate the effect of each individual measurement on the overall estimate and the error or variance of this estimate. Such methods are applied to the Eglin Air Force Base (AFB) Florida site. The benefit of animating surface estimates in data which is taken over time is clearly seen by an example from a site near Phoenix, AZ, where aberrations in the data for one or several years were readily apparent by viewing a smoothed animation.

Finally, a method is proposed for estimating the total amount of contaminant present in a region. The proposed method models the data as a realization of a lognormal stochastic process and then capitalizes on conditional simulation to generate realizations of the modeled process from which the distribution of the total contaminant (or integral of the process) is estimated.

This report was submitted in fulfillment of cooperative agreement No. CR-821906 by Rice University under the sponsorship of the United States Environmental Protection Agency. This report covers a period from 10/01/93 to 03/31/97, and work was completed as of 11/03/98.

Contents

1. Introduction	1
2. Sites and Data	3
2.1 Eglin AFB	3
2.2 Arizona	4
3. Statistical Methods	5
3.1 Nonparametric Regression	5
3.2 Kriging and Variograms	5
3.3 Estimating an Integral via Sample-Mean Monte Carlo	6
4. Eglin AFB: Visualization and Exploratory Analysis	9
4.1 Visualization of Estimated Plumes	9
4.1.1 Two-Dimensional Data	9
4.1.2 Three-Dimensional Data	10
4.2 Error Visualization	11
5. Estimation of Non-Linear Functionals of Random Processes for Environmental Problems	15
5.1 Description of the Problem	15
5.2 Using Monte Carlo to Estimate the Distribution of a Stochastic Integral	16
5.3 Application	17
5.3.1 Discussion of Data	17
5.3.2 Results	29
6. Phoenix, AZ: Visualization with a Time Component	31
6.1 Exploratory Visualization	31
6.2 Animation	31
6.2.1 Trichloroethylene and Dichloroethylene (TCE and DCE)	31
6.2.2 Sulfate Ions	38
6.3 Further Analytical Efforts	41
7. Summary and Conclusions	43
Appendix A. Cross-Validation	45
A.1 Two-dimensional Data	45
A.2 Three-dimensional Data	45
Appendix B. Discussion of Spatial Estimation for Arizona	46
Bibliography	49

List of Figures

2.1	Eglin AFB ground-water data points. Coordinates: depth-axis: 4400 to 5100; width-axis: 4900 to 5600 and vertical-axis: 0 mg/kg to 9.1 mg/kg	3
2.2	Eglin AFB soil data points	4
4.1	Legends for two-dimensional perspective plot contours	10
4.2	Estimate of contaminant plume for Eglin AFB ground-water data	11
4.3	Estimate of soil contamination 7.0 μ g below the water table	12
4.4	Estimate of soil contamination (BTEX) at Eglin AFB	12
4.5	Estimates of ground-water contamination and absolute errors	13
4.6	Estimate of ground-water contamination: contours represent magnitude of error	13
4.7	Smoothed absolute error estimate for Eglin AFB soil data	14
5.1	QQ-plot of logs of Eglin AFB ground-water data	18
5.2	Logs of Eglin AFB ground-water data points	18
5.3	Empirical semivariogram of logged Eglin AFB ground-water data	19
5.4	Empirical semivariograms with rotation angles from 0° on the left to 180° on the right and ratios from 1:25 at the bottom to 2 at the top	19
5.5	Empirical semivariograms with rotation angles from 45° on the left to 135° on the right and ratios from 1:45 at the bottom to 1:55 at the top.	20
5.6	Semivariogram of logged Eglin AFB ground-water data with transformed locations	22
5.7	Kriged surface estimate of logged Eglin AFB ground-water data using rational quadratic variogram details of the integral estimation	22
5.8	Standard errors for kriged surface estimate of logged Eglin AFB ground-water data using a rational quadratic variogram	23
5.9	Surface of a grid simulation	25
5.10	Semivariogram calculated from a grid simulation	25
5.11	Histogram of integral estimates from 1000 samples of size 500: one realization	26
5.12	QQ-plot of integral estimates from 1000 samples of size 500: one realization	26
5.13	Histogram of integral estimates from 1000 samples of size 500: different realizations	27
5.14	Histogram of lower 97.5% integral estimates from 1000 samples of size 500: different realizations	27
5.15	Histogram of logged integral estimates from 1000 samples of size 500: different realizations	28
6.1	TCE prediction surface for 1991. Orientation: depth-axis: 892,600 to 896,800; width-axis: 478,000 to 484,000; vertical-axis: 0 to 2.25	32
6.2	TCE standard errors of prediction for 1991	32
6.3	DCE prediction surface for 1991	33
6.4	DCE standard errors of prediction for 1991	33
6.5	TCE prediction surface for 1992	34
6.6	TCE standard errors of prediction for 1992	34
6.7	DCE prediction surface for 1992	35
6.8	DCE standard errors of prediction for 1992	35

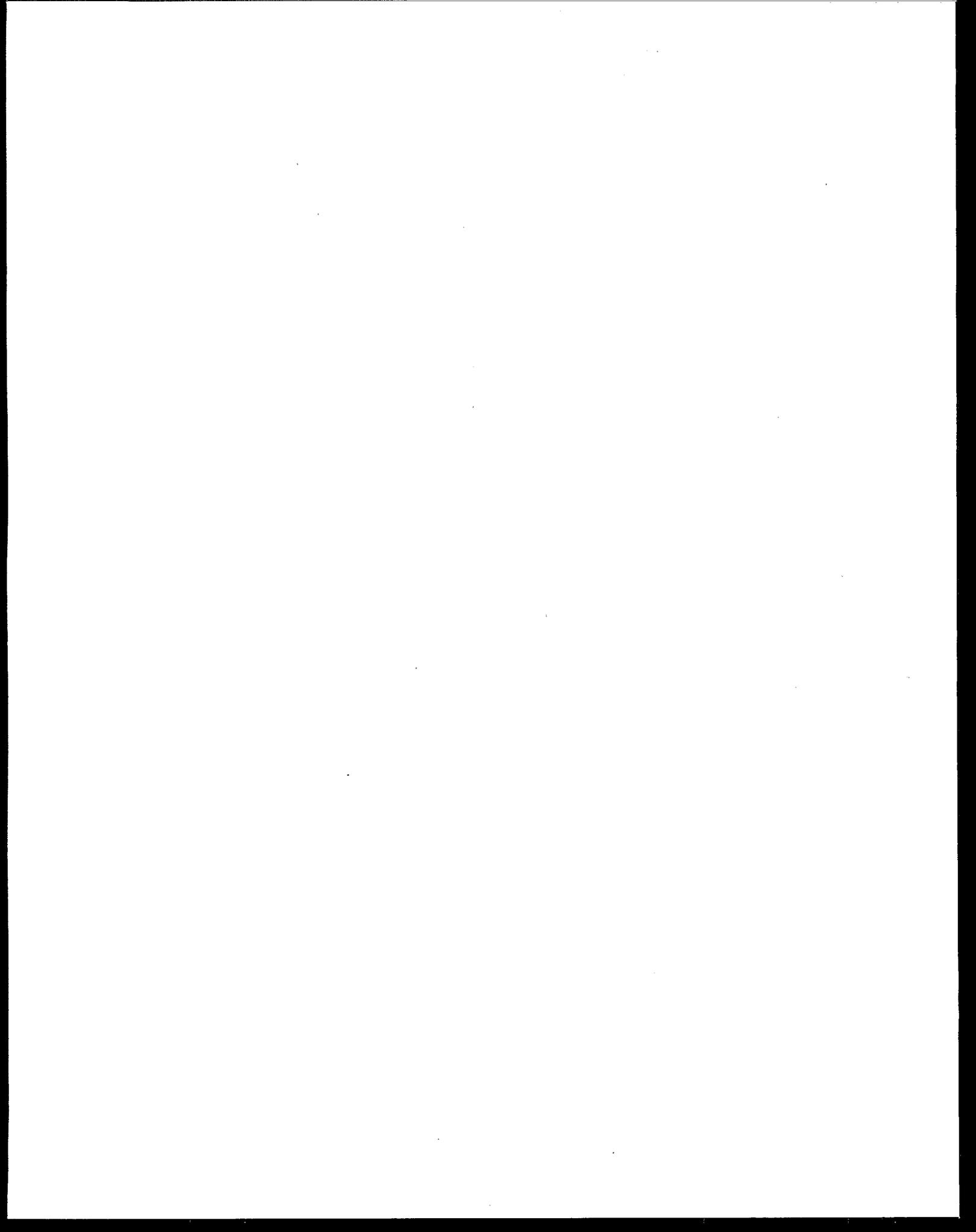
6.9	Legend for prediction surfaces (measurements in <i>mg/l</i>)	36
6.10	Legend for standard errors	36
6.11	TCE and DCE surfaces for 1986	37
6.12	TCE and DCE surfaces for 1988	37
6.13	TCE and DCE surfaces for 1991	38
6.14	TCE and DCE surfaces for 1993	39
6.15	SO ₄ ²⁻ surface for 1986	39
6.16	SO ₄ ²⁻ surface for 1988	40
6.17	SO ₄ ²⁻ surface for 1991	40
A.1	Bandwidth selection for ground-water data	45
B.1	Classical empirical variogram for 1990 TCE	46
B.2	Mean γ values for 1990 TCE	47

Tables

Table 5.1	Statistics of Integral Estimates for 1000 Realizations	29
Table 5.2	Means of Integral Estimates for 1000 Realizations	29

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Chapter 1

Introduction

Understanding the plume of any contaminant is a multi-faceted problem. Often data is limited and modeling exercises are tedious. To aid the environmental researcher, we present several techniques for capitalizing on the measurements of the level of contaminant in soil samples from a region. Our techniques rely on visual displays of statistical estimates of the contaminant plume. We explore two- and three-dimensional estimation and visualization techniques and ways to examine related contaminants. Furthermore, we propose a method for quantification of the total amount of contaminant within a region. Both of these methods are investigated in the context of a site specific example, but the tools generalize to other similar problems.

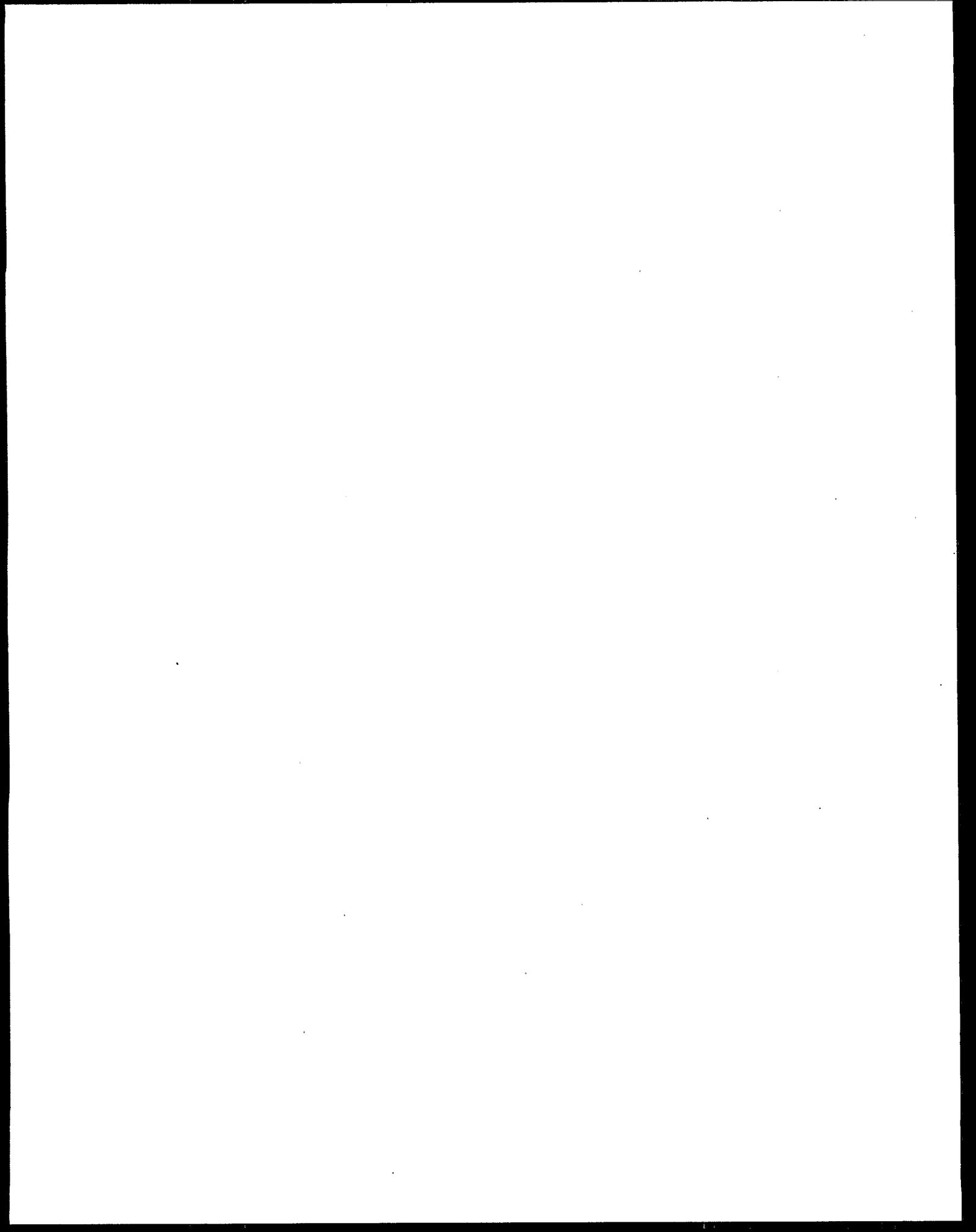
As a simple method for displaying surface estimates from field data, exploratory visualization of the Eglin AFB in Section 4.1 was performed using nonparametric regression to produce the surface estimates. This methodology requires estimation of only one parameter, the bandwidth, as opposed to the several parameters required by the more complicated art of variogram fitting used in geostatistical modeling. Surface estimates were obtained for both two- and three-dimensional data for the Eglin AFB site, using the program *Geomview* on a Silicon Graphics machine to facilitate display and animation. *Geomview* allows the viewer to rotate images in real time, which aids greatly in examining the surface (i.e., looking for peaks and valleys, etc.). For data in two dimensions, the third dimension (i.e., the z direction) may be used to plot the surface estimate as a perspective plot. Color contours on the surface can be set to levels of interest to highlight areas where the contamination is above a fixed level. This tool can be useful in cases where environmental regulations require contamination to be below some specific level, to identify regions of high contaminant concentration, and to follow the movement of a contaminant over time. In an analogous fashion, for three-dimensional visualization, shell contours are plotted at certain levels to illustrate regions of higher concentrations.

Estimates of prediction errors in both the two-dimensional and three-dimensional setting provide an understanding of the differing levels of uncertainty of the estimate of the level of the contaminant over the region. In the case of Eglin AFB ground water, we also use visual tools in conjunction with cross-validation to ascertain the effect each of the data values has on the estimate of the level of contaminant for the region. An animation of estimates produced excluding individual data points, alternated with the overall surface estimate, lends insight to the question of where to obtain new samples. This sort of display also helps us to determine the level of error in our estimates of the contaminant plume.

A second site providing a different type of complexity was examined from a statistical estimation and visualization perspective. This second site, in Arizona, yields observations of several contaminants collected over a period of several years. Animations of estimates capitalizing on the temporal component clearly illustrate major trends and aberrations in the data, which can then be investigated more closely. Also, there were several different contaminant substances measured at the Arizona site, such as TCE, DCE, and SO_4^{2-} . The behavior of these contaminants is expected to be interrelated. We present suggestions on how to best visualize simultaneously two or more related substances in order to highlight possible relationships among the series. The Arizona site also includes a common problem in that the region where measurements were taken increases over time. This problem is addressed here, along with some possible solutions.

Another primary focus of this research is to answer the question of how much total contamination is present at a site and how to best estimate this quantity given soil core samples from the site. It is important when producing such estimates to also understand the level of uncertainty in the estimate, in other words to obtain the standard error of the estimate. A byproduct of carefully implemented geostatistical methods such as *kriging* is standard errors for the estimated mean level over the region. Estimation of total contaminant involves estimation of the integral of the modeled process over a region. We pursue estimation of the total contaminant for Eglin AFB. The level of ground water BTEX was modeled as a realization of a lognormal stochastic process, and estimates of the distribution of the integral were produced by Monte-Carlo simulation of the process conditional on the observed data.

The data used in this research, from Eglin AFB and a site near Phoenix, AZ, are presented in Chapter 2. Chapter 3 contains discussion of the statistical methods used, including estimation by nonparametric regression and kriging. Chapter 4 contains results for Eglin AFB, including both exploratory data analysis and estimation of total contaminant. Chapter 6 contains discussion of the visualization and animation for the Arizona site, including discussions of temporal data and visualization of two related substances. Finally, Chapter 7 contains conclusions and suggestions for future research.



Chapter 2

Sites and Data

2.1 Eglin AFB

In Chapters 4 and 5, we consider data from Eglin AFB, an example of a shallow aquifer in sandy soil. A leak of 30,000 - 40,000 gallons of JP-4 jet fuel was detected at Eglin AFB in Florida by Air Force personnel in 1984 (Boeckenhauer, *et al.*, 1995). The contamination measured here is from BTEX, including benzene, toluene, ethylbenzene, and *m*-, *o*-, and *p*-xylene, which are typically contained in petroleum fuels and are hazardous substances regulated by the U.S. Environmental Protection Agency (Sweed, *et al.*, 1996).

Two data sets are available for this site, namely: (1) Ground-water BTEX concentrations in two dimensions, measured in $\mu\text{g/L}$ and (2) Soil BTEX concentrations in three dimensions, measured in mg/kg . Also, for the exploratory analysis, we used the soil data which are approximately 7.0 and 7.6 ft below the water table as two different two-dimensional data sets. The 22 ground-water data points were collected by researchers from Rice University in March 1993 using a cone penetrometer. These data range from 0.001 to over 9mg/L . A plot of the ground-water data is shown in Figure 2.1.

Anaerobic soil cores were collected in March and July, 1993, and March, 1994. The soil data set contains 336 points at 20 different locations, with values ranging from 0 to approximately 750mg/kg . A plot of the three-dimensional soil data points is shown in Figure 2.2. The actual vertical range of the region is 21.6 ft , whereas the longitude encompasses 230.3 ft and latitude 286.4 ft . The X s connected by the dotted line indicate the location of the source of contaminant. The larger blocks denote observations of measured concentration exceeding 25mg/kg , whereas the smaller blocks depict observations with measurements between 0 and 25mg/kg . Also, the location of the water table is shown with stripes. It is observed from this figure that very few of the data points actually have values greater than 25mg/kg (only 16 of the 336), and *all* of these lie below the water table.

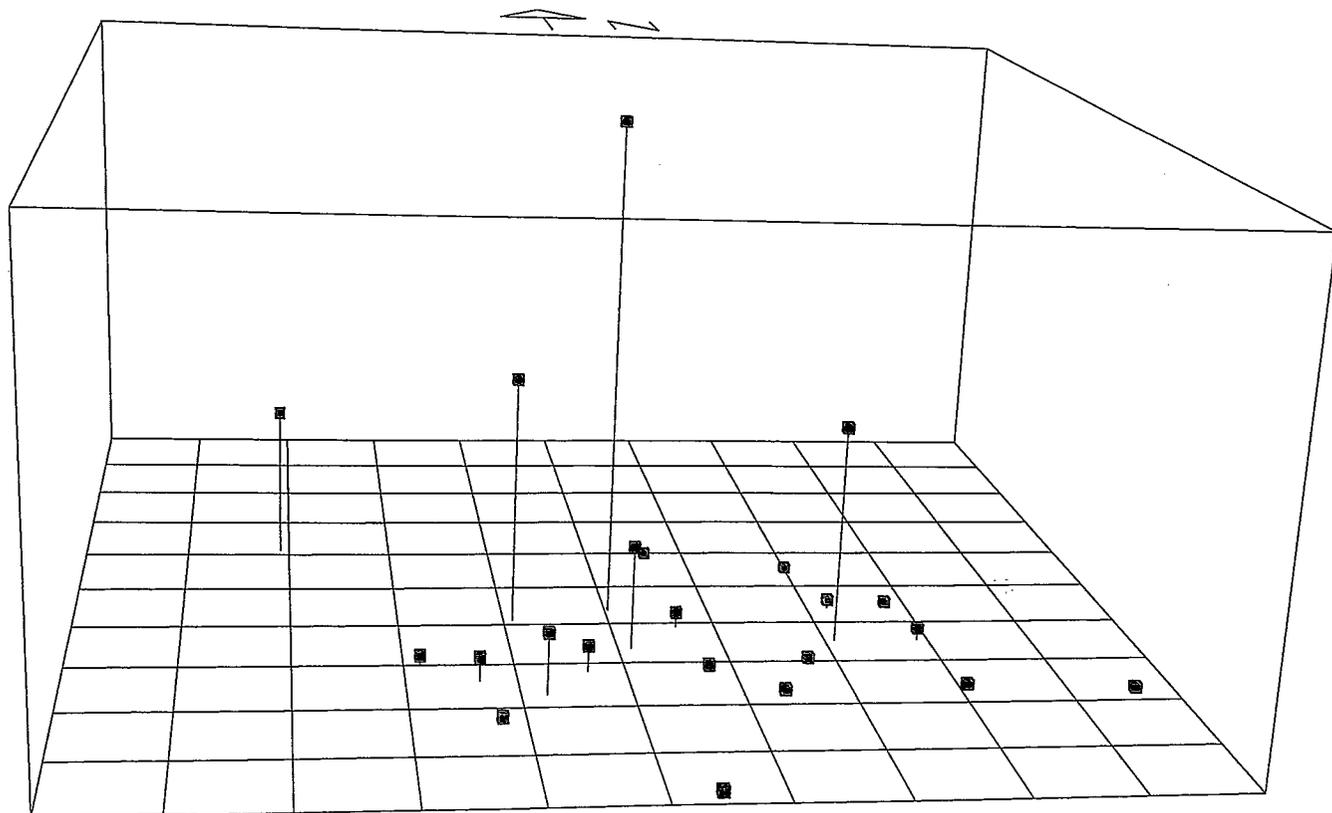


Figure 2.1 Eglin AFB ground-water data points. Coordinates: depth-axis: 4400 to 5100; width-axis: 4900 to 5600 and vertical-axis: 0 mg/kg to 9.1 mg/kg.

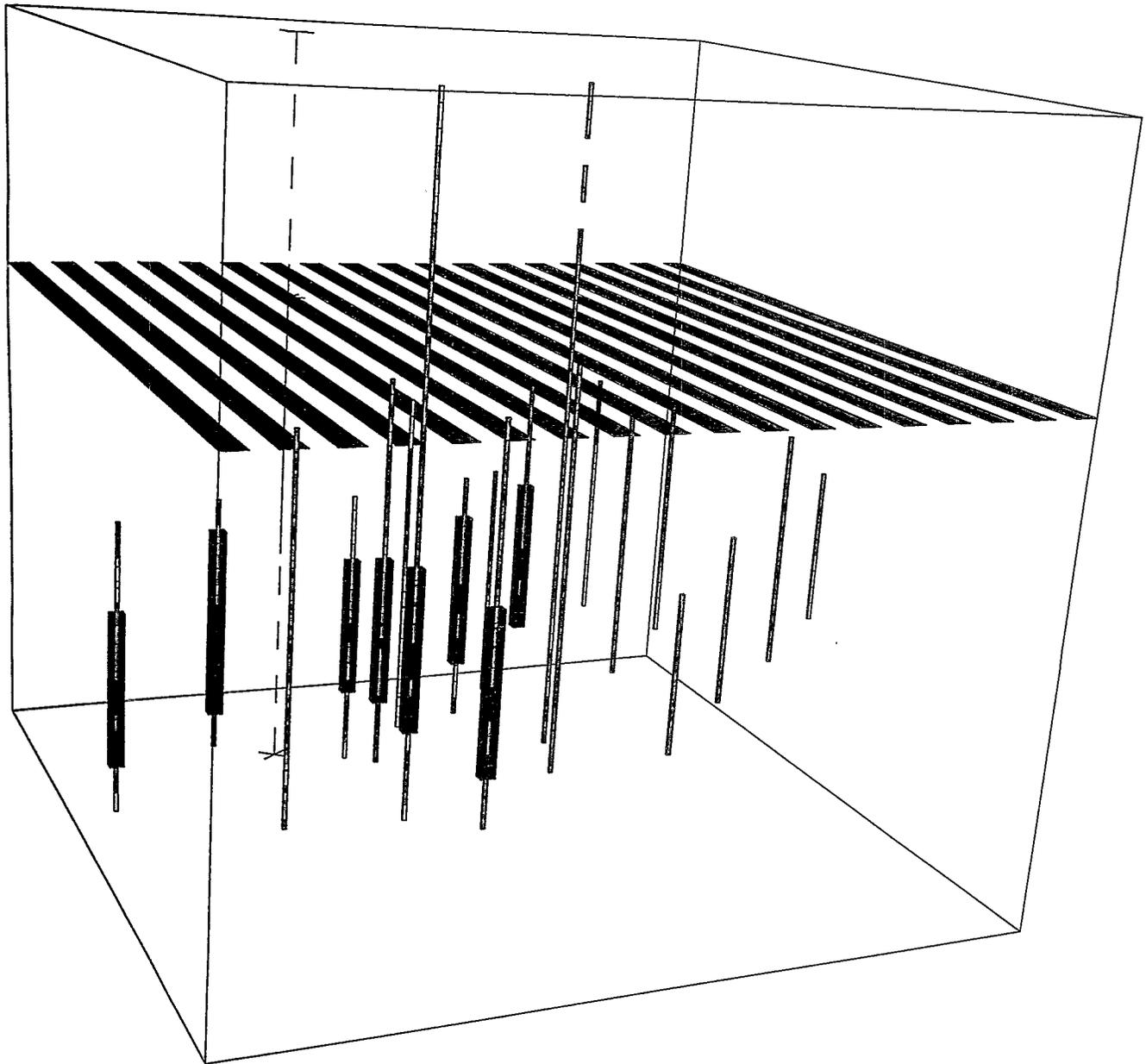


Figure 2.2 Eglin AFB soil data points.

2.2 Arizona

In Chapter 6, we consider data from a contaminated site near Phoenix, AZ. Contaminants measured include trichloroethylene (TCE), dichloroethylene (DCE), and sulfate (SO_4^{2-}), all measured in $\mu\text{g/L}$. Other measured contaminants contained somewhat sparse data and were not used at this time. The DCE "measurements" are actually sums of measured values of 1,1-DCE and 1,2-DCE, so the measurement locations here are only used if measurements of *both* of these are available. These data were gathered from 1985 to 1993.

Chapter 3

Statistical Methods

3.1 Nonparametric Regression

For the exploratory analysis of Eglin AFB in Section 4.1, we used *nonparametric regression* to produce a surface estimate of the plume. The model used for the contaminant plume is $u(\mathbf{x}) = f(\mathbf{x}) + \varepsilon(\mathbf{x})$ where:

- \mathbf{x} = a point in the region of interest,
- $u(\mathbf{x})$ = the observed level of contaminant at \mathbf{x} ,
- $f(\mathbf{x})$ = the true level of contaminant at \mathbf{x} , and
- $\varepsilon(\mathbf{x})$ = random noise in the measurement process.

The model assumes:

- The observation locations $\mathbf{x}_1, \dots, \mathbf{x}_n$ are randomly chosen.
- The unknown function $f(\cdot)$ is twice continuously differentiable. Note that $f(\cdot)$ is not a random process.
- The random noise $\varepsilon(\mathbf{x}_1), \dots, \varepsilon(\mathbf{x}_n)$ is independent, but not necessarily identically distributed.

An estimate of $f(\mathbf{x})$ over the region of interest can be obtained via nonparametric regression methods (Scott, 1992) and is given by:

$$\hat{f}(x) = \sum_{i=1}^n u_i w_h(\mathbf{x}, \mathbf{x}_i) \quad (3.1)$$

where the weights are defined as:

$$w_h(\mathbf{x}, \mathbf{x}_i) = \frac{K_h(x - x_i)}{\sum_{j=1}^n K_h(x - x_j)} \quad (3.2)$$

and $u_i = u(\mathbf{x}_i)$. The function $K_h(\cdot)$ is referred to as the scaled *kernel* function with *bandwidth*, or smoothing parameter, h . Note that the bandwidth determines the smoothness of the surface estimate; a larger bandwidth yields a smoother estimate. For some standardized (or unscaled) kernel function $K(\cdot)$, we define $K_h(\cdot)$ as $K_h(t) = K(t/h)/h$, so as h increases, the value of $t/h = (x - x_i)/h$ decreases.

3.2 Kriging and Variograms

Another method which we will use to estimate contaminant levels over the region is the geostatistical spatial prediction method known as *kriging*. A complete and thorough exposition of geostatistical methods is given in (Cressie, 1993). A very brief overview is provided here for purposes of introduction and definition of notation. The general idea of kriging is to first use the observed levels of a contaminant to produce a model of the spatial covariance structure of the process. This spatial covariance model is then used to obtain the "optimal" predictor $\hat{Z}(s_0)$ of $Z(s_0)$, the value of the random process at s_0 . This predictor is $E[Z(s_0)|\mathbf{Z}]$, which is precisely the same as $\rho^0(\mathbf{Z}; s_0)$ in (5.2) in the case where $g(\cdot)$ is simply $g(\mathbf{Z}) = Z$.

Assume that the data $\mathbf{z} = (z(s_1), \dots, z(s_n))$ are a sample from a realization of the stochastic process $\{Z(s) : s \in A\}$. In order to do inference from the data, we need to make some assumptions. A common practice is to assume *second-order stationarity*. That is, assume that

$$E[Z(s)] = \mu \quad \forall s \in A \quad (3.3)$$

or that $F_z(z) \equiv Pr(Z(s) \leq z)$ does not depend on s and

$$cov(Z(s_i), Z(s_j)) = C(s_i - s_j) \quad \forall s_i, s_j \in A, \quad (3.4)$$

i.e., $cov(Z(s_i), Z(s_j))$ depends only on the vector $s_i - s_j$. Furthermore, if

$$cov(Z(s_i), Z(s_j)) = C(|s_i - s_j|) \quad \forall s_i, s_j \in A, \quad (3.5)$$

i.e., $cov(Z(s_i), Z(s_j))$ depends only on the *distance* $|s_i - s_j|$, then the process is said to be *isotropic*.

If second-order stationarity holds, a convenient way to model the covariance structure of the process is through use of a *variogram* function

$$\text{var}(Z(s_i) - Z(s_j)) = 2\gamma(s_i - s_j) \quad \forall s_i, s_j \in A, \quad (3.6)$$

The function $\gamma(s_i - s_j)$ is referred to as the *semivariogram*. Note that it is easy to show that $\gamma(h) = \gamma(-h)$ and $\gamma(\mathbf{0}) = 0$. If we have:

$$\lim_{h \rightarrow 0} \gamma(h) = c_0 > 0 \quad (3.7)$$

then c_0 is what is known as a *nugget effect*. This may be due either to some microscale variation or to measurement error. The term *nugget effect* comes from spatial prediction's origins in mining, and refers to a variation caused by small *nuggets* of ore. Regardless, in all real data, there is some measurement error and so we would be remiss to model our process without a nugget effect. On the other end, as $|\mathbf{h}| \rightarrow \infty$, the semivariogram converges to the process variance. This follows easily by noting that we assume that the covariance between two values of the process diminishes to zero as the distance between them increases.

In the case that the process is isotropic; i.e., the spatial covariance between values of the process depends *only* on the distance between the observations, there are a number of standard variogram models available (Cressie, 1993). However, if the process is *anisotropic*, it is sometimes possible to transform the locations so that an isotropic variogram model remains appropriate. Specifically, such a transformation is possible in cases of *geometric anisotropy*; i.e., where rotating and scaling the locations produces an isotropic process. For example, it is typically the case with ground-water data that the correlation is higher for points a distance h apart if they lie in the direction of ground-water flow rather than perpendicular to it. In this case, the variogram is of the form:

$$2\gamma(\mathbf{h}) = 2\gamma_0(|\mathbf{B}\mathbf{h}|) \quad \mathbf{h} \in A \subset \mathfrak{R}^d \quad (3.8)$$

where \mathbf{B} is a $d \times d$ matrix and γ_0 is an isotropic variogram. We will be using this type of transformation on the Eglin AFB ground-water contamination data where $d=2$. In the case $d=2$, the matrix \mathbf{B} is given by:

$$\mathbf{B} = \begin{pmatrix} \cos^2(\theta) + r \sin^2(\theta) & (1-r) \sin(\theta) \cos(\theta) \\ (1-r) \sin(\theta) \cos(\theta) & \sin^2(\theta) + r \cos^2(\theta) \end{pmatrix} \quad (3.9)$$

meaning that θ is the angle clockwise from North at which the scale is multiplied by r . The other axis is then the one which is perpendicular to this, and the scale in this direction is not altered. For example, then, if we were working with ground-water data where the flow was along the northwest-southeast direction, we might use $\theta \cong 135$ deg and some $r > 1$.

Assuming the modeled spatial covariance structure of the random process, we can now obtain optimal predictions. If our optimization criteria is minimization of the squared-error loss then the optimal predictor of the random process at any point \mathbf{s}_0 is given by the expectation of the random process conditional on the observed values of the process; in other words, the best predictor of $Z(\mathbf{s}_0)$ is $p(Z; \mathbf{s}_0) = E(Z(\mathbf{s}_0) | Z)$, where Z denotes the vector of data as in (Boeckenhauer, 1996). In the case that $Z(\cdot)$ is a Gaussian process, this predictor is linear. Here we will be using the form of spatial prediction known as *ordinary kriging* (Cressie, 1993) which requires the two assumptions:

1. There is a constant mean, i.e.

$$Z(\mathbf{s}) = \mu + \delta(\mathbf{s}) \quad (3.10)$$

for $\mathbf{s} \in A$ and $\mu \in \mathfrak{R}$ unknown.

2. The predictor is linear in the observations, i.e.

$$p(Z; \mathbf{s}_0) = \sum_{i=1}^n \lambda_i Z(\mathbf{t}_i) \quad (3.11)$$

where the observations are at locations $\mathbf{t}_1, \dots, \mathbf{t}_n$ and $\sum_{i=1}^n \lambda_i = 1$. (Recall that this predictor is an estimate of $E[Z(\mathbf{s}_0) | Z(\mathbf{t}_1), \dots, Z(\mathbf{t}_n)]$.)

Requiring $\sum_{i=1}^n \lambda_i = 1$ guarantees uniform unbiasedness, i.e. $E(p(Z; \mathbf{s}_0)) = \mu = E(Z(\mathbf{s}_0))$. For further information on optimal prediction using the *kriging equations*, see (Cressie, 1993).

3.3 Estimating an Integral via Sample-Mean Monte Carlo

The question of the total amount of contaminant within a given region is equivalent to estimating the integral over the region of the estimated spatial process for this contaminant. Monte Carlo methods provide an estimate of the integral (see also (Rubinstein, 1981) and (Hammersley and Handscomb, 1964)) by viewing the integral as an expectation and simulating the sample mean as an estimate of this expectation. For example, suppose we wish to estimate the integral over a region A of some function $q(\mathbf{s})$:

$$\Phi = \int_A q(\mathbf{s}) ds \quad (3.12)$$

The basis of this method is to represent the integral Φ as the expected value of a random variable. For example, suppose that \mathbf{S} is a random variable which has density $f_{\mathbf{S}}(\mathbf{s})$ on \mathcal{A} . We may then rewrite the integral Φ in (3.12) as:

$$\Phi = \int_A q(\mathbf{s}) ds = \int_A \frac{q(\mathbf{s})}{f_{\mathbf{S}}(\mathbf{s})} f_{\mathbf{S}}(\mathbf{s}) ds = E \left[\frac{q(\mathbf{S})}{f_{\mathbf{S}}(\mathbf{S})} \right] \quad (3.13)$$

provided that $f_{\mathbf{S}}(\mathbf{s}) > 0$ when $q(\mathbf{s}) \neq 0$.

In particular, suppose \mathbf{S} is uniform on \mathcal{A} . That is, \mathbf{S} has density

$$f_{\mathbf{S}}(\mathbf{s}) = \frac{1}{|\mathcal{A}|} I_{\mathcal{A}}(\mathbf{s}) \quad (3.14)$$

where

$$I_{\mathcal{A}}(\mathbf{s}) = \begin{cases} 1 & \text{if } \mathbf{s} \in \mathcal{A} \\ 0 & \text{otherwise} \end{cases} \quad (3.15)$$

is the indicator function on \mathcal{A} and $|\mathcal{A}|$ is the norm of \mathcal{A} (e.g., the area or volume of \mathcal{A} if \mathcal{A} is two- or three-dimensional, respectively). We may then simplify the integral in (3.13)

$$\Phi = \int_A q(\mathbf{s}) ds = E \left[\frac{q(\mathbf{s})}{f_{\mathbf{S}}(\mathbf{s})} \right] = E \left[\frac{q(\mathbf{s})}{1/|\mathcal{A}|} \right] = |\mathcal{A}| E[q(\mathbf{S})] \quad (3.16)$$

To use this method to estimate Φ , then, we will

1. Generate a "large" (say p) number of locations, s_1, \dots, s_p uniformly over the region \mathcal{A} .
2. Evaluate $q(\mathbf{s})$ at each of these locations, yielding $q(s_1), \dots, q(s_p)$.
3. Compute the sample mean of these evaluations to yield an estimate of $E[q(\mathbf{S})]$, i.e. $\frac{1}{p} \sum_{j=1}^p q(s_j)$.
4. Use the sample mean in (3.) to estimate the integral Φ , or

$$\hat{\Phi} = \frac{|\mathcal{A}|}{p} \sum_{j=1}^p q(s_j) \quad (3.17)$$

The error inherent in this method relates to the randomness of the sampled sites and the number of sites which we sample. Specifically, the variance of the integral estimate for the function q is given by:

$$\begin{aligned} \text{Var}(\Phi) &= \text{Var} \left(\frac{|\mathcal{A}|}{p} \sum_{j=1}^p q(s_j) \right) \\ &= \frac{|\mathcal{A}|^2}{p^2} \text{Var} \left(\sum_{j=1}^p q(s_j) \right) \end{aligned} \quad (3.18)$$

This variance may be estimated by:

$$\begin{aligned} \hat{\text{Var}}(\hat{\Phi}) &= \frac{|\mathcal{A}|^2}{p^2} ps^2 \\ &= \frac{|\mathcal{A}|^2 s^2}{p} \end{aligned} \quad (3.19)$$

where s^2 is the sample variance of $q(s_1), \dots, q(s_p)$.

In order to estimate the total level of contaminant say for the Eglin AFB, we model the spatial process of interest. Using our model as the truth, we can generate a p -dimensional Multivariate Normal random vector with the appropriate mean structure

and spatial covariance structure as given by our estimated model (see, for example, Johnson, 1987; Stewart, 1973). This simulated random vector is then used in the above algorithm to ascertain the total amount of contaminant present, and the standard error of this estimate.

Chapter 4

Eglin AFB: Visualization and Exploratory Analysis

Our exploratory analysis of the observations of BTEX from Eglin AFB provides an understanding of the location and shape of the contaminant plume. For the two-dimensional data, perspective plots of the surface estimate with color contours visually display both the level of contamination and the rate of change over the region. The color contours can be set to specific concentrations of interest, such as regulatory levels. In the three-dimensional case, nested contour visualization is used to provide immediate characterization of the plume. Again, the contours could be keyed to concentrations of interest. Such exploratory analyses are greatly enhanced by on-line manipulations of the visual tools provided. For example, it is possible to rotate the surfaces to search for high levels of contamination which may be visible only from certain vantage points. Furthermore, color facilitates identification of trouble spots. However, even the gray-scale static versions of the plots presented here are useful for providing visual understanding of the plume.

The surface estimates for the exploratory visualization were produced using *nonparametric regression*, as discussed in Section 3.1. In order to obtain an accurate surface estimate of the plume, it is necessary to choose appropriate bandwidths to produce the nonparametric regression estimate. (Recall that the larger the bandwidth, the smoother the final surface estimate will be.) Appendix A contains the details of bandwidth selection, via cross-validation, for both the two-dimensional and three-dimensional Eglin AFB data.

Properties of spatial estimates and/or nonparametric regression estimates rely on asymptotic theory which, due to the small number of observations available, is certainly not the situation with the data at hand. Therefore, we explore the robustness of our estimate by examining the change in the estimate as sample points are removed from the estimation process. The uses of this examination are two-fold: (1) a better understanding of the magnitude of the error of our estimates is obtained, and (2) areas where additional observations are needed are highlighted. In other words, intuitively, we would take additional observations in the region where the estimated level of contamination changed the most as data was removed. If removing an observation has little effect on the estimate resulting in a small error, additional data would not be needed in that region. This result was visualized in two ways:

1. by viewing an animation of the estimated surface alternated with surfaces estimated by the removal of one of the sample points, and
2. by visualizations of the absolute differences (errors) between the surface estimated without point i and the measured value at point i .

The animation in case (1) is very useful when viewed on the SGI, but does not appear here. Case (2) appears in Section 4.2.

By viewing a smoothed version of the absolute error of our plume estimate, both in the two-dimensional and three-dimensional cases, it is clear where additional observations are needed. One suggestion for future sampling sites would be to sample in the region where both the estimated level of contamination and the error associated with the estimate are high. Of course, any measure of *error* or the amount of information contained in the data could be displayed in a similar fashion.

4.1 Visualization of Estimated Plumes

The program *Geomview* for an SGI was used to display plume estimates of the BTEX concentration. *Geomview* was written at the NSF Geometry Center, University of Minnesota, and is available through anonymous *ftp* from *ftp.geom.umn.edu*. The program *ashreg*, a modification of *ashn* (Scott, 1992), was used to produce plume estimates from the three-dimensional data. A biweight kernel was used in all cases.

4.1.1 Two-Dimensional Data

Figure 4.2 contains a plot of the estimated plume for the Eglin AFB ground-water data. Figure 4.1 shows the legends for these contour levels and those for the later figures, signifying estimated concentrations of:

$$\begin{array}{llll} (a) & 5000 & \leq & \hat{u} < 10000 \\ (b) & 2000 & \leq & \hat{u} < 5000 \\ (c) & 1000 & \leq & \hat{u} < 2000 \\ (d) & 500 & \leq & \hat{u} < 1000 \\ (e) & 100 & \leq & \hat{u} < 500 \\ (f) & 10 & \leq & \hat{u} < 100 \\ (g) & 0 & < & \hat{u} < 10 \\ (h) & & & \hat{u} = 0 \\ (i) & & & \text{No data} \end{array} \quad (4.1)$$

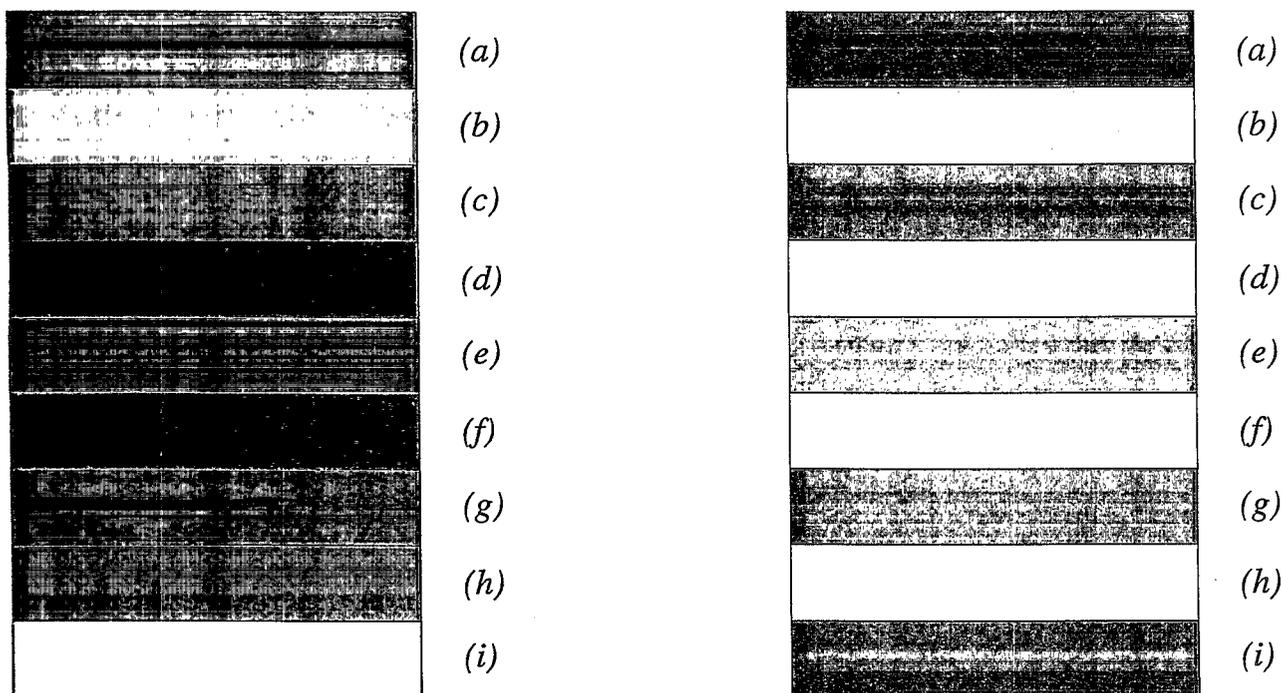


Figure 4.1 Legends for two-dimensional perspective plot contours.

where all of the concentrations are in $\mu\text{g/L}$. The level labeled *No data* includes areas where there is no estimate as we are too far from any of the measured points for the given bandwidth. (Note that, for the black and white figures, some of the lower levels are shown in the same shade, but we are primarily interested in areas where there are *high* concentrations, and these are distinctly different.) The same legend applies to the plot of the estimated plume for the Eglin AFB soil data at a depth of approximately 7.0 ft given in Figure 4.3, except that here the concentrations are:

(c)	50	\leq	\hat{u}	$<$	100
(d)	10	\leq	\hat{u}	$<$	50
(e)	5	\leq	\hat{u}	$<$	10
(f)	1	\leq	\hat{u}	$<$	5
(g)	0	$<$	\hat{u}	$<$	1
(h)			\hat{u}	$=$	0
(i)					<i>No data</i>

with all measurements in mg/kg . (Note that at this particular depth, the estimated concentration does not exceed 50mg/kg .)

For both of the two-dimensional plots, the actual data locations are marked on the grid at the top of the plot. The large point which is connected to the perspective plot by a vertical line is the mode of the estimate. An arrow pointing north indicates the orientation of the plot.

4.1.2 Three-Dimensional Data

Figure 4.4 contains a plot of the estimated plume for the Eglin AFB soil data. Two different levels of contamination are represented, with the lower (outer) shell being sliced so that we can see the higher (inner) one. The outer and inner shells represent concentration levels of approximately 0.73 and 7.33mg/kg , respectively. Also, the location of the water table and the source are clearly marked.

In an on-line version of the 3-D visualization of the plume, nested contours can be displayed using the transparency feature of the SGI and Geomview. This allows the use of solid color nested contours, where the inner shells can be seen through the outer ones. The use of transparency and the ability to rotate the graph greatly enhance the informative 7.0 \hat{f} below the Water Table value of the plot to the user.

4.2 Error Visualization

We simultaneously display a perspective plot of the two-dimensional ground-water BTEX plume estimate and the absolute errors of this estimate in Figure 4.5. Note that the heights of these two plots are on the same scale. The contours for the errors, using the legend in Figure 4.1, are the same as given in 4.1 except for levels (a) and (b):

$$\begin{aligned} (a) \quad & 3000 \leq \hat{u} < 5000 \\ (b) \quad & 2000 \leq \hat{u} < 3000 \end{aligned}$$

with errors in absolute $\mu\text{g}/\text{L}$. In Figure 4.6, we show a perspective plot of the ground-water data where the contours are determined by the smoothed absolute errors. By combining the plume estimate and the absolute errors into a single plot, we more readily identify regions of high concentration and regions with a large amount of uncertainty in the estimated value.

To visualize the errors for the three-dimensional soil data, we simply took the absolute errors as calculated for cross-validation in A.2 (i.e. $|u_1 - \hat{u}_1|, \dots, |u_n - \hat{u}_n|$) and plotted a smoothed contour shells (see Figure 4.7). Here the outer and inner shells represent contaminant concentrations of approximately 0.48 and 4.76 mg/kg , respectively.

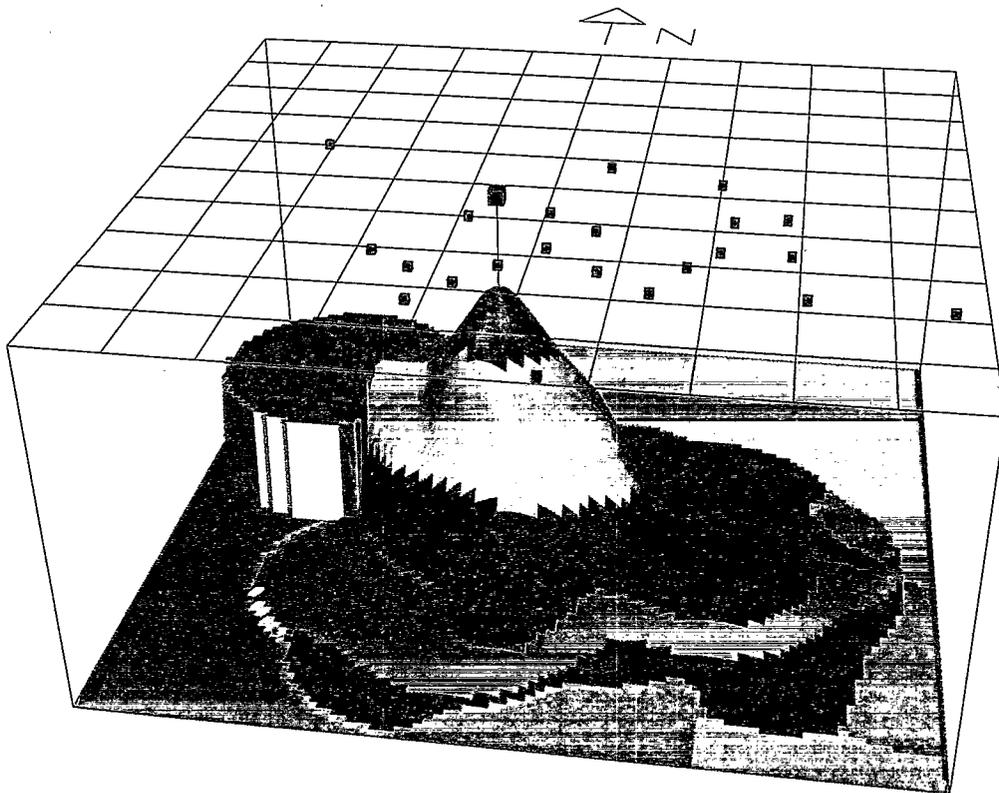


Figure 4.2 Estimate of contaminant plume for Eglin AFB ground-water data.

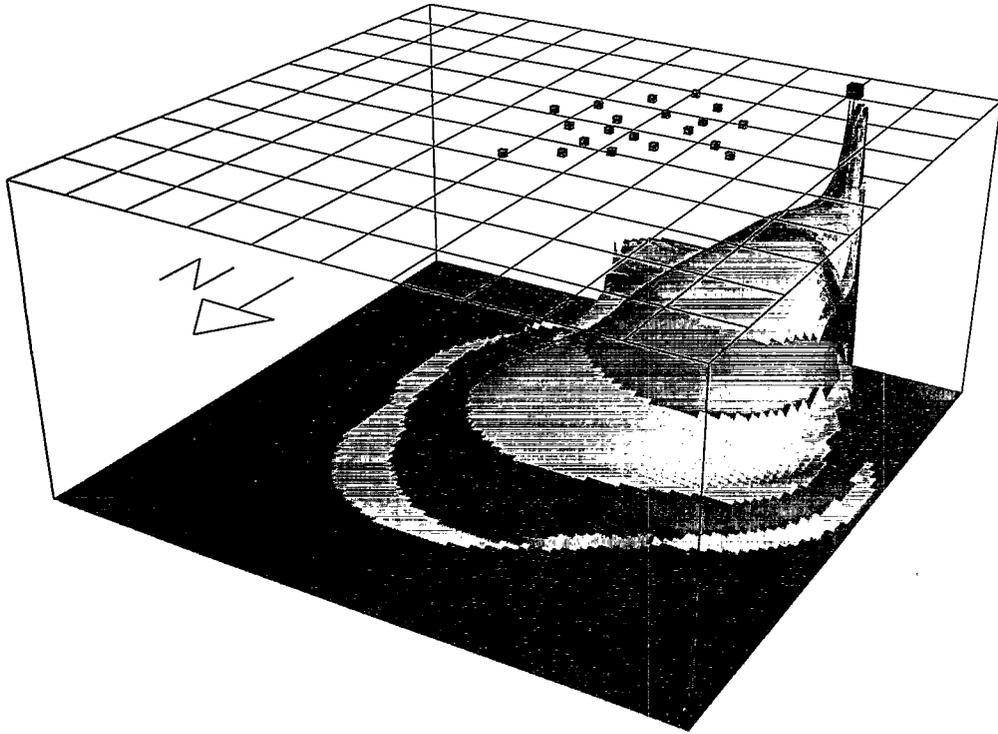


Figure 4.3 Estimate of soil contamination 7.0 *f* below the water table.

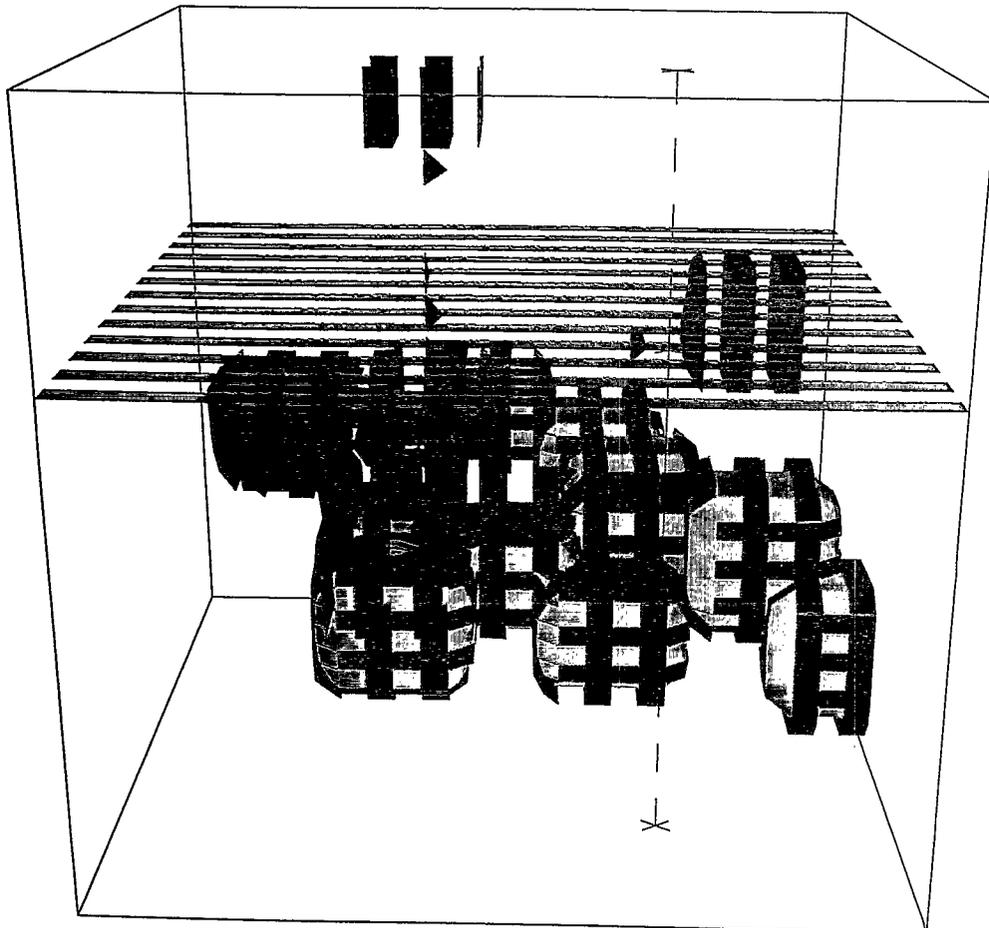


Figure 4.4 Estimate of soil contamination (BTEX) at Eglin AFB.

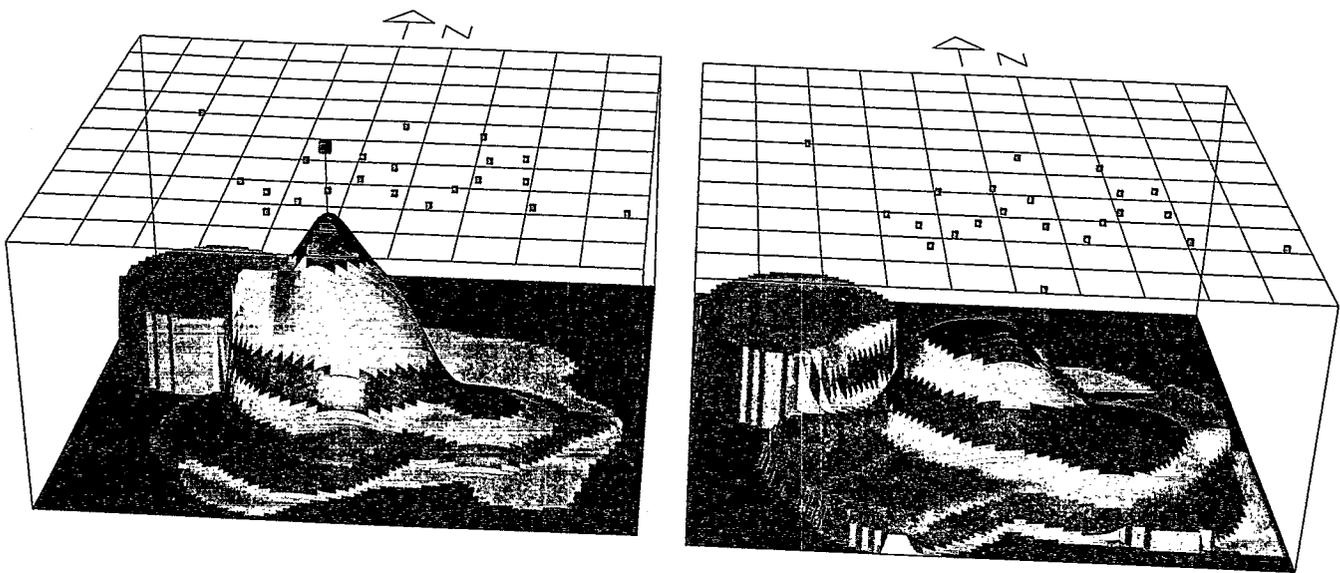


Figure 4.5: Estimates of ground-water contamination and absolute errors.

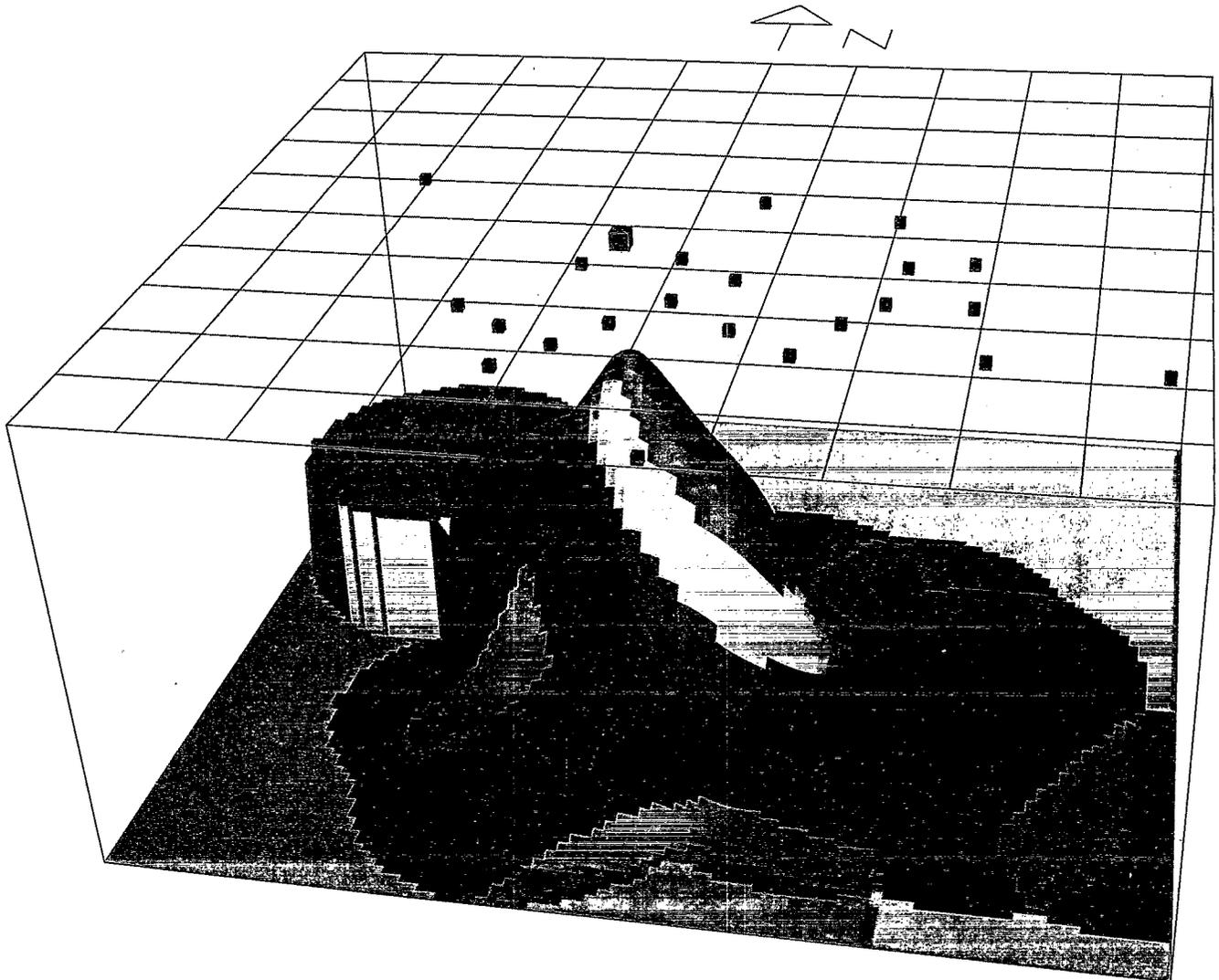


Figure 4.6 Estimate of ground-water contamination: contours represent magnitude of error.

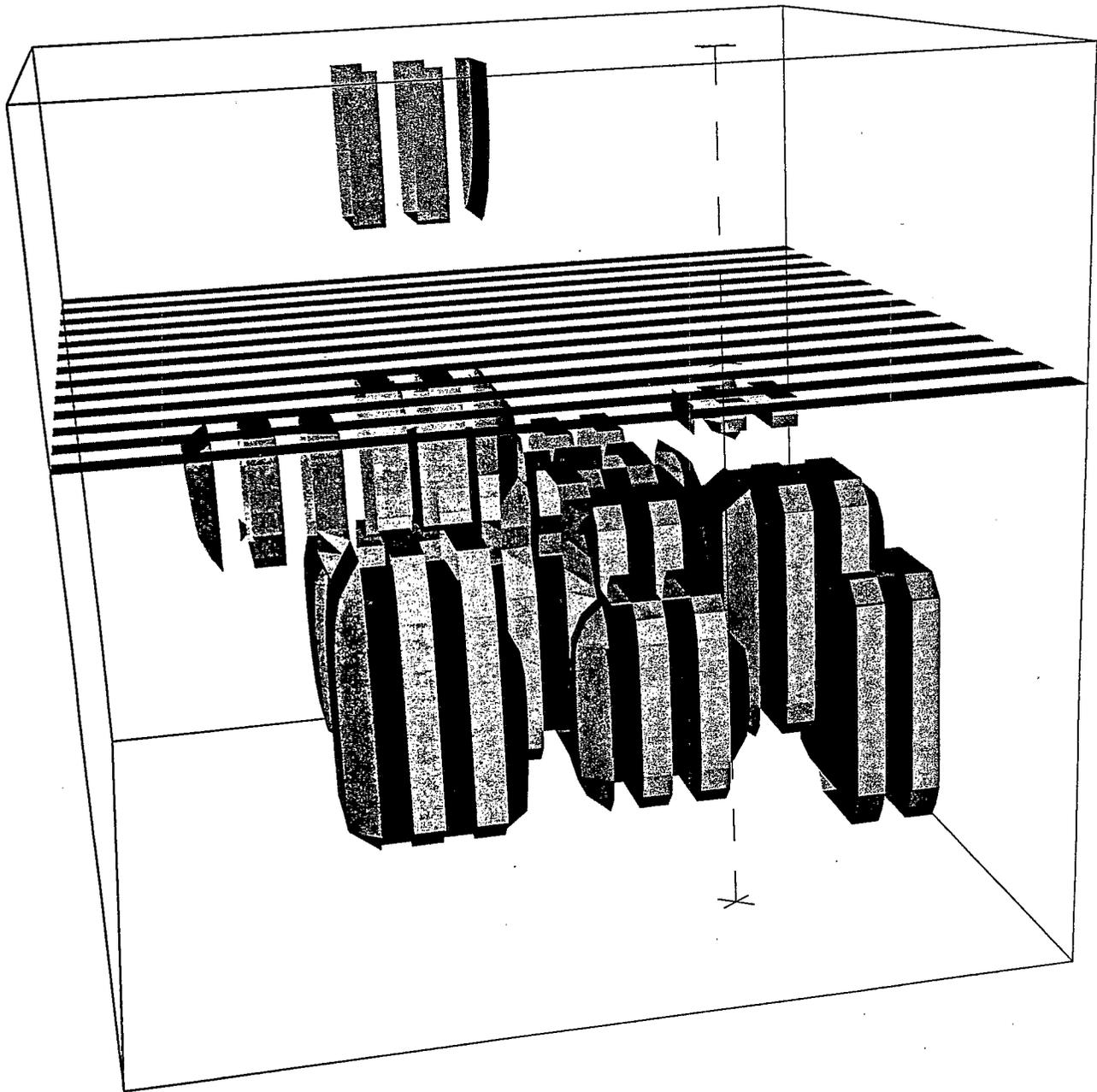


Figure 4.7 Smoothed absolute error estimate for Eglin AFB soil data.

Chapter 5

Estimation of Non-Linear Functionals of Random Processes for Environmental Problems

In analyzing environmental sampling data, it is often of interest to estimate some function of the data. For example, one may be interested in the maximum concentration attained within some region, the location of this maximum, the region for which the concentration exceeds some set value, or the total amount of contaminant present in a region. For example, government regulations on levels of ambient ozone typically involve exceedence of some threshold deemed unsafe for human beings at *any* location within a region (Cox, et al., 1995). In this case, one would wish to estimate the maximum concentration attained in the region of interest. In the case where one is attempting to clean up ground water or soil contamination, it is of interest to know the total amount of contaminant present in a region. The estimation of total contaminant involves estimating an integral over a region and is what will be addressed in this section.

In this chapter, we will model the Eglin AFB ground-water BTEX observations as a realization of a stochastic process using the methods described in §3.2. The goal, then, will be to estimate the distribution of the integral of the process over some set region. Now in the case where this process is Gaussian, estimation of this distribution is a solved problem. However, it is commonly the case that environmental data are *lognormal* or well approximated by a lognormal distribution. Such is the case for the Eglin AFB BTEX observations.

The approach taken here is to estimate the integral of the lognormal process by Monte Carlo simulation of the process conditional on the data. The "conditional simulation" referred to here is similar to that discussed by Englund and Heravi (Englund, et al., 1995) in reference to Deutsch and Journel (Deutsch, et al., 1993). That is, one fits a semivariogram model (Cressie, 1993) to the data, then simulates from this model at some locations of interest. The actual measurements are honored at measured locations, possibly with some error variation. Englund and Heravi discuss the simulation as being along a regular grid; here we will be discussing simulation at random locations.

5.1 Description of the Problem

As previously stated, estimation of the total amount of contaminant present in some region is equivalent to estimation of the stochastic integral $Y = \int_A X(s) ds$ where $\langle X(s) \rangle$ is some random process, based on some (possibly noisy) observations

$x(s_1), \dots, x(s_n)$ where $x(s_i) = X(s_i) + \varepsilon_i$ and $\varepsilon_i \stackrel{i.i.d.}{\sim} N(0, \sigma_\varepsilon^2)$. The definition of a stochastic integral is given in (Boeckenhauer, 1996). In particular, we are interested in a point estimate of Y and an interval estimate (i.e., prediction interval). For the point estimate of a general function of the process $g(X)$, assume initially squared error loss:

$$L(g(X), p(x; g(X))) = (g(X) - p(x; g(X)))^2 \quad (5.1)$$

where x is the vector of data and $g(\bullet)$ is some function of $\langle X \rangle$. Then the optimal predictor (i.e., the predictor $p(\bullet)$ which minimizes $E[L(\bullet)|x]$) is:

$$p^o(x; g(X)) = E[g(X)|x] \quad (5.2)$$

(Cressie, 1993). In particular, then, assuming squared error loss, the optimal predictor of the integral Y is

$$p^o(x; g(X)) = E[Y|x] = E\left[\int_A X(s) ds | x\right] \quad (5.3)$$

Now if $Z(s) = X(s)$ is a Gaussian process, then it is shown in (Boeckenhauer, 1996) that the conditional distribution of Y given Z is normal, and formulas for the mean and variance are given. While these formulas for the conditional mean and variance involve the nontrivial task of calculating integrals of the mean and covariance functions, it is nonetheless in theory a solved problem.

However, suppose that instead $\langle X(s) \rangle$ is a lognormal process. That is, $X(s) = e^{Z(s)} \forall s \in A$, where $\langle Z(s) \rangle$ is a Gaussian process. (Note, here we will actually be using base 10 logs, so we will instead define $X(s) = 10^{Z(s)}$, but this does not affect the argument.) Now we can estimate $E[\int_A Z(s) ds | z]$ as above for the logged process. However, since $\exp(\bullet)$ is a convex function, we have by Jensen's Inequality (Lehmann, 1983),

$$\begin{aligned} E\left[\int_A X(s) ds | x\right] &= E\left[\int_A \exp(Z(s)) ds | x\right] \\ &= \int_A (E[\exp(Z(s)) | x]) ds \\ &= \int_A (\exp(E[Z(s) | x])) ds \end{aligned} \quad (5.4)$$

provided $\text{var}(Z(s)|\mathbf{x}) > 0$, so we cannot simply use the conditional mean of the $\langle Z \rangle$ process to obtain the conditional mean of the $\langle X \rangle$ process. Furthermore, the distribution of the integral in this case will definitely *not* be normal, so some other method must be used to produce prediction intervals.

5.2 Using Monte Carlo to Estimate the Distribution of a Stochastic Integral

The integral which we estimate here is not merely the integral of a function, but rather the integral of a random process over a region, and thus is itself a random variable. We will still be able to use the method discussed in Section 3.3, but instead of evaluating the function at each location, we will simulate the value of the process at each location by generating from the model. We will actually simulate *several* realizations of the process, which will then give us an estimate of the *conditional distribution* of the integral, given the data.

The first step is to use our transformed observations (base 10 log) to produce a model for the process using the geostatistical methods in Section 3.2 and (Cressie, 1993). Secondly, we will generate uniform locations over the region of interest, \mathcal{A} , as discussed in Section 3.3. Variation is introduced here, as discussed in Section 3.3, because we are using observations of the process at only certain locations in \mathcal{A} to estimate the integral over the entire region \mathcal{A} . We must then calculate the covariance matrix and mean vector from the geostatistical model for these particular locations.

To simulate a realization of the random process, we first generate a multivariate normal process based on the mean and covariance obtained from our geostatistical modeling, then we exponentiate the simulated observations. From this realization, we may find the average as discussed in Section 3.3 to produce an estimate of the integral of *that realization*. That is, if we generated p locations $\mathbf{s}_{1,1}, \dots, \mathbf{s}_{1,p}$ uniformly in \mathcal{A} , then simulated values $z_1(\mathbf{s}_{1,1}), \dots, z_1(\mathbf{s}_{1,p})$ at these locations from the Geostatistical model, we are estimating the integral

$$\Phi_1 = \int_{\mathcal{A}} 10^{z_1(s)} ds \quad (5.5)$$

where $10^{z_1(s)}$, $\mathbf{s} \in \mathcal{A}$ denotes this realization. We then estimate the integral of the realization in the manner discussed in §3.3:

$$\hat{\Phi}_1 = \frac{|\mathcal{A}|}{p} \sum_{j=1}^p 10^{z_1(\mathbf{s}_{1,j})} \quad (5.6)$$

The variance of the integral estimate for the realization, conditional on the data and the realization, may be estimated by

$$\begin{aligned} \text{Var}(\hat{\Phi}_1) &= \text{Var} \left(\frac{|\mathcal{A}|}{p} \sum_{j=1}^p 10^{z_1(\mathbf{s}_{1,j})} \right) \\ &= \frac{|\mathcal{A}|^2 s^2}{p} \end{aligned} \quad (5.7)$$

as in (3.19). To estimate the variance of the integral of the process, notice that

$$\begin{aligned} \text{Var}[\hat{\Phi}|\mathbf{x}] &= \text{Var} \left[E[\hat{\Phi}|X(\cdot), \mathbf{x}] | \mathbf{x} \right] + E \left[\text{Var}[\hat{\Phi}|X(\cdot), \mathbf{x}] | \mathbf{x} \right] \\ &= \text{Var}[\Phi|\mathbf{x}] + E \left[\text{Var}[\hat{\Phi}|X(\cdot)] | \mathbf{x} \right] \end{aligned} \quad (5.8)$$

(Recall that \mathbf{x} is the vector of data.) An unbiased estimate of $E \left[\text{Var}[\hat{\Phi}|X(\cdot)] | \text{data} \right]$ is obtained from the sample mean of the

variances of the $\hat{\Phi}_i$, $i = 1, \dots, m$. Also, $\text{Var}[\hat{\Phi}|\mathbf{x}]$ may be estimated by the sample variance of the integral estimates from the realizations. Sampling from a distribution which is not uniform may decrease the variance of the estimate in some cases, however, it is the large variation between the integral estimates from different realizations which should be a cause of concern. This latter error can only be reduced by either (1) improving the model, or (2) gathering additional data.

The above steps are repeated to obtain a large number of realizations thereby reducing error introduced by Monte Carlo estimation. For each simulation i , $i = 1, \dots, m$, we:

1. Generate p locations $\mathbf{s}_{i,1}, \dots, \mathbf{s}_{i,p}$ uniformly in \mathcal{A} .
2. For these locations, calculate the covariance matrix and mean vector, conditional on the data, using the geostatistical model.

3. Generate multivariate normal data $z_1(\mathbf{s}_{i1}), \dots, z_1(\mathbf{s}_{ip})$ using this mean vector and covariance matrix, and exponentiate them (using the same base as for the logs we took of the data to produce the model).
4. Produce an estimate of the integral

$$\Phi_i = \int_A 10^{z_i(s)} ds \quad (5.9)$$

using the sample-mean Monte Carlo method, i.e.

$$\hat{\Phi}_i = \frac{|A|}{p} \sum_{j=1}^p 10^{z_i(\mathbf{s}_{ij})} \quad (5.10)$$

We may then get an estimate of the mean of the integral of the process

$$E[\Phi|x] = E\left[\int_A 10^{Z(s)} ds|x\right] \quad (5.11)$$

where x again denotes the vector of data, by, for example, taking the mean

$$\hat{E}[\Phi|x] = \frac{1}{m} \sum_{i=1}^m \hat{\Phi}_i \quad (5.12)$$

More importantly, we are able to estimate the conditional distribution of the integral and get prediction intervals using the quantiles of the $\hat{\Phi}_i$. We may also estimate the variance of the integral

$$\begin{aligned} Var[\Phi|x] &= Var[\hat{\Phi}|x] - E[Var[\hat{\Phi}|X(\bullet), x]|x] \\ &= \hat{Var} \hat{\Phi}_1, \dots, \hat{\Phi}_m - \frac{1}{m} \sum_{i=1}^m \hat{Var}(\hat{\Phi}_i) \end{aligned} \quad (5.13)$$

as discussed above.

5.3 Application

5.3.1 Discussion of Data

A QQ-plot of the log of the ground-water BTEX data from Eglin AFB, Figure 5.1, indicates that lognormality is a reasonable assumption in this instance. For further reference, we also plot the log of the data at the sampled spatial locations (Figure 5.2).

We now discuss the covariance modeling and integral estimation for the Eglin AFB site using the ground-water data introduced in Section 2.1. Recall that these data appear to be lognormal. In Section 5.3.1, we will estimate a variogram from the log 10 data to model the covariance structure, as discussed in Section 3.2. Section 5.3.1 contains details regarding integral estimation for this data, and thus estimation of the total amount of contaminant.

Variogram Estimation

Before performing spatial estimation on any data, we must first model the covariance structure of the data. The empirical semivariogram for the logged Eglin AFB ground-water data is shown in Figure 5.3. While this semivariogram does, in general, seem to increase with distance as expected, it nonetheless is rather undesirable. In particular, there is high variability, which (a) will make it difficult to estimate well with a variogram model and (b) will cause any estimates made from such a model to have large error variance.

It should be noted that the above variogram was done assuming that the data was *isotropic*, that is, that the covariance of the process at two locations depends only on the distance between these locations and not the direction. In fact, this does not really appear to be the case here, as Figure 5.2 seems to indicate that the plume extends along the northwest-southeast direction, due to the fact that the "large" observations seem to fall about this line. So it is possible here that we can get a better variogram, and thus a better fit, by first transforming the coordinate axes through a rotation and then scaling one of the axes. This allows us to take (this particular type of) anisotropic data and model it using a standard one-dimensional, isotropic variogram model. Using the Splus spatial module function *anisotropy.plot*, we are able to try various rotations and scalings of the coordinate axes in an attempt to produce a more appropriate variogram. Examples of these empirical variograms, along with loess smooth lines, are shown in Figures 5.4 and 5.5. Note that a number of these are obviously bad choices, as they do not even have γ increase with distance. We are looking for something with the points "well-clustered" about an *increasing* line. We concluded the best

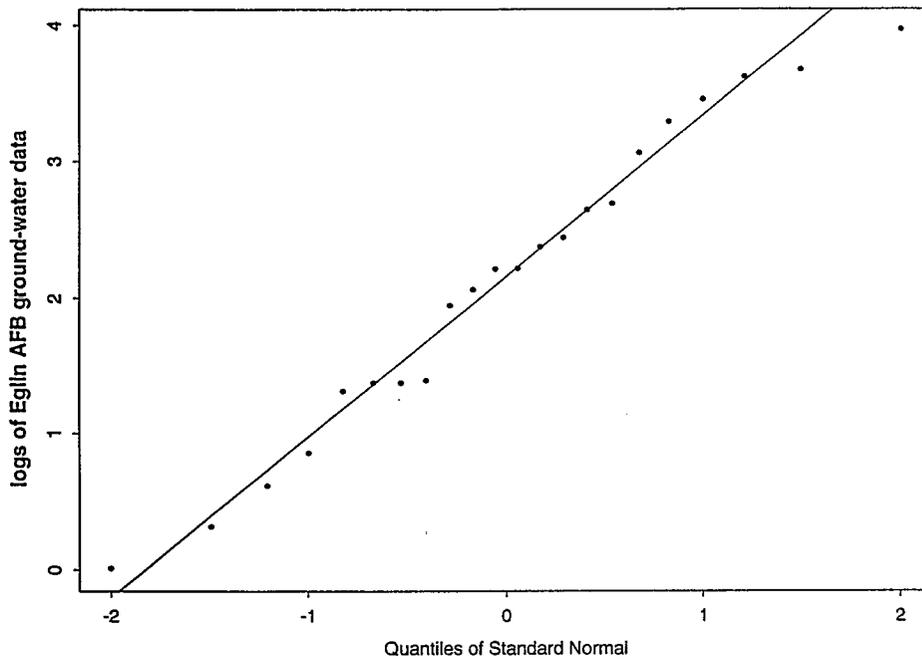


Figure 5.1 QQ-plot of logs of Eglin AFB ground-water data.

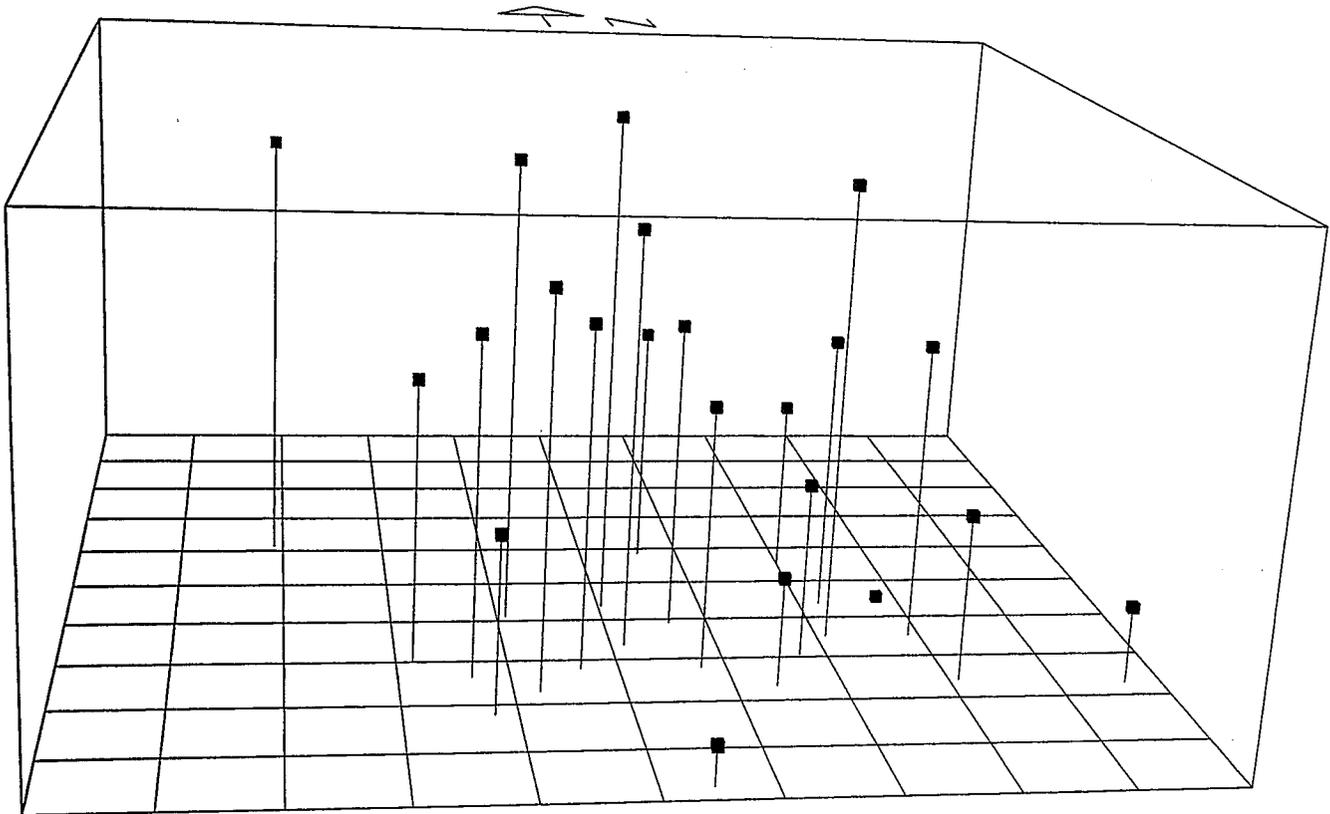


Figure 5.2 Logs of Eglin AFB ground-water data points.

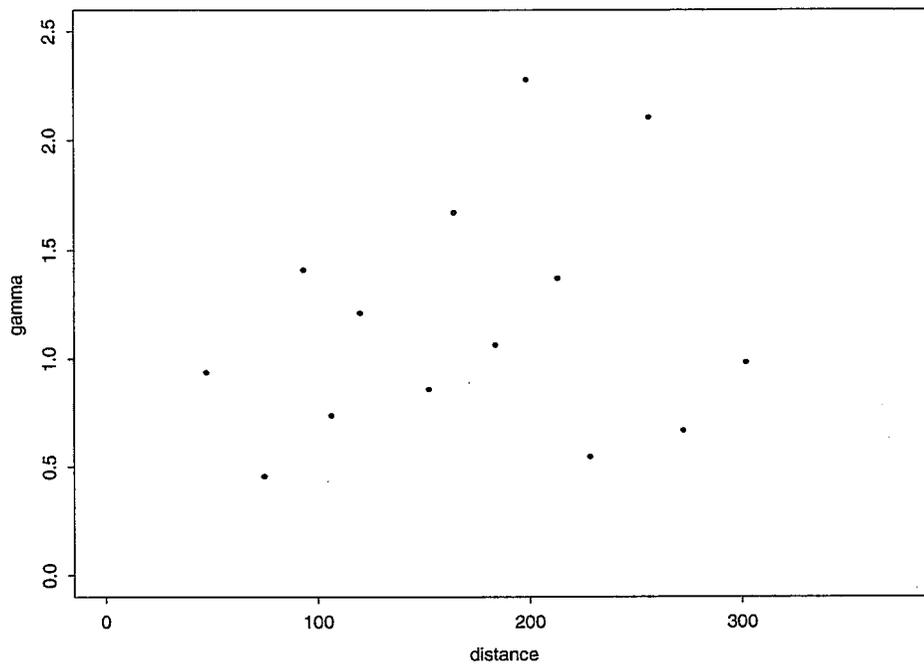


Figure 5.3 Empirical semivariogram of logged Eglin AFB ground-water data.

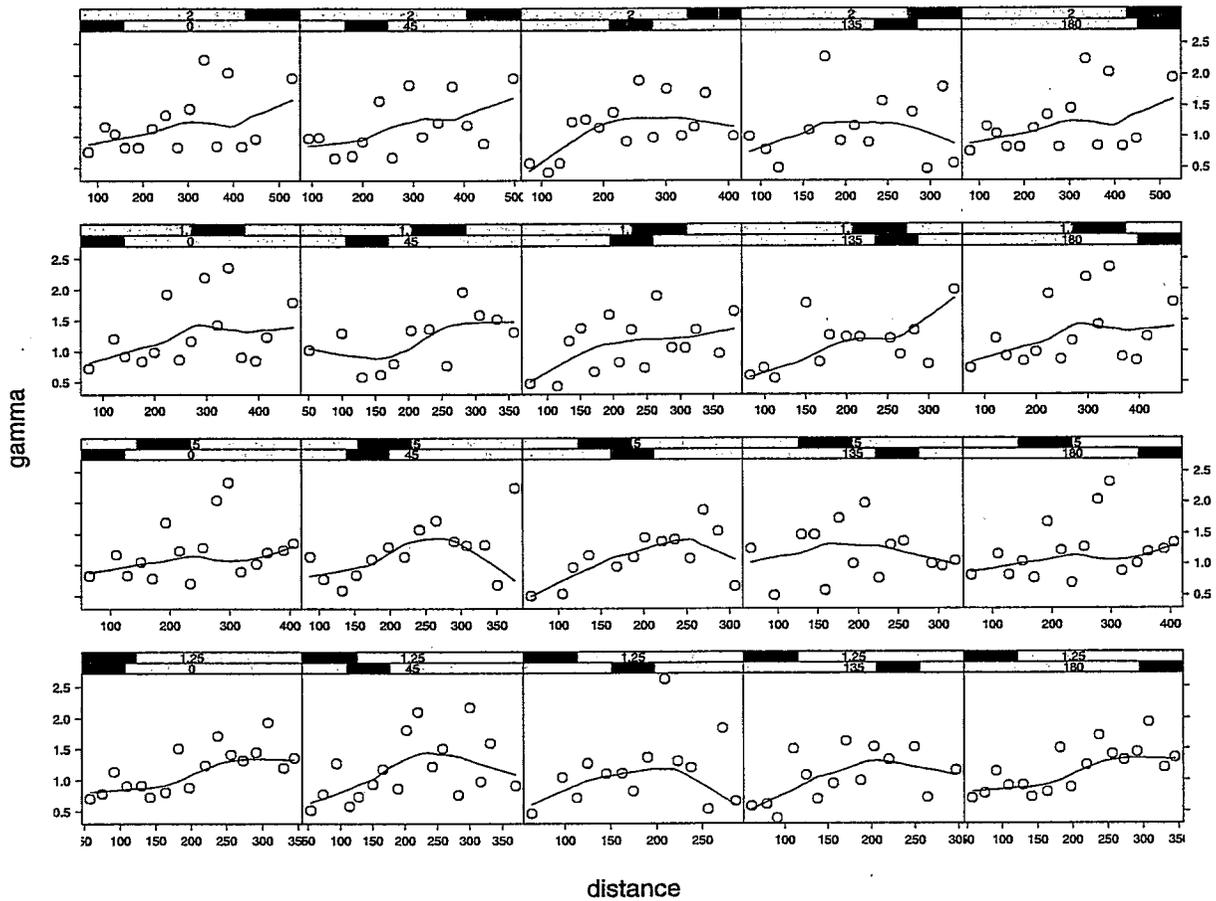


Figure 5.4 Empirical semivariograms with rotation angles from 0° on the left to 180° on the right and ratios from 1:25 at the bottom to 2 at the top.

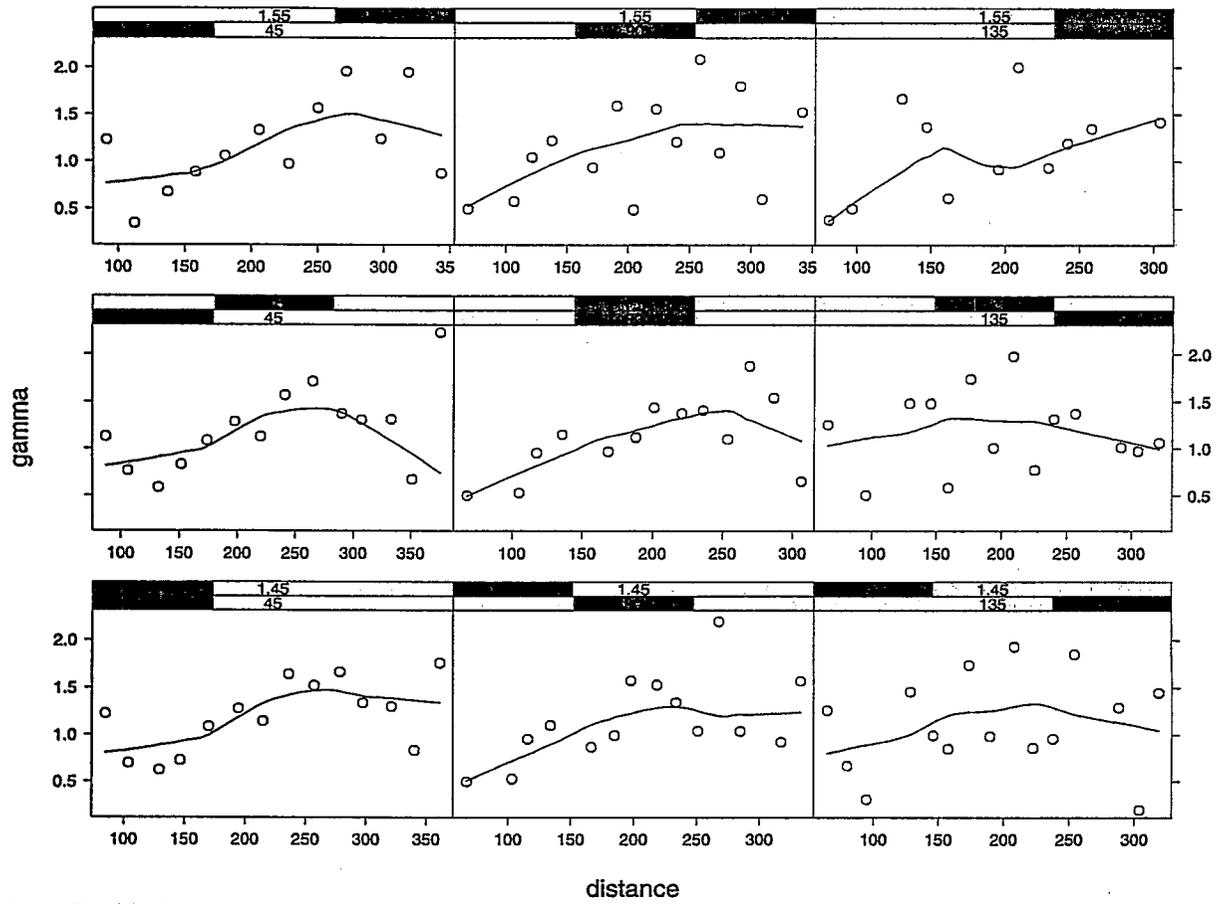


Figure 5.5 Empirical semivariograms with rotation angles from 45° on the left to 135° on the right and ratios from 1:45 at the bottom to 1:55 at the top.

option was a rotation angle of 45° and an axis ratio of 1.45. That is, for the i^{th} data point at location $(x[i], y[i])$, we multiply the location by the matrix \mathbf{B} where

$$\begin{aligned} \mathbf{B} &= \begin{pmatrix} \cos^2(45) + 1.45 \sin^2(45) & (1 - 1.45) \sin(45) \cos(45) \\ (1 - 1.45) \sin(45) \cos(45) & \sin^2(45) + 1.45 \cos^2(45) \end{pmatrix} \\ &= \begin{pmatrix} 1.225 & -0.225 \\ -0.225 & 1.225 \end{pmatrix} \end{aligned} \quad (5.14)$$

as in (3.9). This empirical semivariogram, along with two different semivariogram models, is shown in Figure 5.6. The spherical semivariogram, with the formula

$$\gamma(h) = \begin{cases} 0 & h = 0 \\ c_0 + c_s \left(1.5 * (h/a_s) - .5 * (h/a_s)^3 \right) & 0 < h \leq a_s \\ c_0 + c_s & h \geq a_s \end{cases}$$

(Cressie, 1993) was produced with nugget $c_0 = 0$, (partial) sill $c_s = 1.51$, and range $a_s = 325$. This model appears as the dashed line in Figure 5.6. The rational quadratic semivariogram has formula

$$\gamma(h) = \begin{cases} 0 & h = 0 \\ c_0 + \frac{c_r * h^2}{1 + h^2/a_r} & h > 0 \end{cases} \quad (5.15)$$

(Cressie, 1993) and was calculated with nugget $c_0 = 0.19$, $c_r = 1/14580$, and $a_r = 24750$. This variogram model appears as the solid line in the figure. In both cases, h refers to the *distance* (in the transformed space) between the data points. The two variogram models appear very similar for most distances in Figure 5.6, but are different in the tails. While either one would likely work reasonably well, we chose to use the rational quadratic model as it produces a plausible variogram which has a positive nugget effect (and a nugget effect of zero would assume that there was no measurement error, which is certainly an unreasonable assumption). The kriged surface estimate produced using this variogram model is shown in Figure 5.7 and the standard error surface is depicted in Figure 5.8. The kriging here was done using the spatial module of S-PLUS (MathSoft, 1995), which estimated the constant mean to be $\mu = 1.55344$ on the \log_{10} scale.

Details of the Integral Estimation

Programs to estimate the integral for the Eglin AFB ground-water data were written in the C programming language and appear in (Boeckenhauer, 1996). The method is essentially that described in Section 5.2. That is, for each of M realizations of the process, we simulate values at N locations within the region, where N and M are contained in the file constants.h. The main program, contained in runsim.c, first uses the data locations to produce Σ_{11} , the covariance matrix for these locations. As discussed above, the locations are first corrected for geometric anisotropy by multiplying each pair of locations $\mathbf{t}_i = (x, y)$ by the matrix \mathbf{B} in (5.14). Then the distance (in transformed space) between each pair of points is calculated, followed by the covariance between the locations using the rational quadratic model selected above. Specifically, notice that since we are assuming the data are of the form

$$z(\mathbf{t}_i) = Z(\mathbf{t}_i) + \varepsilon_i \quad i = 1, \dots, 22 \quad (5.16)$$

where ε_i and ε_j are independent for $i \neq j$ and $Z(\mathbf{t})$ is independent of ε_i for every i and j , we have

$$\begin{aligned} \text{Cov}(z(\mathbf{t}_i), z(\mathbf{t}_j)) &= \text{Cov}(Z(\mathbf{t}_i) + \varepsilon_i, Z(\mathbf{t}_j) + \varepsilon_j) \\ &= \text{Cov}(Z(\mathbf{t}_i), Z(\mathbf{t}_j)) + \text{Cov}(Z(\mathbf{t}_i), \varepsilon_j) + \text{Cov}(\varepsilon_i, Z(\mathbf{t}_j)) + \text{Cov}(\varepsilon_i, \varepsilon_j) \\ &= \text{Cov}(Z(\mathbf{t}_i), Z(\mathbf{t}_j)) + \text{Cov}(\varepsilon_i, \varepsilon_j) \\ &= \begin{cases} \text{Cov}(Z(\mathbf{t}_i), Z(\mathbf{t}_j)) & \text{if } i \neq j \\ \text{Var}(Z(\mathbf{t}_i)) + \text{Var}(\varepsilon_i) & \text{if } i = j \end{cases} \end{aligned} \quad (5.17)$$

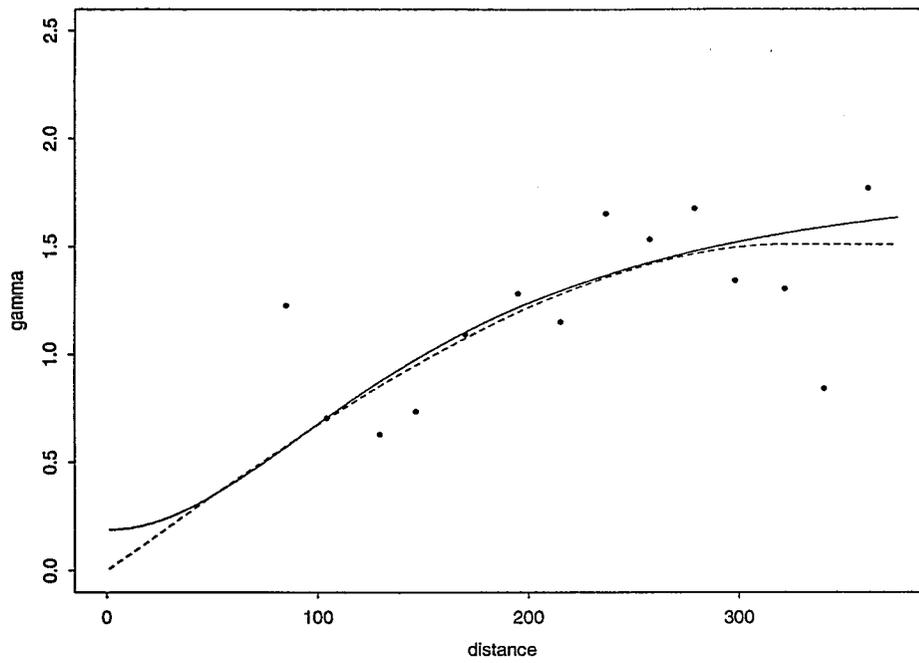


Figure 5.6 Semivariogram of logged Eglin AFB ground-water data with transformed locations.

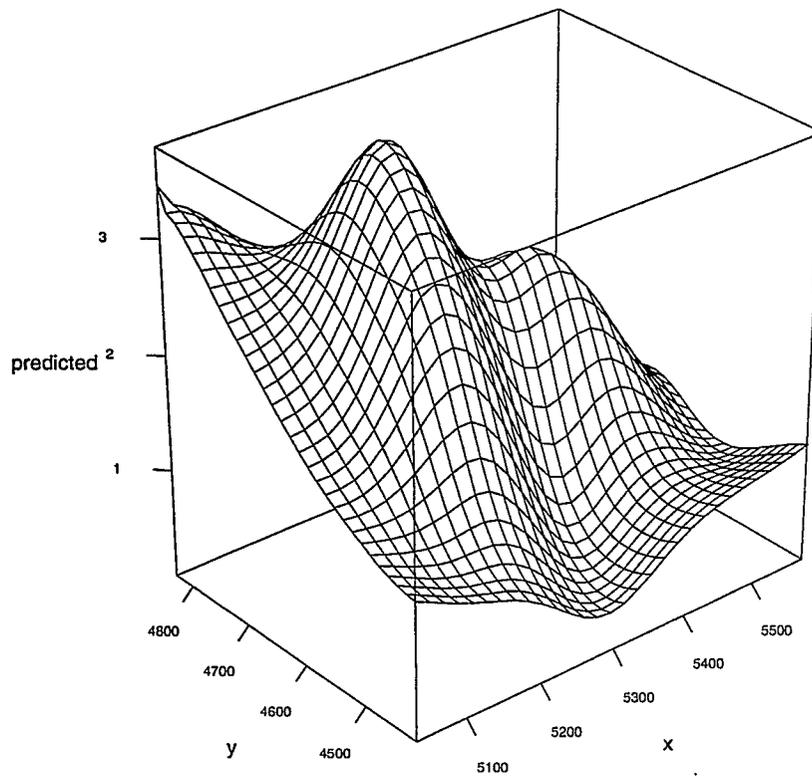


Figure 5.7 Kriged surface estimate of logged Eglin AFB ground-water data using rational quadratic variogram details of the integral estimation.

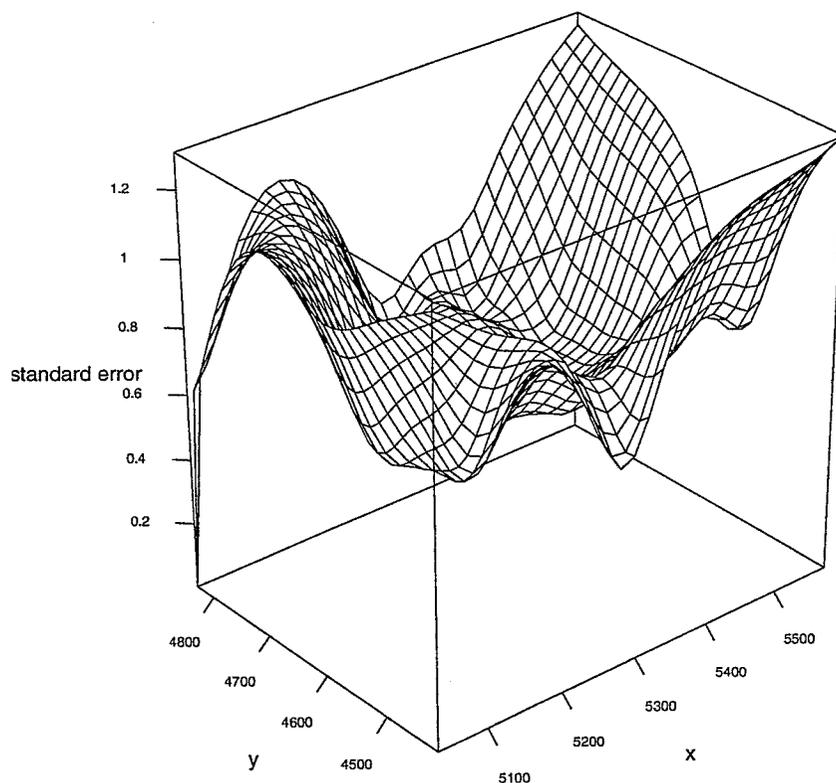


Figure 5.8 Standard errors for kriged surface estimate of logged Eglin AFB ground-water data using a rational quadratic variogram.

Recall that we are using the rational quadratic model. So letting $h = |\mathbf{t}_i - \mathbf{t}_j|$ (i.e., h is the distance between locations i and j after transforming locations), we have:

$$\text{Cov}(Z(\mathbf{t}_i), Z(\mathbf{t}_j)) = C(h) = c_r a_r - \frac{c_r * h^2}{1 + h^2/a_r} \quad (5.18)$$

and

$$\text{Var}(\varepsilon_i) = c_0 \quad (5.19)$$

(i.e., the nugget effect). Thus the i, j^{th} element of Σ_{11} is given by:

$$\begin{aligned} (\Sigma_{11})_{i,j} &= \text{Cov}(z(\mathbf{t}_i), z(\mathbf{t}_j)) \\ &= \begin{cases} c_r a_r - \frac{c_r h^2}{1 + h^2/a_r} & = \frac{c_r a_r}{1 + h^2/a_r} & \text{for } i \neq j \\ c_0 + c_r a_r - \frac{c_r * h^2}{1 + h^2/a_r} & = c_0 + c_r a & \text{for } i = j \end{cases} \end{aligned} \quad (5.20)$$

Recall that $c_0 = 0.19$, $c_r = 1/14580$, and $a_r = 24750$ were the parameters used for our model in the previous section.

The function *sim*, contained in *sim.c*, is then called M times, each time producing a sample from a realization of the process of size N . For each simulation, we first generate N locations uniformly over the region using the function *loc* in *loc.c*, first generating all of the x values, then all of the y s. Then the function *cov*, contained in *cov.c* is used to calculate the conditional mean vector and covariance matrix for these generated locations given the data. Using standard multivariate normal theory (Mardia, et al., 1979), we first calculate the unconditional matrix for the generated locations using the rational quadratic model. Letting s_1, \dots, s_N be the simulated sampling locations, this yields the $N \times N$ matrix Σ_{22} where the i, j^{th} element is given by

$$\begin{aligned}
 (\Sigma_{22})_{i,j} &= \text{Cov}(z(s_i), z(s_j)) \\
 &= \text{Cov}(Z(s_i), Z(s_j)) \\
 &= C(|(s_i - s_j)\mathbf{B}|) \\
 &= c_r a_r - \frac{c_r h^2}{1 + h^2/a_r} \\
 &= \frac{c_r a^2}{1 + h^2/a_r}
 \end{aligned} \tag{5.21}$$

where h is the distance between the locations after transformation; i.e., $h = |s_i \mathbf{B} - s_j \mathbf{B}| = |(s_i - s_j)\mathbf{B}|$. Similarly, we calculate the $N \times N$ cross-covariance matrix Σ_{21} with the i, j^{th} element given by:

$$\begin{aligned}
 (\Sigma_{21})_{i,j} &= \text{Cov}(z(s_i), z(t_j)) \\
 &= \text{Cov}(Z(s_i), Z(t_j) + \epsilon_j) \\
 &= \text{Cov}(Z(s_i), Z(t_j)) + \text{Cov}(Z(s_i), \epsilon_j) \\
 &= C(|(s_i - t_j)\mathbf{B}|) \\
 &= c_r a_r - \frac{c_r h^2}{1 + h^2/a_r} \\
 &= \frac{c_r a^2}{1 + h^2/a_r}
 \end{aligned} \tag{5.22}$$

with h in this case being $h = |s_i \mathbf{B} - t_j \mathbf{B}| = |(s_i - t_j)\mathbf{B}|$. We then can find the conditional covariance matrix

$$\Sigma = \Sigma_{22} - \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{21}^T \tag{5.23}$$

and the conditional mean vector

$$\mu = \mu \mathbf{1}_N + \Sigma_{21} \Sigma_{11}^{-1} (\mathbf{Z} - \mu \mathbf{1}_n) \tag{5.24}$$

where $\mathbf{1}_N$ ($\mathbf{1}_n$) is a vector of 1s of length N (n), and μ is the constant mean as estimated by the kriging (1.55344) and \mathbf{Z} is the vector of \log_{10} observations. Calculation of $\Sigma_{11}^{-1} \Sigma_{21}^T$ was accomplished with the use of the LAPACK function *dpsv* (Anderson, et al., 1992).

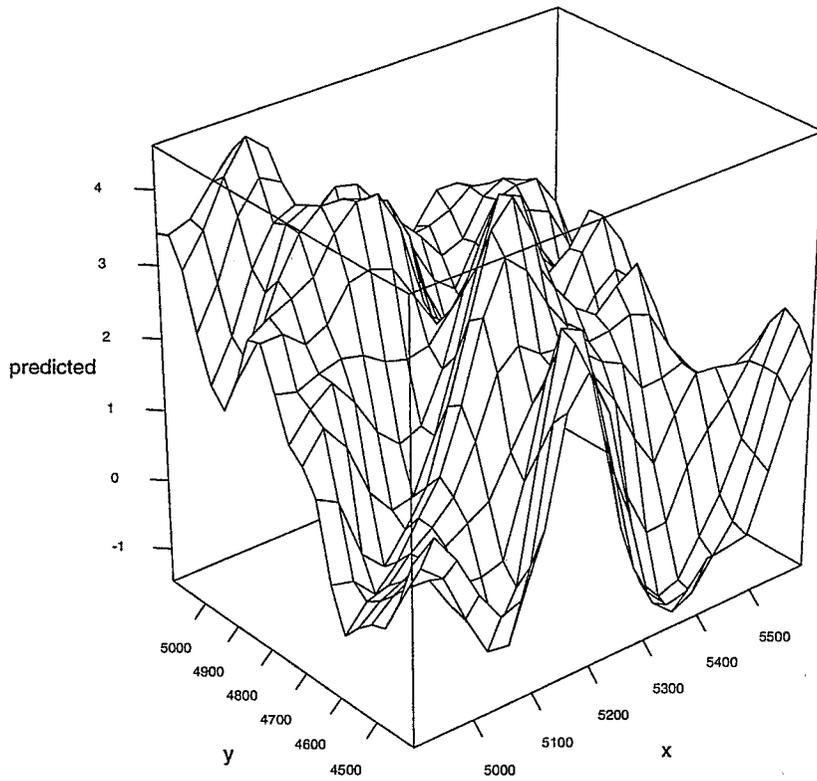


Figure 5.9 Surface of a grid simulation.

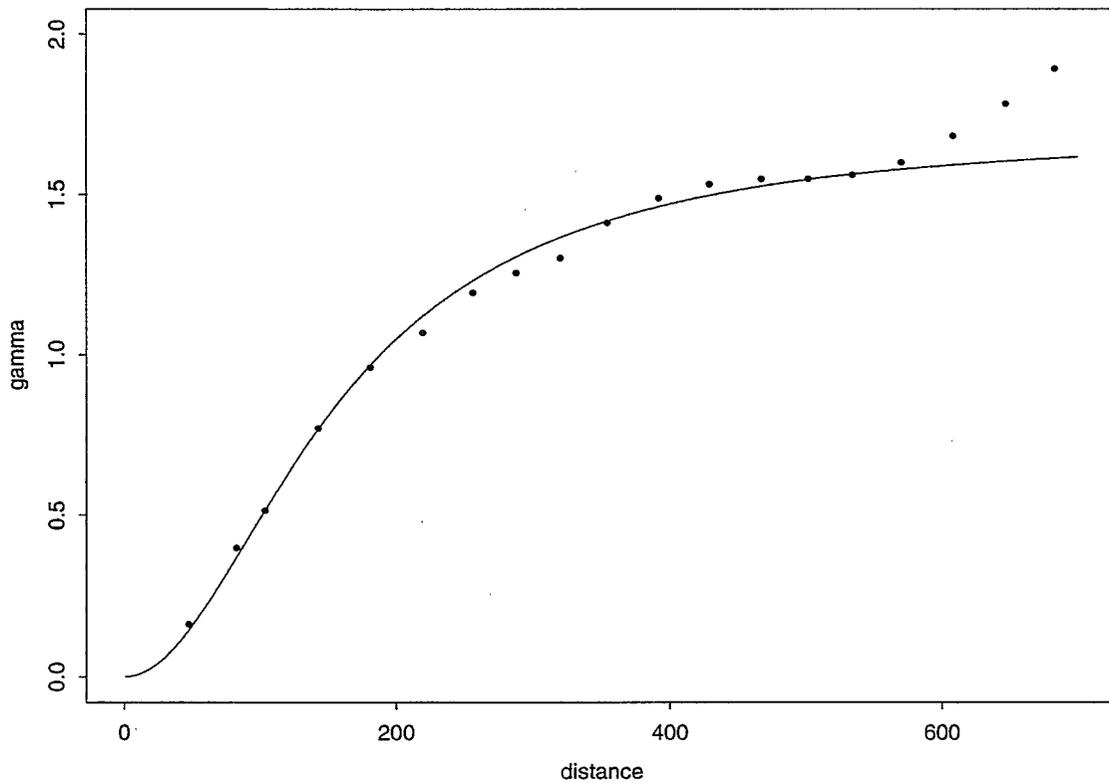


Figure 5.10 Semivariogram calculated from a grid simulation.

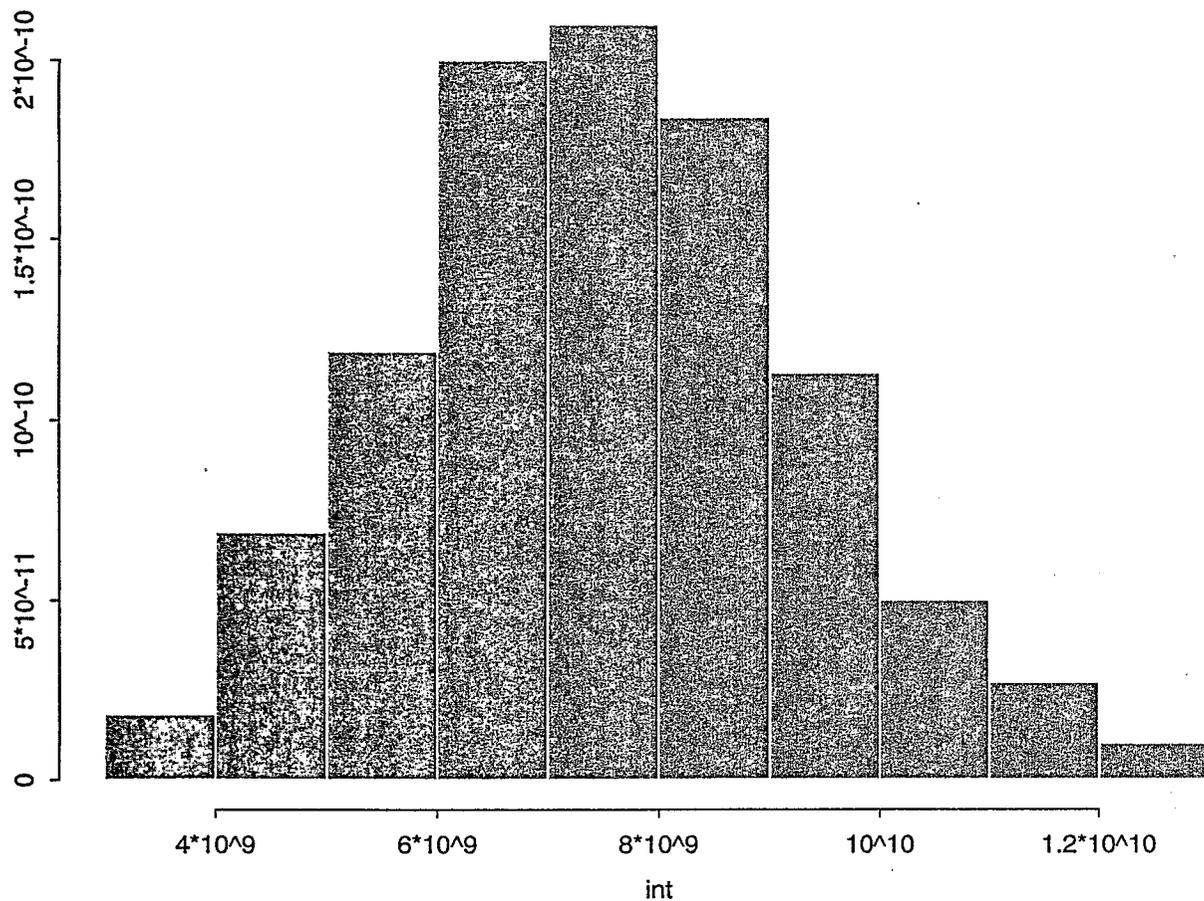


Figure 5.11 Histogram of integral estimates from 1000 samples of size 500: one realization.

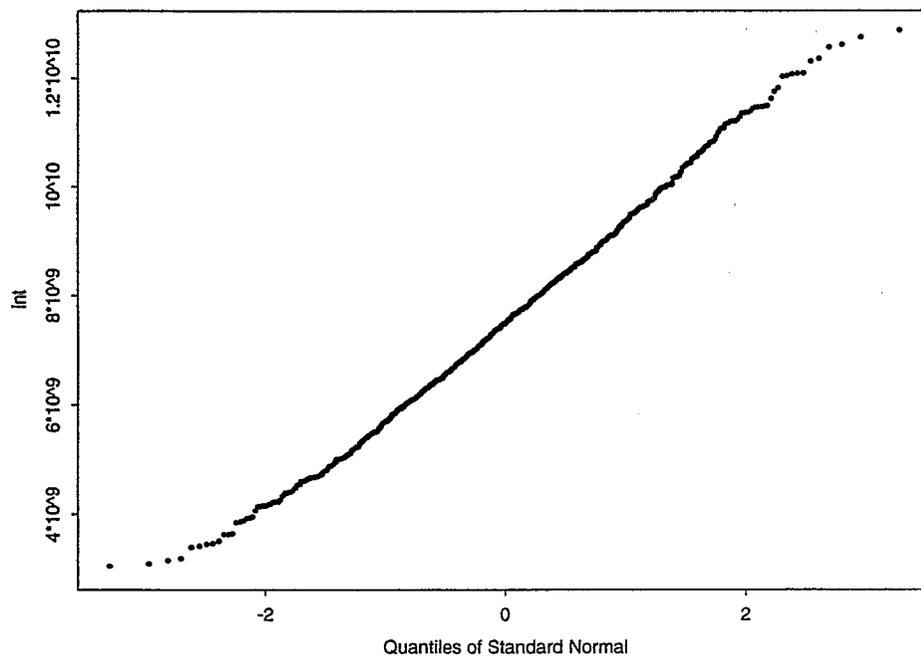


Figure 5.12 QQ-plot of integral estimates from 1000 samples of size 500: one realization.

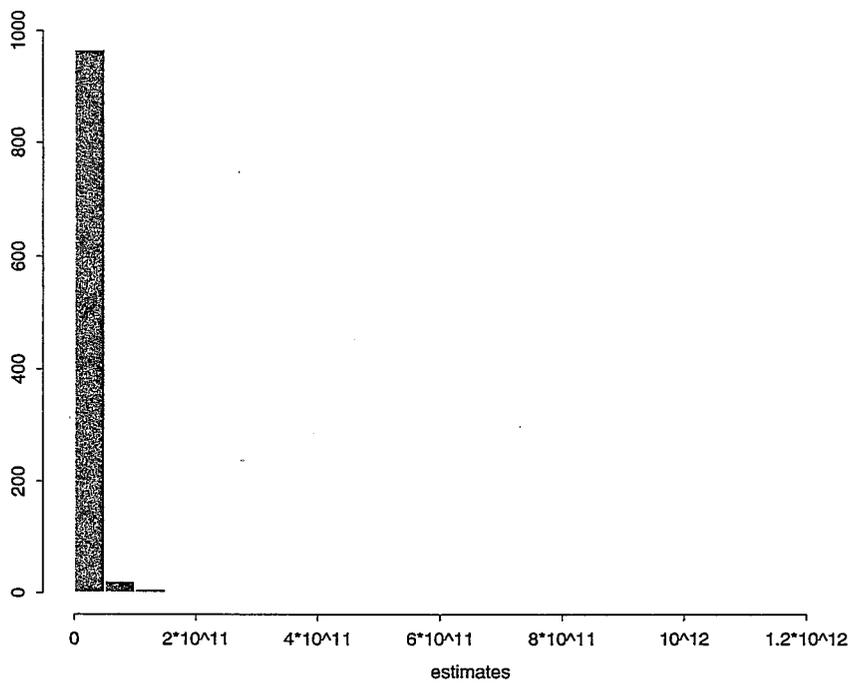


Figure 5.13 Histogram of integral estimates from 1000 samples of size 500: different realizations.

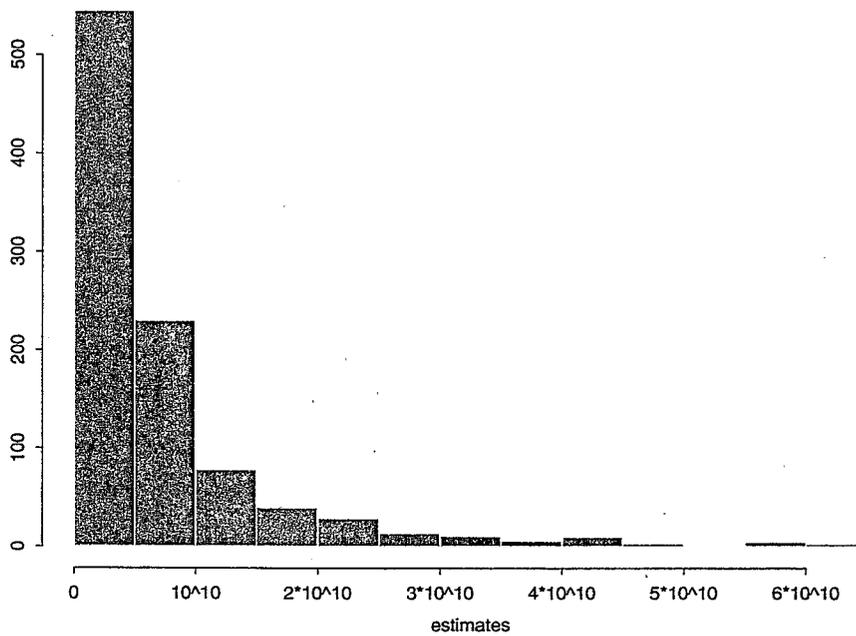


Figure 5.14 Histogram of lower 97.5% integral estimates from 1000 samples of size 500: different realizations.

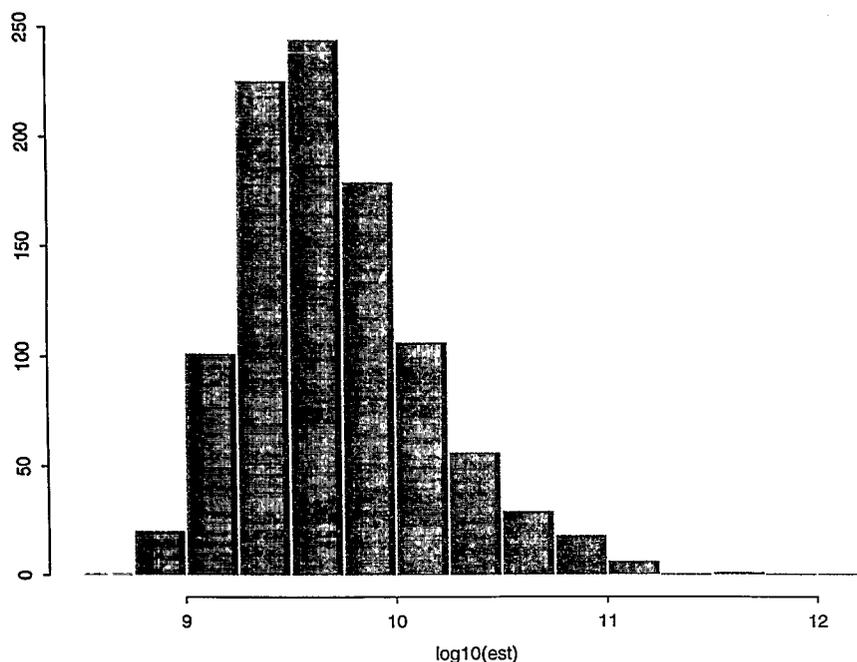


Figure 5.15 Histogram of logged integral estimates from 1000 samples of size 500: different realizations.

The function *sim* then calls the function *multnorm*, located in *multnorm.c*, which uses μ and Σ to generate multivariate normal random variables from $N_N(\mu, \Sigma)$. We first generate an N -vector \mathbf{Y} of standard normal random variates, i.e. $\mathbf{Y} \sim N(0, \mathbf{I}_N)$ where $\mathbf{0}_N$ is a p -vector of zeroes and \mathbf{I}_N is the $p \times p$ identity matrix. This is done using the function *gauss* (Reilly, 1995) in *boxmu1.c*. The lower triangular Cholesky decomposition matrix \mathbf{L} is calculated by using the LAPACK function *dpptrf* (Anderson, et al., 1992). (Recall that \mathbf{L} is the unique lower triangular matrix such that $\Sigma = \mathbf{L}\mathbf{L}^T$). Finally, we calculate $\mathbf{X} = \mathbf{L}\mathbf{Y} + \mu$. Since *dpptrf* calculates \mathbf{L} in packed format (Anderson, et al., 1992), it was necessary to write code to do the matrix multiplication. This was done using as few operations as possible.

Now predictions of the process at the simulated locations are obtained by letting $Z(\mathbf{s}_j) = 10^{x(\mathbf{s}_j)} = 10^{X_j}$. The integral of the realization is then estimated by

$$\hat{\Phi} = \frac{k^2 |A|}{N} \sum_{j=1}^N Z(\mathbf{s}_j) \quad (5.25)$$

as discussed in §3.3. Note that in this case A is rectangular, so $|A|$ is easy to calculate. The constant $k=3.048$ refers to the number of dm/ft , since the (x,y) locations are in ft and the concentration predictions $Z(\mathbf{s}_j)$ are in $\mu g/L$. Since this region is only 2-dimensional, the integral estimate here is in $\mu g/dm$, and would need to be multiplied by a depth in dm to give an estimate of the total amount of contaminant. Also, the variance of the integral estimate is calculated in the manner discussed in §3.3.

However, instead of calculating $\hat{\text{var}}(\hat{\Phi}_i) = (k^4 |A|^2 / N^2) \hat{\text{var}}\left(\sum_{j=1}^N 10^{z_i(\mathbf{s}_{i,j})}\right)$, it is calculated as

$$\hat{\text{var}}(\hat{\Phi}_i) = (1/N^2) \hat{\text{var}}\left(\sum_{j=1}^N W_{i,j}\right) = (1/N) \mathbf{s}_{W_i}^2 \quad (5.26)$$

where $W_{i,j} = k^2 |A| 10^{z_i(\mathbf{s}_{i,j})}$ and $\mathbf{s}_{W_i}^2$ is the sample variance of $W_{i,1}, \dots, W_{i,N}$. This amounts to the same thing but is easier to program, as we can then use the integral estimate in calculating the sample variance.

This entire procedure is performed M times and the resulting integral estimates from the realizations are then used to estimate the conditional distribution of the integral of the process, given the data. A point estimate of the integral may be found by, for example, taking the mean of the integral estimates for the realizations. Approximate $100(1-\alpha)\%$ prediction intervals may be found by using the $\alpha/2$ and $1-\alpha/2$ quantiles of the simulated integral estimates.

5.3.2 Results

As a quick assessment that our computer code is simulating the desired process, we generate, from the assumed model, a single realization over a 20x20 grid which encompasses the region, where the x -values range from 4900 to 5600 and the y -values range from 4400 to 5100. A perspective plot of this single realization is given in Figure 5.9. The realization behaves as one might expect given the conditional mean shown in Figure 5.7. Also, the empirical variogram of this realization compares well to the rational quadratic variogram model used to generate the data (see Figure 5.10).

Recall that the estimate of the integral for a realization, as discussed in §3.3, is given by

$$\hat{\Phi} = \frac{|A|}{N} \sum_{j=1}^N q(\mathbf{s}_j) \quad (5.27)$$

where the $q(\mathbf{s}_j)$, $j=1, \dots, N$ are the values of realization at locations $\mathbf{s}_1, \dots, \mathbf{s}_N$. Noting that this is in fact a sample mean of the $|A|q(\mathbf{s}_j)$, $j=1, \dots, N$, we have by the central limit theorem that, for a single realization, the estimate of the integral should have a normal distribution as $N \rightarrow \infty$. We would like to check the integral estimates produced from samples of a *single realization* to see that this is in fact the case.

Ideally, we would like to be able to take a large number of samples from a single realization of size P , where the samples are sufficiently sized for the asymptotics to “kick in” (say $N=500$ or 1000). However, since we are simulating the realization, we must simulate all of the values of the realization which we wish to sample together initially. If there are P such values of the realization, this means that we must not only calculate a $P \times P$ covariance matrix, but must then calculate the Cholesky decomposition of this matrix. As P gets large, near singularities (i.e., singularities within machine precision) in the conditional covariance matrix Σ cause the Cholesky decomposition routine to fail. The largest value of P for which the code could be successfully run with any consistency was 2000, which does not allow for a great number of independent samples of size 500, to say the least.

In lieu of independent samples we rely on dependent samples; i.e., samples which share some of the same realization values. A single realization of size 2000 was simulated and subsamples of size 500 were obtained from the 2000. The subsampling was performed with replacement. So each sample is then a sample from this realization taken at 500 independent uniform locations over the region. From each of these samples, an integral estimate was calculated using the integral estimate (5.25). Figure 5.11 shows a histogram of the integral estimates taken from 1000 such samples. The histogram appears to be approximately normal. Figure 5.12 contains a qq-plot of the 1,000 integral estimates. The qq-plot is very close to a straight line, although a bit off in the tails. Again, this indicates that these integral estimates are approximately normally distributed. Also, the integral estimate produced by the entire realization was approximately 7.548×10^9 , which is also very close to the center of the histogram and the median of the integral estimates from the samples. Thus, the distribution of integral estimates for samples from a single realization appears to be fairly normal, as it should be.

Finally, to actually estimate the distribution of the integral, we generated samples of 500 from each of 1000 different realizations. Figure 5.13 shows a histogram of the 1000 different integral estimates. This histogram is obviously *very* skewed, to the extent that we cannot see any of the detail in the lower part of the histogram, where most of the values reside. Figure 5.14 shows a histogram of the lower 97.5% of these estimates and Figure 5.15 shows a histogram of the \log_{10} estimates. These allow us to see more detail in the lower part of the histogram. Note that the units for the estimates are $\mu\text{g}/\text{dm}$, and they would have to be multiplied by a measurement of depth in dm to provide an estimate of total contaminant for a *three*-dimensional region. Tables 5.1 and 5.2 contain summary statistics about the integral estimates for the realizations. We can see the effect of the skewness in these summary statistics. For example, the value of the sample mean is more than *twice* the value of the sample median. Furthermore, the values of the $\alpha\%$ trimmed means *rapidly* approach the value of the median as α increases.

Table 5.1 Statistics of Integral Estimates for 1000 Realizations

minimum	0.025 quantile	median	0.975 quantile	maximum
5.604×10^8	1.034×10^9	4.527×10^9	6.354×10^{10}	1.252×10^{12}

Table 5.2 Means of Integral Estimates for 1000 Realizations

mean	5% trimmed mean	10% trimmed mean	20% trimmed mean
1.204×10^{10}	7.776×10^9	6.849×10^9	5.946×10^9

Recall that we said in Section 5.1 that the conditional mean (i.e., the mean calculated above) was an optimal estimate of the integral under squared error loss. Now either the median or any of the means could be used as a point estimate of the integral of the process. In particular, in the case of absolute error loss

$$L(g(X), p(x; g(X))) = |g(X) - p(x; g(X))| \quad (5.28)$$

the median is actually optimal. However, due to the high skewness and the large difference between the median and the mean, we would do well to exercise caution in our choice. More investigation is necessary to determine which of these is more representative of the truth, or if some other statistic would be better, or if what is "better" depends on the particular application.

It is important to reiterate here that even though the distribution of integral estimates from samples from *one* realization is quite normal, the distribution of the integral of the process is not even close to normal. However, this is not surprising as these are two entirely different distributions. The first is the distribution of estimates for a realization with variation coming only from the "sampling error", i.e. the error induced by estimating a value of the integral for a region with only a finite number of points. The second involves this sampling error, along with the actual variation of the process.

As the distribution of the integral is not normal, we obviously cannot use typical normal prediction intervals. We may, however, use quantiles of the distribution to get estimated prediction intervals for the integral of the process. For example, for a 95% prediction interval, we may use the values in Table 5.1 to get an interval of $(1.034 \times 10^9 ; 6.354 \times 10^{10})$. Note, however, that this interval still involves the aforementioned sampling error.

The variances for the integral estimates for the realizations, $\hat{\Phi}_i$, were estimated as discussed in Section 5.2. The estimated standard deviations ranged from 5.645×10^7 to 4.602×10^{11} . However, for the lower 97.5% of the integral estimates, the largest estimated standard deviation was 1.708×10^{10} , nearly 30 times smaller than the overall maximum. This would lead us to suspect that the highest integral estimates for realizations come about due to one or two very high simulated values in that realization, thus increasing the variance of the sample from the realization tremendously. Further investigation is necessary to determine if this is in fact the case.

The variance of the integral is estimated here as discussed in Section 5.2. That is

$$\text{Var}[\Phi|\mathbf{x}] = \text{Var}[\hat{\Phi}|\mathbf{x}] - E[\text{Var}[\hat{\Phi}|X(\cdot)]|\mathbf{x}] \quad (5.29)$$

where $\text{Var}[\hat{\Phi}|\mathbf{x}]$ may be estimated by the sample variance of the integral estimates from the realizations and an unbiased estimate of $E[\text{Var}[\hat{\Phi}|X(\cdot)]|\mathbf{data}]$ is obtained by taking the sample mean of the variances of the $\hat{\Phi}_i$, calculated from the 1000 realizations as discussed above. In this example, this yields

$$\text{Var}[\Phi|\mathbf{x}] = 2.423 \times 10^{21} - 2.796 \times 10^{20} \cong 2.143 \times 10^{21} \quad (5.30)$$

So the estimated standard deviation of the integral is $\sqrt{\text{Var}[\Phi|\mathbf{x}]} = 4.629 \times 10^{24}$. It is of concern here that this value is actually *larger* than the estimated mean of the integral of 1.204×10^{10} . This is caused by the large variation between the integral estimates for the different realizations, and the high skewness of the distribution.

Chapter 6

Phoenix, AZ: Visualization with a Time Component

In this chapter, we use methods of kriging and related spatial estimation (Cressie, 1993) to study various concentration plumes at a site near Phoenix, Arizona. Since we have data from several years for this site, we are able to incorporate time into our analysis. In all cases, the plots were intended to represent a yearly average, so *all* of the data from each year was used. In cases where there was more than one measurement for a particular location in a year, the average of these values was used. In Section 6.1, we do an exploratory visualization of contaminant levels, along with accuracy assessments in the form of prediction standard errors. In Section 6.2, we present portions of animations of contaminants together, including a method for animation of two possibly related contaminants.

6.1 Exploratory Visualization

Figures 6.1, 6.3, 6.5, and 6.7 show "prediction" surfaces for TCE and DCE concentrations for two selected years. The predictions were done using the log of the data, so these surfaces are on a log scale. Figures 6.2, 6.4, 6.6, and 6.8 show the corresponding standard error surfaces. The x and y coordinates are the same for all of the plots in this section and the next, with the z coordinates varying slightly. The legends for the z coordinates are given in Figures 6.9 and 6.10 for the prediction surfaces and error surfaces, respectively.

Figures 6.9 and 6.10 indicate the color codes for different levels of concentrations and standard errors. (Note that the legend for the prediction surfaces in Figure 6.9 refers to the level of the original data, rather than the log of the data.) Predicted values tend to be most accurate in the neighborhood of wells where the data were taken, which explains the downward spikes in the standard error surfaces. (That is, each small downward spike represents an observation well location.)

One sees, when comparing TCE concentration maps (Figures 6.1 and 6.5 for the years 1991 and 1992, respectively) with the corresponding DCE concentrations (Figures 6.3 and 6.7), that both substances are highest in the northeast portion of the region, and the TCE plume drops off more quickly than the DCE plume. This suggests scavenging of TCE to create DCE over time as the plume is transported from northeast to southwest. Thus, a map of the ratio of concentration of DCE to TCE should show a large increase moving down the plume, but the sum of the two concentrations might be relatively constant, assuming the region is relatively "closed." Of course, conclusions drawn from such displays would have to be tempered by the accuracy of the estimated quantities.

6.2 Animation

6.2.1 Trichloroethylene and Dichloroethylene (TCE and DCE)

Since it is suspected that the TCE and DCE plumes are somehow interrelated, it is desirable to plot the two together in such a way as to make the relationship (if it exists) more visible. With this in mind, animation of the TCE and DCE data is accomplished by combining the estimated concentration plots for each on the same plot. This allows the two substances to be easily animated together in time, which in turn should facilitate our attempts to see relationships between the levels of the two substances through space and time. The animation has been performed using the measured data from the years 1985 to 1993, as discussed in Section 2.2.

Spatial estimation, via kriging, was then performed on the *logs* (base 10) of the *yearly* data. (See Appendix B for a brief discussion of the spatial modeling and an explanation of the problems there encountered.) For the animation, interpolations were done in between the years (5 time slices between each pair of years), allowing a smoother progression which aids greatly in seeing general trends in the data.

Examples of the plots used in the animation are shown in Figures 6.11, 6.12, 6.13, and 6.14, representing the years 1986, 1988, 1991, and 1993, respectively. The TCE surface is the upper one in all of the plots and the DCE the lower. The size of the region is approximately 18000 ft^2 in the E-W direction and 8300 ft^2 in the N-S direction. All plots are shown on the \log_{10} scale; e.g., the purple regions which are labeled as 1 to 2 on the scale are regions where the estimated contaminant level is between 10 and 100 $\mu\text{g/L}$.

These plots all confirm our assumption that the values of the contaminants are generally highest in the Northeast region, where the source is located. These plots help to point out some general features in the data, as well as introducing some new questions. In particular, Figure 6.13 would seem to indicate that there is a ridge of high values of contaminant along a line from East-Northeast to West-Southwest, along with some low values next to this region of high values. Investigation into the site properties yielded the information that the ground-water flow is generally from E-NE to W-SW, so it would appear that the contaminant levels are highest along a direct line from the source in the direction of ground-water flow, perhaps indicating very slow dispersion of the contaminants through other means. The 1986 plot, Figure 6.11, is representative of the earlier years in that data were only taken in an area relatively close to the source. In later years, gradually points were added farther to the west of the source. (There were none added to the east, presumably since it was unexpected that the contaminant would spread greatly in a direction counter to the direction of ground-water flow.) By 1993, both contaminants appear to have dissipated greatly, and many of the mild variations seen are likely due to measurement error. Figure 6.12, from 1988, shows lower values of

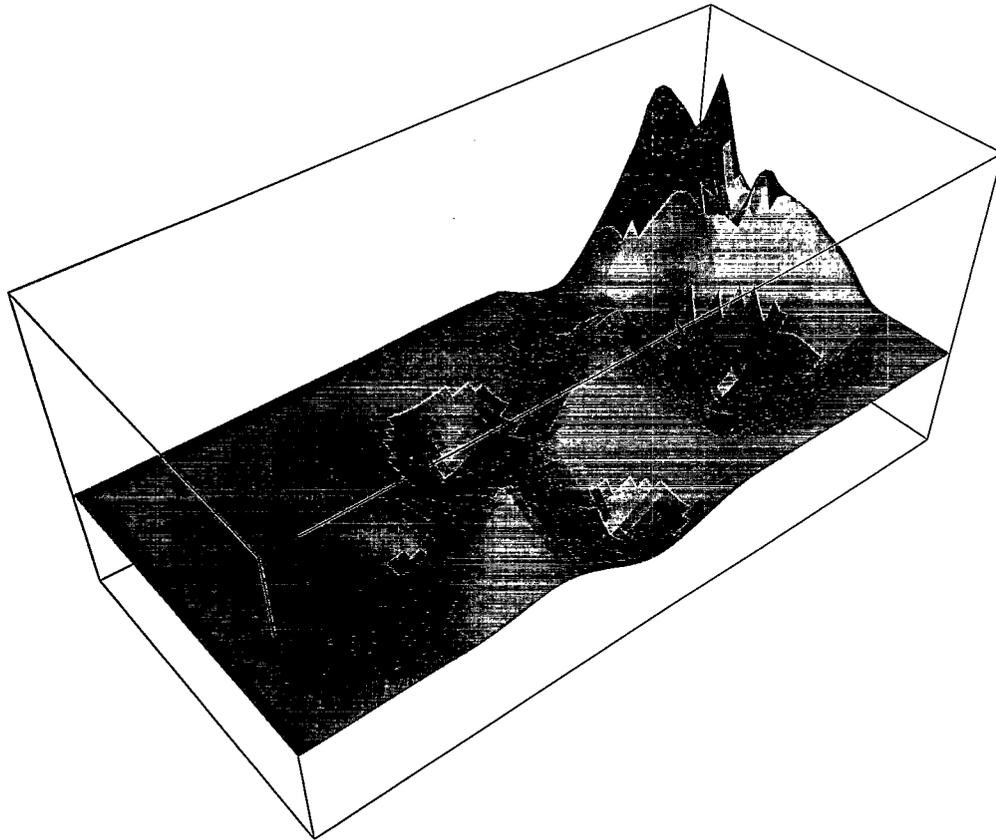


Figure 6.1 TCE prediction surface for 1991. Orientation: depth-axis: 892,600 to 896,800; width-axis: 478,000 to 484,000; vertical-axis: 0 to 2.25.

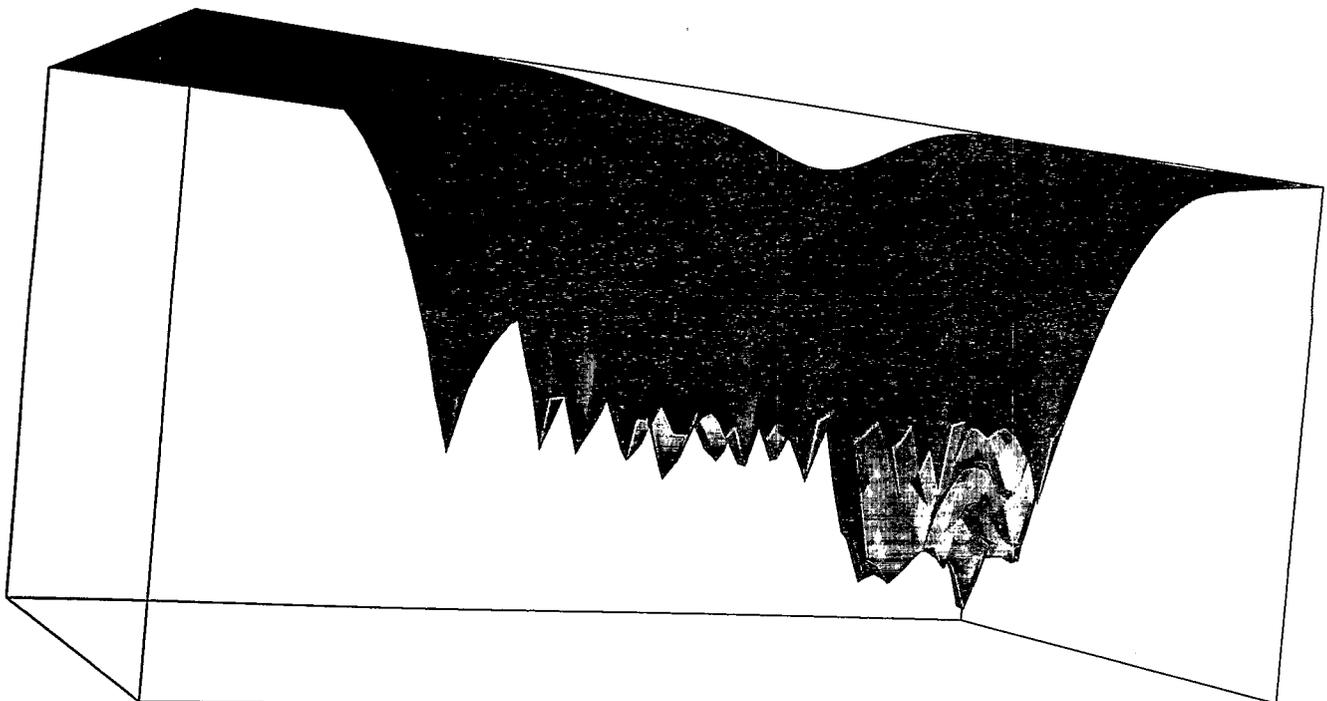


Figure 6.2 TCE standard errors of prediction for 1991.

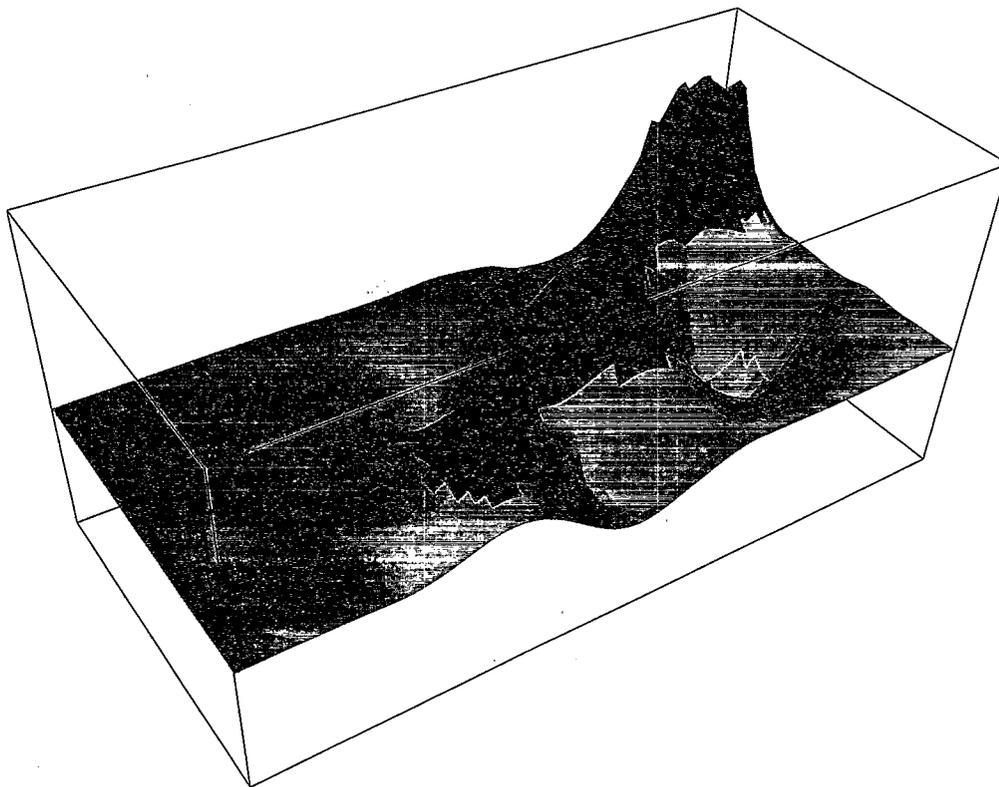


Figure 6.3 DCE prediction surface for 1991.

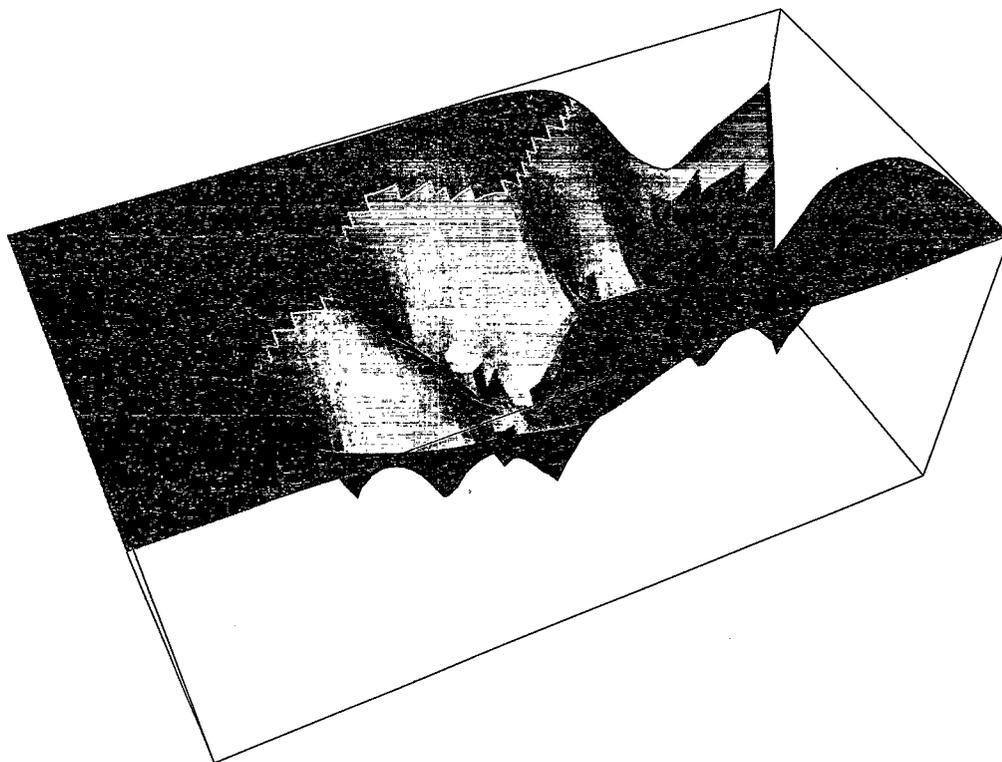


Figure 6.4 DCE standard errors of prediction for 1991.

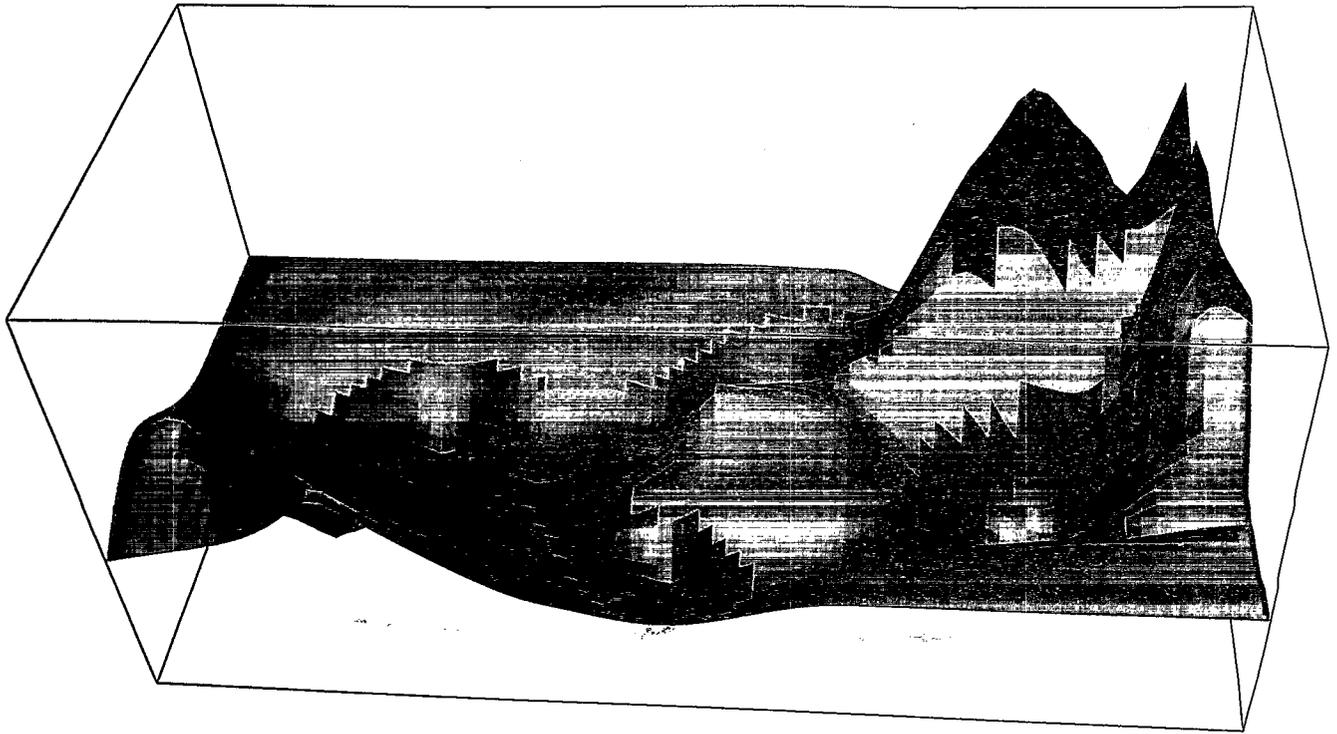


Figure 6.5 TCE prediction surface for 1992.

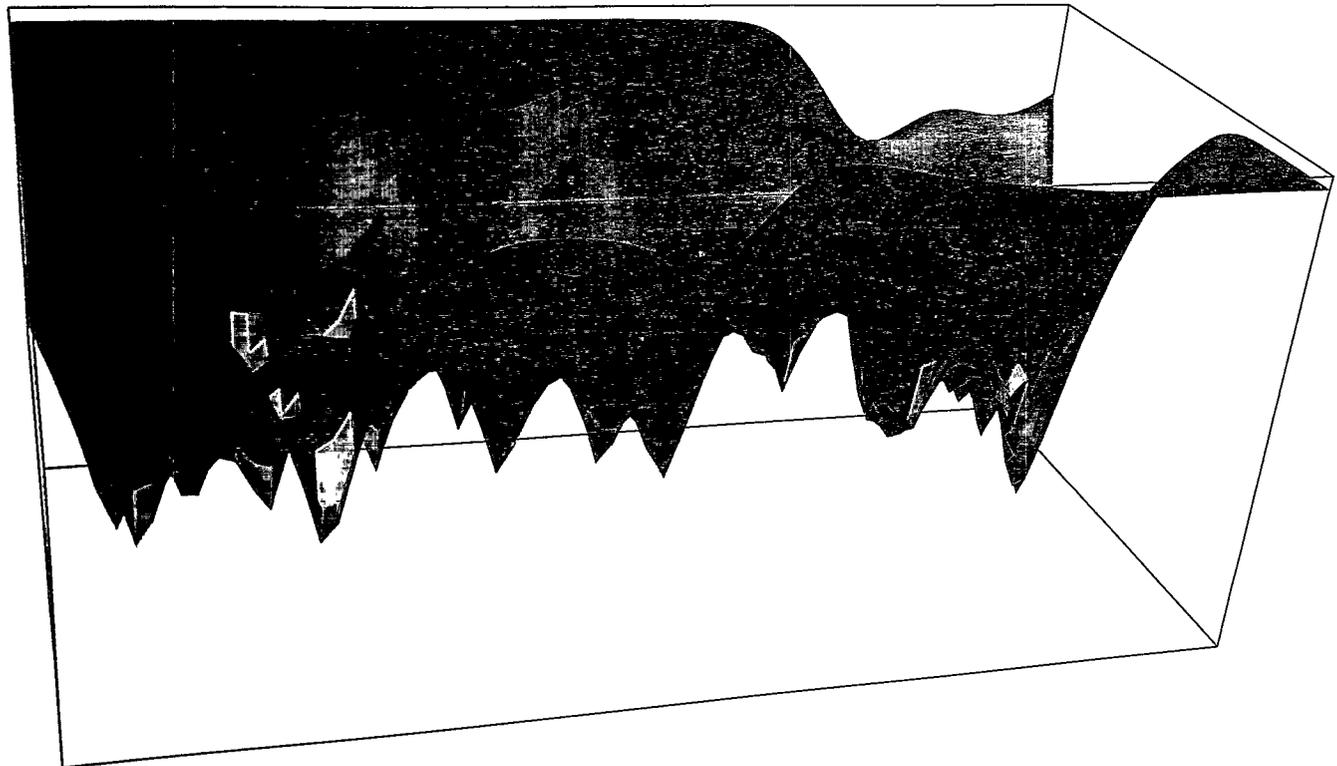


Figure 6.6 TCE standard errors of prediction for 1992.

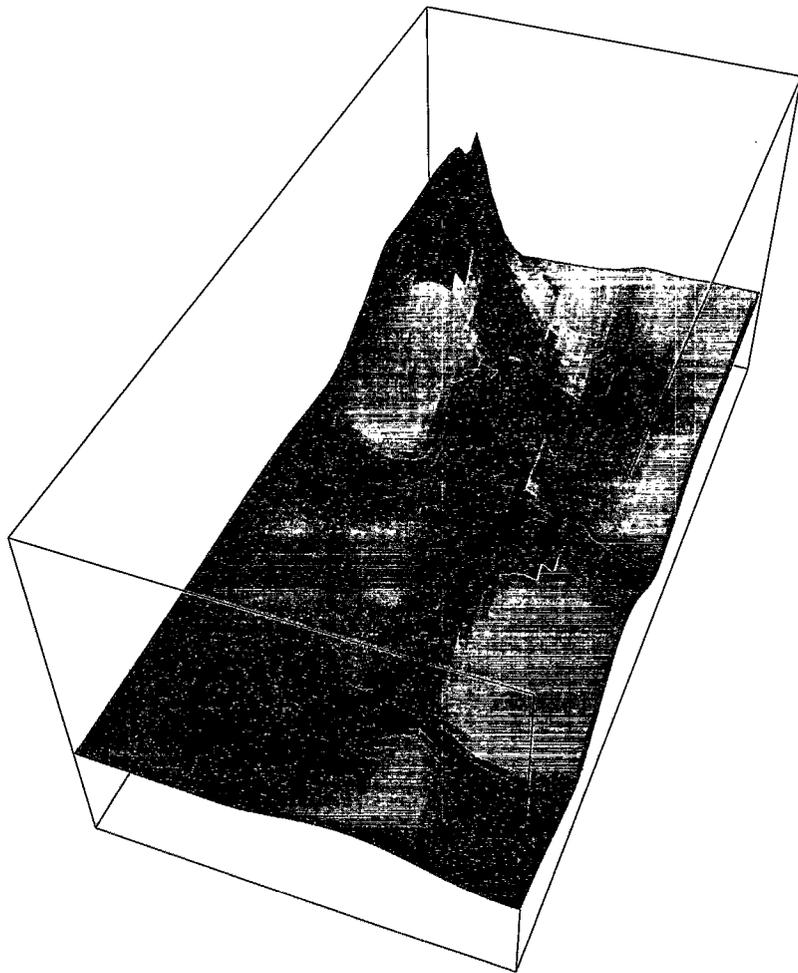


Figure 6.7 DCE prediction surface for 1992.

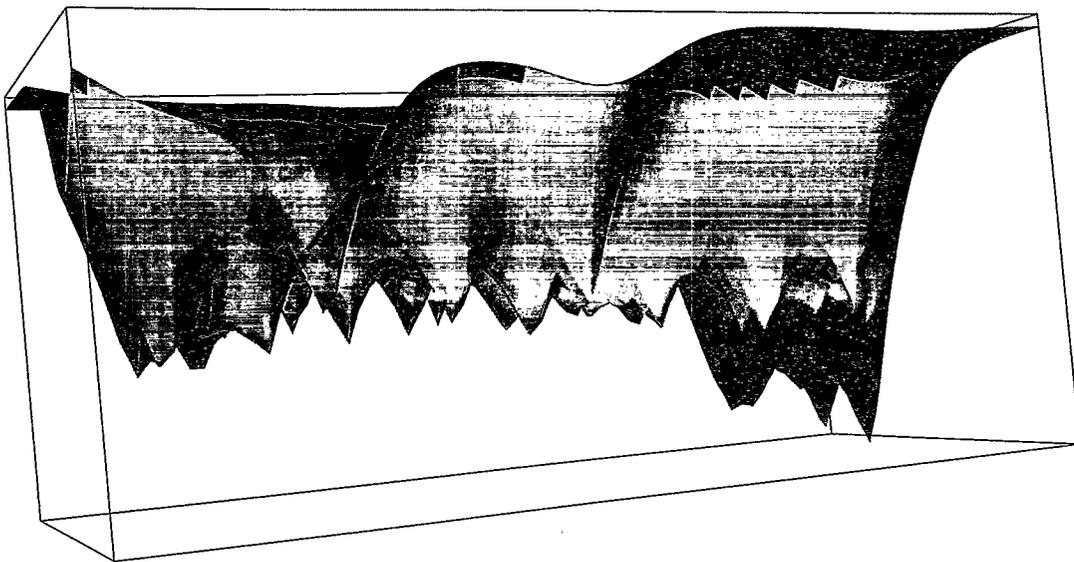


Figure 6.8 DCE standard errors of prediction for 1992.

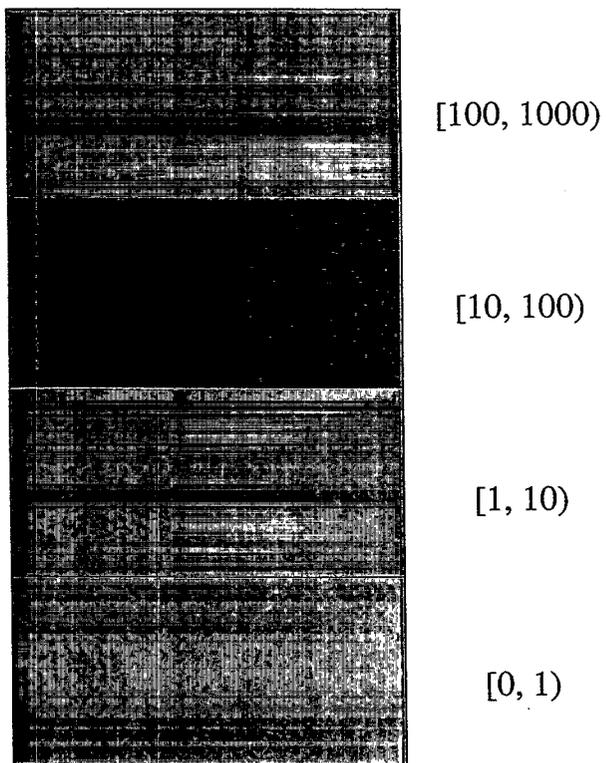


Figure 6.9 Legend for prediction surfaces (measurements in *mg/L*).

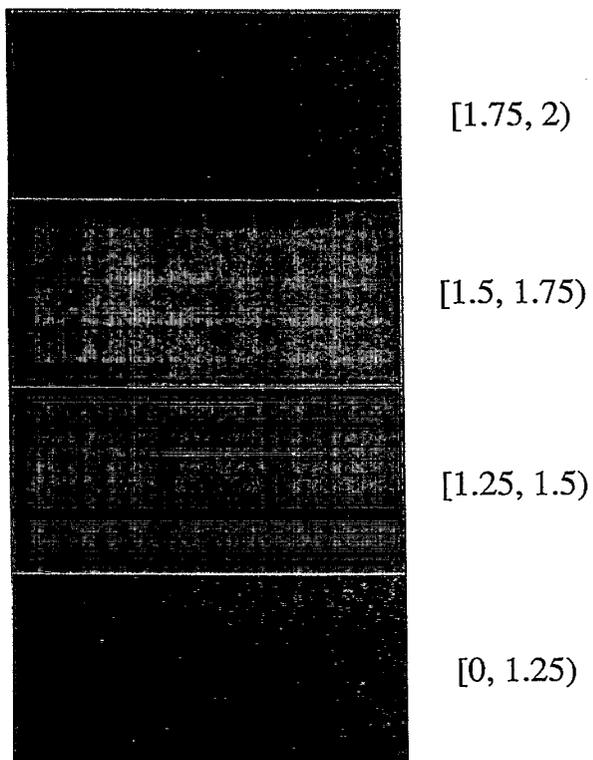


Figure 6.10 Legend for standard errors.

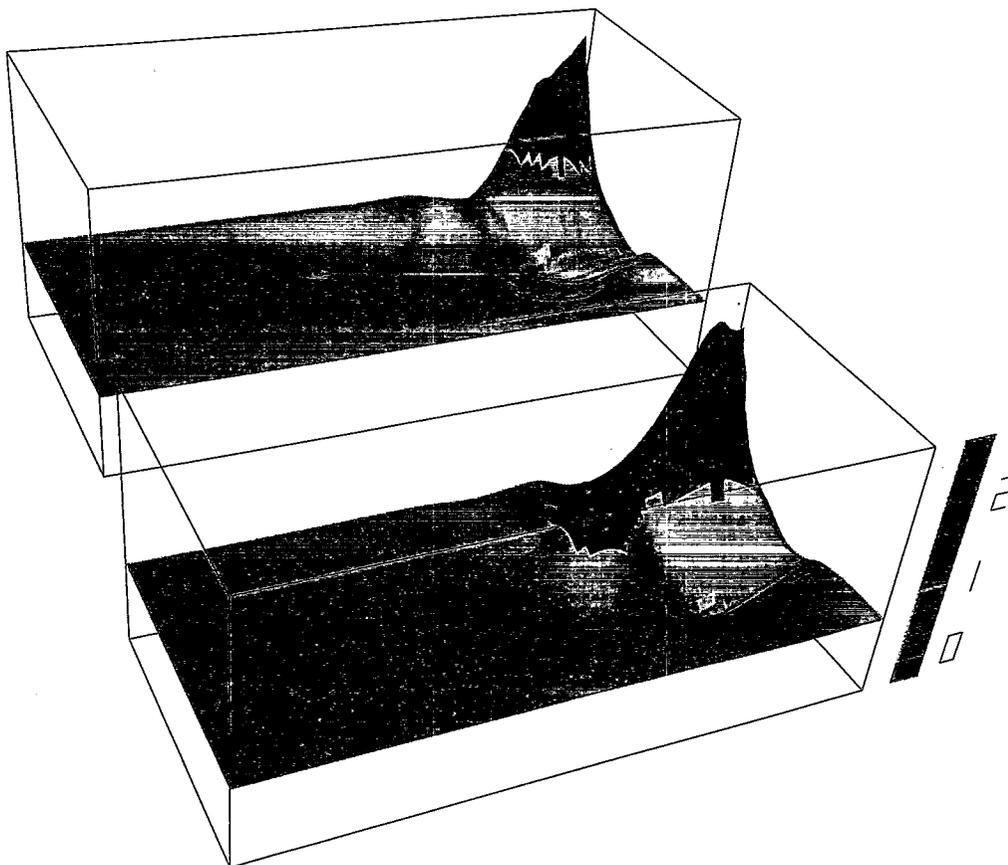


Figure 6.11 TCE and DCE surfaces for 1986.

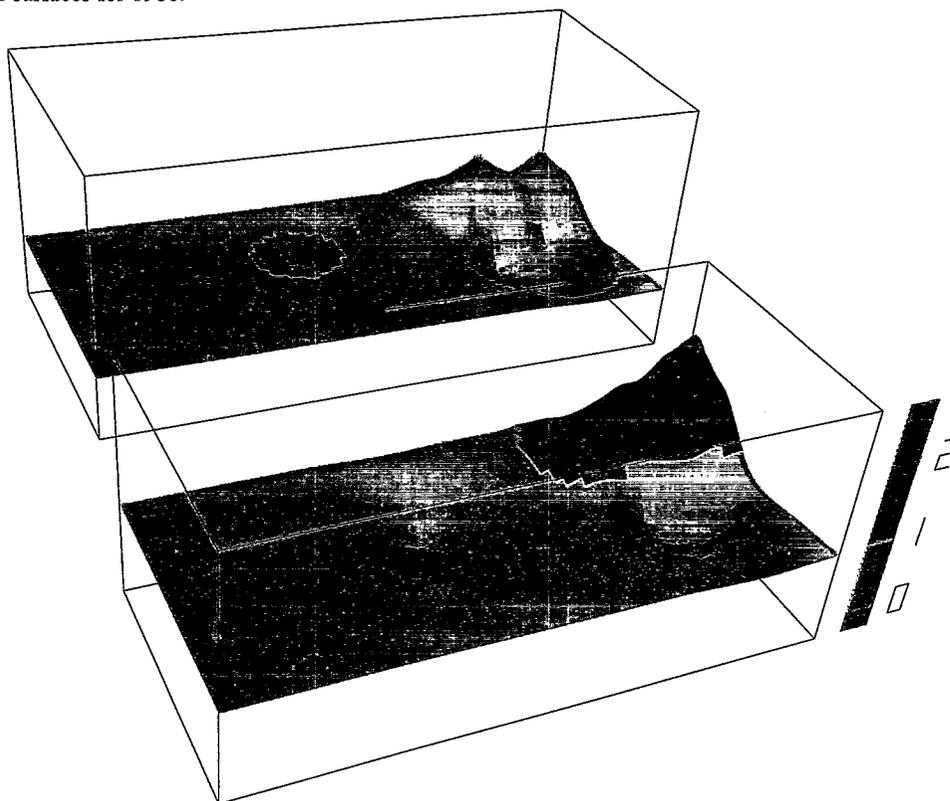


Figure 6.12 TCE and DCE surfaces for 1988.

this occurred. It has been supposed that perhaps an excessive amount of rainfall in this year would have diluted the concentrations of contaminant in the ground water, but it should be noted that this is definitely only suspicion and further investigation is necessary. In any event, however, animation of the spatial estimates through time allowed us to easily pick up on this seeming aberration.

6.2.2 Sulfate Ions

Measurements of sulfate ions (SO_4^{2-}) are of interest due to a supposed connection between levels of SO_4^{2-} , TCE, and DCE.

That is, anaerobic bacteria which consume SO_4^{2-} also consume TCE, converting it into DCE. It is believed that regions of low sulfate, dubbed "sulfate holes," indicate the presence of such bacteria. If this is true, we also would expect to see TCE drop in these regions. There are much fewer sulfate data than there are TCE and DCE data, to the extent that there are insufficient data in several of the years to do a reasonable surface estimate. For this reason, SO_4^{2-} surfaces were produced only for the years 1985 through 1989, inclusive, and 1991. As there was some concern that the large flat sections of the surfaces in the portions of the region with no data might be somewhat misleading, a new visualization technique was tried with the SO_4^{2-} data. For each year, the surface was only plotted in the area where there *were* data, with a bounding box to indicate the region and keep all years on the same scale. The success of this approach is perhaps mixed. It does indeed make it very clear in what regions we do not have any good estimates due to lack of data. However, it also makes it nearly impossible to interpolate between years to produce a smooth animation, and in fact increases the "jumpy" effect seen when viewing the surfaces in chronological order. (This is not such a problem with the sulfate data, as the time gap makes them not entirely suitable for animation, anyway.) Again, the plots are all on a \log_{10} scale with the same color contours as for TCE and DCE.

Figures 6.15, 6.16, and 6.17 contain examples of these SO_4^{2-} surfaces. These surfaces have several interesting features. In all three, we see a small peak in sulfate levels near the source of TCE and DCE contamination. Also, in all three, we see one or more "sulfate holes" near to this peak. This indicates that perhaps TCE is being converted to DCE near to the source, which would lead to TCE values dropping off more rapidly than DCE as distance from the source increases. Efforts to see if such a relationship exists will be discussed further in Section 6.3. Figure 6.16 reveals another interesting and somewhat odd feature of

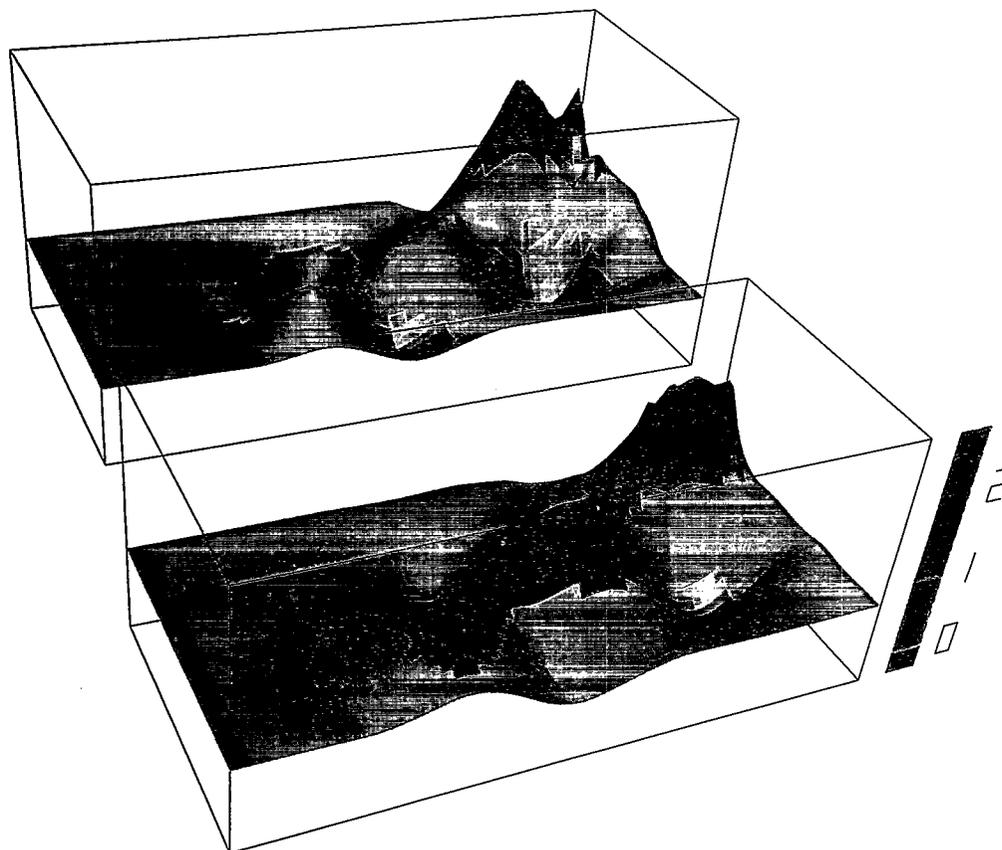


Figure 6.13 TCE and DCE surfaces for 1991.

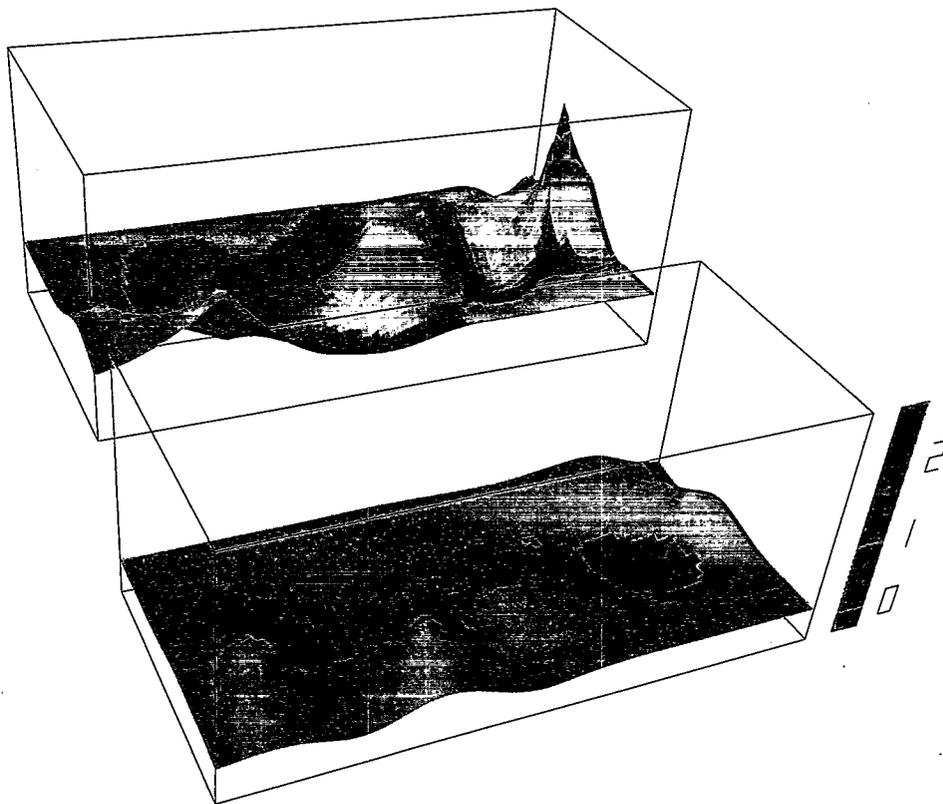


Figure 6.14 TCE and DCE surfaces for 1993.

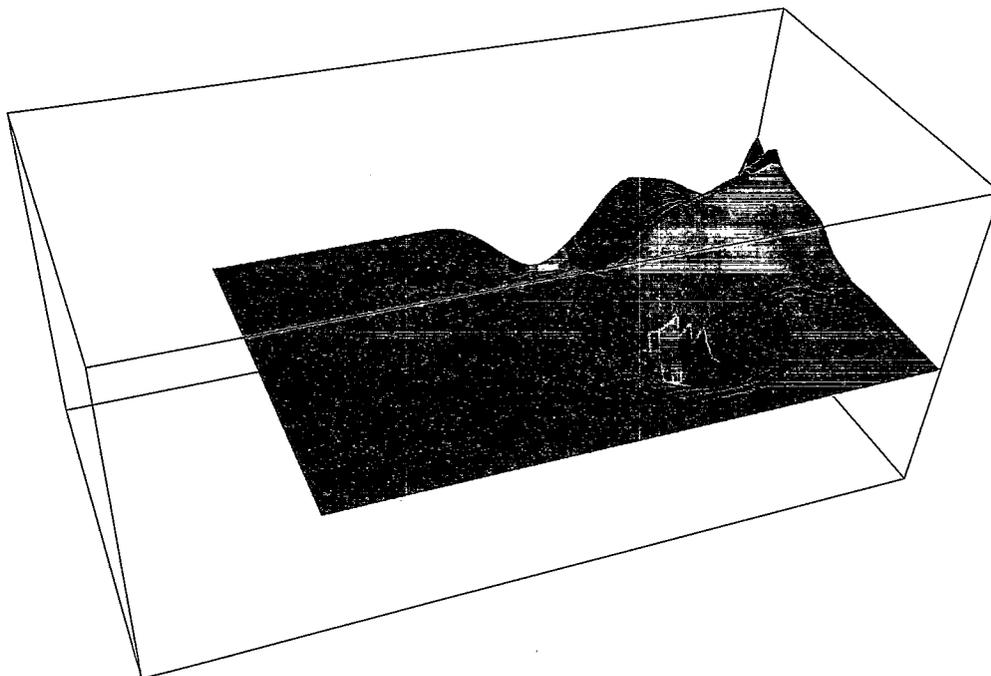


Figure 6.15 SO_4^{2-} surface for 1986.

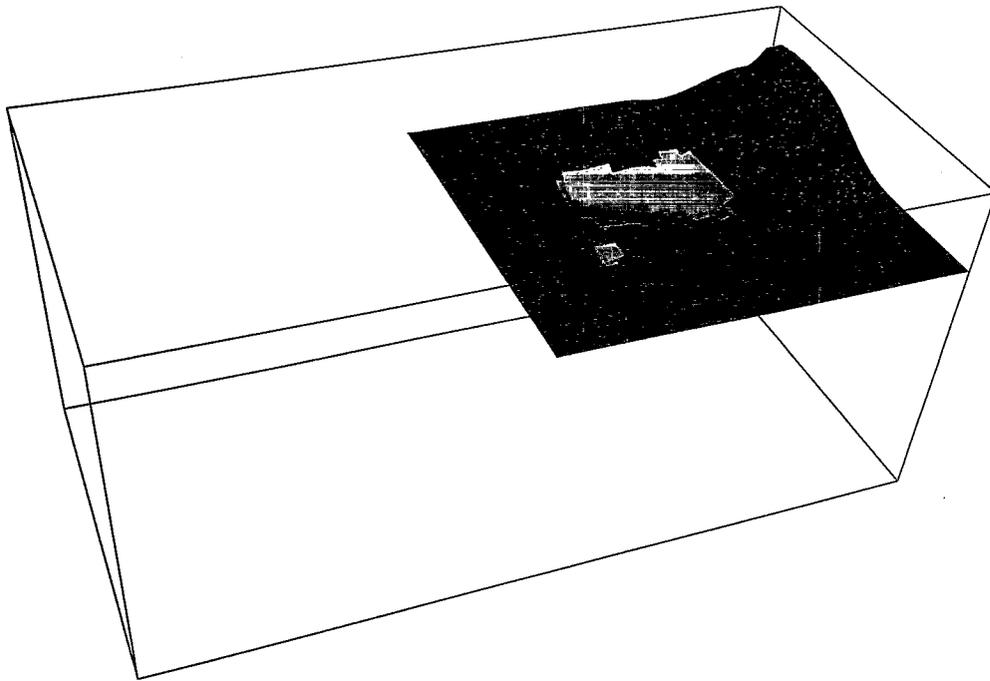


Figure 6.16 SO_4^{2-} surface for 1988.

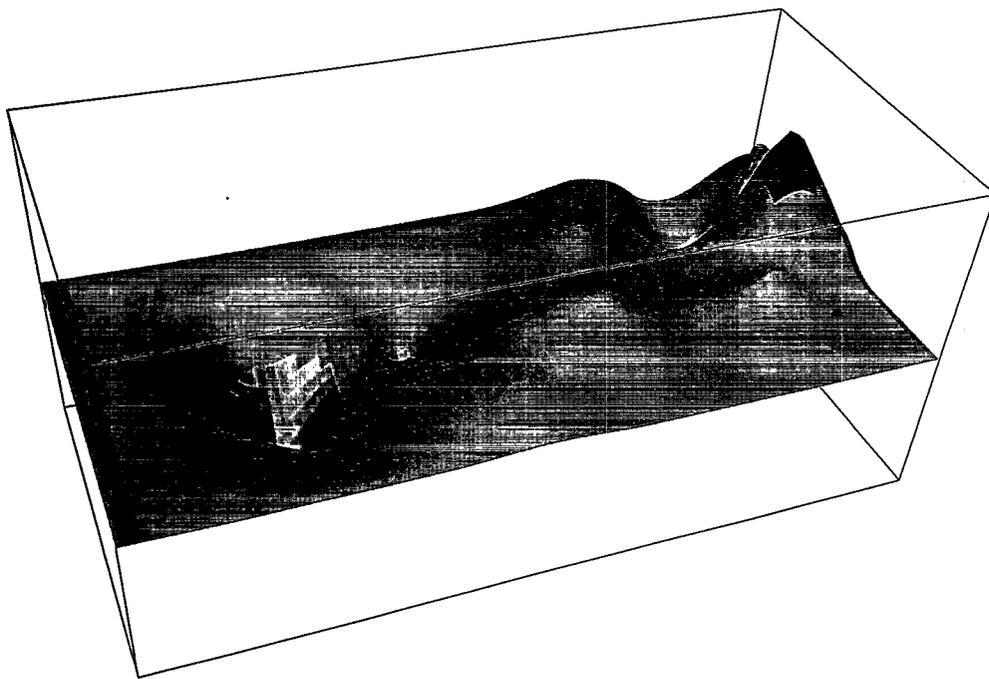


Figure 6.17 SO_4^{2-} surface for 1991.

the sulfate data. The overall sulfate levels for the years 1987, 1988, and 1989 over the region are significantly higher than for the other years studied. We have not yet been able to identify a reason for this, but it certainly seems to warrant further investigation.

6.3 Further Analytical Efforts

As mentioned previously, the region for which there were data available increased as time progressed. Specifically, in the earlier years (e.g., 1985), there were data points only relatively close to the source. Later, more data points were added to the south and especially to the west. This can create some problems with analysis, so it was decided following a conversation with Dr. Joe Hughes that we should try to do local analyses using some smaller region around the source. It is hoped that this will help us to better understand the chemical and transport processes at work. We expect that

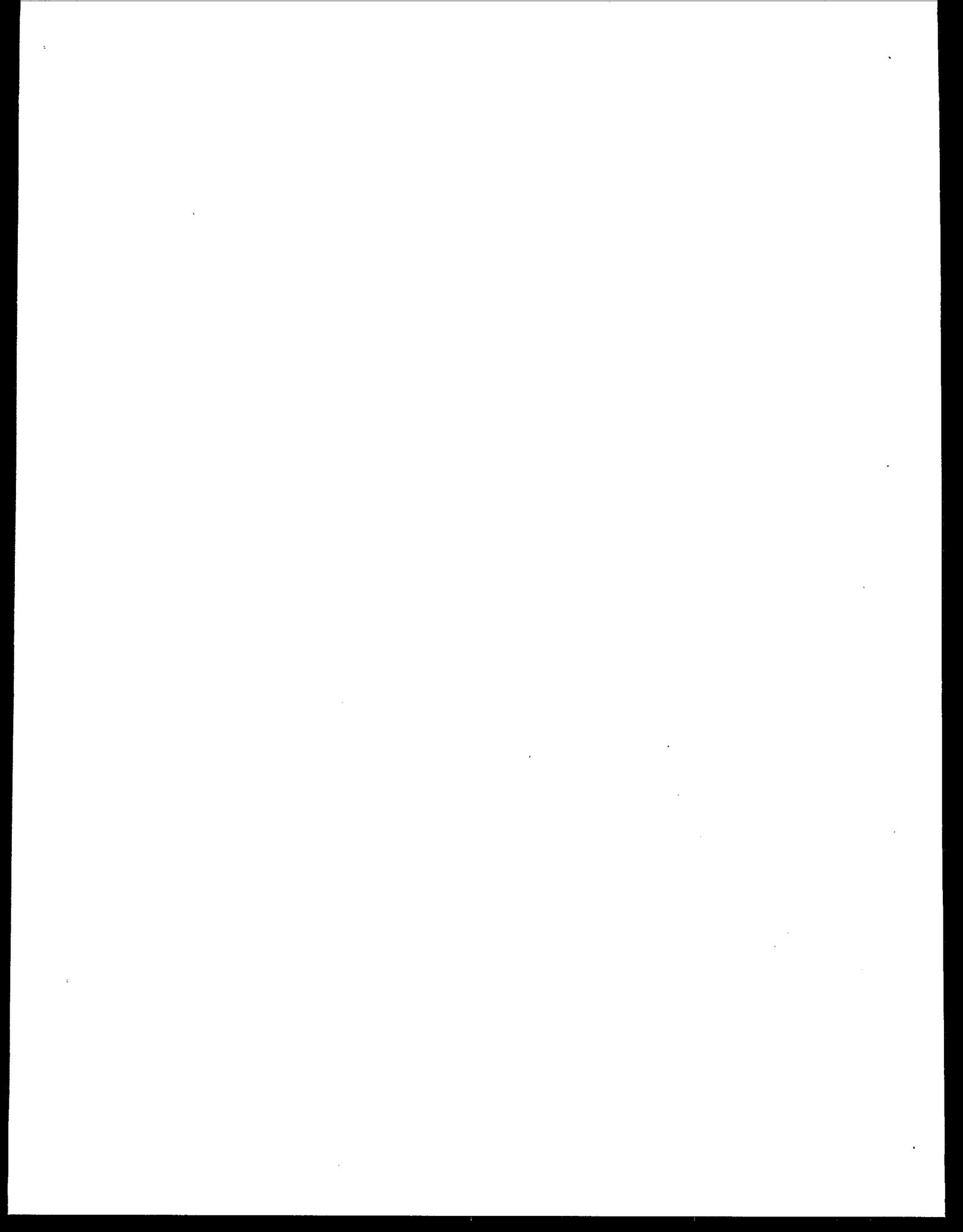
- TCE should decrease in regions of high sulfate due to the likely presence of sulfate-consuming bacteria in these regions, and that
- TCE and SO_4^{2-} should decrease quicker with distance from the source than DCE.

Two different types of local analyses were attempted. The first involves simply using only a small rectangular region around the source; e.g., the Northeast corner of the total region. The other involves using a relatively narrow region from the source and extending in the direction of flow. For this second method, we then want to do spatial estimates of contaminant (i.e., \log_{10} of TCE, DCE, and SO_4^{2-}) vs. the following:

1. distance from the source,
2. time since Jan. 1, 1985 and distance from the source, and
3. time since Jan. 1, 1985 and distance from the source at time 0.

As the region chosen in this case is narrow, the distance from the source is approximately equal to the distance from the source along the line of flow. This method seems reasonable because the primary method of transport of contaminant in this system is ground-water flow, with dispersion being decidedly less. So if the speed of ground-water flow is s ft/day, then the contaminant present a distance st from the source in the direction of flow on day t should have been at the source on day 0. This is precisely the motivation for the third case listed above, for which we calculate $d' = d - st$, the estimated distance from the source at time 0.

Unfortunately, there is one problem with this latter method which has not yet been resolved: it is not entirely clear where the source of contaminant is. The general vicinity is certainly known, but to pinpoint an "exact" location allowing us to place a narrow strip about the source has proved to be a difficult problem. It is possible that the source is in fact a large area and would not be well approximated by a point source. From recent investigations, what appears likely is that there are at least 2 point sources approximately 500 - 1000 ft apart. (We have hypothesized this after noticing that in the general vicinity of the source, there are two clusters of measurement locations which both contain very high levels of TCE. As it is common to place large numbers of wells near a known source, the presence of two sources known to previous investigators seems a logical hypothesis.) This presents some unforeseen problems and is what has led us to consider the first method mentioned; i.e., doing more standard estimation on a small region about the source.



Chapter 7

Summary and Conclusions

Site characterization and estimation of contaminant plumes is a complex problem which requires the compilation by the environmental researcher of many sources of information. Observations on the contaminant level over the region are expensive and sometimes difficult to obtain. In this research effort, we suggested several methods of examining such valuable data to further the researcher's understanding of the environmental problem under study.

Based on observational data, we explored analytical methods for estimating the level and extent of the contaminant plume. Nonparametric regression methods proved useful for quick summaries of the contaminant plume, whereas the more difficult to implement geostatistical methods were required for quantitative measures of the contaminant plume, such as the total amount of contaminant present.

In addition to exploring the analytical issues associated with estimation of the contaminant plume and functionals of this plume, we investigated how best to display this information through visualization methods. Two and three-dimensional perspective plots with color contours proved useful in our investigation. To associate the error in the estimated plume with the estimated level of the plume, we suggest associating the height of the perspective plot with the estimated level of contaminant and the color contours with the estimated amount of observed error in the estimate.

Our investigations also found that animation of the estimated level of contaminants or estimated errors was a useful exploratory tool. For the Eglin data, surface estimates produced with all but one point are animated alternately with the surface estimate using all the data points. This allows us to readily see the effect each data point has on the surface estimate. For points whose absence produces a large change in the surface estimate, it may be desirable to take additional samples near this point to help stabilize the estimate in this area; estimates of the prediction errors at these points are also useful for this reason. Animations through time, with smoothing, were used for the Arizona data allowing quick identification of atypical behavior in time. Also for the Arizona site, we investigated methods of simultaneously animating two related substances. Simultaneous animations of TCE and DCE helped identify the relationship between these two substances. Furthermore, we examined the issue of a growing region or plume. Both of these issues are the focus of further research.

We proposed in Section 5 a method for estimating the integral of a random process in the case where the process is lognormal by modeling the process through geostatistical methods and simulating the process conditional on the data. This is useful for estimating the total amount of contaminant present in a region. When implemented on the Eglin ground water observations for BTEX, this method produced reasonable point estimates but large confidence intervals. Large confidence intervals are to be expected from such a small number of observations, however we are hopeful that further research into improved statistical methods can yield tighter confidence intervals for small sample sizes.

Future Research

This work has surfaced a number of topics which would be appropriate for future research. It is still an open question how to best view two possibly related substances to see how they are related. For the TCE and DCE data from Arizona, it was thought that examining the ratio of the two substances might be useful, but this did not seem to reveal very much. An examination of functions of two such substances so they may be viewed as a single surface seems like a promising idea, however.

For the sulfate data from Arizona, we attempted to deal with the issue of an increasing design region over time, due to more information, and interest, on the part of those taking observations. Attempts to plot various portions of the estimated surface, dependent on the region, seem to be of dubious value. The idea of estimating a small region near the source, or perhaps estimating along the line of ground-water flow from the source, as discussed in Section 6.3, is a promising idea. The lack of a well-defined source in this instance made such an examination difficult, but such a method could certainly still be examined for this and other data.

The method for estimating the integral discussed in Section 5 is promising, but reductions of variance and better prediction intervals are areas which need to be addressed. Specifically, if one looks at the values obtained for the integral estimates and their standard deviations, one notices that in fact the standard deviations are *extremely* high. In particular, recall that if we use the mean of the integral estimates for the realizations as a point estimate for the integral of the process, we get an estimate of total contaminant of 1.204×10^{10} . However, the estimated variance of this value is then the mean of the variances for the realizations, giving a variance of 2.796×10^{20} , and a standard deviation of 1.672×10^{10} . That is, the estimated standard deviation of total concentration is actually *higher* than the estimated concentration. It is possible that by sampling locations using some distribution other than a uniform, i.e. *importance sampling* (Rubinstein, 1981), may yield integral estimates with a smaller variance. For example, we may wish to sample from a smaller, possibly non-rectangular region where the data are more dense. Or we may wish to sample with higher probability along the direction of geometric anisotropy than in the perpendicular direction. At any rate, it is desirable to investigate ways of reducing the variance of the integral estimates, and this is a topic of current research for some of the authors of this report.

For the prediction intervals, we used what are referred to as *equal tail* intervals. That is, the interval is a two-tailed interval with equal probability in either of the tails. This is not always the best type of interval to use, and particularly may not be in the case

of such an asymmetric distribution. It would be worthwhile to investigate other types of intervals, particularly those known as *highest posterior density* (HPD) regions (Casella and Berger, 1990). In this case, the $1 - \alpha$ interval is chosen so as to be as short as possible. Specifically, if the posterior density is denoted by π , the $1 - \alpha$ HPD region is given by $\{x: \pi(x) \geq c\}$ where c is such that $1 - \alpha = \int_{\{x: \pi(x) \geq c\}} \pi(x) dx$. Also, the prediction intervals discussed here are actually *too large*, as they contain additional variation due to Monte Carlo sampling error. To get better prediction intervals, this factor needs to be corrected for.

Finally, it was mentioned at the beginning of Section 5 that there are actually *several* nonlinear functionals of random processes which are of interest to estimate. The integral of the process is the only one of these which we have investigated in detail to this point. Other functions which are of interest are:

- the maximum concentration attained within a region,
- the location where this maximum concentration occurs, and
- the region for which the concentration exceeds some set value.

These other three are quantities which are of interest for various types of environmental contamination and these warrant further investigation. Further, in ozone modeling, it is common to use a square root transform rather than a log transform as in Carroll et al., 1997. Thus it is also of interest to estimate the total contaminant in the case where the process is transformed by a square root rather than a log.

Appendix A

Cross-Validation

In all cases, it is assumed that bandwidths in the x and y directions should be the same, i.e. $\underline{h} = (h_x, h_y)$ where h_x is the bandwidth in the longitude and latitude directions and h_y is the bandwidth in the vertical direction. We will use \underline{h} to denote either h_x or (h_x, h_y) depending on whether the estimate is in 2-D or 3-D, respectively. The bandwidths were chosen by minimizing over \underline{h}

$$SSE(\underline{h}) = \sum_{i=1}^n (u_i - \hat{u}_{i,\underline{h}})^2$$

where n is the number of data points, u_i is the i^{th} observation, and $\hat{u}_{i,\underline{h}}$ is the nonparametric regression estimate, based on bandwidth \underline{h} , of the value at the i^{th} data point obtained when this point is removed. (Note: $\hat{u}_{i,\underline{h}} = \hat{f}(x_i)$ from 4.1.)

A.1 Two-dimensional Data

For the ground-water data, a single cross-validation was performed on bandwidths varying from 100 to 250 \hat{z} in increments of ten. As seen in Figure A.1, the bandwidth selected here is 120 \hat{z} . See 4.1 for a plot of the estimated plume.

Similarly, a cross-validation was performed for two-dimensional soil data from Eglin at approximate depths of 7.0 and 7.6 \hat{z} below the water table. In both of these cases, the minimization of $SSE(\underline{h})$ was performed by a grid search from 100 to 250 \hat{z} in increments of ten. The bandwidth chosen for the depth of 7.0 \hat{z} is 170 \hat{z} , while 230 \hat{z} was chosen for the depth of 7.6 \hat{z} . See 4.1 for a plot of the estimated plume at a depth of 7.0 \hat{z} .

In addition to an estimate of the contaminant plume, we also visualize a smoothed estimate of the absolute error of this estimate as each data point is removed. A cross-validation of the absolute errors for the ground-water data resulted in a bandwidth of 130 \hat{z} , which is close to the 120 \hat{z} found for the plume estimate. The plots for visualizing the error are given in Section 4.1.

A.2 Three-dimensional Data

For the three-dimensional soil data, we needed to perform cross-validation in both the x and y directions and the z direction. (Here the x direction is longitude, the y direction is latitude, and the z direction is distance above or below the water table.) First we performed cross-validation in the x and y directions, allowing the bandwidth in the z direction to vary along with the bandwidth in the x and y directions. This yielded an x and y bandwidth of 24 \hat{z} . Then we examined the $SSE(\underline{h})$ using x and y bandwidths varying from 20 to 40 \hat{z} (which includes the minimum of 24 \hat{z}), and six different z bandwidths ranging from approximately 1.5 to approximately 3. This caused us to choose an xy bandwidth of approximately 24 \hat{z} and a z bandwidth of approximately 1.8 \hat{z} .

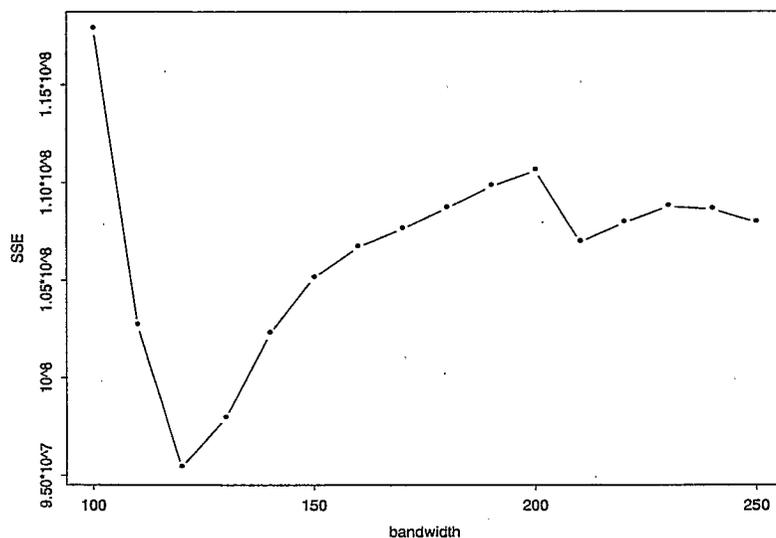


Figure A.1 Bandwidth selection for ground-water data.

Appendix B

Discussion of Spatial Estimation for Arizona

There were a number of difficulties encountered when doing the spatial estimates of TCE, DCE, and SO_4^{2-} for the Arizona site. The biggest problem was finding suitable variogram models. It was decided that it would be most reasonable to find only one variogram model for each substance, which would be used for all years of data. Many of the classical empirical variograms with standard default binwidths, etc., produced totally unreasonable variograms (e.g., variograms which were flat or indicated stronger correlation between points which were a long ways apart than for points which were close together). For example, consider the classical empirical variogram for 1990 TCE, shown in Figure B.1. This plot is highly variable and shows a general *decreasing* trend, whereas a variogram should be generally *increasing*. Cressie's robust variogram estimator did not usually solve these problems. It was conjectured that the high variability could largely be due to low numbers of pairs of data points at many of the higher distances. To combat this, we binned the data point pairs into groups with equal *numbers of pairs*, rather than equal width bins as in the classical estimator. We tried taking both means and medians within these groups, analogous to the classical and robust estimators. A plot of the mean case for the 1990 TCE data is shown in Figure B.2. Apart from the last bin, where the data point pairs used are so far apart in distance as to be suspicious anyway, this empirical variogram estimator looks much better than the classical one. Specifically, it is *much* less variable and has a decidedly increasing trend. Using this type of empirical variogram estimator, then, spherical variogram models were fit first for each year (and each substance). Then, from these, a variogram model for each substance was chosen which would be "best" in most years, and hopefully reasonable in all. This is intended to allow us to get satisfactory variogram estimates even for those years which do not contain much data and to provide a more unified approach.

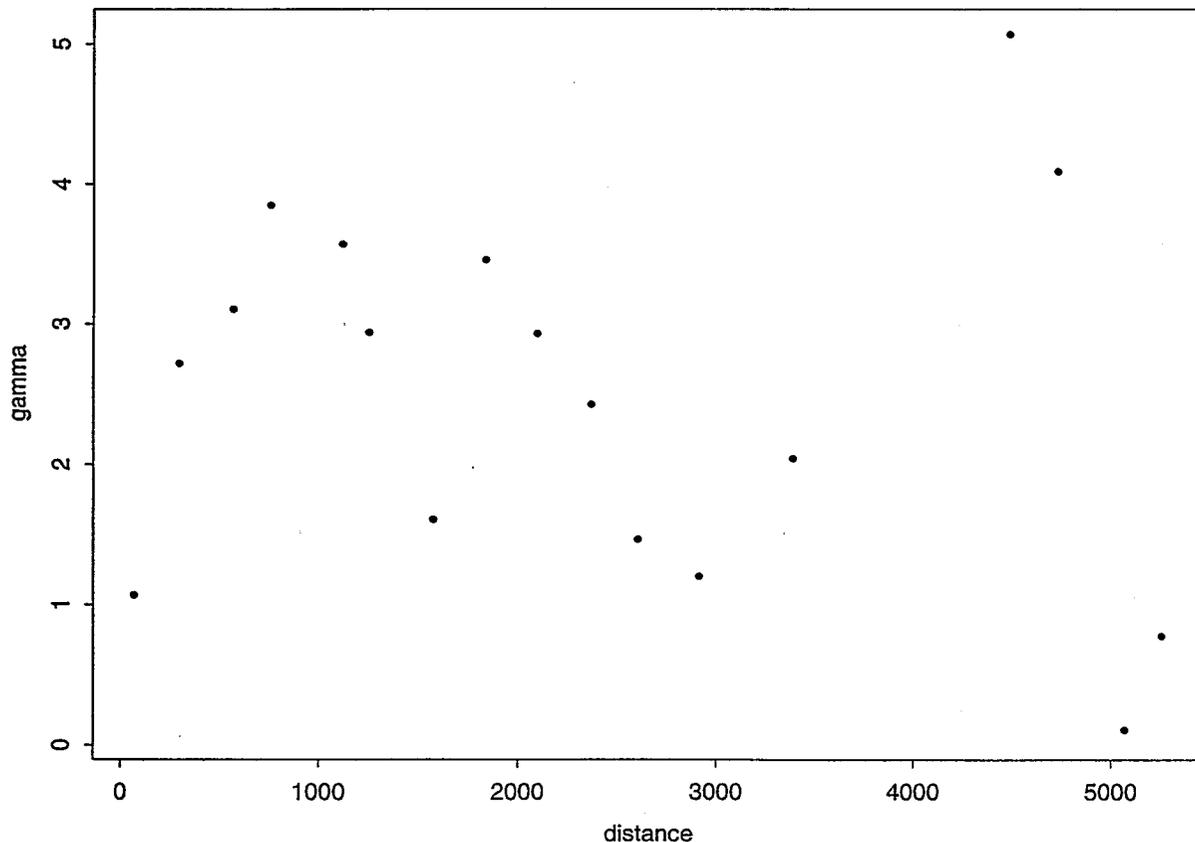


Figure B.1 Classical empirical variogram for 1990 TCE.

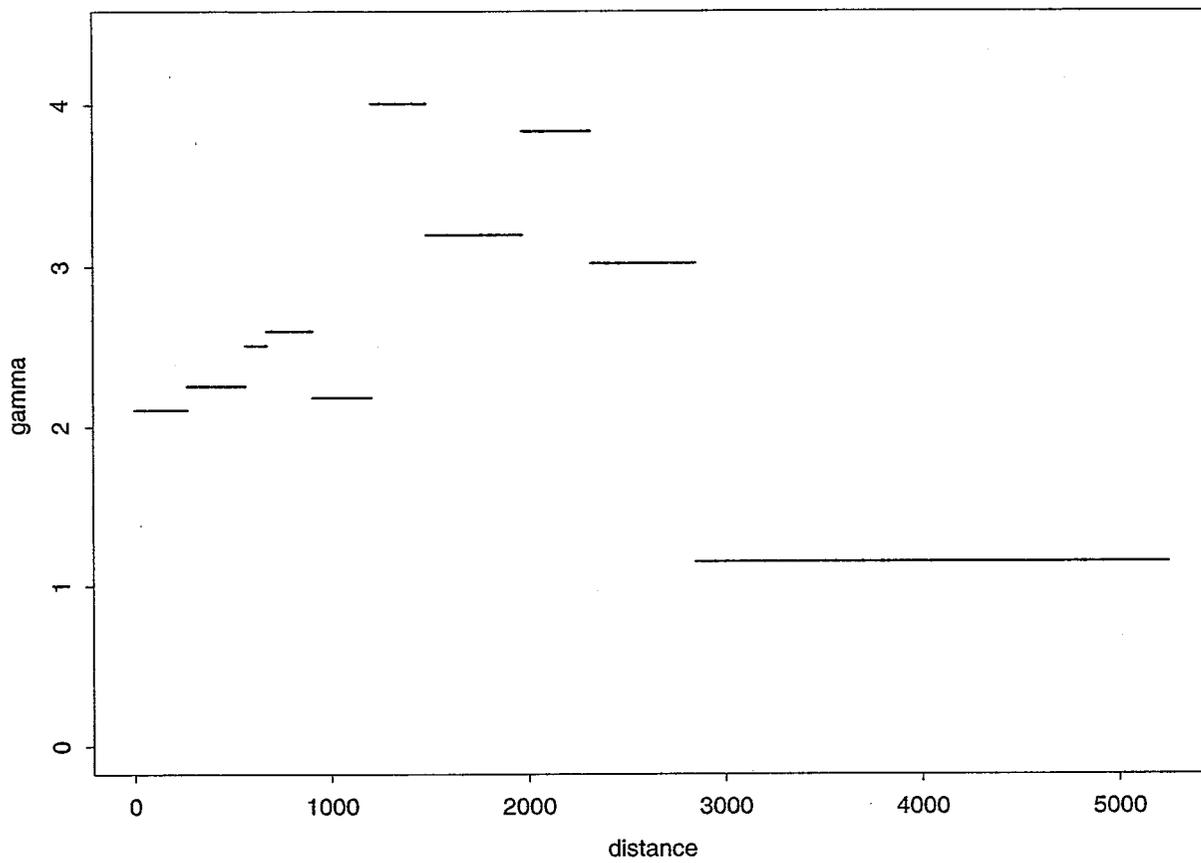
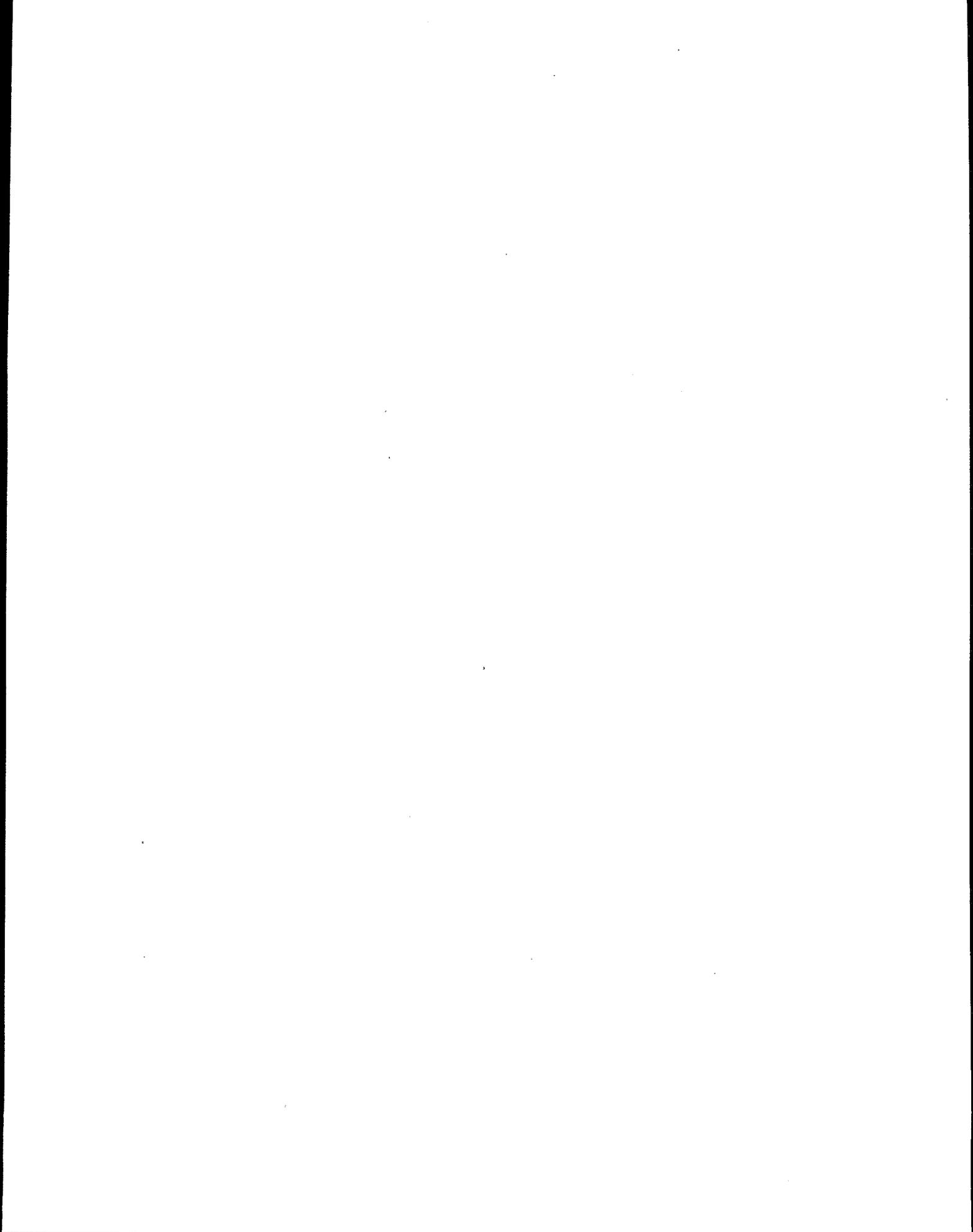
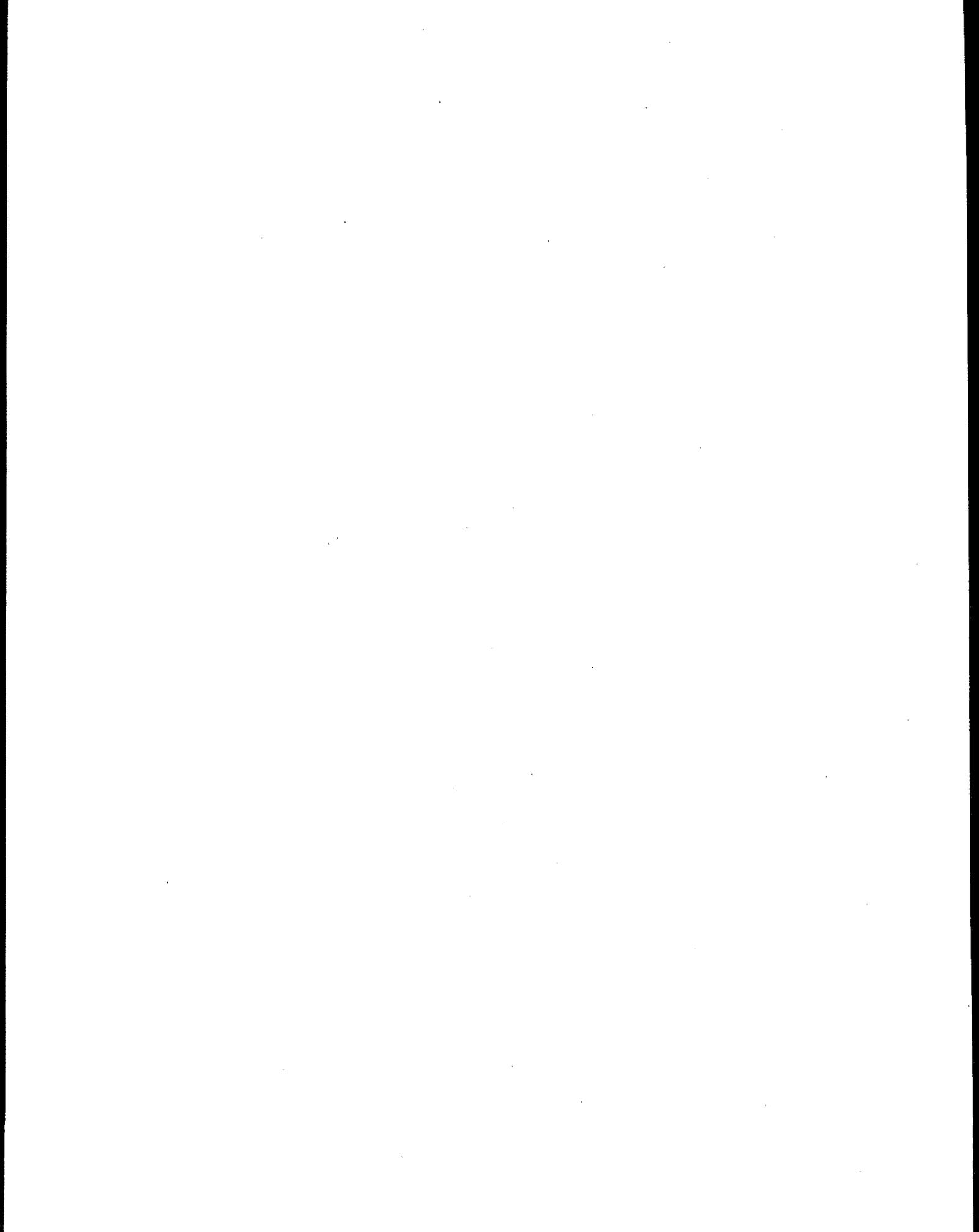


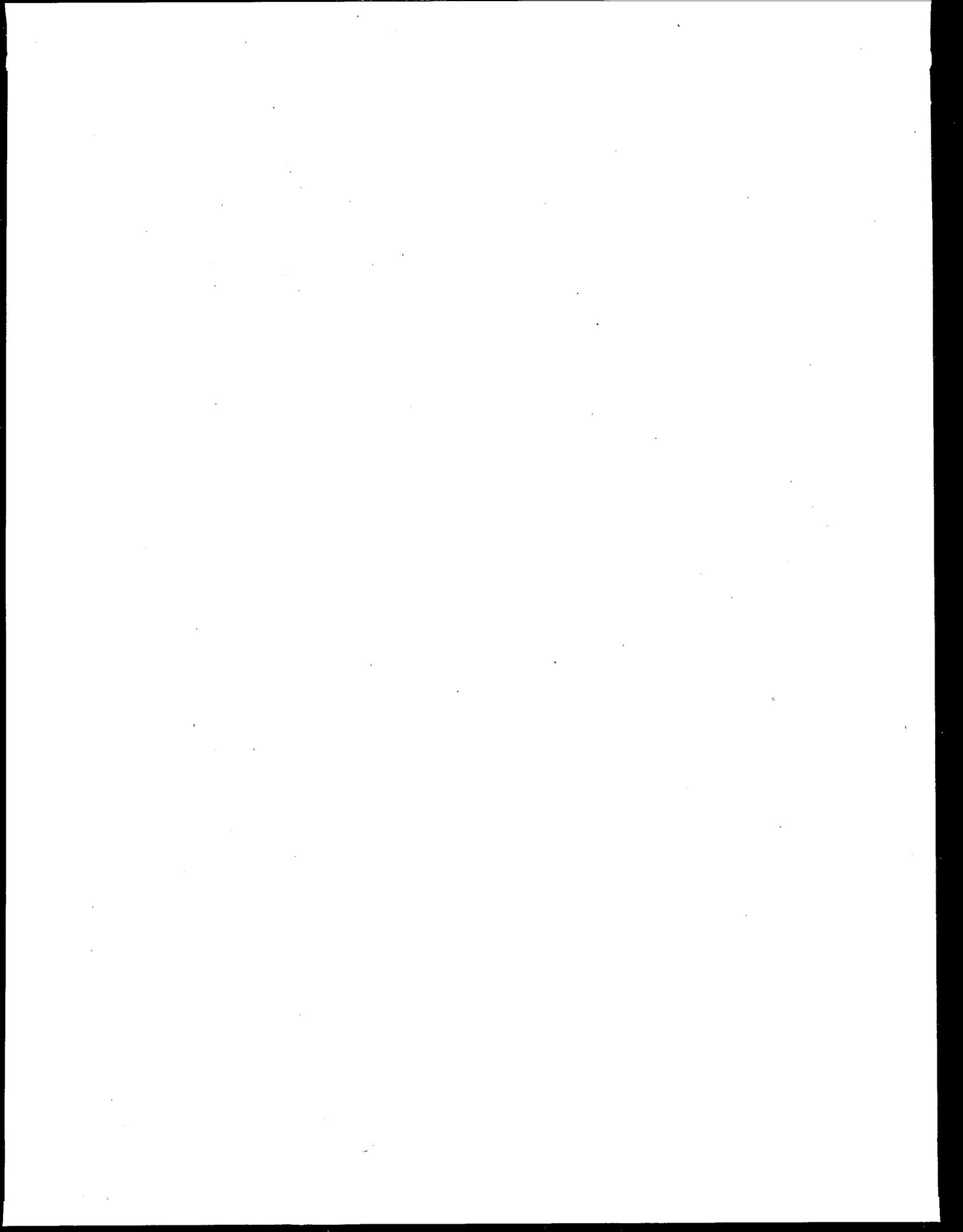
Figure B.2 Mean γ values for 1990 TCE.



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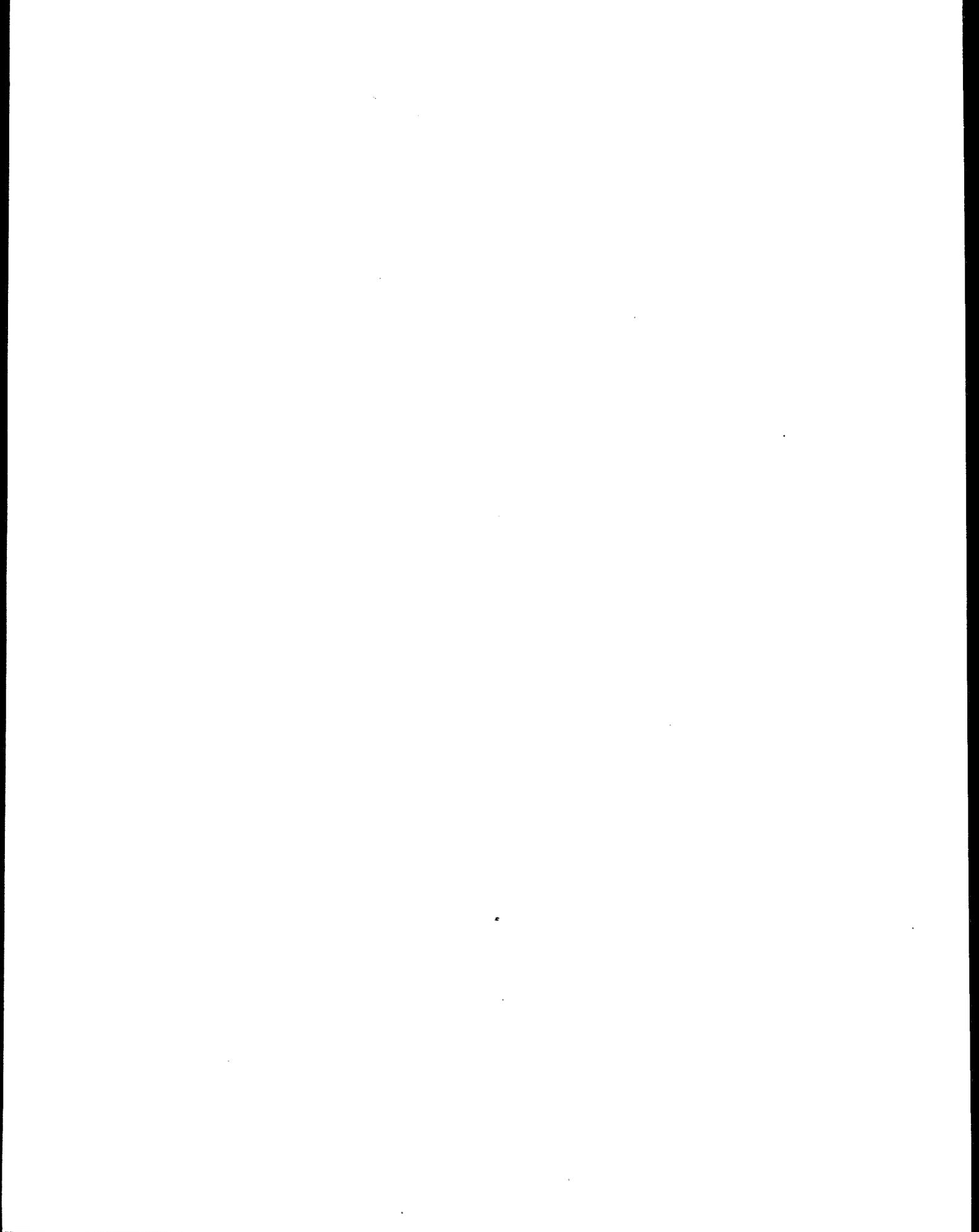
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Interim Reregistration Eligibility Decision (IRED)

Propetamphos



EPA Propetamphos Facts

EPA has assessed the risks of propetamphos and reached an Interim Reregistration Eligibility Decision (IRED) for this organophosphate (OP) pesticide. Provided that the risk mitigation measures outlined in this document are adopted, propetamphos fits into its own "risk cup"; that is, its aggregate risks are within acceptable levels. Propetamphos is also eligible for reregistration, pending a full reassessment of the cumulative risk from all OPs.

Propetamphos is an insecticide used indoors for the control of insects, such as ants, cockroaches, fleas and termites. Propetamphos residues in food and drinking water do not pose risk concerns. Additionally, risks are low to workers who mix, load, and apply propetamphos at commercial and residential use sites. There are also no environmental risk concerns. However, there are post-application risk concerns for adults, and especially children entering areas treated with propetamphos. With mitigation canceling all residential use, propetamphos fits into its own "risk cup". With other mitigation measures, propetamphos' worker risks also will be below levels of concern for reregistration.

EPA is reviewing the OP pesticides to determine whether they meet current health and safety standards. OPs need decisions about their eligibility for reregistration under FIFRA. Additional OPs with residues in food, drinking water, and other non-occupational exposures also must be reassessed to make sure they meet the new Food Quality Protection Act (FQPA) safety standard.

EPA's next step under the Food Quality Protection Act (FQPA) safety standard is to complete a cumulative risk assessment and risk management decision encompassing all the OP pesticides, which share a common mechanism of toxicity. The interim decision on propetamphos cannot be considered final until this cumulative assessment is complete. Further risk mitigation may be necessary at that time.

The OP Pilot Public Participation Process

The organophosphates are a group of related pesticides that affect the functioning of the nervous system. They are among EPA's highest priority for review under the Food Quality Protection Act.

EPA is encouraging the public to participate in the review of the OP pesticides. Through a six-phased pilot public participation process, the Agency is releasing for review and comment its preliminary and revised scientific risk assessments for individual OPs. (Please contact the OP Docket, telephone 703-305-5805, or see EPA's web site, www.epa.gov/pesticides/op.)

EPA is exchanging information with stakeholders and the public about the OPs, their uses, and risks through Technical Briefings, stakeholder meetings, and other fora. USDA is coordinating input from growers and other OP pesticide users.

Based on current information from interested stakeholders and the public, EPA is making interim risk management decisions for individual OP pesticides, and will make final decisions through a cumulative OP assessment.

The propetamphos IRED was made through the OP pilot public participation process, which increases transparency and maximizes stakeholder involvement in EPA's development of risk assessments and risk management decisions. EPA worked extensively with affected parties to reach the decisions presented in this IRED document, which concludes the OP pilot process for propetamphos.

Uses

- Propetamphos is an OP insecticide used indoors for the control of insects, primarily ants, cockroaches, fleas, and termites. Propetamphos may be applied at indoor residential, medical, commercial, and industrial buildings and equipment, such as homes, apartments, stores, schools, hospitals, offices and factories. It may also be used in food service establishments where there is no contact with food, and where no processing, packing, or warehousing of food occurs.
- Total annual usage is low, and estimated at 90,000 pounds active ingredient. The typical rate of dilution varies from 0.5% to 1.0% active ingredient solution. Propetamphos is applied as a water dilution through a compressed air sprayer, often with a low pressure hand wand.

Health Effects

Propetamphos can cause cholinesterase inhibition in humans; that is, it can overstimulate the nervous system causing nausea, dizziness, confusion, and at very high exposures (e.g., accidents or major spills), respiratory paralysis and death.

Risks

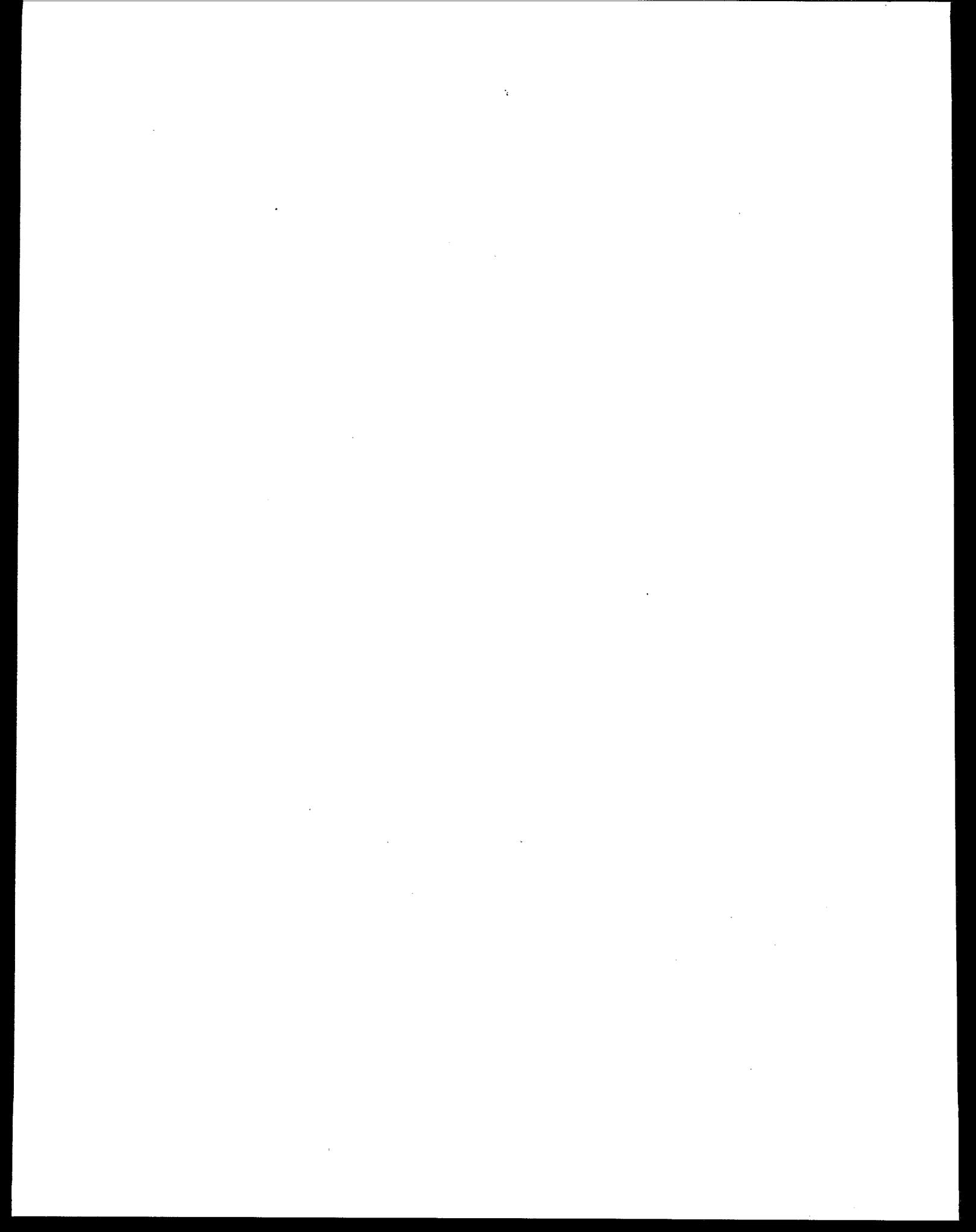
- Dietary exposures from food are not of concern for the entire U.S. population, including infants and children, provided food is removed or covered prior to an area being treated. Because propetamphos is only used indoors, exposure from drinking water sources is not expected.
- Risks are low, but still of concern for workers who mix, load, and apply propetamphos at commercial and residential use sites.
- Risks are of concern for adults, and especially children, from combined dermal, inhalation, and (for children only) oral routes of post-application exposure from re-entering areas treated with propetamphos.
- Because propetamphos is used indoors, exposure to the environment is not expected, and therefore, ecological risks are not of concern to the Agency.

In order to support an IRED for propetamphos, the following risk mitigation measures are necessary:

- To mitigate dietary (food) risks:
 - for use in food service establishments, all food must be either covered or removed prior to the area being treated.
- To mitigate worker risks:
 - reduce the maximum rate of dilution from 1.0% to 0.5% active ingredient solution;
 - applicators must wear personal protective equipment consisting of a long-sleeve shirt, long pants, shoes and socks, and chemical-resistant gloves; and
 - only protected handlers may be in the area during applications.
- To mitigate non-occupational risks to persons re-entering treated areas (post-application risks):
 - cancel all residential uses;
 - prohibit use in structures children and the elderly occupy, such as or including homes, schools, day-cares, hospitals, nursing homes (except for areas of food service when food is covered or removed prior to treatment);
 - cancel all spot, broadcast, and termiticide treatment; and
 - restrict the method of application to crevice treatment only, as defined in OPPTS 860.1460 Food Handling.

Next Steps

- Numerous opportunities for public comment were offered as this decision was being developed. The Propetamphos IRED, therefore, is issued in final (see www.epa.gov/REDs/ or www.epa.gov/pesticides/op) without a formal public comment period. The docket remains open, however, and any comments submitted in the future will be placed in this public docket.
- To effect risk mitigation as quickly as possible, time frames for making the changes described in the Propetamphos IRED are shorter than those in a usual RED. All labels need to be amended to include the above mitigation and submitted to the Agency within 90 days after issuance of this IRED.
- For propetamphos, tolerances for residues in food commodities will remain in effect and unchanged until a full reassessment of the cumulative risk assessment for all OP pesticides is completed. Upon completion of the cumulative risk assessment, EPA will issue its final tolerance reassessment decision for propetamphos and may request further risk mitigation measures. For all OPs, raising and/or establishing tolerances will be considered once a cumulative assessment is completed.





UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

OFFICE OF
PREVENTION, PESTICIDES
AND TOXIC SUBSTANCES

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OCT 31 2000

Dear Registrant:

This is to inform you that the Environmental Protection Agency (hereafter referred to as EPA or the Agency) has completed its review of the available data and public comments received related to the preliminary and revised risk assessments for the organophosphate (OP) pesticide propetamphos. The public comment period on the revised risk assessment phase of the reregistration process is closed. Based on comments received during the public comment period and additional data received from the registrant, the Agency revised the human health and environmental effects risk assessments and made them available to the public on December 1, 1999. This action brought an end to Phase 4 of the OP Public Participation Pilot Process developed by the Tolerance Reassessment Advisory Committee, and initiated Phase 5 of that process. During Phase 5, all interested parties were invited to participate and provide comments and suggestions on ways the Agency might mitigate the estimated risks presented in the revised risk assessments. This public participation and comment period commenced on December 1, 1999, and closed on February 1, 2000.

Based on its review, EPA has identified risk mitigation measures that the Agency believes are necessary to address the human health risks associated with the current use of propetamphos. The EPA is now publishing its interim decision on the reregistration eligibility of and risk management decision for the current uses of propetamphos and its associated human health and environmental risks. The reregistration eligibility and tolerance reassessment decisions for propetamphos will be finalized once the cumulative assessment for all of the OP pesticides is complete. The enclosed "Interim Reregistration Eligibility Decision for Propetamphos," which was approved September 29, 2000, contains the Agency's decision on the individual chemical propetamphos.

A Notice of Availability for this Interim Reregistration Eligibility Decision (IRED) for propetamphos is being published in the *Federal Register*. To obtain a copy of this IRED document, please contact the OPP Public Regulatory Docket (7502C), US EPA, Aerial Rios Building, 1200 Pennsylvania Avenue NW, Washington, DC 20460, telephone (703) 305-5805. Electronic copies of the IRED and all supporting documents are available on the Internet. See <http://www.epa.gov/pesticides/op>.

The IRED is based on the updated technical information found in the propetamphos public docket. The docket not only includes background information and comments on the Agency's preliminary risk assessments, it also now includes the Agency's revised risk assessments: *Updated Revised*

Preliminary Risk Assessment: Propetamphos, June 7, 1999; *Updated Occupational and Residential Dermal Exposure Assessment* addendum, September 27, 2000; *EFED Integrated Science Chapter for Propetamphos*, December 2, 1997; and *Propetamphos Errata Sheet For EFED Chapter*, January 12, 1999; and a document summarizing the Agency's Response to Comments. The Response to Comments document addresses corrections to the preliminary risk assessments submitted by chemical registrants, as well as responds to comments submitted by the general public and stakeholders during the comment period on the risk assessment. The docket will also include comments on the revised risk assessment, and any risk mitigation proposals submitted during Phase 5. For propetamphos, a proposal was submitted by Wellmark International, the technical registrant. Mitigation suggestions were also submitted by the National Pest Management Association (NPMA).

This document and the process used to develop it are the result of a pilot process to facilitate greater public involvement and participation in the reregistration and/or tolerance reassessment decisions for OP pesticides. As part of the Agency's effort to involve the public in the implementation of the Food Quality Protection Act of 1996 (FQPA), the Agency is undertaking a special effort to maintain open public dockets on the OP pesticides and to engage the public in the reregistration and tolerance reassessment processes for these chemicals. This open process follows the guidance developed by the Tolerance Reassessment Advisory Committee (TRAC), a large multi-stakeholder body that advised the Agency on implementing the new provisions of the FQPA. The reregistration and tolerance reassessment reviews for the OP pesticides are following this new process.

Please note that the propetamphos risk assessment and the attached IRED concern only this particular OP pesticide. This IRED presents the Agency's conclusions on the dietary risks posed by exposure to propetamphos alone. The Agency has also concluded its assessment of the ecological and worker risks associated with the use of propetamphos. Because the FQPA directs the Agency to consider available information on the basis of cumulative risk from substances sharing a common mechanism of toxicity, such as the toxicity expressed by the OPs through a common biochemical interaction with cholinesterase enzyme, the Agency will evaluate the cumulative risk posed by the entire OP class of chemicals after completing the risk assessments for the individual OPs. The Agency is working towards completion of a methodology to assess cumulative risk and the individual risk assessments for each OP are likely to be necessary elements of any cumulative assessment. The Agency has decided to move forward with individual assessments and to identify mitigation measures necessary to address those human health and environmental risks associated with the current uses of propetamphos. The Agency will issue the final tolerance reassessment decision for propetamphos and finalize decisions on the reregistration eligibility once the cumulative assessment for all of the OPs is complete.

This document contains a generic and a product-specific Data Call-In(s) (DCI) that outline(s) further data requirements for this chemical. Note that a complete DCI, with all pertinent instructions, is being sent to registrants under separate cover. Additionally, for product-specific DCIs, the first set of required responses to is due 90 days from the receipt of the DCI letter. The second set of required responses is due eight months from the date of the DCI.

In this IRED, the Agency has determined that propetamphos will be eligible for reregistration provided

current uses of propetamphos may pose unreasonable adverse effects to human health and the environment, and that such effects can be mitigated with the risk mitigation measures identified in this IRED. Accordingly, the Agency recommends that registrants implement these risk mitigation measures immediately. Section IV of this IRED describes labeling amendments for end-use products and data requirements necessary to implement these mitigation measures. Instructions for registrants on submitting revised labeling and the time frame established to do so can be found in Section V of this document.

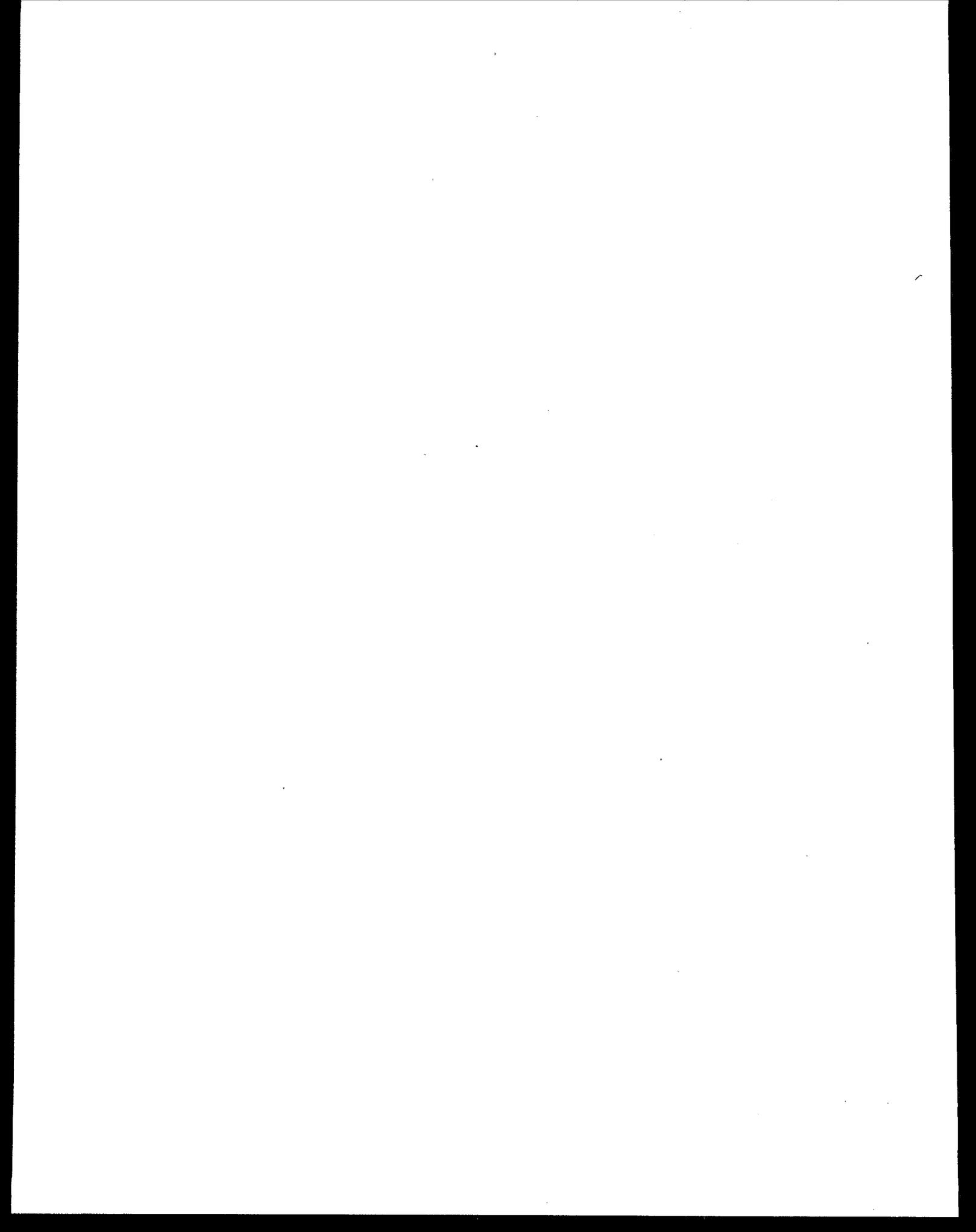
Should a registrant fail to implement any of the risk mitigation measures outlined in this document, the Agency will continue to have concerns about the risks posed by propetamphos. Where the Agency has identified any unreasonable adverse effect to human health and the environment, the Agency may at any time initiate appropriate regulatory action. At that time, any affected person(s) may challenge the Agency's action.

If you have questions on this document or the label changes necessary for reregistration, please contact the Special Review and Reregistration Division Chemical Review Manager, Gary Mullins at (703) 308-8044. For questions about product reregistration and/or the Product DCI that accompanies this document, please contact Karen Jones at (703) 308-8047.



Lois A. Rossi, Director
Special Review and
Reregistration Division

Attachment



**INTERIM REREGISTRATION
ELIGIBILITY DECISION
for
PROPETAMPHOS**

Case No. 2550

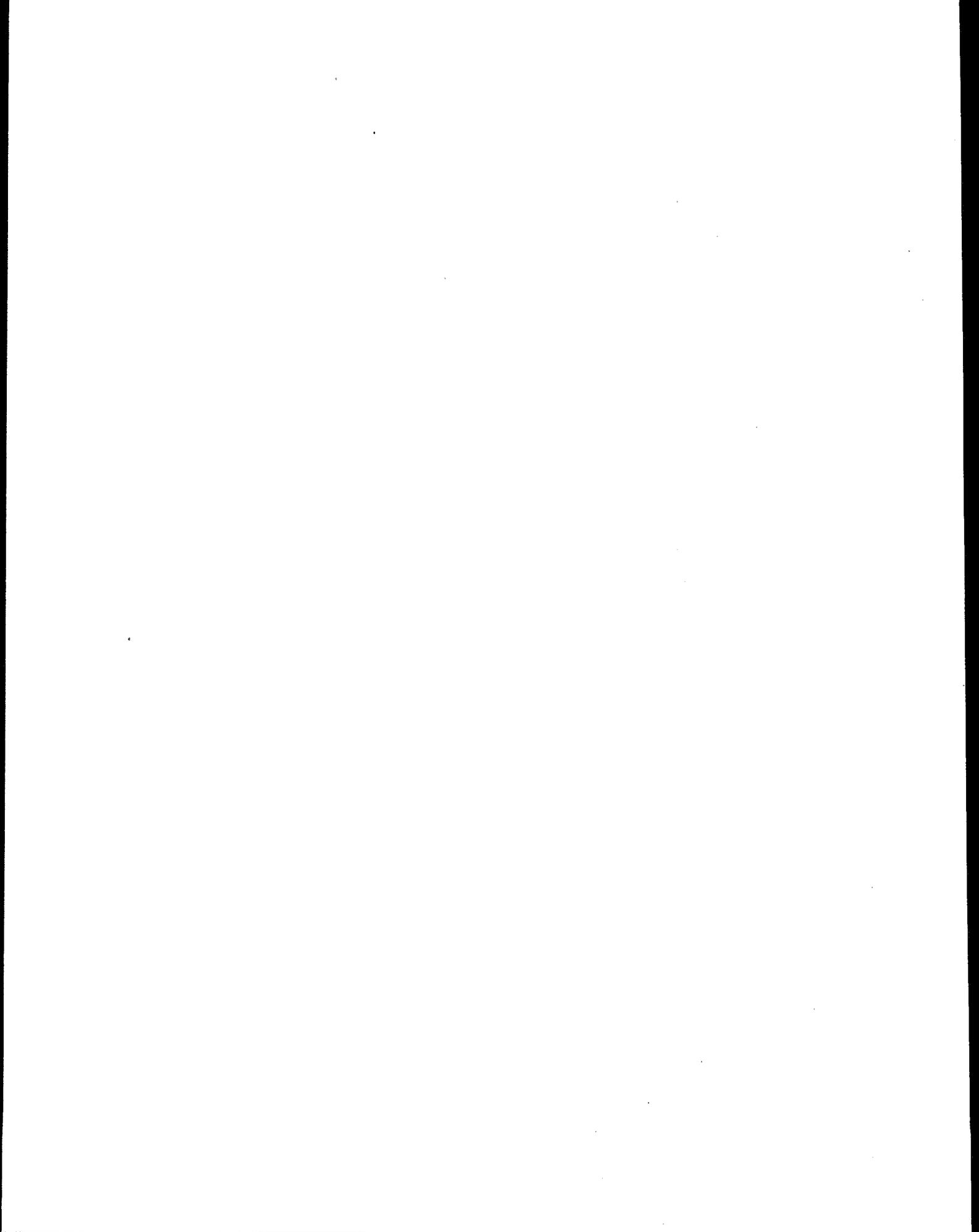


TABLE OF CONTENTS

Executive Summary	ii
I. Introduction	1
II. Chemical Overview	3
A. Regulatory History	3
B. Chemical Identification	3
C. Use Profile	4
D. Estimated Usage of Pesticide	5
III. Summary of Propetamphos Risk Assessment	7
A. Human Health Risk Assessment	7
1. Dietary Risk from Food	7
a. Toxicity	7
b. FQPA Safety Factor	8
c. Population Adjusted Dose (PAD)	9
d. Hazard Determination	9
e. Cancer Determination	9
f. Acute Dietary (Food) Risk	10
g. Chronic Dietary (Food) Risk	10
2. Dietary Risk from Drinking Water	11
3. Occupational and Residential Risk	11
a. Toxicity	11
b. Hazard Determination	12
c. Exposure	13
d. Occupational and Residential Risk Summary	15
4. Aggregate Risk	18
5. Human Incident Reports	19
B. Environmental Risk Assessment	20
IV. Interim Risk Management and Reregistration Decision	21
A. Determination of Interim Reregistration Eligibility	21
B. Summary of Phase 5 Comments and Responses	22
C. FQPA Assessment	23
1. "Risk Cup" Determination	23
2. Tolerance Summary	23
3. Endocrine Disruptor Effects	24

D.	Regulatory Rationale	25
1.	Human Health Mitigation Measures	25
a.	Dietary (Food and Drinking Water) Risk	25
b.	Occupational Risk	25
c.	Residential (Post-Application) Risk	26
2.	Environmental Risk Mitigation Measures	27
E.	Label Amendments	27
V.	What Registrants Need to Do	29
A.	Manufacturing-Use Products	29
1.	Additional Generic Data Requirements	29
2.	Labeling for Manufacturing-Use Products	30
B.	End-Use Products	30
1.	Product-Specific Data Requirements	30
2.	Labeling for End-Use Product	31
C.	Existing Stocks	31
D.	Labeling Changes Summary Table	32
VI.	Related Documents and How to Access Them	37
A:	Use Patterns Eligible For Reregistration	41
B:	Table Of Generic Data Requirements And Studies Used To Make The Interim Reregistration Decision	43
C:	Technical Support Documents	47
D:	Citations Considered To Be Part Of The Database Supporting the Interim Reregistration Eligibility Decision (Bibliography)	49
E:	Generic Data Call-In	59
F:	Product Specific Data Call-In	63
G:	List of Registrants Sent this Data Call-In	71
H:	List of Related Documents and Electronically Available Forms	73

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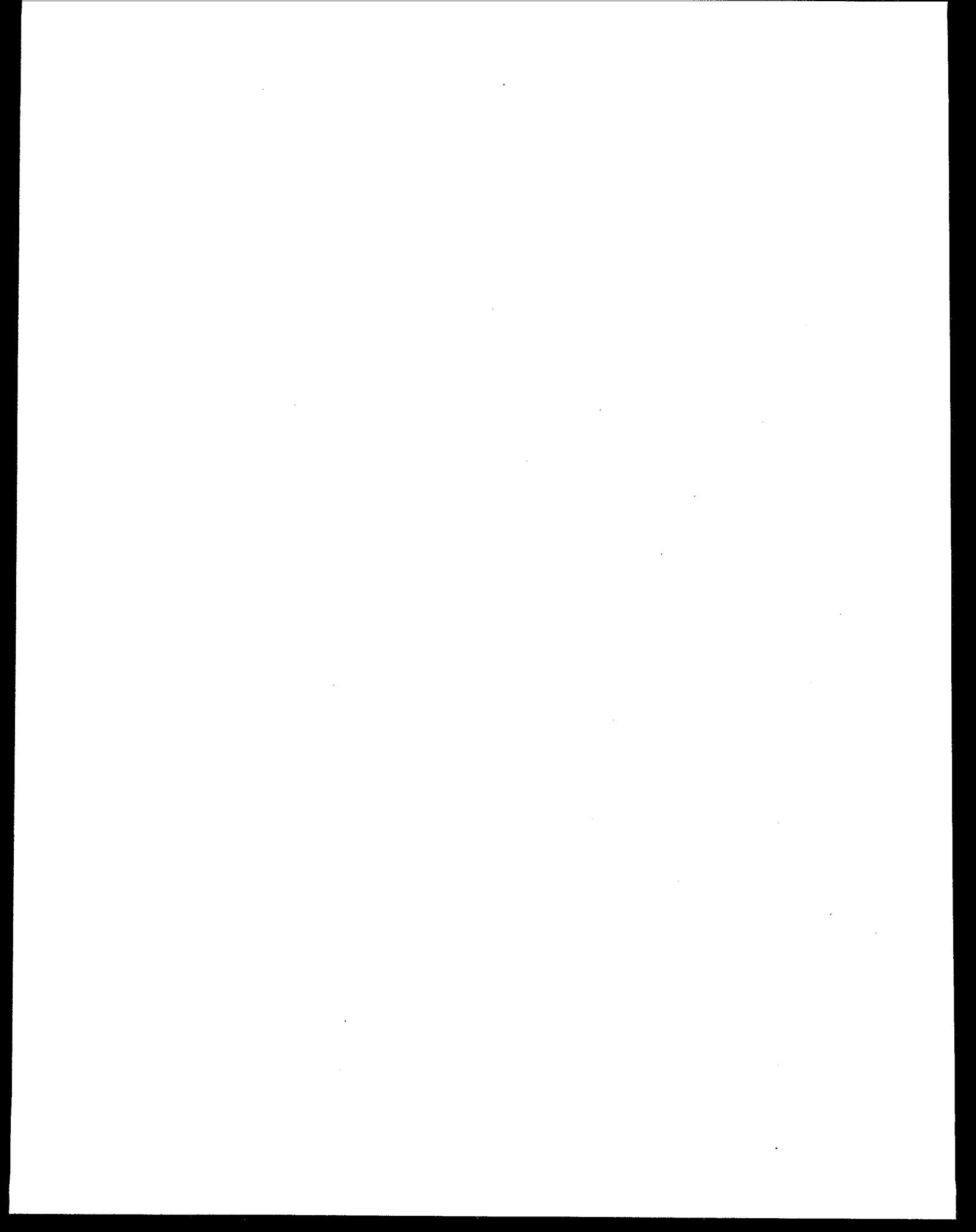
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Glossary of Terms and Abbreviations

ai	Active Ingredient
aPAD	Acute Population Adjusted Dose
AR	Anticipated Residue
ARI	Aggregate Risk Index
C/CPAS	Certified/Commercial Pesticide Applicator Survey
CFR	Code of Federal Regulations
ChEI	Cholinesterase inhibition
cPAD	Chronic Population Adjusted Dose
CSF	Confidential Statement of Formula
DCI	Data Call-In
DEEM	Dietary Exposure Evaluation Model
EC	Emulsifiable Concentrate Formulation
EDSP	Endocrine Disrupter Screening Program
EDSTAC	Endocrine Disrupter Screening and Testing Advisory Committee
EPA	Environmental Protection Agency
EP	End-Use Product
ExpoSAC	Exposure Science Advisory Committee
FIFRA	Federal Insecticide, Fungicide, and Rodenticide Act
FFDCA	Federal Food, Drug, and Cosmetic Act
FHEs	Food Handling Establishments
FSEs	Food Service Establishments
FQPA	Food Quality Protection Act
FR	Federal Register
GLN	Guideline Number
GC	Gas Chromatography
GC/MSD	Gas Chromatography/Mass Spectrometry Detection
HED	Health Effects Division
IDS	The OPP Incident Data System
IPM	Integrated Pest Management
IREL	Interim Reregistration Eligibility Decision
LC ₅₀	Median Lethal Concentration. A statistically derived concentration of a substance that can be expected to cause death in 50% of test animals. It is usually expressed as the weight of substance per weight or volume of water, air or feed, e.g., mg/l, mg/kg or ppm.
LD ₅₀	Median Lethal Dose. A statistically derived single dose that can be expected to cause death in 50% of the test animals when administered by the route indicated (oral, dermal, inhalation). It is expressed as a weight of substance per unit weight of animal, e.g., mg/kg.
LOD	Limit of Detection
LOAEL	Lowest Observed Adverse Effect Level
MCCEM	Multi-Chamber Concentration and Exposure Model
mg/kg/day	Milligram Per Kilogram Per Day
MOE	Margin of Exposure
MRID	Master Record Identification (number). EPA's system of recording and tracking studies submitted.
MUP	Manufacturing-Use Product

Glossary of Terms and Abbreviations

NA	Not Applicable
NHGUS	National Home and Garden Pesticide Use Survey
NOAEL	No Observed Adverse Effect Level
NPMA	National Pest Management Association
NPTN	National Pesticide Telecommunications Network
OPIDN	Organophosphate Induced Delayed Neurotoxicity
OP	Organophosphate
OPP	EPA Office of Pesticide Programs
OPPTS	EPA Office of Prevention, Pesticides and Toxic Substances
PAD	Population Adjusted Dose
PAM	Pesticide Analytical Manual
PCC	Pest Control Centers
PCO	Pest Control Operator
PHED	Pesticide Handler's Exposure Data
PPE	Personal Protective Equipment
ppm	Parts Per Million
QUA	Quantitative Usage Assessment
RBC	Red Blood Cell
RED	Reregistration Eligibility Decision
RfD	Reference Dose
SAP	Science Advisory Panel
SF	Safety Factor
SOP	Standard Operating Procedure
TGAI	Technical Grade Active Ingredient
TRAC	Tolerance Reassessment Advisory Committee
USDA	United States Department of Agriculture
UF	Uncertainty Factor
UV	Ultraviolet
WPS	Worker Protection Standard

Executive Summary

Propetamphos is an organophosphate (OP) insecticide registered by Wellmark International for the control of insects indoors. Target pests include ants, cockroaches, fleas, and termites in buildings and structures. Propetamphos may be applied at indoor residential and medical sites, such as homes, apartment buildings, stores, schools or hospitals. It may also be used in food service establishments, commercial, and industrial buildings. Based upon available pesticide usage information between the years 1990 and 1997, average annual domestic use at approximately 90,000 lbs of active ingredient per year.

EPA has completed its review of public comments and has revised the risk assessments and developed interim risk management decisions for propetamphos. The decisions outlined in this document do not include the final tolerance reassessment decision for propetamphos. For propetamphos, the only tolerance for residues in food commodities will remain unchanged. The final tolerance reassessment decision for this chemical will be issued once the cumulative assessment for all the OPs is complete. The Agency may need to pursue further risk management measures for propetamphos once the cumulative assessment is finalized.

The revised risk assessments are based on review of the required target data base supporting the use patterns of currently registered products and new information received. The Agency invited stakeholders to provide proposals, ideas or suggestions on appropriate interim mitigation measures before the Agency issued its risk mitigation decision on propetamphos. After considering the revised risks, as well as mitigation proposed by Wellmark International, the technical registrant of propetamphos, mitigation suggestions by the National Pest Management Association, and comments from other interested parties, EPA developed its interim risk management decision for uses of propetamphos that pose risks of concern. This decision is discussed fully in this document. Results of the risk assessments, and necessary label amendments to mitigate those risks, are presented in this interim reregistration eligibility decision (IRED).

Overall Risk Summary

EPA's human health risk assessment for propetamphos indicates some risk concerns. Dietary (food and drinking water) risk is not expected for all populations and is not of concern to the Agency. Additionally, risks are low to workers who mix, load, and apply propetamphos at commercial and residential use sites. However, there are post-application risk concerns for adults, and especially children entering areas treated with propetamphos. Also, there are no environmental risk concerns.

To mitigate risks of concern posed by the uses of propetamphos, EPA considered the mitigation proposal submitted by the technical registrant, as well as comments and mitigation suggestions from other interested parties, and has decided on a number of label amendments to address the residential risk concerns. Results of the risk assessments, and the necessary label amendments to mitigate those risks, are presented in this IRED.

Dietary (Food and Drinking Water)

There are no acute dietary (food) risks associated with propetamphos, and chronic (food) dietary exposure for propetamphos residues is not expected. Because propetamphos is only used indoors, exposure from drinking water sources are not expected and no drinking water assessment was conducted. Provided that the label is amended to require that food is covered or removed prior to treatment, no further mitigation measures are necessary at this time for dietary (food and drinking water) exposure to propetamphos.

Occupational

Based on a proposed maximum dilution rate of 0.5 % solution of active ingredient, and the addition of minimum personal protective equipment (PPE) consisting of single-layer clothing and chemical-resistant gloves, both dermal and inhalation risks to applicators are low and not of concern to the Agency.

Residential

Risks resulting from use of propetamphos in the residential setting are of concern. Combined risks (oral, inhalation, and dermal routes of exposure) for residential broadcast (flea) treatment using propetamphos are high for adults, and especially high for children. Combined risks (dermal and oral (hand-to-mouth)) for residential spot treatment, and crack and crevice applications using propetamphos are high for children, but dermal risks are low for adults. Because of these risk concerns, the registrant has agreed to voluntarily cancel all residential uses of propetamphos.

Chronic residential inhalation exposure to propetamphos is possible because of the termiticide use of this pesticide, however, dermal or incidental oral exposure is not anticipated based on the use pattern (gallery treatment). Based on a conservative exposure assessment, chronic inhalation risks are high for adults and children, and are of concern to the Agency. In response, the registrant has informed the Agency that it does not support the continued registration of termiticide use for propetamphos and has voluntarily canceled this use.

Ecological Risk

Ecological risks associated with propetamphos use are not of concern to the Agency. Because all currently registered uses of propetamphos are limited to indoor use, exposure to nontarget terrestrial and aquatic plants and animals are not expected.

For the uses of propetamphos, the Agency has determined that, with the adoption of all of the label amendments noted in this document, these uses may continue until the outcome of the cumulative assessment of all OPs has been decided.

The Agency is issuing this IRED for propetamphos, as announced in a Notice of Availability published in the *Federal Register*. This IRED includes guidance and time frames for complying with any necessary label changes for products containing propetamphos. There is no comment period for this document, and the time frames for compliance with the necessary changes outlined in this document are shorter than those given in previous REDs. As part of the process discussed by the Tolerance Reassessment Advisory Committee, which sought to open up the process to interested parties, the

Agency's risk assessments for propetamphos have already been subject to numerous public comment periods, and a further comment period for propetamphos was deemed unnecessary. Phase 6 of the pilot process does not include a public comment period; however, for some chemicals, the Agency may provide for another comment period, depending on the content of the risk management decision. With regard to complying with the requirements in this document, the Agency has shortened this time period so that the risks identified herein are mitigated as quickly as possible. Neither the tolerance reassessment nor the reregistration eligibility decision for propetamphos can be considered final, however, until the cumulative risk assessment for all OP pesticides is complete.

I. Introduction

The Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) was amended in 1988 to accelerate the reregistration of products with active ingredients registered prior to November 1, 1984. The amended act calls for the development and submission of data to support the reregistration of an active ingredient, as well as a review of all submitted data by the U.S. Environmental Protection Agency (referred to as EPA or "the Agency"). Reregistration involves a thorough review of the scientific database underlying a pesticide's registration. The purpose of the Agency's review is to reassess the potential hazards arising from the currently registered uses of the pesticide; to determine the need for additional data on health and environmental effects; and to determine whether the pesticide meets the "no unreasonable adverse effects" criteria of FIFRA.

On August 3, 1996, the Food Quality Protection Act of 1996 (FQPA) was signed into law. This Act amends FIFRA to require tolerance reassessment of all existing tolerances. The Agency decided that, for those chemicals that have tolerances and are undergoing reregistration, the tolerance reassessment will be initiated through this reregistration process. It also requires that by 2006, EPA must review all tolerances in effect on the day before the date of the enactment of the FQPA, which was August 3, 1996. FQPA also amends the Federal Food, Drug, and Cosmetic Act (FFDCA) to require a safety finding in tolerance reassessment based on factors including an assessment of cumulative effects of chemicals with a common mechanism of toxicity. Propetamphos belongs to a group of pesticides called OPs, which share a common mechanism of toxicity by affecting the nervous system by inhibiting cholinesterase. Although FQPA significantly affects the Agency's reregistration process, it does not amend any of the existing reregistration deadlines. Therefore, the Agency is continuing its reregistration program while it resolves the remaining issues associated with the implementation of FQPA.

This document presents the Agency's revised human health and ecological risk assessments; and the interim decision on the reregistration eligibility of propetamphos. It is intended to be only the first step in the reregistration process for propetamphos. The Agency will eventually proceed with its assessment of the cumulative risk of the OP pesticides and issue a final reregistration eligibility decision for propetamphos.

The implementation of FQPA has required the Agency to revisit some of its existing policies relating to the determination and regulation of dietary risk, and has also raised a number of new issues for which policies need to be created. These issues were refined and developed through collaboration between the Agency and the Tolerance Reassessment Advisory Committee (TRAC), which was composed of representatives from industry, environmental groups, and other interested parties. The TRAC identified the following science policy issues it believed were key to the implementation of FQPA and tolerance reassessment:

- Applying the FQPA 10-Fold Safety Factor
- Whether and How to Use "Monte Carlo" Analyses in Dietary Exposure Assessments
- How to Interpret "No Detectable Residues" in Dietary Exposure Assessments
- Refining Dietary (Food) Exposure Estimates

- Refining Dietary (Drinking Water) Exposure Estimates
- Assessing Residential Exposure
- Aggregating Exposure from all Non-Occupational Sources
- How to Conduct a Cumulative Risk Assessment for Organophosphate or Other Pesticides with a Common Mechanism of Toxicity
- Selection of Appropriate Toxicity Endpoints for Risk Assessments of Organophosphates
- Whether and How to Use Data Derived from Human Studies

The process developed by the TRAC calls for EPA to provide one or more documents for public comment on each of the policy issues described above. Each of these issues is evolving and in a different stage of refinement. Some issue papers have already been published for comment in the Federal Register and others will be published shortly.

In addition to the policy issues that resulted from the TRAC process, the Agency issued on September 29, 2000 a Pesticide Registration Notice (PR 2000-9) that presents EPA's approach for managing risks from OP pesticides to occupational users. The Worker PR Notice describes the Agency's baseline approach to managing risks to handlers and workers of OP pesticides. Generally, basic protective measures such as closed mixing and loading systems, enclosed cab equipment, or protective clothing, as well as increased restricted entry intervals will be necessary for most uses where current risk assessments indicate a risk and such protective measures are feasible. The policy also states that the Agency will assess each pesticide individually, and based upon the risk assessment, determine the need for specific measures tailored to the potential risks of the chemical. The measures included in this IRED are consistent with that draft Pesticide Registration Notice.

This document consists of six sections. Section I contains the regulatory framework for reregistration, as well as descriptions of the process developed by TRAC for public comment on science policy issues for the OP pesticides and the worker risk management PR notice. Section II provides a profile of the use and usage of the chemical. Section III gives an overview of the revised human health and environmental effects risk assessments resulting from public comments and other information. Section IV presents the Agency's interim decision on reregistration eligibility and risk management decisions. Section V summarizes the label changes necessary to implement the risk mitigation measures outlined in Section IV. Section VI provides information on how to access related documents. Finally, the Appendices A list the use patterns eligible for reregistration; B, the necessary studies for reregistration; and C, the bibliography listing citations of all studies considered relevant to the IRED document. The revised risk assessments are not included in this document, but are available on the Agency's web page www.epa.gov/oppsrrd1/op, and in the Public Docket.

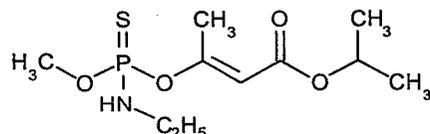
II. Chemical Overview

A. Regulatory History

Propetamphos technical was first registered to Sandoz Crop Protection (Company No. 11273) by the Agency in December 1980. In March 1981, the first end-use product was registered as a non-food/non-feed use for indoor structural pest control. In 1983, a food/feed use in food/feed handling establishments was registered. This permitted propetamphos to be used in food processing facilities (mills, dairies, etc.), meat and poultry plants, food processing facilities (packing, canning, bottling, etc.), food and/or feed warehouses, and food service establishments. The regulations to permit residues in food/feed resulting from application in food handling establishment were announced in the Federal Register Notice of November 23, 1983 (48 FR 52902). The registrations were transferred to Zoecon Industries (Company No. 2724) in 1984. On June 23, 1997, the company name was subsequently changed to Wellmark International (retaining the same company number of 2724).

In 1998, all propetamphos labels were amended to delete the food and feed handling establishment uses, except food service establishment uses where food is prepared and served (e.g., restaurants).

B. Chemical Identification



Propetamphos is a yellowish oily liquid with a boiling point of 87-89°C. Propetamphos is practically insoluble in water (110 mg/L at 20° C), but is completely miscible in most organic solvents including acetone, chloroform, diethyl ether, ethanol, hexane, and xylene. The vapor pressure of propetamphos is 2.6×10^{-7} mm Hg at 25°C.

- Chemical Name: ((e)-)-methylethyl 3-[[[(ethylamino)methoxyphosphinothioyl]oxy]-2-butenate)
- Common Name: Propetamphos
- Chemical family: Organophosphate
- CAS registry number: 31218-83-4
- OPP chemical code: 113601

- Empirical formula: $C_{10}H_{20}NO_4PS$
- Molecular weight: 281.3 g
- Trade and other names: Catalyst™, Saffrotin™, Zoecon™
- Basic manufacturer: Wellmark International

C. Use Profile

Type of Pesticide

Propetamphos is an insecticide used for indoor structural pest control. The following is a summary of propetamphos use sites:

Indoor Food/Non-Food: There are no food uses of propetamphos, however, propetamphos may be used in food service establishments. Application is limited to spot and crack and crevice treatments. Food service establishments may include restaurants, cafeterias, taverns, delicatessens, mess halls, school and institutional dining areas, hospitals, mobile canteens, vending machines, groceries and markets. Indoor non-residential non-food areas (may include eating establishments, office buildings, commercial and industrial premises and equipment) where there is no contact with food, and where no food processing, packing, and no food and/or feed warehousing occurs.

Residential: Propetamphos is used inside residential homes on carpets (limited to broadcast applications for fleas) and other surfaces, on hard surfaces (e.g., floors, counters, walls), spot applications (areas up to 2' X 2'), crack and crevice (primarily for cockroach control), and galleries for termites (e.g., crawl spaces, foundations).

Public Health: According to the National Center of Infectious Diseases of the Centers for Disease Control and Prevention, "propetamphos is not used regularly as an insecticide in public health programs in the United States." Propetamphos is not on the Agency's proposed listing of Public Health Pesticides.

Other Non-Food: Propetamphos is used in pet living/sleeping quarters, and in institutional/medical and veterinary facilities.

Target Pests

Propetamphos is used to control silverfish, cockroaches, earwigs, beetles, fleas, ants, termites, ticks, other indoor insects, and spiders.

Formulation Types

There are three current registered products that contain propetamphos: one manufacturing-use product (MUP) (EPA Reg. No. 2724-313) containing 90% active ingredient (ai), and two end-use products (EPs). One EP consists of a 46.5% ai emulsifiable concentrate (Zoecon 8718 EW, EPA Reg. No. 2724-449) formulation, and the other is an 18.9% ai soluble concentrate (Zoecon 9001 EW, EPA

Reg. No. 2724-450) formulation. Only Zoecon 9001 EW is currently manufactured and used in the United States, whereas Zoecon 8718 EW is manufactured for export only and has never been sold in the United States. The registrant has voluntarily canceled the Zoecon 8718 EW product registration. There are no section 24(c) special local need registered propetamphos products or uses.

Method and Rates of Application

Propetamphos is applied as a water dilution through a compressed air sprayer, often with a low pressure hand wand. Termite applications use a crack and crevice or injection tube nozzle. For general surface application, propetamphos is applied at a rate of 0.5% ai in a fine spray. Approximately 1 gallon of finished spray is used per 1500 square feet for broadcast application. For spot, and crack and crevice applications, propetamphos is applied as a 0.5 to 1.0 % ai solution. For spray applications, propetamphos is applied as a 1.0% ai spray. Gallery (termite) applications are applied at a 1.0% ai spray using low pressure equipment. For all applications, additional treatment may be repeated as needed, but not more than once every 7 days, and not to exceed 2 treatments in a 30-day period.

Use Classification

The 46.5 % ai emulsifiable concentrate formulation (Zoecon 8718 EW, EPA Reg. No. 2724-449) is classified as a restricted-use product, due to acute oral and dermal toxicity. The 18.9 % ai soluble concentrate product (Zoecon 9001 EW, EPA Reg. No. 2724-450) is not classified as a restricted use product.

D. Estimated Usage of Pesticide

This section summarizes the best estimates available for the pesticide uses of propetamphos, based on available pesticide usage information between the years 1990 and 1997. Total annual usage has been estimated at 90,000 lbs ai/year. About 70% of this total annual propetamphos usage is applied to residential areas (by Pest Control Operators (PCOs)), while the remaining 30% is applied to various commercial sites. About 90% of application is carried out by PCOs, while most of the remaining 10% of applications are by not-for-hire applicators, such as maintenance workers.

An estimated 1.2% of all residences, and 3.3% of all food handling establishments are treated with propetamphos each year (food service establishments are a subset of food handling establishments, and annual treatment based on this use alone would be less than 3.3%). Estimates of propetamphos use (lbs ai) are based on the 1993 Certified/Commercial Pesticide Applicator Survey (C/CPAS), 1992 National Home and Garden Pesticide Use Survey (NHGPUS), and other proprietary data sources. The quantitative usage assessment for propetamphos is provided in Table 1.

Table 1. Quantitative Usage Assessment for Propetamphos (Based on 1990-1997 data)^a

Use Site	Propetamphos		Area Treated		Calculated Percent Treated		Total Pounds ai Applied (000)	Application Rates (lbs ai) ^c		
	Total Units ^b		Likely Average	Likely Maximum	Likely Average	Likely Maximum		Likely Average	lbs ai/yr/unit	#app/yr
Residential	90 Million Homes		1.1 Million Sq. ft.	3.3 Million Sq. ft.	1.2%	3.7%	63	0.059	1	0.059
Commercial Buildings Total	63 Billion Sq. ft.									
Food Handling Establishments	1.6 Billion Sq. ft.		55 Million Sq. ft.	169 Million Sq. ft.	3.3%	10.1%	22	0.586	10	0.059
Other Commercial Buildings	61.4 Billion Sq. ft.		14 Million Sq. ft.	41 Million Sq. ft.	0.8%	2.4%	5	0.586	10	0.059
Total							90			

^a Estimates of propetamphos use (lbs ai) are based on the 1993 Certified/Commercial Pesticide Applicator Survey (C/CPAS), 1992 National Home and Garden Pesticide Use Survey (NHGPUS), and other proprietary data sources.

^b Based on Statistical Abstract of the United States, 1992, Total Number of Occupied Housing Units Table #1223. Total Number of Commercial Buildings is 4,523 million.

^c Residential application rates based on ~1,500 sq. ft./home.

III. Summary of Propetamphos Risk Assessment

Following is a summary of EPA's revised human health and ecological risk findings and conclusions for the OP pesticide propetamphos, as fully presented in the documents: *Updated Revised Preliminary Risk Assessment: Propetamphos*, June 7, 1999; *Updated Occupational and Residential Dermal Exposure Assessment addendum*, September 27, 2000; *EFED Integrated Science Chapter for Propetamphos*, December 2, 1997; and *Propetamphos Errata Sheet For EFED Chapter*, January 12, 1999. The purpose of this summary is to assist the reader by identifying the key features and findings of these risk assessments, and to better understand the conclusions reached in the assessments.

The risk assessment summaries presented here form the basis of the Agency's risk management decision for propetamphos only; the Agency must complete a cumulative assessment of the risks of all the OP pesticides before any final decisions can be made.

A. Human Health Risk Assessment

EPA issued its preliminary risk assessments for propetamphos on December 15, 1998. In response to comments and studies submitted during Phase 3, the risk assessments were updated and refined and were included in the revised risk assessment and addendum, dated June 7, 1999 and September 27, 2000, respectively. This risk assessment serves as the basis for this IRED. Major revisions to the human health risk assessment are listed below:

1. Dietary Risk from Food

a. Toxicity

The Agency has reviewed all submitted toxicity studies and has determined that the toxicity database for propetamphos is complete, and that it supports an interim reregistration eligibility determination for all currently registered uses. Further details on the toxicity of propetamphos can be found in the June 7, 1999 Human Health Risk Assessment and the September 27, 2000 addendum. A brief overview of the studies used for the dietary risk assessment is outlined in Table 2.

The toxicity data base provides evidence that cholinesterase inhibition is the most sensitive toxicological observation in laboratory animals. Propetamphos, like other OPs, has anticholinesterase and neurotoxic effects in all species tested, including dogs, rabbits, rats, and mice. Signs of neurotoxicity, such as muscle tremors, fasciculations and cholinesterase inhibition (ChEI) have been observed in acute, subchronic, chronic and developmental/reproductive toxicity studies. Propetamphos did not, however, induce organophosphate induced delayed neurotoxicity in hens when orally dosed as part of a delayed neurotoxicity study. Propetamphos is acutely toxic via the oral route of exposure and is classified as a toxicity category II, based on an oral rat study (MRID 41607417) with a Lethal Dose (LD_{50}) = 116.1 mg/kg in males and Lethal Dose (LD_{50}) = 96.4 mg/kg in females.

The subchronic and chronic toxicity studies demonstrate that propetamphos inhibits cholinesterase activity in plasma, red blood cells (RBC), and/or brain in rats, dogs, and mice. Clinical signs associated with cholinesterase activity inhibition were observed and included ataxia, tremors, salivation, constricted pupils, and dyspnea. Propetamphos was not toxic to the visual system of dogs in a chronic toxicity study.

There is no evidence of increased susceptibility for infants and children, based on adequate developmental toxicity studies in rats and rabbits and an adequate two-generation reproduction study in rats. Following *in utero* exposures, no developmental toxicity was seen in rats. In the rabbit study, developmental toxicity occurred only at a dose that also caused maternal toxicity. In the two-generation rat reproductive toxicity study, offspring toxicity was only seen in the presence of maternal systemic toxicity.

The Agency has concluded that there are no metabolites of toxicological concern and that the residues to be regulated in food commodities will consist of propetamphos *per se*.

b. FQPA Safety Factor

The FQPA Safety Factor Committee determined that the 10x FQPA safety factor should be removed (equivalent to 1x), based on the following factors:

- In prenatal developmental toxicity studies following *in utero* exposure in rats and rabbits, there was no evidence of developmental effects being produced in fetuses at lower doses as compared to maternal animals nor was there evidence of an increase in severity of effects at or below maternally toxic doses.
- In the pre/post natal two-generation reproduction study in rats, there was no evidence of enhanced susceptibility in pups when compared to adults (i.e., effects noted in offspring occurred at maternally toxic doses or higher).
- There was no evidence of abnormalities in the development of the fetal nervous system in the pre/post natal studies.
- There was no concern for positive neurological effects from the available neurotoxicity studies or for histopathology in the central nervous system from the other toxicological studies (e.g., subchronic rat, chronic dog, chronic rat and mouse).
- The toxicology data base is complete, and there are no data gaps according to the Subdivision F Guideline requirements.
- Adequate actual data, surrogate data, and/or modeling outputs are available to satisfactorily assess dietary and residential exposure.

c. Population Adjusted Dose (PAD)

The PAD is a term that characterizes the dietary risk of a chemical, and reflects the Reference Dose (RfD), either acute or chronic, that has been adjusted to account for the FQPA safety factor (i.e., RfD ÷ FQPA safety factor). The RfD is the level of daily exposure to a pesticide residue which is believed to have no significant deleterious effects. In the case of propetamphos, the FQPA safety factor is 1; therefore, the acute and chronic RfDs are equal to the acute and chronic PADs, respectively. A risk estimate that is less than 100% of the acute or chronic PAD does not exceed the Agency's risk concern.

d. Hazard Determination

Cholinesterase inhibition was the toxicity endpoint chosen for the acute and chronic dietary endpoints. For risk assessments describing acute oral exposures, the dose selected was the no observed adverse effect level (NOAEL) of 0.05 mg/kg/day based on brain cholinesterase inhibition at a lowest observed adverse effect level (LOAEL) of 0.1 mg/kg/day observed in the 4-week oral toxicity study in mice. An uncertainty factor of 100 (10x for inter-species extrapolation and 10x for intra-species variation) and an FQPA safety factor of 1x was applied to the NOAEL, therefore, the acute PAD is 0.0005 mg/kg/day.

For the chronic dietary risk assessment, the dose selected for risk assessment was the NOAEL of 0.05 mg/kg/day based on plasma cholinesterase inhibition at a LOAEL of 0.1 mg/kg/day observed in the 1-year chronic toxicity and carcinogenicity study in mice. An uncertainty factor of 100 (10x for inter-species extrapolation and 10x for intra-species variation) and an FQPA safety factor of 1x was applied to the NOAEL, therefore, the chronic PAD is 0.0005 mg/kg/day. This toxicity and endpoint selection information is summarized in Table 2.

Table 2. Toxicology Endpoints for Dietary Risk

Exposure Scenario	Dose (mg/kg/day)	Endpoint	UF	FQPA SF	PAD (mg/kg/day)
Acute Dietary	NOAEL = 0.05 mg/kg/day (4-week oral mouse study)	Brain cholinesterase inhibition (ChEI)	100	1	0.0005
Chronic Dietary	NOAEL = 0.05 mg/kg/day (mouse chronic feeding/ carcinogenicity study)	Brain, RBC, and plasma ChEI	100	1	0.0005

e. Cancer Determination

The Agency has classified propetamphos as "not likely to be a human carcinogen." This classification is based on the lack of evidence of carcinogenicity in male and female rats and in male and female mice when tested at dose levels that caused cholinesterase inhibition and, therefore, were judged to be adequate to assess the carcinogenic potential of propetamphos. Additionally, propetamphos was non-mutagenic both *in vivo* and *in vitro*.

f. Acute Dietary (Food) Risk

Acute dietary risk considers all food that is eaten in one day (in this instance, by the individual who consumed the most) and maximum, or high-end residue values in the food. It is the Agency's policy that acute dietary exposure analysis does not take into account food handling establishments. Residues resulting from pesticide use in food handling establishments (or food service establishments—a subset of food handling establishments) are not likely to result in incidental contamination of all foods at tolerance levels on a uniform and consistent basis, and not all foods consumed by an individual in a day are likely to have come from a food handling establishment. Therefore, an acute dietary (food) exposure and risk assessment is not needed for pesticides having only food handling establishment tolerances, such as propetamphos.

g. Chronic Dietary (Food) Risk

Because a tolerance is required for pesticides used for treatments of food service establishments, the Agency assesses chronic dietary (food) exposure, due to concerns of inadvertent residues on food in food service establishments when sprayed applications are made. Chronic dietary (food) exposure is calculated using the average consumption value for food and average residue values on those foods over a 70-year lifetime. Chronic dietary exposure is then compared with the chronic PAD (cPAD). The cPAD is the dose at which an individual could be exposed over the course of a lifetime and no adverse health effects would be expected. The chronic dietary risk estimate is expressed as percent of the cPAD. A risk estimate that is less than 100% of the cPAD does not exceed the Agency's level of risk concern.

For propetamphos, a Tier III chronic dietary exposure assessment was conducted based upon anticipated residues and the estimate of 11% of food handling establishments being treated with propetamphos. Magnitude of the residue data showed that propetamphos residues were non-detectable (<0.01 ppm) in/on foods that were held in closed containers. Therefore, anticipated residues of 0.005 ppm ($\frac{1}{2}$ Limit Of Detection (LOD)) were used in the Tier III chronic dietary assessment.

Also, this chronic dietary assessment was conducted prior to refinements to the quantitative usage assessment (QUA) in Table 1. Since the time of this analysis, the percent of food handling establishments treated with propetamphos has been lowered from 11% to 3.3%. Incorporating this refined usage information into the analysis will lower the chronic dietary risks. Presently, the chronic dietary risks are low, thus, further refinements to the chronic dietary analysis to reflect this usage information were not conducted.

The Tier III chronic analysis, based on non-detectable residues on foods held in covered containers during pesticide application, indicates that chronic dietary (food) exposure and risk estimates for propetamphos are below the Agency's level of concern. Refer to Table 3 for the propetamphos chronic dietary risk estimates.

Table 3. Chronic Dietary Risk of Propetamphos^a For Covered Food

Population Subgroups	Exposure (mg/kg/day)	Chronic Risk (% cPAD)
U.S. Population	0.000030	6 %
Non-nursing infants (< 1 year old)	0.000104	21 %
Children (1-6 years old)	0.000061	12 %

^a Expressed in terms of propetamphos *per se*.

As indicated above, the chronic dietary assessment is based on no detectable residues. It is the Agency's policy to use ½ LOD, which is 0.005 ppm for propetamphos, to estimate dietary risk when no residues are detected. Realistically, provided foods are covered or removed prior to treatment of the area, actual chronic (food) dietary risk for treatment in food service establishments may be as low as zero.

2. Dietary Risk from Drinking Water

Propetamphos is presently not registered for use on food/feed crops, potable water, or aquatic food, and is not expected to be released to water. Therefore, exposure from drinking water sources is not expected and no drinking water risk assessment was conducted.

3. Occupational and Residential Risk

Occupational workers can be exposed to propetamphos through mixing, loading, and applying, or re-entering treated sites. Residents or homeowners can be exposed to propetamphos through entering or performing other activities in treated areas. Occupational handlers of propetamphos include pest control operators (PCOs) who mix, load, and apply pesticides. Risk for all of these potentially exposed populations is measured by a Margin of Exposure (MOE), which determines how close the occupational or residential exposure comes to a NOAEL, or, if necessary, by the Aggregate Risk Index (ARI), which is a way to aggregate MOEs that have dissimilar target MOEs. For propetamphos, dermal and oral MOEs greater than 100, inhalation MOEs greater than 300, and ARIs that are greater than 1.0 are not of concern to the Agency.

a. Toxicity

In summary, propetamphos is acutely toxic *via* the oral and dermal routes of exposure, has low inhalation toxicity, is not a skin or eye irritant, and is not a dermal sensitizer. Propetamphos, technical, is placed in toxicity category II for acute oral and dermal toxicity, category III for acute inhalation, and category IV for acute eye and skin irritation. A summary of the acute toxicity profile of propetamphos is provided in Table 4.

Table 4. Acute Toxicity Profile of Propetamphos

Study Type	MRID No.	Results	Toxicity Category
Acute Oral-Rat	41607417	LD ₅₀ = 116.1 mg/kg, males LD ₅₀ = 96.4 mg/kg, females	II
Acute Dermal-Rabbit	41607418	LD ₅₀ = 486.4 mg/kg, both sexes combined	II
Acute Inhalation-Rat	41529301	LC ₅₀ = 1.5 mg/L, males LC ₅₀ = 0.69 mg/L, females	III
Primary Eye Irritation	41607419	Negative for eye irritation	IV
Primary Skin Irritation	41607420	Negative for dermal irritation	IV
Dermal Sensitization	41607412	Negative for dermal sensitization	N/A

b. Hazard Determination

For the short- and intermediate-term (< 30 days) dermal risk assessment, the dose selected was the NOAEL of 1.25 mg/kg/day, based on brain cholinesterase inhibition at a LOAEL of 2.5 mg/kg/day observed in the 21-day dermal toxicity study in rats. Due to concerns of rapid detoxification of some OPs when rabbits are used for dermal toxicity tests, and thereby sometimes underestimating risk, the registrant conducted a 21-day dermal toxicity study in rats. The Agency has recently received the 21-day dermal toxicity study in rats, and has conducted a preliminary review. The Agency is currently conducting a final review of the study and is confident that the NOAEL is 1.25 mg/kg/day and will be selected by the Agency's Hazard Identification and Assessment Review Committee. An MOE of greater than 100 (10x for inter-species extrapolation and 10x for intra-species variation) does not exceed the Agency's level of concern for these risk assessments. Because a dermal study was used to determine the toxicity endpoint, a dermal absorption factor is not necessary.

For the intermediate- (> 30 days) and long-term dermal risk assessment, the dose selected was the NOAEL of 0.08 mg/kg/day, based on RBC cholinesterase inhibition at a LOAEL of 0.17 mg/kg/day observed in the 6-month subchronic toxicity study in dogs. An MOE of greater than 100 (10x for inter-species extrapolation and 10x for intra-species variation) does not exceed the Agency's level of concern for these risk assessments. However, based on current use patterns, it is expected that applicators will not be continuously exposed to propetamphos for greater than 30 days. Therefore, the dermal risk assessment is based on the short- and intermediate-term (< 30 days) toxicity endpoint discussed above and listed in Table 5.

For inhalation exposure (of any duration), the dose selected for risk assessment was the LOAEL of 4.7 mg/kg/day based on plasma cholinesterase inhibition at this dose in a 14-day rat inhalation toxicity study. Because a NOAEL was not established in this study, an extra uncertainty factor of 3x was applied. Therefore, a MOE of greater than 300 (10x for inter-species extrapolation, 10x for intra-species variation, and 3x for use of LOAEL) does not exceed the Agency's level of concern for these risk assessments. A summary of the toxicological endpoints, and other factors used in the occupational and residential risk assessments for propetamphos are listed below in Table 5.

For the oral ingestion (children) route of exposure, the toxicological endpoint was based on a 4-week oral mouse study. This study is further described in Section III. A.1.d Hazard Determination for human dietary risk (see Table 2).

Table 5. Summary of Toxicological Endpoints for Occupational and Residential Risks

Assessment	Dose (mg/kg/day)	Endpoint	Study	Absorption factor	Target MOE
Short- and Intermediate term dermal (<30 days)	NOAEL = 1.25	Brain cholinesterase inhibition (ChEI)	21-day dermal rat	N/A	100
Intermediate-term dermal (>30 days)	NOAEL = 0.08	RBC ChEI at 4 weeks. This is supported by a NOAEL of 0.05 mg/kg/day for brain ChEI in a 4-week mouse study	6-month oral dog study	100	100
Long-term dermal (>180 days)					
Oral ingestion (children)	NOAEL = 0.05	Brain ChEI	4 week oral mice	N/A	100
Inhalation (Any time period)	LOAEL = 4.7	Plasma ChEI in both sexes. No NOAEL established.	14-day inhalation rat	100	300

c. Exposure

Occupational Exposure

Chemical-specific exposure data for handlers were not available for propetamphos, so risks to pesticide handlers were assessed from data derived from the Pesticide Handlers Exposure Database (PHED), using standard assumptions based on the exposure scenarios and types of equipment supported by current labeling. The basic premise of PHED is that the chemical formulation (i.e., soluble concentrate) and method of application are the major determinants of pesticide exposure, rather than chemical specific properties. PHED is a database containing exposure data for surrogate chemicals used in a number of different formulations and application scenarios. The occupational exposure assessment was conducted for a worker who not only mixes, but loads and applies this insecticide in one day (with the assumption that one worker may perform all three tasks in a day and, therefore, will have additive exposures from all three tasks). The quality of the data and exposure factors represent the best sources of data currently available to the Agency for completing these kinds of assessments. The exposure factors (e.g., body weight, amount ai treated per day, protection factors, etc.) are all standard values that have been used by the Agency over several years. For more information about PHED and the data used for each scenario, see the *Updated Revised Preliminary Risk Assessment: Propetamphos*, June 7, 1999 and the *Updated Occupational and Residential Dermal Exposure Assessment* addendum, September 27, 2000, which is available in the public docket and on the Internet.

Anticipated use patterns and application methods, range of application rates, and typical rate of coverage were derived from current labeling. Application rates specified on propetamphos labels range from 0.5 to 1.0% concentration of active ingredient per gallon of finished solution. One gallon of finished

spray (at a diluted solution of 0.5%) will typically cover 1500 square feet for broadcast application. There are no restrictions on the label stipulating how much product may be used in any given day.

Occupational handler exposure assessments are conducted by the Agency using different levels of personal protection. The Agency typically evaluates all exposures with minimal protection and then adds additional protective measures using a tiered approach to obtain an appropriate MOE (i.e., going from minimal to maximum levels of protection). The lowest tier is represented by the baseline exposure scenario, followed by, if needed (i.e., MOEs are less than 100 for dermal exposure and MOEs are less than 300 for inhalation exposure), increasing levels of risk mitigation to include personal protective equipment (PPE). Currently, there is no requirement for PPE on the propetamphos labels. The levels of protection that formed the basis for calculations of occupational exposure from propetamphos activities include:

- Baseline: Long-sleeved shirt and long pants, shoes and socks.
- Minimum PPE: Baseline + chemical resistant gloves.
- Maximum PPE: Coveralls over long-sleeved shirt and long pants, shoes and socks, and chemical-resistant gloves.

Residential Exposure

Residential exposure is assessed by determining how a person could come into contact with a pesticide in and around a home. There are no registered homeowner uses for propetamphos at the present time. However, post-application exposure is possible as a result of PCO indoor broadcast (flea control) or spot, and crack and crevice (e.g., cockroach, ant, cricket control) applications. Since propetamphos is used strictly indoors, and only applied by PCOs, residential exposure to propetamphos takes place when people come into contact with post-application residues either by touching, breathing, or ingesting them. Therefore, residential post-application exposure scenarios were considered for the broadcast, spot, and crack and crevice use scenarios.

Where available, chemical-specific post-application exposure data have been used for these scenarios. When no chemical-specific data is available, the post-application exposure assessment is based on the newly proposed Standard Operating Procedures (SOPs) for Residential Exposure Assessments and recommended approaches by the Agency's Health Effects Division (HED), Exposure Science Advisory Committee (ExpoSAC). The newly proposed SOPs for Residential Exposure Assessments alter the residential post-application scenario assumptions. Compared with the previous SOPs, the newly proposed SOPs are expected to better represent residential exposure, but are still considered to be high-end, screening level assumptions.

For the post-application scenario resulting from the indoor broadcast use (carpet treatment for flea control), residential exposures were estimated using a chemical-specific (Jazzercise) post-application study. Because there are no chemical-specific studies measuring post-application exposures resulting from the spot, and crack and crevice use of propetamphos, the proposed Residential SOPs were used to assess exposure.

To assess chronic inhalation exposure resulting from the termiticide use, the Agency utilized the Multi-Chamber Concentration and Exposure Model (MCCEM), as outlined in the SOPs for Residential Exposure Assessments. The MCCEM is a model that is capable of calculating indoor air concentrations and the corresponding exposure assessments for chronic scenarios. The MCCEM contains a database of various default house data that are needed to complete each calculation, such as air exchange rates, geographically based inter-room air flows, and house/room volumes.

d. Occupational and Residential Risk Summary

Occupational Risk

An occupational exposure assessment was conducted for a worker who mixes, loads, and applies propetamphos (one worker is considered to perform all three tasks). The Aggregate Risk Index (ARI) is a way to aggregate MOEs that have dissimilar target MOEs. Because the target MOE for dermal exposure is 100 and the target MOE for inhalation exposure is 300, an ARI method to combine the MOEs is necessary. ARIs that are greater than 1.0 are not of concern to the Agency. As indicated in Table 6, the ARIs are greater than 1.0 for all occupational use scenarios and are, therefore, not of concern.

Table 6. Occupational Mixer/Loader/Applicator Risk Assessment

Use Scenario		Dermal MOEs ^a		Inhalation MOEs ^b	ARIs ^c	
		Minimum PPE	Maximum PPE	No Respirator	Minimum PPE	Maximum PPE
Low Pressure Handwand, Broadcast or Crack and Crevice	5 homes/day, 0.5% ai	625	740	>8400	>5.1	>5.8
	10 apartments/day, 0.5% ai	310	370	>8400	>2.8	>3.3
	5 homes/day, 1.0% ai	310	370	>8400	>2.8	>3.3
	10 apartments/day, 1.0% ai	160	180	8400	1.5	1.7
Gallery Injection Treatment for Termites	1 gal, 1% ai	3000	4500	>6.3E5	>30	>45
	2 gal, 1% ai	1500	2200	>6.3E5	>15	>22
	3 gal, 1% ai	1000	1500	6.3E5	10	15

^a Dermal NOAEL = 1.25 mg/kg/day, (21-day dermal rat study).

^b Inhalation NOAEL = 0.027 mg/L = 4.7 mg/kg/d (14 day inhalation toxicity study in rats).

^c ARI < 1 is of concern to the Agency.

Residential Risk

Most residential exposures to propetamphos are from entering or performing some activity on treated areas. Post-application exposure was assessed on the same day the pesticide was applied, since it was assumed that homeowners could contact treated areas immediately after application.

Similarly with the occupational risk assessment, because the target MOEs for propetamphos are 100 for dermal and oral exposure, and 300 for inhalation, an ARI method to combine the MOEs for residential risk is necessary. ARIs that are greater than 1.0 are not of concern to the Agency.

Broadcast Application

As indicated in Table 7, the dermal MOEs for both adults and children are significantly below the target MOE of 100. Incidental oral exposures (hand-to-mouth) for children is also below the target MOE of 100. However, inhalation MOEs are above the target MOE of 300 for adults and children. Therefore, the combined (ARI) exposure from broadcast carpet treatment is less than 1.0 and of concern to the Agency. Because a chemical-specific exposure study is available (Jazzersize study using 0.5% Saftrotin solution), the Agency has a high level of confidence in these exposure and risk estimates. A summary of these risk estimates are provided in Table 7.

Table 7. Summary of Dermal, Inhalation, and Oral MOEs for Broadcast Carpet Treatment

Population	Dermal MOE ^a	Inhalation MOE ^b	Oral MOE ^c	ARI ^d
Adults	10	3900	N/A	0.1
Children	2	1400	0.4	0.003

^a Dermal NOAEL = 1.25 mg/kg/day, (21-day dermal rat study).

^b Inhalation NOAEL = 0.027 mg/L = 4.7 mg/kg/d (14 day inhalation toxicity study in rats).

^c Acute Oral NOAEL = 0.05 mg/kg/d (4 week oral toxicity study in mice).

^d ARI < 1 is of concern to the Agency.

Spot, and Crack and Crevice Application

Chemical specific data were not available depicting exposures resulting from the spot, and crack and crevice application. The residential post-application exposure assessment for the crack and crevice/spot treatment application of propetamphos was conducted using the proposed revisions to the Residential Exposure Assessment SOPs.

The following considerations and assumptions were used to estimate post-application exposure and risk from spot, and crack and crevice applications, based on the proposed reduced maximum application rate and current label instructions for spot, and crack and crevice (i.e., spot applications to baseboards):

- a proposed maximum rate of dilution of 0.5% ai solution
- one quart of diluted material would be used to treat a 2,500 ft² home
- based on chemical-specific data, only 0.5% of the residue on carpet is dislodgeable using the hand roller method
- only 1% of the residue is dislodgeable on hard surfaces
- post-application exposure was assessed on the same day the pesticide was applied, since it is assumed that homeowners could contact the treated surfaces immediately after application.
- the duration of exposure is assumed to be 8 hours per day for carpet and 4 hours for hard surfaces
- the mean dermal transfer coefficient was assumed to be 16,700 cm²/hr for adults and 6,000 cm²/hr for children
- for children incidental hand-to-mouth exposures, the surface area of the hand put into the mouth was assumed to be 20 cm² with 20 events/hr, and this activity lasts 2 hours

At the proposed maximum dilution rate of 0.5% ai solution, the dermal MOEs for adults are above the target MOE of 100. Dermal and oral (hand-to-mouth) MOEs for children are below the target MOE

of 100. Because the dermal and oral target MOEs are the same (100), the MOEs for both routes of exposure can be combined to assess risks to children. Therefore, dermal risks to adults are not of concern, and risks to children are of concern to the Agency. Table 8 summarizes the risk results from spot, and crack and crevice applications of propetamphos.

Table 8. Residential Post-Application Risks from Crack and Crevice/Spot Treatment Use

Scenario	Population	Dermal MOE ^a	Oral MOE ^b	Combined MOE
Exposure from residue deposition on carpet	Children	80	50	31
	Adult	140	NA	
Exposure from residue deposition on hard surfaces	Children	80	23	18
	Adult	140	NA	

^a Dermal MOE based on NOAEL = 1.25 mg/kg/day (21-day rat dermal toxicity study)

^b Oral MOEs based on NOAEL = 0.05 mg/kg/day (4-week oral mouse study)

Termiticide Application

Chronic residential inhalation exposure to propetamphos is possible because of the termiticide use of this pesticide. Dermal or incidental oral exposure is not anticipated based on the use pattern (gallery treatment). The exposure assessment for the gallery treatment is based on the Multi-Chamber Concentration and Exposure Model (MCCEM), as outlined in the SOPs for Residential Exposure Assessments.

The termiticide assessment represents a conservative Tier I estimate of exposure. It is assumed that 100% gallery treatment (i.e., applied inside the home) technique is a source for offgassing for long-term inhalation exposure. Based on this conservative (Tier I) exposure assessment, chronic inhalation MOEs for adults and children were 150 and 48 respectively. Because the chronic inhalation MOEs were below the target MOE of 300, the inhalation exposure from termiticide use of propetamphos is of concern to the Agency. This risk information is summarized in Table 9.

Table 9. Residential Chronic Post-Application Risks from Termiticide Use

Scenario	Population	Inhalation MOE ^a
Chronic exposure from termiticide use	Adult	150
	Children	48

^a MOEs based on LOAEL = 47 mg/kg/day (14-day inhalation rat study)

Because the Agency does not have chemical-specific termiticide use data for propetamphos, the actual use pattern of propetamphos (gallery injections with sealing of holes in dry wall) may well result in less than 100% of the total amount applied being available as a source. This model is intended to be a conservative screening scenario because it assumes 21 hours of residential exposure in a generic house with a moderate air exchange rate. The application of a 1% solution was also assumed. Because of these factors, the risk estimates provided in Table 9 are considered to be an overestimate and actual risk resulting from termiticide applications are expected to be much lower.

4. Aggregate Risk

An aggregate risk assessment looks at the combined risk from dietary exposure (food and drinking water routes) and residential exposure (dermal and inhalation exposure, and incidental hand-to-mouth oral exposure for children). For propetamphos, all individual and combined MOEs must be greater than the target MOE (i.e., 100 for dermal and oral, and 300 for inhalation), and the ARI must be greater than 1 to be not of concern to the Agency. Results of the aggregate risk assessment are summarized here, and are further discussed in *Propetamphos Updated Revised Preliminary Risk Assessment*, June 7, 1999 and *Updated Occupational and Residential Dermal Exposure Assessment* addendum, September 27, 2000.

Acute Aggregate Risk

Acute aggregate exposure assessments take into account acute dietary food and drinking water exposures. An acute aggregate risk assessment is not needed because only food handling establishment tolerances are established for propetamphos. Residues resulting from pesticide use in food handling establishments are not likely to result in incidental contamination of all foods at tolerance levels on a uniform and consistent basis, and not all foods consumed by an individual in a day are likely to have come from a food handling establishment. Also, based on the nature of propetamphos uses (in buildings and structures), residues are not expected in drinking water; therefore, an acute aggregate assessment of risk is not necessary.

Short-Term Aggregate Risk

Short-term aggregate risk takes into account short-term residential exposures (dermal and inhalation for adults), and dermal, inhalation and oral [incidental hand-to-mouth] for children, combined with chronic dietary (food) exposure. Because propetamphos is not expected in drinking water, the dietary component of the aggregate risk assessment is based on food exposure only. As indicated in Table 3, there are no chronic dietary food concerns (provided that foods are removed or covered during applications).

For broadcast carpet treatments, the ARIs for adults (combined MOEs for dermal and inhalation) for residential post-application exposure are less than 1.0 and, therefore, are of concern (see Table 7). The ARIs for children (combined MOEs for dermal, inhalation and oral [incidental hand-to-mouth] exposure) for residential post-application exposure are also less than 1.0 and are of concern (see Table 7). The ARIs are 0.1 and 0.003 for adults and children, respectively. Therefore, an aggregate risk assessment with dietary exposure was not be conducted.

For spot, and crack and crevice treatments, dermal MOEs for residential post-application exposure to adults were above the target MOE. Therefore, an aggregate assessment with chronic dietary (food) exposure was conducted and the resultant aggregate risks are not of concern. For children, combined dermal and oral (hand-to-mouth) MOEs for all scenarios are below the target MOE and are of concern (see Table 8). Therefore, an aggregate risk assessment with dietary exposure to children was not be conducted.

Chronic Aggregate Risk

Aggregate chronic risk estimates consider chronic dietary (food) and chronic residential (termiticide) exposure scenarios. Provided foods are covered or removed prior to application of propetamphos in food service establishments, chronic dietary (food) risk estimates for propetamphos are not of concern to the Agency.

For chronic inhalation exposure resulting from the termiticide use, post-application inhalation MOEs for children (48) and adults (150) are well below the inhalation target MOE of 300. Therefore, the aggregate chronic risk estimate was not conducted and is of concern to the Agency. However, as indicated in the previous section, this chronic inhalation risk assessment represents a conservative Tier I estimate of exposure, and actual risks are expected to be lower.

5. Human Incident Reports

OPs as a group, have a well documented and disproportionately higher rate of poisonings than other pesticides. The incident reports associated with propetamphos are disproportionately higher than other pesticides used interiorly in both the number of indoor incidents reported, and in the number of incidents involving PCOs. Incident reports from the following sources were reviewed for their potential relationship to propetamphos exposure:

- The OPP Incident Data System (IDS)
- Poison Control Centers (PCCs)
- The National Pesticide Telecommunications Network (NPTN)
- California Pesticide Illness Surveillance Program (1982-1995)

Based on data from the NPTN, reported poisoning incidences involving propetamphos have steadily declined between the years 1984 and 1998. Incidents where propetamphos was the only source of exposure or where it was the only cholinesterase inhibitor and the symptoms were consistent with cholinesterase inhibition were included. It is not clear at this point whether that decline is due to a lower odor formulation or due to the reduction in usage of propetamphos products, or a change in use pattern. However, three recent cases reported in California and submitted to EPA's Incident Data System (one in July of 1999, two in March of 2000) suggest that offensive odor continues to be a serious problem for propetamphos products. The specific cause of many of the reported effects from these incidents and others could be odor, due to constituents other than the active ingredient.

In 235 out of 301 detailed descriptions of cases submitted to the California Pesticide Illness Surveillance Program (1982-1995), propetamphos was used alone and was judged to be responsible for the health effects. Only cases with a definite, probable or possible relationship were reviewed. Propetamphos ranked 7th as a cause of systemic poisoning in California and 36th as a cause of hospitalization. Non-occupational exposure and residue from structural applications was associated with the overwhelming majority (88%) of the poisonings. Symptoms of these illnesses included difficulty breathing, chest tightness, shortness of breath, mental confusion, nausea, dizziness, headaches, vomiting, and eye irritation. Also common were cluster poisonings where large groups of office workers were

exposed, poisonings due to workers returning to offices that did not receive proper ventilation, and incidences where there was improper dilution by the applicator. Additionally, cluster poisonings have been reported where there was no evidence of either poor ventilation or label violations. The total number of poisoning cases related to structural pest control applications appears excessive when compared to the extent of use. The main concern with propetamphos appears to be inappropriate use or misuse by PCOs indoors. Most of the more serious poisonings appear to involve misuse, especially improper dilution, application in enclosed spaces with bystanders present, inadequate ventilation of structures before occupants are readmitted, and site inappropriate applications. A number of illnesses occurred despite the apparent adherence to label directions. In some of these cases, it appears symptoms are brought on by the offensive odor of the compound. This was supported by the finding that only one case out of 235 needed hospitalization. It should be recognized that individuals developing symptoms brought on by odor effects are poisonings by definition. Cholinesterase depression, though a useful indicator for exposure, does not have to be present to prove that poisoning has occurred. If odors are offensive enough to cause illness and to seek medical attention, then the circumstances that lead to such morbidity should be examined so that risk reduction measures can be identified and implemented.

Poison Control Center data were obtained and reviewed for all pesticides for the years 1993-96. This review reported on 199 exposures to propetamphos alone. Thirteen of the OP insecticides used in residential settings were ranked on a variety of hazard measures. Propetamphos ranked in the top three highest, and higher than any other OP except phosmet. Propetamphos ranked first for proportion of exposures and symptomatic cases that were due to environmental residue. As with the California data, Poison Control Center data suggests that propetamphos ranks high due to problems associated with exposure to residues as a result of inappropriate use by PCOs.

In summary, propetamphos continues to rank high in the total number of poisoning cases related to problems likely to be associated with exposure to residues and inappropriate use by PCOs, and appears excessive when compared to the extent of use. In a nationwide survey of residential and commercial PCO use, which estimated the total number of pounds of active ingredient of propetamphos applied indoors compared to a total of 9,232,000 pounds active ingredient for all pesticides used indoors, propetamphos accounted for only one percent of indoor use but accounted for 10 percent of the systemic poisonings.

B. Environmental Risk Assessment

Because all currently registered uses of propetamphos are limited to indoor use, exposure to nontarget terrestrial and aquatic plants and animals is not expected. Therefore, no ecological risk assessment was conducted for propetamphos.

IV. Interim Risk Management and Reregistration Decision

A. Determination of Interim Reregistration Eligibility

Section 4(g)(2)(A) of FIFRA calls for the Agency to determine, after submissions of relevant data concerning an active ingredient, whether products containing the active ingredients are eligible for reregistration. The Agency has previously identified and required the submission of the generic (i.e., an active ingredient specific) data required to support reregistration of products containing propetamphos active ingredients. Appendix A identifies the use patterns eligible for reregistration that the Agency has reviewed as part of its determination of reregistration eligibility of propetamphos.

The Agency has completed its assessment of the occupational and ecological risks associated with the use of pesticides containing the active ingredient propetamphos, as well as a propetamphos-specific dietary risk assessment that has not considered the cumulative effects of OPs as a class. Based on a review of these generic data and public comments on the Agency's preliminary risk assessments for the active ingredient propetamphos, EPA has sufficient information on the human health and ecological effects of propetamphos to make interim decisions as part of the tolerance reassessment process under FFDCA and reregistration under FIFRA, as amended by FQPA. The Agency has determined that propetamphos is eligible for reregistration provided that: (i) current data gaps and additional data needs are addressed; (ii) the risk mitigation measures outlined in this document are adopted, and label amendments are made to reflect these measures; and (iii) the cumulative risk assessment for the OPs support a final reregistration eligibility decision. Label changes are described in Section IV. Appendix B identifies the generic data requirements that the Agency reviewed as part of its interim determination of reregistration eligibility of propetamphos, and lists the submitted studies that the Agency found acceptable.

Although the Agency has not yet completed its cumulative risk assessment for the OPs, the Agency is issuing this interim assessment now in order to identify risk reduction measures that are necessary to support the continued use of propetamphos.

Based on its current evaluation of propetamphos alone, the Agency has determined that propetamphos products, unless labeled and used as specified in this document, would present risks inconsistent with FIFRA. Accordingly, should a registrant fail to implement any of the risk mitigation measures identified in this document, the Agency may take regulatory action to address the risks concerns from use of propetamphos.

At the time that a cumulative assessment is conducted, the Agency will address any outstanding risk concerns. For propetamphos, if all changes outlined in this document are incorporated into the labels, then all risks will be mitigated. But, because this is an IRED, the Agency will take further actions to finalize the reregistration eligibility decision for propetamphos after assessing the cumulative risk of the OP class. Such an incremental approach to the reregistration process is consistent with the Agency's goal of improving the transparency of the reregistration and tolerance reassessment processes. By evaluating each OP in turn and identifying appropriate risk reduction measures, the Agency is addressing the risks from the OPs in as timely a manner as possible.

Because the Agency has not yet completed the cumulative risk assessment for the OPs, this IRED does not specifically address the reassessment of the existing propetamphos food residue tolerances as called for by the Food Quality Protection Act (FQPA). When the Agency has completed the cumulative assessment, propetamphos tolerances will be reassessed. At that time, the Agency will reassess propetamphos along with the other OP pesticides to complete the FQPA requirements and make a final reregistration eligibility determination. By publishing this interim decision on reregistration eligibility and requesting mitigation measures now for the individual chemical propetamphos, the Agency is not deterring or postponing FQPA requirements, rather, EPA is taking steps to assure that uses which exceed FIFRA's unreasonable risk standard do not remain on the label indefinitely, pending completion of assessment required under the FQPA. This decision does not preclude the Agency from making further FQPA determinations and tolerance-related rulemakings that may be needed on this pesticide or any other in the future.

If the Agency determines, before finalization of the RED, that any of the determinations described in this IRED are no longer appropriate, the Agency will pursue appropriate action, including but not limited to, reconsideration of any portion of this IRED.

B. Summary of Phase 5 Comments and Responses

When making its interim reregistration decision, the Agency took into account all comments received during Phase 5 of the OP Pilot Process. As stated previously, a mitigation proposal was received from the registrant, Wellmark International, a summary of which is outlined below. Several other comments on mitigation were also received from the National Pest Management Association (NPMA), as well as approximately thirty comments from commercial pest companies and other interested stakeholders. A general summary of the majority of the comments received indicate a concern that propetamphos continue to be available as one more additional tool in Integrated Pest Management (IPM) programs, where a variety of chemicals are rotated to reduce potential resistance to any one type of chemical. Additionally, most comments made the statement that propetamphos is particularly effective in the control of heavy pest infestations, when other chemicals are not as efficacious.

Wellmark International's submission on proposed mitigation measures included the following:

- cancel the restricted-use product Zoecon 8718 EW (EPA Reg. No. 2724-449)
- amend the Catalyst end-use product label (EPA Reg. No. 2724-450) to state that foods must be covered or removed during application in food handling establishments
- specify for Pest Control Operator (PCO) use only
- add personal protective equipment requirements
- conduct a 21-day dermal toxicity study in rats to refine the dermal NOAEL

The registrant also provided comments on data from the National Pesticide Telecommunications Network (NPTN), suggesting that the decline in the number of reports from 1984-91 (35 calls per year) to the later time period, 1995-98 (7 calls per year) is due to the introduction of a low odor formulation. The original formula, Safroten EC (EPA Reg. No. 2724-314), had volatile sulfides, which the registrant contends were largely responsible for the adverse effects reported (i.e., nausea, headaches and eye

effects). A new formulation replaced this product in 1995. However, the Agency believes the comparison made between 1984-91 NPTN data and 1995-98 data may not be appropriate. This information suggests that there has been a recent decline in the number of propetamphos incidents, but may only represent a decline in the number of propetamphos incidents reported, which may be the result of a change in reporting. It is not clear at this point whether the decline in number of propetamphos incidents reported is due to a lower odor formulation, a reduction in usage of propetamphos products, or a change in use pattern.

C. FQPA Assessment

1. "Risk Cup" Determination

As part of the FQPA tolerance reassessment process, EPA assessed the risks associated with this OP. The assessment was for this individual OP, and does not attempt to fully reassess these tolerances as required under FQPA. FQPA requires the Agency to evaluate food tolerances on the basis of cumulative risk from substances sharing a common mechanism of toxicity, such as the toxicity expressed by the OPs through a common biochemical interaction with the cholinesterase enzyme. The Agency will evaluate the cumulative risk posed by the entire class of OPs once the methodology is developed and the policy concerning cumulative assessments is resolved.

EPA has determined that risk from exposure to propetamphos is within its own "risk cup." In other words, if propetamphos did not share a common mechanism of toxicity with other chemicals, EPA would be able to conclude today that the tolerances for propetamphos meet the FQPA safety standards. In reaching this determination EPA has considered the available information on the special sensitivity of infants and children, as well as the chronic and acute food exposure. An aggregate assessment was conducted for exposures through food, residential uses, and drinking water. Results of this aggregate assessment indicate that the human health risks from these combined exposures are considered to be within acceptable levels; that is, combined risks from all exposures to propetamphos "fit" within the individual risk cup. Therefore, for propetamphos, the tolerances remain in effect and unchanged until a full reassessment of the cumulative risk from all OPs is completed.

2. Tolerance Summary

Propetamphos is not registered for use on plants (either food or feed crops). The only food or feed-related use is the spot, and crack and crevice treatment of food service establishments. Tolerances for propetamphos residues in food commodities exposed to the insecticide during treatment of food or feed handling establishments are established at 0.1 ppm and are expressed in terms of propetamphos *per se*, ((e)-)-methylethyl 3-[[[(ethylamino) methoxyphosphinothioyl]oxy]-2-butenate), [40 CFR §180.541].

The qualitative nature of the residue in food commodities is adequately understood based upon metabolism studies examining the degradation of [C¹⁴] propetamphos in tomato juice, butter, bread, and hamburger meat. Adequate analytical methodology is available for enforcing tolerances and collecting data on propetamphos residues in food commodities. A gas chromatography/flame photometric detection enforcement method for determining propetamphos on fruit, meats, milk, and vegetables is listed in the

Pesticide Analytical Manual (PAM), Vol. II, as method I. The registrant also submitted a gas chromatography/mass spectrometry detections method (GC/MSD) for tolerance enforcement. This method has been successfully validated by the Agency. The validated limit of quantitation (LOQ) is 0.1 ppm and the limit of detection (LOD) is 0.01 ppm.

Reregistration requirements for magnitude of the residue in food handling establishments are fulfilled. Adequate data (obtained using the GC/MSD analytical method) are available depicting residues of propetamphos in representative food commodities (apples, beer, bologna, bread, butter, flour, hamburger, lettuce, macaroni, milk, Rice Krispies®, and sugar) exposed, in open and closed containers on tables, to propetamphos treatments reflecting the registered use pattern for food handling areas.

Tolerance Listed Under 40 CFR §180.541:

Registration requirements for data depicting residues of propetamphos in/on food commodities following applications representative of the use in food handling establishments are fulfilled, and sufficient data are available to ascertain the adequacy of the established tolerance for residues in/on food commodities. The available data indicate that the current 0.1 ppm tolerance for residues of propetamphos in food commodities is appropriate, based on the validated LOQ of the analytical method.

3. Endocrine Disruptor Effects

EPA is required under the FFDCFA, as amended by FQPA, to develop a screening program to determine whether certain substances (including all pesticide active and other ingredients) "may have an effect in humans that is similar to an effect produced by a naturally occurring estrogen, or other such endocrine effects as the Administrator may designate." Following the recommendations of its Endocrine Disruptor Screening and Testing Advisory Committee (EDSTAC), EPA determined that there were scientific bases for including, as part of the program, the androgen and thyroid hormone systems, in addition to the estrogen hormone system. EPA also adopted EDSTAC's recommendation that the program include evaluations of potential effects in wildlife. For pesticide chemicals, EPA will use FIFRA and, to the extent that effects in wildlife may help determine whether a substance may have an effect in humans, FFDCFA authority to require the wildlife evaluations. As the science develops and resources allow, screening of additional hormone systems may be added to the Endocrine Disruptor Screening Program (EDSP).

When the appropriate screening and/or testing protocols being considered under the Agency's EDSP have been developed, propetamphos may be subjected to additional screening and/or testing to better characterize effects related to endocrine disruption.

D. Regulatory Rationale

The following is a summary of the rationale for managing risks associated with the use of propetamphos. Where labeling revisions are warranted, specific language is set forth in the summary tables of Section V of this document. The Agency has determined that the mitigation measures discussed below, combined with additional amendments to the label, will reduce risks to workers, homeowners and children to an acceptable level, and that unreasonable adverse effects are unlikely to result from such use. Provided the following risk mitigation measures are incorporated into amended labels for propetamphos, the Agency finds that all remaining registered uses of propetamphos are eligible for interim reregistration, pending a cumulative assessment of the OPs.

1. Human Health Mitigation Measures

a. Dietary (Food and Drinking Water) Risk

Acute Dietary (Food)

Acute dietary exposure and risk assessment is not necessary for propetamphos, a pesticide having only food handling establishment tolerances. Therefore, there are no acute dietary (food) mitigation measures necessary for propetamphos.

Chronic Dietary (Food)

The chronic dietary risk of propetamphos from food residues does not exceed the Agency's level of concern, provided that language stating food be removed or covered prior to pesticide application is added to the product labels.

Drinking Water

Because propetamphos is not expected to be released to water, exposure to drinking water is not expected. Therefore, there are no drinking water mitigation measures necessary for propetamphos.

b. Occupational Risk

As indicated in Table 6, the ARIs are greater than 1.0 for all occupational use scenarios and are, therefore, not of concern. These risk estimates are based on a reduced dilution rate of 0.5% ai solution (from 1.0% ai), and applicators wearing personal protective equipment (PPE) consisting of a long-sleeve shirt, long pants, shoes and socks, and gloves. Because PPE statements are not on the current propetamphos label, the Agency has included as a mitigation measure that product labels be amended to state that applicators must wear PPE consisting of a long-sleeve shirt, long pants, shoes and socks, and chemical-resistant gloves. Additionally, to further mitigate these risks, the following measures are necessary:

- Reduce the maximum rate of dilution to 0.5% ai solution.
- Require that only protected handlers may be in the area during applications.

The dermal exposure component of the occupational risk assessment is based on the recently received 21-day dermal toxicity study in rats. Based on a preliminary review of the study, the Agency has determined that the NOAEL = 1.25 mg/kg/day based on brain cholinesterase inhibition at a LOAEL of 2.5 mg/kg/day. The Agency is currently conducting a final review of the study and is confident of its determination and that it will be selected by the Agency's Hazard Identification and Assessment Review Committee.

c. Residential (Post-Application) Risk

Broadcast Applications

As indicated in Table 7, the dermal MOEs for both adults and children are significantly below the target MOE of 100. Incidental oral exposures (hand-to-mouth) for children is also below the target MOE of 100. However, inhalation MOEs are above the target MOE of 300 for adults and children. Therefore, the combined (ARI) exposure from broadcast carpet treatment is less than 1.0 for all populations and of concern to the Agency. Because these risk estimates are based on a chemical-specific exposure study, the Agency has a high level of confidence in these exposure and risk estimates. Because of these risk concerns, broadcast carpet treatment with propetamphos products shall be prohibited and removed from the label.

Spot, and Crack and Crevice Applications

As indicated in Table 8, for crack and crevice/spot treatment, dermal MOEs for residential post-application exposure to adults were above the target MOE. Therefore, an aggregate assessment with chronic dietary (food) exposure was conducted and the resultant aggregate risks are not of concern. For children, combined dermal and oral (hand-to-mouth) MOEs for all scenarios are below the target MOE and are of concern (see Table 8). To mitigate these risks to children and other potentially sensitive populations, the following measures are necessary:

- Cancel all residential uses.
- Prohibit use in structures children and the elderly occupy, such as or including homes, schools, day-cares, hospitals, nursing homes, with the exception of areas of food service within those structures, when food is covered or removed prior to treatment.

Additionally, provided that a crack and crevice treatment meets the following application restrictions (as defined in OPPTS 860.1460 Food Handling): "*crack and crevice treatment is application of small amounts of pesticides into crack and crevices in which pests hide or through which they may enter a building. Openings of this type commonly occur at expansion joints, between different elements of construction, and between equipment and floors. These openings may lead to voids such as hollow walls, equipment legs and bases, conduits, motor housings, and junction or switch boxes.*", dermal and inhalation exposure and risk to persons re-entering the treated area is expected to be negligible. To further mitigate these risks from non-residential uses, the following measures are also necessary:

- Cancel all spot treatment applications and restrict its use to crack and crevice treatment only, as defined in OPPTS 860.1460 Food Handling.
- The product may only be used for crack and crevice treatment in food service establishments (e.g., restaurants, taverns, delicatessens, mess halls, mobile canteens, around vending machines, grocery stores and markets-where there is no contact with food) including schools, hospitals and nursing homes in food service areas only; indoor non-food areas (e.g., office buildings, commercial, and industrial premises and equipment); and non-food areas of eating establishments where there is no contact with food, and where no food processing, packing, and no food and/or feed warehousing occurs.

Termiticide Applications

Chronic residential inhalation exposure to propetamphos is possible because of the termiticide use of this pesticide. Dermal or incidental oral exposure is not anticipated based on the use pattern (gallery treatment). Based on the exposure assessment, chronic inhalation MOEs for adults and children are 150 and 48, respectively. This risk information is summarized in Table 9. Because the chronic inhalation MOEs are below the target MOE of 300, the inhalation exposure from termiticide use of propetamphos is of concern to the Agency. However, as discussed previously, this chronic inhalation risk assessment represents a conservative Tier I estimate of exposure and actual risks are expected to be lower. Consequently, the registrant has informed the Agency that it does not support the continued termiticide use and has requested voluntarily cancellation of the termiticide use for propetamphos.

2. Environmental Risk Mitigation Measures

Because all currently registered uses of propetamphos are limited to indoor use, exposure to nontarget terrestrial and aquatic plants and animals is not expected. Therefore, no ecological risk mitigation measures are necessary for propetamphos.

E. Label Amendments

Provided the following risk mitigation measures are incorporated in their entirety into labels for propetamphos-containing products, the Agency finds that all remaining registered uses of propetamphos would be eligible for reregistration, pending a cumulative assessment of the OPs. The regulatory rationale for each of the mitigation measures outlined below is discussed in the previous section of this IRED. Also, in order to remain eligible for reregistration, other use and safety information need to be placed on the labeling of all end-use products containing propetamphos. For specific labeling statements, refer to Section V of this document.

- Cancel all residential uses.
- Prohibit use in structures children and the elderly occupy, such as or including homes, schools, day-cares, hospitals, nursing homes, with the exception of areas of food service within those structures, when food is covered or removed prior to treatment.

- Cancel all spot, broadcast, and termiticide treatments.
- The product may only be used for crack and crevice treatment in food service establishments (e.g., restaurants, taverns, delicatessens, mess halls, mobile canteens, around vending machines, grocery stores and markets-where there is no contact with food) including schools, hospitals and nursing homes in food service areas only; indoor non-food areas (e.g., office buildings, commercial, and industrial premises and equipment); and non-food areas of eating establishments where there is no contact with food, and where no food processing, packing, and no food and/or feed warehousing occurs.
- Amend the label to include the following crack and crevice treatment definition as defined in OPPTS 860.1460 Food Handling: *“crack and crevice treatment is application of small amounts of pesticides into crack and crevices in which pests hide or through which they may enter a building. Openings of this type commonly occur at expansion joints, between different elements of construction, and between equipment and floors. These openings may lead to voids such as hollow walls, equipment legs and bases, conduits, motor housings, and junction or switch boxes.”*
- Reduce the maximum rate of dilution from 1.0% ai to 0.5 % ai solution.
- For food service establishment use, all food must be either covered or removed prior to application of the product.
- Applicators must wear personal protective equipment consisting of a long-sleeve shirt, long pants, shoes and socks, and chemical-resistant gloves.
- For use by Pest Control Operators (PCOs) only.
- Only protected handlers may be in the area during applications.

V. What Registrants Need to Do

A. Manufacturing-Use Products

1. Additional Generic Data Requirements

The generic data base supporting the reregistration of propetamphos for the above eligible uses has been reviewed and determined to be substantially complete. The following confirmatory data in Table 10 are required:

Table 10. Confirmatory Data Requirements

Guideline Test Name	New Guideline No.	Old Guideline No.
Dissociation Constant in Water	OPPTS 830.7370	63-10
Partition coefficient (<i>n</i> -octanol/water), shake flask method	OPPTS 830.7550-70	63-11
Stability to normal and elevated temperatures, metals, and metal ions	OPPTS 830.6313	63-13
UV/Visible Absorption	OPPTS 830.7050	none

Chemistry Studies

Pertinent product chemistry data requirements remain unfulfilled for the Wellmark International 90% T/TGAI concerning stability, pH, UV/visible absorption, and octanol/water partition coefficient (OPPTS 830.6313, 830.7370, 830.7050, and 830.7550-70). The registrant must submit the data required in the attached data summary tables for the 90% T/TGAI, and either certify that the suppliers of beginning materials and the manufacturing process for the propetamphos technical grade active ingredient (TGAI) have not changed since the last comprehensive product chemistry review or submit a complete updated product chemistry data package.

Neurotoxicity Studies

A Data Call-In (DCI) Notice has been sent to registrants of OP pesticides currently registered under FIFRA (August 6, 1999 64FR42945-42947, August 18 64FR44922-44923). DCI requirements included acute, subchronic, and developmental neurotoxicity studies. The Agency has received acceptable acute (MRID 43403901) and subchronic (MRID 43403902 and 43995601) neurotoxicity studies, therefore, the DCI referenced above only refers to the developmental neurotoxicity study for propetamphos. After further consideration of the risk mitigation measures discussed in Section IV of this IRED and other factors discussed below, the requirement for the developmental neurotoxicity study is waived, provided the registrant complies with the necessary label amendments and annual limit of 25,000 pounds of propetamphos active ingredient sold or distributed. If the registrant sell or distributes more than 25,000 pounds of propetamphos active ingredient within any calendar year, the registrant will be required to submit to the Agency the developmental neurotoxicity study. The following factors were considered for waiving these studies:

- Based on the risk assessments and limited use pattern of propetamphos, there are no dietary (food and water), occupational, or ecological risk concerns.

- There is no evidence of neuropathology in the acute and subchronic studies; chronic dog study; and no organophosphate induced delayed neurotoxicity (OPIDN) in the hen study. Also, there is no evidence of increased susceptibility, based on adequate developmental toxicity and reproduction studies. Therefore, the FQPA Safety Factor for propetamphos was removed (equivalent to 1x).
- The use of propetamphos will be restricted to (non-residential) crack and crevice only treatment in food service establishments; indoor non-food areas; and non-food areas of eating establishments where there is no contact with food, and where no food processing, packing, and no food and/or feed warehousing occurs. All residential uses will be canceled, thereby significantly reducing potential exposure to children.
- Provided propetamphos is restricted to PCO use for crack and crevice only treatment (excluding baseboard and spot treatment applications), and because the low vapor pressure of propetamphos (2.6×10^{-7} mm Hg at 25°C) will significantly limit the volatilization of the compound, exposure to persons re-entering treated areas is not expected to occur.
- Provided all foods are covered or removed prior to treatment of food service establishments, there is no expectation of detectable residues on food.
- To assure that potential exposure to propetamphos does not increase significantly beyond current levels, the amount of propetamphos active ingredient shall be limited to 25,000 pounds.

2. Labeling for Manufacturing-Use Products

To remain in compliance with FIFRA, manufacturing-use product (MUP) labeling should be revised to comply with all current EPA regulations, PR Notices, and applicable policies. The MP labeling should bear the labeling contained in Table 11 at the end of this section.

B. End-Use Products

1. Product-Specific Data Requirements

Section 4(g)(2)(B) of FIFRA calls for the Agency to obtain any needed product-specific data regarding the pesticide after a determination of eligibility has been made. Registrants must review previous data submissions to ensure that they meet current EPA acceptance criteria and if not, commit to conduct new studies. If a registrant believes that previously submitted data meet current testing standards, then the study MRID numbers should be cited according to the instructions in the Requirement Status and Registrants Response Form provided for each product. A product-specific DCI, outlining specific data requirements, accompanies this IRED.

2. Labeling for End-Use Product

Labeling changes are necessary to implement measures outlined in Section IV. Specific language to incorporate these changes is specified in the Table 11 at the end of this section.

C. Existing Stocks

Registrants may generally distribute and sell propetamphos products bearing old labels/labeling for 12 months from the date of the issuance of the RED document. Persons other than the registrant may generally distribute or sell such products for 24 months from the date of the issuance of this interim RED. However, existing stocks time frames will be established case-by-case, depending on the number of products involved, the number of label changes, and other factors. Refer to "Existing Stocks of Pesticide Products; Statement of Policy"; Federal Register, Volume 56, No. 123, June 26, 1991.

The Agency has determined that registrants may distribute and sell propetamphos products bearing old labels/labeling for 8 months from the date of issuance of this IRED. Persons other than the registrant may distribute or sell such products for 18 months from the date of the issuance of this IRED. Registrants and persons other than the registrant remain obligated to meet pre-existing label requirements and existing stocks requirements applicable to products they sell or distribute.

D. Labeling Changes Summary Table

Table 11: Summary of Labeling Changes for Propetamphos		
Description	Amended Labeling Language	Placement on Label
Needed on all MUPs	<p>Manufacturing-Use Products</p> <p>“Only for formulation into an insecticide for the following use(s): For indoor, non-residential crack and crevice treatments only for the following use areas:</p> <ul style="list-style-type: none"> • food service establishments (e.g. restaurants, taverns, delicatessens, mess halls, mobile canteens, around vending machines, grocery stores and markets where there is no contact with food, and when food is removed or covered prior to treatment), including schools, hospitals and nursing homes in food service areas only; • indoor non-food areas (e.g., office buildings; commercial; and industrial buildings and warehouses; and institutions, except those where children and the elderly occupy, such as and including schools, day-cares, hospitals, and nursing homes); and • non-food areas of eating establishments where there is no contact with food, and where no food processing, packing, and no food and/or feed warehousing occurs.” 	Directions for Use
One of these statements may be added to a label to allow reformulation of the product for a specific use or all additional uses supported by a formulator or user group	<p>“The product may be used to formulate products for any use(s) not listed on the MP label if the formulator, user group, or grower has complied with U.S. EPA submission requirements regarding support of such use(s).”</p> <p>“The product may be used to formulate products for any additional use(s) not listed on the MP label if the formulator, user group, or grower has complied with U.S. EPA submission requirements regarding support of such use(s).”</p>	Directions for Use

Table 11: Summary of Labeling Changes for Propetamphos

Description	Amended Labeling Language	Placement on Label
Environmental Hazards Statements Needed by the RED and Agency Label Policies	<p>"This chemical is toxic to fish, aquatic invertebrates and other wildlife, and poses a risk to reproduction of birds. Do not discharge effluent containing this product into lakes, streams, ponds, estuaries, oceans or other waters unless in accordance with the requirements of a National Pollutant Discharge Elimination System (NPDES) permit and the permitting authority has been notified in writing prior to discharge. Do not discharge effluent containing this product to sewer systems without previously notifying the local sewage treatment plant authority. For guidance contact your state Water Board or Regional Office of the EPA."</p>	Precautionary Statements following Hazards to Humans and Domestic Animals
End-Use Products		
Protective Clothing Requirements Established by the IRED for Liquid Products	<p>"Personal Protective Equipment (PPE) Mixers, loaders, applicators, and other handlers must wear:</p> <ul style="list-style-type: none"> • Long-sleeve shirt, long pants • Shoes plus socks • Chemical-resistant gloves" (<i>registrant inserts correct chemical-resistant material</i>) <p>Note: PPE that is established on the basis of Acute Toxicity of the end-use product must be compared to the active ingredient PPE in this document. The more protective PPE must be placed in the product labeling. For guidance on which PPE is considered more protective, see PR Notice 93-7.</p>	Towards the end of the Hazards to Humans and Domestic Animals section, following Precautionary Statements
User Safety Requirements	<p>"Follow manufacturer's instructions for cleaning/maintaining PPE. If no such instructions for washables exist, use detergent and hot water. Keep and wash PPE separately from other laundry."</p>	At the end of the Hazards to Humans and Domestic Animals section, following the protective clothing requirements

Table 11: Summary of Labeling Changes for Propetamphos		
Description	Amended Labeling Language	Placement on Label
User Safety Recommendations	<p>"User Safety Recommendations</p> <p>Users should wash hands before eating, drinking, chewing gum, using tobacco, or using the toilet.</p> <p>Users should remove clothing/PPE immediately if pesticide gets inside. Then wash thoroughly and put on clean clothing.</p> <p>Users should remove PPE immediately after handling this product. Wash the outside of gloves before removing. As soon as possible, wash thoroughly and change into clean clothing."</p>	Place at the end of the Hazards to Humans and Domestic Animals section, following the user safety requirements. (Must be placed in a box).
Entry Restriction	"Do not enter or allow others to enter until sprays have dried."	Directions for Use

Table 11: Summary of Labeling Changes for Propetamphos

Description	Amended Labeling Language	Placement on Label
<p>General Application Restrictions</p>	<p>For indoor, non-residential crack and crevice treatments only for the following use areas:</p> <ul style="list-style-type: none"> • food service establishments (e.g., restaurants, taverns, delicatessens, mess halls, mobile canteens, around vending machines, grocery stores and markets where there is no contact with food, and when food is removed or covered prior to treatment), including schools, hospitals and nursing homes in food service areas only; • indoor non-food areas (e.g., office buildings; commercial; and industrial buildings and warehouses; and institutions, except those where children and the elderly occupy, such as and including schools, day-cares, hospitals, and nursing homes.); and • non-food areas of eating establishments where there is no contact with food, and where no food processing, packing, and no food and/or feed warehousing occurs. <p>“All food must be removed or covered prior to treatment in food service establishments.”</p> <p>“This product shall only be used for crack and crevice treatment. Crack and crevice treatment is application of small amounts of pesticides into crack and crevices in which pests hide or through which they may enter a building. Openings of this type commonly occur at expansion joints, between different elements of construction, and between equipment and floors. These openings may lead to voids such as hollow walls, equipment legs and bases, conduits, motor housings, and junction or switch boxes.”</p> <p>“This product cannot be used in homes, apartment buildings, or any other residential structure. Also, this product cannot be used in structures where children and the elderly occupy, such as and including schools, day-cares, hospitals, and nursing homes, but</p>	<p>Place this statement in the Directions for Use section under “General Precautions and Restrictions”</p>

Table 11: Summary of Labeling Changes for Propetamphos

Description	Amended Labeling Language	Placement on Label
General Application Restrictions (Continued)	<p>may be used in the food service establishment areas within these structures, provided food is removed or covered prior to treatment.”</p> <p>“For use by Pest Control Operators (PCOs) only.”</p> <p>“Do not apply this product in a way that will contact workers or other persons, either directly or through drift. Only protected handlers may be in the area during applications.”</p> <p>“The maximum rate of dilution is 0.5 % active ingredient solution; * <u> </u> oz. per gallon.”</p> <p>* <i>Registrant inserts correct amount of product based on product formulation.</i></p> <p>“This product may not be reapplied more than once every 7 days, and treatment may not exceed 2 applications in a 30-day period.”</p>	Place this statement in the Directions for Use section under “General Precautions and Restrictions”

Instructions in the Labeling Required section appearing in quotations represent the exact language that must appear on the label. Instructions in the Labeling Required section not in quotes represents actions that the registrant must take to amend their labels or product registrations

VI. Related Documents and How to Access Them

This IRED document is supported by documents that are presently maintained in the OPP docket. The OPP docket is located in Room 119, Crystal Mall #2, 1921 Jefferson Davis Highway, Arlington, VA. It is open Monday through Friday, excluding legal holidays from 8:30 am to 4 pm.

The docket initially contained preliminary risk assessments and related documents as of January 15, 1999. Sixty days later the first public comment period closed. The EPA then considered comments, revised the risk assessment, and added the formal "Response to Comments" document and the revised risk assessment to the docket on December 1, 1999.

All documents, in hard copy form, may be viewed in the OPP docket room or downloaded or viewed via the Internet at the following site: "<http://www.epa.gov/pesticides/op>."

If any of the conditions of this interim decision are not satisfied, including but not limited to the submission of an unacceptable study, missing established deadlines, or failing to amend product labels, the Agency may take other regulatory actions. If the Agency later determines (based upon consideration of the cumulative assessment) that any of the determinations described in this IRED are no longer appropriate, the Agency will pursue appropriate action, including but not limited to, reconsideration of any portion of this IRED.

VII. APPENDICES

Appendix A: Use Patterns Eligible For Reregistration

Table 12. Eligible Use Patterns

PROPETAMPHOS (CASE 2550): USE PATTERNS ELIGIBLE FOR REREGISTRATION					
Application/Type Equipment	Formulation [EPA Reg. No.]	ai Maximum Single App. Rate (lbs)	Maximum No. of Applications	Minimum Retreatment Interval	Restrictions /Comments
Food Service Establishments					
Crack and crevice; air sprayer, with low pressure hand wand, or injection nozzle capable of delivering a pin-stream application	18.90% [2724-450]	0.5% ai solution	No more than 2 applications in 30 days	No more than once in 7 days	Limit re-treatment intervals to not more than 2 treatments per 30 days. For indoor, non-residential crack and crevice treatments only for the following use areas: food service establishments (e.g. restaurants, taverns, delicatessens, mess halls, mobile canteens, around vending machines, grocery stores and markets where there is no contact with food, and when food is removed or covered prior to treatment), including schools, hospitals and nursing homes in food service areas only;
Non-Residential Non-Food Areas					
Crack and crevice; air sprayer, with low pressure hand wand, or injection nozzle capable of delivering a pin-stream application	18.90% [2724-450]	0.5% ai solution	No more than 2 applications in 30 days	No more than once in 7 days	For indoor, non-residential crack and crevice treatments only for the following use areas: indoor non-food areas (e.g., office buildings; commercial; and industrial buildings and warehouses; and institutions, except those where children and the elderly occupy, such as and including schools, day-cares, hospitals, and nursing homes); and non-food areas of eating establishments where there is no contact with food, and where no food processing, packing, and no food and/or feed warehousing occurs.

Appendix B. Table Of Generic Data Requirements And Studies Used To Make The Interim Reregistration Decision

GUIDE TO APPENDIX B

Appendix B contains listing of data requirements which support the reregistration for active ingredients within case #2550 (propramphos) covered by this Interim RED. It contains generic data requirements that apply to propramphos in all products, including data requirements for which a "typical formulation" is the test substance.

The data table is organized in the following formats:

1. Data Requirement (Column 1). The data requirements are listed in the order in which they appear in 40 CFR part 158. The reference numbers accompanying each test refer to the test protocols set in the Pesticide Assessment Guidance, which are available from the National technical Information Service, 5285 Port Royal Road, Springfield, VA 22161 (703) 487-4650.
2. Use Pattern (Column 2). This column indicates the use patterns for which the data requirements apply. The following letter designations are used for the given use patterns.
 - A. Terrestrial food
 - B. Terrestrial feed
 - C. Terrestrial non-food
 - D. Aquatic food
 - E. Aquatic non-food outdoor
 - F. Aquatic non-food industrial
 - G. Aquatic non-food residential
 - H. Greenhouse food
 - I. Greenhouse non-food
 - J. Forestry
 - K. Residential
 - L. Indoor food
 - M. Indoor non-food
 - N. Indoor medical
 - O. Indoor residential
3. Bibliographic Citation (Column 3). If the Agency has acceptable data in its files, this column list the identify number of each study. This normally is the Master Record Identification (MIRD) number, but may be a "GS" number if no MRID number has been assigned. Refer to the Bibliography appendix for a complete citation of the study.

APPENDIX B

(OLD/NEW GUIDELINE) REQUIREMENTS				
OLD	NEW	STUDY	USE PATTERN	CITATION(S)
Product Chemistry				
61-1	830.1550	Chemical Identity	ALL	41607414
61-2A	830.1600	Start. Mat. & Mnfg. Process	ALL	41607414
61-2B	830.1670	Formation of Impurities	ALL	41607414
62-1	830.1700	Preliminary Analysis	ALL	42355803
62-2	830.1750	Certification of limits	ALL	42355802
62-3	830.1800	Analytical Method	ALL	42355803, 42355804
63-2	830.6302	Color	ALL	41607411
63-3	830.6303	Physical State	ALL	41607411
63-4	830.6304	Odor	ALL	41607411
63-5	830.7200	Melting Point	ALL	41607411
63-6	830.7220	Boiling Point	ALL	41607411
63-7	830.7300	Density	ALL	41607411
63-8	830.7840 830.7860	Solubility	ALL	41607408
63-9	830.7950	Vapor Pressure	ALL	41607416
63-13	830.7370	Stability	ALL	42254701
63-17	830.7550	Storage stability	ALL	41997304, 41607402
63-20	830.6320	Corrosion Characteristics	ALL	41997304
ECOLOGICAL EFFECTS				
71-1	830.2100	Acute Avian Oral -Quail/Duck	ALL	00097891, 41607401
71-2A	850.2200	Avian Dietary - Quail	ALL	42144701, 42144702
72-1A	850.1075	Fish Toxicity-Bluegill	ALL	41607409
72-1C	850.1075	Fish Toxicity Rainbow Trout	ALL	41607415
72-2A	850.1010	Invertebrate Toxicity	ALL	41607401, 41607404
TOXICOLOGY				
81-1	870.1100	Acute Oral Toxicity - Rat	ALL	41607417
81-2	870.1200	Acute Dermal Toxicity -Rabbit/Rat	ALL	41607418 45198401
81-3	870.1300	Acute Inhalation Toxicity-Rat	ALL	41529301

OLD	NEW	STUDY	USE PATTERN	CITATION(S)
81-4	870.2400	Primary Eye Irritation -Rabbit	ALL	41607419
81-5	870.2500	Primary Dermal Irritation-Rabbit	ALL	41607420
81-6	870.2600	Dermal Sensitization-Guinea Pig	ALL	41607412, 42194401
81-7	870.6100	Acute Delayed Neurotoxicity - Hen	ALL	42194401, 92150013
82-1B	870.3150	90-Day Feeding - Non-rodent	ALL	00039596
82-2	870.3200	21-Day Dermal -Rabbit/Rat	CLMNO	00052920, 00052921
83-1A	870.4100	Chronic Feeding Toxicity-Rodent	CLMNO	42399001
83-2A	870.4200	Oncogenicity - Rat	CLMNO	42399001
83-4	870.3800	2-Generation Reproduction - Rat	ALL	43039801
84-2A	870.5140	Gene Mutation (Ames Test)	ALL	41607405
84-2B	870.5375	Structural Chromosomal Aberration	ALL	41607406
85-1	870.7485	General Metabolism	ALL	42978201
81-8	870.6200	Acute Neurotoxicity Study	ALL	43403901
85-4-SS	None	6-Mo Ocular Toxicity Study	ALL	43049501
160-5	None	Chemical identity	ALL	41607414
171-2	None	Chemical identity	ALL	41607414
171-4E	860.1380	Storage Stability	ALL	43193303

Appendix C: Technical Support Documents

Additional documentation in support of this Interim RED is maintained in the OPP docket, located in Room 119, Crystal Mall #2, 1921 Jefferson Davis Highway, Arlington, VA. It is open Monday through Friday, excluding legal holidays, from 8:30 am to 4 pm.

The docket initially contained the preliminary risk assessments and related documents as of September 23, 1998. Sixty days later the first public comment period closed. The Agency considered comments on the revised risk assessments and added the formal "Response to Comments" document and the revised risk assessment to the docket on September 24, 1999.

All documents, in hard copy form, may be viewed in the OPP docket room or downloaded or viewed via the Internet at the following site:

www.epa.gov/pesticides/op

Appendix D. Citations Considered To Be Part Of The Database Supporting the Interim Reregistration Eligibility Decision (Bibliography)

GUIDE TO APPENDIX D

1. CONTENTS OF BIBLIOGRAPHY. This bibliography contains citations of all studies considered relevant by EPA in arriving at the positions and conclusions stated elsewhere in the Reregistration Eligibility Document. Primary sources for studies in this bibliography have been the body of data submitted to EPA and its predecessor agencies in support of past regulatory decisions. Selections from other sources including the published literature, in those instances where they have been considered, are included.
2. UNITS OF ENTRY. The unit of entry in this bibliography is called a "study". In the case of published materials, this corresponds closely to an article. In the case of unpublished materials submitted to the Agency, the Agency has sought to identify documents at a level parallel to the published article from within the typically larger volumes in which they were submitted. The resulting "studies" generally have a distinct title (or at least a single subject), can stand alone for purposes of review and can be described with a conventional bibliographic citation. The Agency has also attempted to unite basic documents and commentaries upon them, treating them as a single study.
3. IDENTIFICATION OF ENTRIES. The entries in this bibliography are sorted numerically by Master Record Identifier, or "MRID number". This number is unique to the citation, and should be used whenever a specific reference is required. It is not related to the six-digit "Accession Number" which has been used to identify volumes of submitted studies (see paragraph 4(d)(4) below for further explanation). In a few cases, entries added to the bibliography late in the review may be preceded by a nine character temporary identifier. These entries are listed after all MRID entries. This temporary identifying number is also to be used whenever specific reference is needed.
4. FORM OF ENTRY. In addition to the Master Record Identifier (MRID), each entry consists of a citation containing standard elements followed, in the case of material submitted to EPA, by a description of the earliest known submission. Bibliographic conventions used reflect the standard of the American National Standards Institute (ANSI), expanded to provide for certain special needs.
 - a. Author. Whenever the author could confidently be identified, the Agency has chosen to show a personal author. When no individual was identified, the Agency has shown an identifiable laboratory or testing facility as the author. When no author or laboratory could be identified, the Agency has shown the first submitter as the author.
 - b. Document date. The date of the study is taken directly from the document. When the date is followed by a question mark, the bibliographer has deduced the date from the evidence contained in the document. When the date appears as (19??), the Agency was unable to determine or estimate the date of the document.

c. Title. In some cases, it has been necessary for the Agency bibliographers to create or enhance a document title. Any such editorial insertions are contained between square brackets.

d. Trailing parentheses. For studies submitted to the Agency in the past, the trailing parentheses include (in addition to any self-explanatory text) the following elements describing the earliest known submission:

- 1) Submission date. The date of the earliest known submission appears immediately following the word "received".
- 2) Administrative number. The next element immediately following the word "under" is the registration number, experimental use permit number, petition number, or other administrative number associated with the earliest known submission.
- 3) Submitter. The third element is the submitter. When authorship is defaulted to the submitter, this element is omitted.
- 4) Volume Identification (Accession Numbers). The final element in the trailing parentheses identifies the EPA accession number of the volume in which the original submissions of the study appears. The six-digit accession number follows the symbol "CDL," which stands for "Company Data Library." This accession number is in turn followed by an alphabetic suffix which shows the relative position of the study within the volume.

Appendix D

PROPETAMPHOS BIBLIOGRAPHY

MRID Number

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- 00039596 Klotzsche, C.; Carpy, S.; Luginbuehl, H. (1978) Propetamphos (San 52.139 I): 13-Week Feeding Study in Rats: Report No. 24/77. (Unpublished study including report 47/78, received May 8, 1980 under 11273-EX-19; prepared by Sandoz, Ltd. and Univ. of Bern, Institute for Animal Pathology, submitted by Sandoz, Inc. Crop Protection, San Diego, Calif.; CDL:242462-A)
- 00052919 Goldenthal, E.I.; Wazeter, F.X., Geil, R.G.; et al. (1976) Three Week Dermal Study in Rabbits: IRDC No. 163-373. (Unpublished study received May 5, 1976 under 876-252; prepared by International Research and Development Corp., submitted by Velsicol Chemical Corp., Chicago, Ill.; CDL:228723-G)
- 00052922 Goldenthal, E.I.; Wazeter, F.X.; Geil, R.G.; et al. (1975) Fourteen Day Inhalation Toxicity Study in Rats: IRDC No. 163-334. (Unpublished study received May 5, 1976 under 876-252; prepared by International Research and Development Corp., submitted by Vesical Chemical Corp., Chicago, Ill.; CDL:228723-J)
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- 00085156 Leuschner, F.; Leuschner, A.; Klie, R.; et al. (1978) Two-weeks toxicity of Safrotin in Sprague-Dawley Rats when Administered by Inhalation. (Unpublished study received Nov 1, 1978 under 11273-21; prepared by Laboratorium für Pharmakologie und Toxikologie, West Germany, submitted by Sandoz, Inc. Crop Protection, San Diego, Calif.; CDL:235623-L)
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- 42275801 Ferdinandi, E. (1991) Metabolism, Mass Balance of Radioactivity and Plasma Pharmacokinetics of [carbon 14]-Propetamphos in Male and Female Sprague-Dawley Rats Following its Oral Administration: Lab Project Number: 38804: 1532. Unpublished study prepared by Bio-Research Labs., Ltd. 427 p T-2-10/12/79. Unpublished study prepared by Wildlife International, Ltd. 24 p.
- 42144701 Fink, R.; McCormack, R. (1979) LC50 Determination of Propetamphos in the Mallard Duck: Final Report: Sandoz Project No. T-1389; WI Study No. 131-112; Report T-1-10/12/79. Unpublished study prepared by Wildlife International Ltd. 39 p.
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- 43193301 Lephart, J. (1994) Response to United States Environmental Protection Agency Letter, October 28, 1993, Regarding Propetamphos Residue Studies (Part 1: Method Development): Supplement: Lab Project Number: 1538. Unpublished study prepared by Sandoz Agro, Inc. 13 p.
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- 43403902 Minnema, D. (1994) Subchronic Neurotoxicity Study of Dietary Propetamphos (Technical) in Rats: Final Report: Lab Project Number: HWA 777-141: 9005. Unpublished study prepared by Hazleton Washington, Inc. 488 p.
- 43890201 Cannon, J. (1995) Evaluation of Propetamphos Degradation in Four Food Matrices: Lab Project Number: 3861: 0924-167: 2207. Unpublished study prepared by Midwest Research Institute. 71 p.
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Appendix E. Generic Data Call-In

See attached table for a list of generic data requirements. Note that a complete Data Call-In (DCI), with all pertinent instructions, is being sent to registrants under separate cover.

United States Environmental Protection Agency

Washington, D.C. 20460

DATA CALL-IN RESPONSE

Form Approved

OMB No. 2070-0107
2070-0057

Approval Expires 12/31/00

INSTRUCTIONS: Please type or print in ink. Please read carefully the attached instructions and supply the information requested on this form. Use additional sheet(s) if necessary

1. Company name and Address		2. Case # and Name 2550 Propetamphos Chemical # and Name 113601 Propetamphos		3. Date and Type of DCI GENERIC	
4. EPA Product Registration	5. I wish to cancel this product registration voluntarily	6. Generic Data 6a. I am claiming a Generic Data Exemption because I obtain the active ingredient from the source EPA registration number listed below.	6b. I agree to satisfy Generic Data requirements as indicated on the attached form entitled "Requirements Status and Registrant's Response."	7. Product Specific Data 7a. My product is an MUP and I agree to satisfy the MUP requirements on the attached form entitled "Requirements Status and Registrant's Response."	7b. My product is an EUP and I agree to satisfy the EUP requirements on the attached form entitled "Requirements Status and Registrant's Response."
8. Certification I certify that the statements made on this form and all attachments are true, accurate, and complete. I acknowledge that any knowingly false or misleading statement may be punishable by fine, imprisonment or both under applicable law.		9. Date		11. Phone Number	
Signature and Title of Company's Authorized Representative		10. Name of Company Contact			

United States Environmental Protection Agency
 Washington, D.C. 20460
REQUIREMENTS STATUS AND REGISTRANT'S RESPONSE

Form Approved
 OMB No. 2070-0107
 2070-0057
 Approval Expires 12/31/00

INSTRUCTIONS: Please type or print in ink. Please read carefully the attached instructions and supply the information requested on this form. Use additional sheet(s) if necessary

3. Date and Type of DCI
GENERIC

2. Case # and Name
2550 Propetamphos
 Chemical # and Name **113601**
 Propetamphos

4. Guideline Requirement Number	5. Study Title	6. Use Pattern			7. Test Substance	8. Time Frame	9. Registrant Response
		Progress Reports	1	2			
63-10 63-11 63-13 830.7050	Dissociation Constant Oct/Water partition Coef. Stability U/V Visible Absorption	PROHIBIT				all all all LMN	12 MOS. 12 MOS. 12 MOS. 12 MOS.

10. Certification
 I certify that the statements made on this form and all attachments are true, accurate, and complete.
 I acknowledge that any knowingly false or misleading statement may be punishable by fine, imprisonment or both under applicable law.
 Signature and Title of Company's Authorized Representative _____

11. Date _____
 12. Name of Company Contact _____
 13. Phone Number _____

Appendix F: Product Specific Data Call-In

See attached table for a list of product-specific data requirements. Note that a complete Data Call-In (DCI), with all pertinent instructions, is being sent to registrant under separate cover.

United States Environmental Protection Agency
 Washington, D. C. 20460
 DATA CALL-IN RESPONSE

Form Approved
 OMB No. 2070-0107
 2070-0057

INSTRUCTIONS: Please type or print in ink. Please read carefully the attached instructions and supply the information requested on this form. Use additional sheet(s) if necessary.

1. Company name and Address SAMPLE COMPANY NO STREET ADDRESS NO CITY, XX 00000		2. Case # and Name 2550 Propetamphos		3. Date and Type of DCI PRODUCT SPECIFIC		
4. EPA Product Registration NNNNNN - NNNNN		5. I wish to cancel this product registration voluntarily.	6. Generic Data 6a. I am claiming a Generic Data Exemption because I obtain the active ingredient from the source EPA registration number listed below. N.A.	6b. I agree to satisfy Generic Data requirements as indicated on the attached form entitled "Requirements Status and Registrant's Response." N.A.	7. Product Specific Data 7a. My product is a MUP and I agree to satisfy the MUP requirements on the attached form entitled "Requirements Status and Registrant's Response." N.A.	7b. My product is an EUP and I agree to satisfy the EUP requirements on the attached form entitled "Requirements Status and Registrant's Response." N.A.
8. Certification I certify that the statements made on this form and all attachments are true, accurate, and complete. I acknowledge that any knowingly false or misleading statement may be punishable by fine, imprisonment or both under applicable law. Signature and Title of Company's Authorized Representative _____						
9. Date _____						
10. Name of Company Contact _____						
11. Phone Number _____						

United States Environmental Protection Agency
Washington, D. C. 20460
REQUIREMENTS STATUS AND REGISTRANT'S RESPONSE

Form Approved
OMB No. 2070-0107
2070-0057

INSTRUCTIONS: Please type or print in ink. Please read carefully the attached instructions and supply the information requested on this form. Use additional sheet(s) if necessary.

1. Company name and Address SAMPLE COMPANY NO STREET ADDRESS NO CITY, XX 00000		2. Case # and Name 2550 Propetamphos EPA Reg. No. NNNNNN-NNNNN			3. Date and Type of DCI PRODUCT SPECIFIC ID# NNNNNN-RD-NNNN			7. Test Substance	8. Time Frame	9. Registrant Response
4. Guideline Requirement Number	5. Study Title	1	2	3	PROTOCOL					
830.1550	<u>Prod Chem - Regular Chemical</u> Product identity & composition (1) Description of materials used (1,2) to produce the product Description of production (1,2) process Description of formulation (1,2) process Discussion of formation of (1,3) impurities Preliminary analysis (1,4) Certified limits (1,5) Enforcement analytical method (1) Color (17) Physical state (17) Odor (17)									
830.1600					ABCDEFHIJKLMNO	MP/EP	8 MOS.			
830.1620					ABCDEFHIJKLMNO	MP/EP	8 MOS.			
830.1650					ABCDEFHIJKLMNO	MP/EP	8 MOS.			
830.1670					ABCDEFHIJKLMNO	MP/EP	8 MOS.			
830.1700					ABCDEFHIJKLMNO	MP/EP	8 MOS.			
830.1750					ABCDEFHIJKLMNO	MP/EP	8 MOS.			
830.1800					ABCDEFHIJKLMNO	MP/EP	8 MOS.			
830.6302				ABCDEFHIJKLMNO	MP/EP	8 MOS.				
830.6303				ABCDEFHIJKLMNO	MP/EP	8 MOS.				
830.6304				ABCDEFHIJKLMNO	MP/EP	8 MOS.				

10. Certification
I certify that the statements made on this form and all attachments are true, accurate, and complete.
I acknowledge that any knowingly false or misleading statement may be punishable by fine, imprisonment or both under applicable law.

Signature and Title of Company's Authorized Representative _____

11. Date _____

12. Name of Company Contact _____

13. Phone Number _____

United States Environmental Protection Agency
 Washington, D. C. 20460
REQUIREMENTS STATUS AND REGISTRANT'S RESPONSE

Form Approved

OMB No. 2070-0107
 2070-0057

INSTRUCTIONS: Please type or print in ink. Please read carefully the attached instructions and supply the information requested on this form. Use additional sheet(s) if necessary.

1. Company name and Address SAMPLE COMPANY NO STREET ADDRESS NO CITY, XX 00000		2. Case # and Name 2550 Propetamphos EPA Reg. No. NNNNNN-NNNNN		3. Date and Type of DCI PRODUCT SPECIFIC ID# NNNNNN-RD-NNNN		4. Guideline Requirement Number			5. Study Title	6. Use Pattern	7. Test Substance	8. Time Frame	9. Registrant Response
						Progress Reports	1	2					
830.7000													
830.7050													
830.7100													
830.7300													
830.6314													
830.6315													
830.6316													
830.6317													
830.6319													
830.6320													
830.6321													
870.1100													
870.1200													
870.1300													
870.2400													
870.2500													
870.2600													

Initial to indicate certification as to information on this page (full text of certification is on page one).

Date

United States Environmental Protection Agency
 Washington, D. C. 20460
REQUIREMENTS STATUS AND REGISTRANT'S RESPONSE

Form Approved
 OMB No. 2070-0107
 2070-0057

INSTRUCTIONS: Please type or print in ink. Please read carefully the attached instructions and supply the information requested on this form.
 Use additional sheet(s) if necessary.

4. Guideline Requirement Number	5. Study Title	2. Case # and Name			7. Test Substance	8. Time Frame	9. Registrant Response
		1	2	3			
		2550 Propetamphos EPA Reg. No. NNNNNN-NNNNN					
		Efficacy - Invertebrate Control Agents					
95-11	Premises Treatments Laboratory efficacy evaluation				KLM O EP	8 MOS.	
95-11	Comparative field test				KLM O EP	8 MOS.	

Initial to indicate certification as to information on this page
 (full text of certification is on page one). Date

United States Environmental Protection Agency
Washington, D. C. 20460

FOOTNOTES AND KEY DEFINITIONS FOR GUIDELINE REQUIREMENTS

Case # and Name: 2550 Propetamphos

Key: MP = manufacturing-use product; EP = end-use product; provided formulators purchase their active ingredient(s) from a registered source, they need not submit or cite data pertaining to the purchased product. NOTE: If a product is a 100 percent repackage of another registered product, registrants are not subject to any data requirements identified in the tables.; TE = typical end-use product; TGA = technical grade of the active ingredient; PAI = "pure" active ingredient; PAIRA = "pure" active ingredient, radiolabeled.

Use Categories Key:

A - Terrestrial food crop	B - Terrestrial food feed crop	C - Terrestrial nonfood crop	D - Aquatic food crop	E - Aquatic nonfood outdoor
F - Aquatic nonfood Industrial	G - Aquatic nonfood residential	H - Greenhouse food crop	I - Greenhouse nonfood crop	J - Forestry
K - Residential outdoor	L - Indoor food	M - Indoor nonfood	N - Indoor Medical	O - Indoor residential

Footnotes: [The following notes are referenced in column two (5. Study Title) of the REQUIREMENTS STATUS AND REGISTRANT'S RESPONSE form.]

Prod Chem - Regular Chemical

- 1 Requirements pertaining to product identity, composition, analysis, and certification of ingredients are detailed further in the following sections: *158.155 for product identity and composition (61-1); *158.160, 158.162, and 158.165 for description of starting materials and manufacturing process (61-2); *158.167 for discussion of formation of impurities (61-3); *158.170 for preliminary analysis (62-1); *158.175 for certification of limits (62-2); and *158.180 for enforcement analytical methods (62-3).
- 2 A schematic diagram and/or brief description of the production process will suffice if the pesticide is not already under full scale production and an experimental use permit is being sought.
- 3 If the pesticide is not already under full scale production and an experimental use permit is sought, a discussion of unintentional ingredients shall be submitted to the extent this information is available.
- 4 To support registration of an MP or EP, whether produced by an integrated system or not, the technical grade of Active Ingredient must be analyzed. If the technical grade of Active Ingredient cannot be isolated, a statement of composition of the practical equivalent of the technical grade of Active Ingredient must be submitted. Data on EPs or MPs will be required on a case-by-case basis.
- 5 Certified limits are not required for inert ingredients in products proposed for experimental use.
- 9 Required if test substances are dispersible with water.
- 10 Required if product contains an oxidizing or reducing agent.
- 11 Required if product contains combustible liquids.
- 12 Required if product is potentially explosive.
- 13 Required if product is a liquid.
- 14 Required if product is an emulsifiable liquid and is to be diluted with petroleum solvents.
- 15 Required if end-use product is liquid and is to be used around electrical equipment.
- 17 Not required unless efficacy data are required.

Acute Toxic - Regular Chemical

- 1 Not required if test material is a gas or highly volatile.
- 2 Not required if test material is corrosive to skin or has pH less than 2 or greater than 11.5; such a product will be classified as Toxicity Category I on the basis of potential eye and dermal irritation effects.
- 3 Required if the product consists of, or under conditions of use will result in, an inhalable material (e. g., gas, volatile substances, or aerosol/particulate).
- 4 Required unless repeated dermal exposure does not occur under conditions of use.

United States Environmental Protection Agency
Washington, D. C. 20460

FOOTNOTES AND KEY DEFINITIONS FOR GUIDELINE REQUIREMENTS

Case # and Name: 2550 Propetamphos

Footnotes (cont.):

37 Testing of the EP dilution in addition to the EP or MP is required if it can be reasonably anticipated that the results of such testing may meet the criteria for restriction to use by certified applicators specified in 40 CFR 152.170(b) or the criteria for initiation of special review specified in 40 CFR 154.7 (a)(1).

Efficacy - Invertebrate Control Agents

- 1 The agency has waived all requirements to submit efficacy data for invertebrate control agents for nonpublic health uses. However, each registrant must ensure through testing that his products are efficacious when used in accordance with label directions and commonly accepted pest control practices. The registrant must develop and maintain the relevant data upon which the determination of efficacy is based. The Agency reserves the right to require, on a case-by-case basis (e.g., significant new uses or benefits data in cases of special reviews) submission of efficacy data for any pesticide product, registered or proposed for registration when necessary.
- 2 Comparative product performance data are required to be developed and maintained in the registrant's file and must be submitted to the Agency on a case-by-case basis for risk/benefit analyses such as for public interest findings and cases of special review.
- 3 Efficacy evaluations can be conducted under laboratory, greenhouse, or field conditions.
- 4 Required to be developed and maintained in the Registrant's file for all pests claimed on the label when resistance to the pesticide has been demonstrated.
- 50 Data showing each product is efficacious when used in accordance with label directions and commonly accepted pest control practices must be submitted for the public health pest, cockroaches. The conduction of the efficacy studies must be consistent with the EPA Guidelines (95-11) and Good Laboratory Practices.

Appendix G: List of Registrants Sent this Data Call-In

List of All Registrants Sent This Data Call-In Notice

Case # and Name

2550 Propetamphos

Chemical # and Name

113601 Butenoic acid, 3-((ethylamino)methoxyphosphinothi

Company Number Company Name

002724 WELLMARK INTERNATIONAL

Additional Name

Address

1000 TOWER LANE, SUITE 245

City & State

BENSENVILLE IL

Zip

60106

Appendix H: List of Related Documents and Electronically Available Forms

Pesticide Registration Forms are available at the following EPA internet site:

<http://www.epa.gov/opprd001/forms/>.

Pesticide Registration Forms (These forms are in PDF format and require the Acrobat reader)

Instructions

1. Print out and complete the forms. (Note: Form numbers that are bolded can be filled out on your computer then printed.)
2. The completed form(s) should be submitted in hardcopy in accord with the existing policy.
3. Mail the forms, along with any additional documents necessary to comply with EPA regulations covering your request, to the address below for the Document Processing Desk.

DO NOT fax or e-mail any form containing 'Confidential Business Information' or 'Sensitive Information.'

If you have any problems accessing these forms, please contact Nicole Williams at (703) 308-5551 or by e-mail at williams.nicole@epamail.epa.gov.

The following Agency Pesticide Registration Forms are currently available via the internet:
at the following locations:

8570-1	Application for Pesticide Registration/Amendment	http://www.epa.gov/opprd001/forms/8570-1.pdf
8570-4	Confidential Statement of Formula	http://www.epa.gov/opprd001/forms/8570-4.pdf
8570-5	Notice of Supplemental Registration of Distribution of a Registered Pesticide Product	http://www.epa.gov/opprd001/forms/8570-5.pdf
8570-17	Application for an Experimental Use Permit	http://www.epa.gov/opprd001/forms/8570-17.pdf
8570-25	Application for/Notification of State Registration of a Pesticide To Meet a Special Local Need	http://www.epa.gov/opprd001/forms/8570-25.pdf
8570-27	Formulator's Exemption Statement	http://www.epa.gov/opprd001/forms/8570-27.pdf
8570-28	Certification of Compliance with Data Gap Procedures	http://www.epa.gov/opprd001/forms/8570-28.pdf
8570-30	Pesticide Registration Maintenance Fee Filing	http://www.epa.gov/opprd001/forms/8570-30.pdf

8570-32	Certification of Attempt to Enter into an Agreement with other Registrants for Development of Data	http://www.epa.gov/opprd001/forms/8570-32.pdf
8570-34	Certification with Respect to Citations of Data (in PR Notice 98-5)	http://www.epa.gov/opppmsd1/PR_Notices/pr98-5.pdf
8570-35	Data Matrix (in PR Notice 98-5)	http://www.epa.gov/opppmsd1/PR_Notices/pr98-5.pdf
8570-36	Summary of the Physical/Chemical Properties (in PR Notice 98-1)	http://www.epa.gov/opppmsd1/PR_Notices/pr98-1.pdf
8570-37	Self-Certification Statement for the Physical/Chemical Properties (in PR Notice 98-1)	http://www.epa.gov/opppmsd1/PR_Notices/pr98-1.pdf

Pesticide Registration Kit

www.epa.gov/pesticides/registrationkit/

Dear Registrant:

For your convenience, we have assembled an online registration kit which contains the following pertinent forms and information needed to register a pesticide product with the U.S. Environmental Protection Agency's Office of Pesticide Programs (OPP):

1. The Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) and the Federal Food, Drug and Cosmetic Act (FFDCA) as Amended by the Food Quality Protection Act (FQPA) of 1996.
2. Pesticide Registration (PR) Notices
 - a. 83-3 Label Improvement Program--Storage and Disposal Statements
 - b. 84-1 Clarification of Label Improvement Program
 - c. 86-5 Standard Format for Data Submitted under FIFRA
 - d. 87-1 Label Improvement Program for Pesticides Applied through Irrigation Systems (Chemigation)
 - e. 87-6 Inert Ingredients in Pesticide Products Policy Statement
 - f. 90-1 Inert Ingredients in Pesticide Products; Revised Policy Statement
 - g. 95-2 Notifications, Non-notifications, and Minor Formulation Amendments
 - h. 98-1 Self Certification of Product Chemistry Data with Attachments (This document is in PDF format and requires the Acrobat reader.)

Other PR Notices can be found at http://www.epa.gov/opppmsd1/PR_Notices.

3. Pesticide Product Registration Application Forms (These forms are in PDF format and will require the Acrobat reader.)
 - a. EPA Form No. 8570-1, Application for Pesticide Registration/Amendment
 - b. EPA Form No. 8570-4, Confidential Statement of Formula
 - c. EPA Form No. 8570-27, Formulator's Exemption Statement

- d. EPA Form No. 8570-34, Certification with Respect to Citations of Data
 - e. EPA Form No. 8570-35, Data Matrix
4. General Pesticide Information (Some of these forms are in PDF format and will require the Acrobat reader.)
- a. Registration Division Personnel Contact List
 - 2. Biopesticides and Pollution Prevention Division (BPPD) Contacts
 - 41. Antimicrobials Division Organizational Structure/Contact List
 - d. 53 F.R. 15952, Pesticide Registration Procedures; Pesticide Data Requirements (PDF format)
 - e. 40 CFR Part 156, Labeling Requirements for Pesticides and Devices (PDF format)
 - f. 40 CFR Part 158, Data Requirements for Registration (PDF format)
 - g. 50 F.R. 48833, Disclosure of Reviews of Pesticide Data (November 27, 1985)

Before submitting your application for registration, you may wish to consult some additional sources of information. These include:

1. The Office of Pesticide Programs' Web Site
2. The booklet "General Information on Applying for Registration of Pesticides in the United States," PB92-221811, available through the National Technical Information Service (NTIS) at the following address:

National Technical Information Service (NTIS)
5285 Port Royal Road
Springfield, VA 22161

The telephone number for NTIS is (703) 605-6000. Please note that EPA is currently in the process of updating this booklet to reflect the changes in the registration program resulting from the passage of the FQPA and the reorganization of the Office of Pesticide Programs. We anticipate that this publication will become available during the Fall of 1998.

3. The National Pesticide Information Retrieval System (NPIRS) of Purdue University's Center for Environmental and Regulatory Information Systems. This service does charge a fee for subscriptions and custom searches. You can contact NPIRS by telephone at (765) 494-6614 or through their Web site.
4. The National Pesticide Telecommunications Network (NPTN) can provide information on active ingredients, uses, toxicology, and chemistry of pesticides. You can contact NPTN by telephone at (800) 858-7378 or through their Web site: ace.orst.edu/info/nptn.

The Agency will return a notice of receipt of an application for registration or amended registration, experimental use permit, or amendment to a petition if the applicant or petitioner

encloses with his submission a stamped, self-addressed postcard. The postcard must contain the following entries to be completed by OPP:

Date of receipt
EPA identifying number
Product Manager assignment

Other identifying information may be included by the applicant to link the acknowledgment of receipt to the specific application submitted. EPA will stamp the date of receipt and provide the EPA identifying File Symbol or petition number for the new submission. The identifying number should be used whenever you contact the Agency concerning an application for registration, experimental use permit, or tolerance petition.

To assist us in ensuring that all data you have submitted for the chemical are properly coded and assigned to your company, please include a list of all synonyms, common and trade names, company experimental codes, and other names which identify the chemical (including "blind" codes used when a sample was submitted for testing by commercial or academic facilities). Please provide a CAS number if one has been assigned.

Documents Associated with this RED

The following documents are part of the Administrative Record for this RED document and may be included in the EPA's Office of Pesticide Programs Public Docket. Copies of these documents are not available electronically, but may be obtained by contacting the person listed on the respective Chemical Status Sheet.

- a. Health and Environmental Effects Science Chapters.
- b. Detailed Label Usage Information System (LUIS) Report.