A QUANTITATIVE RISK ASSESSMENT WITH ESTIMATED UNCERTAINTY FOR PESTICIDE USE IN OKLAHOMA

BY

JON S. HANSON

Bachelor of Science

Oklahoma State University

Stillwater, Oklahoma

1993

Submitted to the Faculty of the
Graduate College of the
Oklahoma State University
in partial fulfillment of
the requirements for
the Degree of
MASTER OF SCIENCE
December, 1995

A QUANTITATIVE RISK ASSESSMENT WITH ESTIMATED UNCERTAINTY FOR PESTICIDE USE IN OKLAHOMA

Thesis Approved:

William F. McTernan

Thesis Advisor

Gregory J. Wilber

Kirk D Wells

Thomas C. Collins

Dean of the Graduate College

ACKNOWLEDGMENTS

I would like to express my genuine gratitude to my major advisor, Dr. William McTernan, for his arranging generous financial support, for all the time he spent assisting me, and for his persistent encouragement. I thank him for providing me with this research opportunity. Without his guidance this project could not have been completed.

I would also like to thank my immediate family for their contributions. My father, Dr. Bertil Hanson, provided many excellent suggestions that I feel greatly improved the quality of this work. My mother, Adelia, provided me with moral support and many splendid meals. My brother, Peter, provided solutions to many of the computer difficulties I faced. Without their support this undertaking would have been a much more formidable task.

I would also like to thank Dr. Jim Crisswell in Entomology Department for allowing me access to their computer containing the IRIS data base.

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CHAPTER I

INTRODUCTION

Background

The agricultural community is now dependent upon chemical control of pests through the use of pesticides (Furtick, 1976). Pesticides are materials that are toxic to pests in some stage of their life cycle. Their use is necessary in order to economically provide the large volume of crops required by our society (Furtick, 1976). Each year thousands of tons of these chemicals are applied to farmland throughout the U.S. Five hundred thousand tons of active ingredients were applied in 1991 (Pimentel and Acquay, 1992). The amount applied has more than doubled since 1984 (OTA, 1984).

Pesticides contain many different chemicals and their impact on soil, water, and air contamination is substantial. When these chemicals accumulate in the environment they may become available for absorption by higher animals (including human beings) that were not the intended target organisms. In some cases this could effect the health of the organism adversely (Connell and Miller, 1984). Sixty-seven thousand non-fatal pesticide poisonings were reported in 1990 (Pimentel and Acquay, 1992).

Finding optimal ways to reduce the hazards associated with potentially harmful chemicals is a challenging engineering problem. Ideally, what one would like to do as an engineer is show that some combinations of ingredients in the picture that consists of assorted pesticides, different irrigation techniques, different soils, and different levels of exposure are less hazardous to people than others.

Routes of Exposure

People can be exposed to hazardous chemicals in many ways. They may drink or bathe in water that has been contaminated, breath air that has been contaminated, or be exposed to soil that carries pesticide residues.

When pesticides are applied, they are either sprayed onto the crop canopy or are applied directly onto or into the ground (Yaron, 1989). They do not necessarily remain stationary. Pesticides can move through the environment by diffusion, mass flow, volatilization, and/or may be transported on adsorbed particles (Yaron, 1989). As pesticides move through the environment they undergo physical, chemical and biological transformations, but often retain their toxic properties (Yaron, 1989). If the pesticides do not degrade rapidly they may migrate downward to the water table, possibly resulting in contaminated groundwater. If this groundwater is used as a water source

the contaminants may be piped directly into residences, where people will drink and bathe in them. Contaminants may also volatilize from the groundwater being used to cook with or shower in, allowing people to inhale them.

Contaminated groundwater is not the only way for people to be exposed to pesticides. Pesticides can also pollute the atmosphere. The chemicals can become airborne through the mechanisms of volatilization or they may be adsorbed on to soil particles which then become airborne as the wind picks them up. If people inhale these pollutants as vapors or dust emissions it can present a health hazard. People can also be exposed to these chemicals by coming into contact with contaminated soil. The chemicals can be absorbed by the body, directly through the skin.

Figure 1-1 exhibits the routes of exposure that were considered in this effort. These include drinking water, dermal uptake during shower, inhalation during shower, inhalation of soil emissions, dermal contact with soil, and soil ingestion.

Exposure to these chemicals may affect people differently. People come in all shapes and sizes and have many different habits. These factors all compound the

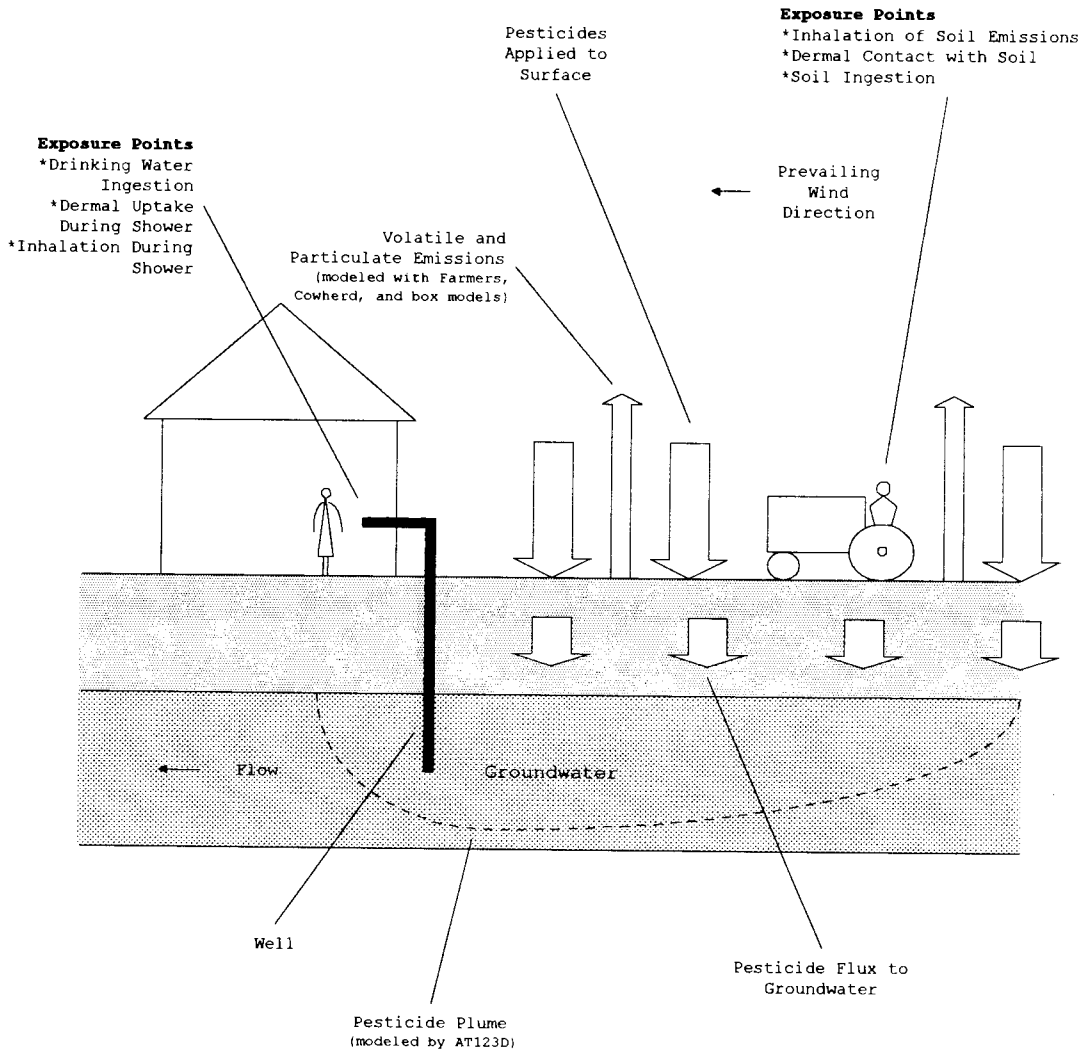


Figure 1-1 The exposure route that were used for this study

difficulty of determining just how big a risk people face from coming into contact with these chemicals.

Hazard Index

The dangers faced by a population exposed to contaminants can be quantified by using hazard quotients for non-carcinogenic effects and cancer risk probabilities for carcinogenic effects (U.S.EPA, 1989). The hazard quotient is defined as the ratio of an exposure level over a specified time period to a toxicity value for that substance (U.S.EPA, 1989). The sum of hazard quotients for each exposure pathway is known as the hazard index (U.S.EPA, 1989). When the hazard index exceeds one, there is the potential for health to be effected (U.S.EPA, 1989). It should be noted that the hazard index is a measure of the potential for non-carcinogenic effects and it is not a probabilistic risk.

Cancer risk values are estimated as the probability of an individual developing cancer over a lifetime as a result of exposure to the potential carcinogen (U.S.EPA, 1989). None of the pesticides in this study are considered to be carcinogens by the U.S.EPA, for which reason cancer risk probabilities were not given special consideration in this study.

Reference Doses

The reference dose (RfD) is the EPA's preferred toxicity value for evaluating non-carcinogenic effects resulting from exposure to contaminants (U.S.EPA, 1989). In order to determine a RfD value a review committee established by the EPA gathers all available studies examining the toxicity of a chemical. These studies are examined for scientific merit and any differences between studies are reconciled. An overall evaluation is reached and the EPA identifies the experimental exposure level representing the highest level tested at which no adverse effects were demonstrated. This highest "no-observed-adverse-effect level" (NOAEL) is the key to deriving a RfD. The RfD is calculated using this equation (U.S.EPA, 1989):

$$RfD = \frac{NOAEL}{\sum UF_{1..n} \times MF} \qquad (1\text{-}1)$$

where

UF = uncertainty factors
MF = modifying factor

Uncertainty

The discussion of uncertainty is an important part of any environmental risk assessment. A decision-maker can evaluate whether hazard index estimates are the highest likely to occur based on the sources and degree of uncertainty. Uncertainties about the numerical results of

environmental risk assessments are generally large, often as large as an order of magnitude or greater (U.S.EPA, 1989). Some sources of uncertainty include absence of accurate field data, model applicability and assumptions, toxicity values, and parameter uncertainty. The last is of particular concern to this study.

Parameter value uncertainty is the uncertainty in the results of a risk assessment that arises from variability in the parameters used during the calculations of chemical fate and transport and human intake. It can be quantified by performing a sensitivity analysis. In a sensitivity analysis the values of parameters that are suspected to have an influence on the uncertainty are varied. The degree to which changes in the input variables affect changes in the output can then be compared for different input variables. The variable with the highest ratio of change in the output to change in the input would be the variable to which the model is most sensitive.

The overall uncertainty in a model can be quantified by using Monte Carlo analysis. The output from a Monte Carlo analysis results in a distribution of exposures and the assessor can identify the value corresponding to any specified percentile (U.S.EPA, 1989). Monte Carlo analysis is discussed further, later in this chapter.

The Purpose of this Study

The present study concerns the problem of characterizing and quantifying risks posed to human health by long term exposure to pesticidal substances used on crops. It focuses on conditions in Caddo County, Oklahoma, but in principal the same kind of study could be done for any agricultural locale.

As will be shown in the following pages, an attempt was made to identify variables representing the toxicity of pesticidal substances and degrees of exposure to them that have the most significant effect on risks to human health. Once these variables were identified, the uncertainty in the hazard index that they influenced was qualitatively estimated by performing an uncertainty analysis using American Petroleum Institute's Decision Support System.

Identification of exposure related variables and examination of the assumptions that affected the uncertainty in the hazard index were key parts of this study. The study summarized and quantified uncertainty associated with key exposure-related parameters and discussed how differences in pesticides, soil type and crops produced different hazard indexes.

Hopefully this study will provide information that will assist in performing risk assessments and lead to a better

understanding of the degree to which health hazards can be reasonably reduced. Also, it is hoped that this information can contribute to better irrigation management practices.

Site Selection

Caddo County, Oklahoma was chosen for this investigation because farming practices there are undergoing a change. Many of the farmers are moving from non-irrigated

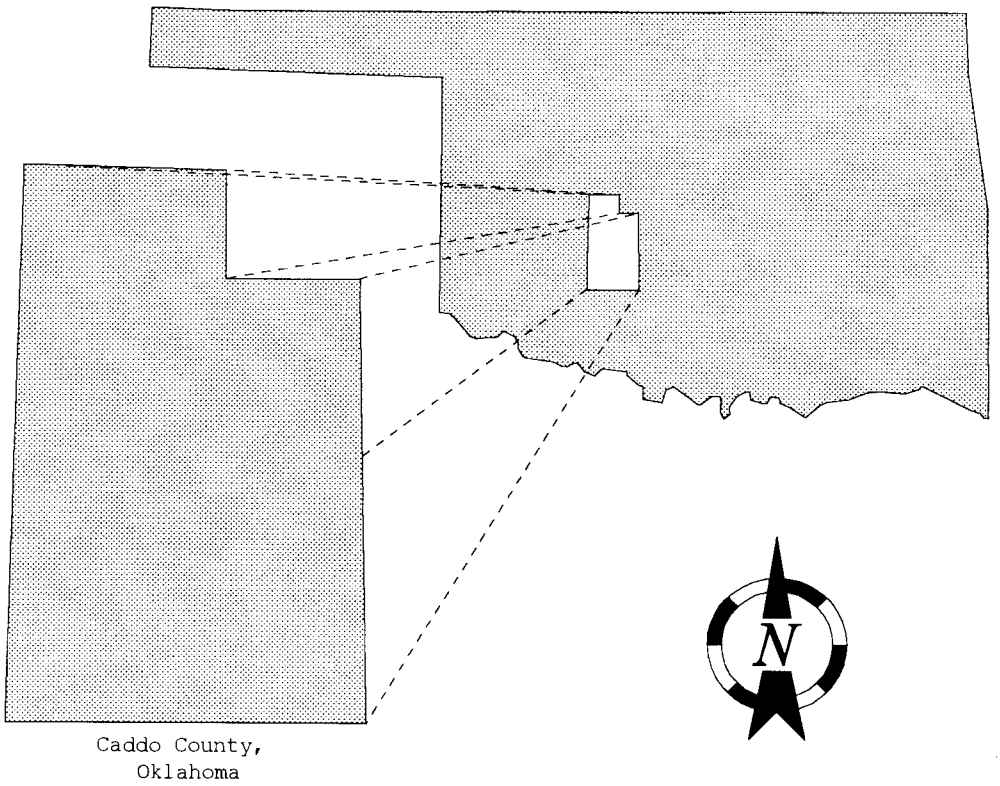


Figure 1-2

crops to crops that require irrigation but turn a higher profit. The irrigated area in this county has risen from 44,439 acres (U.S. Dept. of Commerce, 1989) to 48,636 acres (U.S. Dept. of Commerce, 1994), reflecting this change. With increasing irrigation there is an increased chance of pesticides leaching to groundwater and being discharged to surface waters (McTernan and Mize, 1991). This increased chance of ground and surface water contamination has the possibility of exposing humans to an increased risk of adverse health effects.

Consequently the problem arises of reconciling the farmers wish for a more profitable kind of farming with the more general goal of minimizing the risk to human health. A risk assessment that is well done can be very useful when confronting this problem. It is a goal of this study to provide information that will lead to more reliable risk assessments and lead to a more complete understanding of the results. This, it is hoped, will contribute to a better understanding of irrigation management practices that are tolerable from a public health viewpoint.

American Petroleum Institute's Decision Support System

APIDSS Version 1.0 was the primary tool used for this study. It is a computer software package that provides an

easy to use interface to a combination of publicly available models. It was developed to assist in the estimation of human exposure and risk from contaminated sites. The software brings together several well known fate and transport models: Sesoil and Jury for unsaturated zone modeling, AT123D for groundwater transport modeling, and Sesoil, Jury, Farmers and Thibodeaux's air emission models which are linked to a box or Gaussian air dispersion model (Farmer, et al. 1980, Pasquill, 1961, Yeh, 1981, API, 1994). The program then uses the receptor point concentrations provided by the fate and transport models to estimate the exposure and the subsequent risk to humans for several exposure routes. The models utilized by this study are discussed in greater detail in Chapter III.

The APIDSS package might not be completely appropriate for this study because it was originally designed for use with petroleum-related chemicals. Also pesticides are applied by spraying or surface application, this means that air is the first medium through which the chemicals move. This is not accounted for in the models included with APIDSS, and thus was not accounted for in this effort.

The Monte Carlo Technique

APIDSS includes the option to perform a Monte Carlo analyses around the Fate and Transport models as well as for the Chemical Intake and Risk Calculation models. A Monte Carlo simulation is the process of repeatedly solving a model's equation(s). It allows the user to enter the statistical parameters needed to describe the distribution of each parameter. The computer selects randomly from these probability distributions describing each variable every time the equation/model is solved.

A Monte Carlo simulation can be described by the following:

$$C = f(x_{1..n}) \qquad (1\text{-}2)$$

where

C is the concentration of contaminant at a receptor point

f is a function representing a fate and transport model

$x_{1..n}$ represents the vector of all of the parameters required by the model

At least one of the parameters represented by $x_{1..n}$ must defined by a statistical distribution. When equation 1-2 is solved repeatedly, the resulting values can be grouped into cumulative probability distributions, from which an assessor can estimate the value corresponding to any specified

percentile. For example, the 95th percentile upperbound receptor point concentration or hazard index can be estimated.

It is this feature that allows the uncertainty to be quantified. If the results of a model have a very large standard deviation the cumulative distribution function will have a very steep slope and there will be significant uncertainty. If the standard deviation is small the cumulative distribution function will have a more gradual slope, thus revealing to the modeler that there is less uncertainty in the results. Further, if this type of analysis is applied sequentially to each of the critical transport or exposure variables, the relative amount of uncertainty associated with each variable can be identified. This type of stochastic sensitivity analysis can be employed to assign relative probabilities to these uncertainties.

CHAPTER II

METHODOLOGY AND RISK ASSESSMENT BASICS

This study was conducted in two distinct phases: a risk assessment and an uncertainty analysis. The first phase of the study involved determining hazard indexes for many different possible agronomic alternatives common in Caddo County. These alternatives consisted of four kinds of crops, three types of soils, six pesticides, and two irrigation practices. The soils were classified by their SCS hydrologic soil grouping. A type soils are the most permeable and D type the least. The crops were peanuts, alfalfa, wheat, and cotton. The two irrigation methods were full or none. The pesticides are discussed later in this chapter. All of these alternatives were defined in Mills (1994).

A risk assessment was performed for each combination of these alternatives. In order to complete this phase the methods for performing a risk assessment as explained in Risk Assessment Guidance for Superfund (U.S.EPA, 1989) and in the APIDSS manual (1994) were followed.

In Phase 2, the uncertainty in the hazard index that arose from variation in individual parameters was calculated. This was done using the Monte Carlo techniques described in Chapter I and later in this chapter.

Each component of a typical risk assessment and how each step was performed for this study are discussed below. The procedures used to complete Phase 2 are also explained.

Phase 1: Risk Assessment

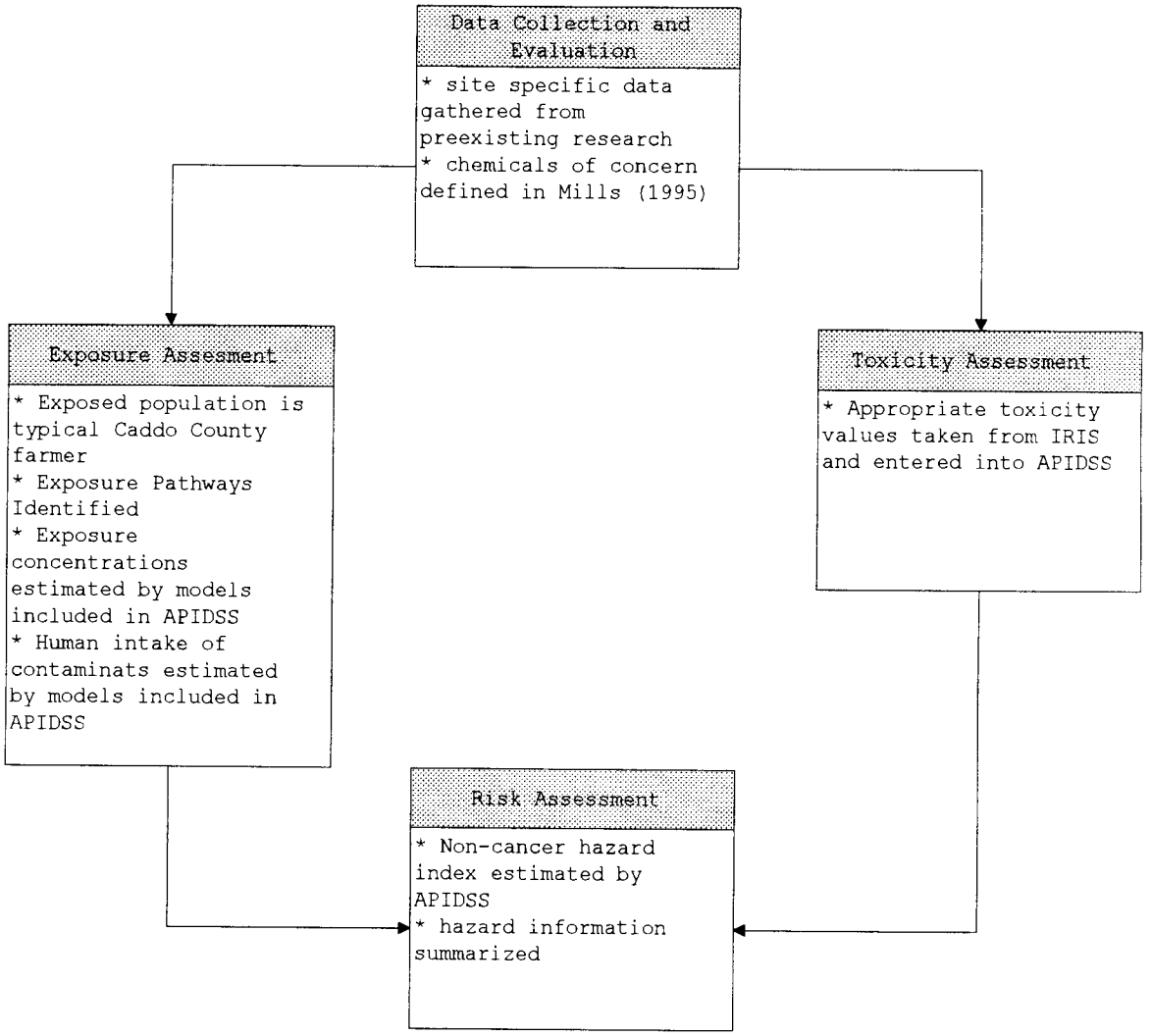
The main objective of this aspect of the study was to characterize the risks to human health brought about by the use of the various agronomic alternatives listed above on crops in Caddo County, Oklahoma using risk assessment methods.

There were four fundamental steps in the risk assessment process. They were data collection and analysis, exposure assessment, toxicity assessment, and risk characterization. Figure 2-1 shows each of these steps and what was done for each step in this study.

Data Collection and Analysis

This step involves the gathering of site specific data relevant to the evaluation of risks to human health (U.S.EPA, 1989). This includes identification of hazardous substances present at the site and their release rates into the environment. It also includes gathering information on

Figure 2-1 The steps in a risk assessment and what was done for each step in this study (U.S.EPA, 1989)



the characteristics of the local environment that might effect the fate and transport of the chemicals.

The data reflecting the characteristics of the local environment are discussed in Chapter III in the sections on configuring the models. This information was compiled from existing sources (Tanaka and Davis, 1963, Upthegrove, 1989, Shonfelt *et al.*, 1991, API, 1994, and Das, 1990). It included permeability, hydraulic conductivity, hydraulic gradient, etc. Compiling this information was the first step of this study.

The pesticides of concern to this study, defined by Mills (1994), are Malathion, 2,4-D, Furadan, Lasso, Treflan, and Prowl. These pesticides were chosen because they are among some of the most commonly used in Oklahoma (Criswell, 1982). This study assumes that only one of these pesticides is present for any scenario. The application rates of these chemicals were defined by Mills (1994). They are given as loading rates (kg/hectare/day) to the unsaturated zone and the groundwater table. To enter these loading rates into the models used by APIDSS it was necessary to convert them to kg/yr entering the qroundwater and mg/kg for the concentration in the unsaturated zone. Conversion of these loading rates to kg/yr and mg/kg was accomplished as follows on the basis of farm size and geometry.

pesticide loading rate to aquifer:

$$\frac{kg}{yr} = \frac{kg}{ha \times d} \times \frac{365d}{yr} \times \frac{203.96ha}{farm} \qquad (2\text{-}1)$$

where

203.96 ha/farm is the avg. farm size in Caddo County (U.S. Dept. of Commerce, 1994).

pesticide concentration in unsaturated zone:

$$\frac{mg}{kg} = \frac{kg}{ha \times d} \times \frac{1(10)^6 mg}{kg} \times \frac{ha}{10{,}000m^2} \times \frac{m^3}{1800kg} \times \frac{1}{m} \qquad (2\text{-}2)$$

Tables 2-1 through 2-6 include Mills' data and the converted values. The letters in the far left column (PAF, PAO etc.) represent the cases modeled by Mills. The first letter represents the crop grown (P for peanuts). The second letter is the soil type and the third letter is the irrigation practice (F for full O for none).

Table 2-1 Data used for input to AT123D and soil emission and volatilization models (from Mills, 1994
Cases involving Lasso

Scenario		*Unsaturated zone conc.*			*Vadose zone loading rate*		
		kg/ha/d	mg/kg	std. dev.	kg/ha/d	kg/yr	std. dev.
	+1 std. dev.	2.00E-01	0.011111		2.00E-11	1.49E-06	
PAF	mean	0.1	0.005556	0.00501	1.10E-11	8.19E-07	6.33E-07
	-1 std. dev.	0.02	0.001111		3.00E-12	2.23E-07	
	+1 std. dev.	2.00E-01	0.011111		2.00E-11	1.49E-06	
PAO	mean	0.1	0.005556	0.00501	1.10E-11	8.19E-07	6.33E-07
	-1 std. dev.	0.02	0.001111		3.00E-12	2.23E-07	
	+1 std. dev.	3.76E-01	0.020889		7.42E-12	5.52E-07	
PBF	mean	3.70E-01	0.020556	0.000333	7.37E-12	5.49E-07	4.49E-09
	-1 std. dev.	3.64E-01	0.020222		7.30E-12	5.43E-07	
	+1 std. dev.	3.76E-01	0.020889		5.10E-12	3.8E-07	
PBO	mean	3.70E-01	0.020556	0.000333	5.06E-12	3.77E-07	2.98E-09
	-1 std. dev.	3.64E-01	0.020222		5.02E-12	3.74E-07	
	+1 std. dev.	3.21E-01	0.017833		2.10E-14	1.56E-09	
PDF	mean	3.21E-01	0.017833	3.21E-05	2.10E-14	1.56E-09	0
	-1 std. dev.	3.20E-01	0.017778		2.10E-14	1.56E-09	
	+1 std. dev.	5.10E-01	0.028333		3.30E-14	2.46E-09	
PDO	mean	4.00E-01	0.022222	0.007837	2.60E-14	1.94E-09	6.76E-10
	-1 std. dev.	2.30E-01	0.012778		1.50E-14	1.12E-09	

Table 2-2 Data used for input to AT123D and soil emission and volatilization models(from Mills, 1994)
Cases involving Furadan

Scenario		*Unsaturated zone conc.*			*Vadose zone loading rate*		
		kg/ha/d	mg/kg	std. dev.	kg/ha/d	kg/yr	std. dev.
	+1 std. dev.	2.00E-01	0.011111		2.20E-04	16.37829	
AAF	mean	0.1	0.005556	0.004243	1.00E-04	7.444677	6.823159
	-1 std. dev.	0.05	0.002778		4.00E-05	2.977871	
	+1 std. dev.	2.00E-01	0.011111		2.20E-04	16.37829	
AAO	mean	0.1	0.005556	0.004243	1.00E-04	7.444677	6.051901
	-1 std. dev.	0.05	0.002778		6.50E-05	4.83904	
	+1 std. dev.	6.44E-01	0.035778		1.00E-02	744.4677	
ABF	mean	6.42E-01	0.035667	0.00014	9.94E-03	740.0009	5.228969
	-1 std. dev.	6.39E-01	0.0355		9.86E-03	734.0452	
	+1 std. dev.	6.44E-01	0.035778		1.00E-02	744.4677	
ABO	mean	6.42E-01	0.035667	0.00014	9.94E-03	740.0009	5.228969
	-1 std. dev.	6.39E-01	0.0355		9.86E-03	734.0452	
	+1 std. dev.	5.72E-01	0.031778		3.90E-03	290.3424	
ADF	mean	5.72E-01	0.031778	3.21E-05	3.90E-03	290.3424	0.429819
	-1 std. dev.	5.71E-01	0.031722		3.89E-03	289.5979	
	+1 std. dev.	5.72E-01	0.031778		3.90E-03	290.3424	
ADO	mean	5.72E-01	0.031778	3.21E-05	3.90E-03	290.3424	0.429819
	-1 std. dev.	5.71E-01	0.031722		3.89E-03	289.5979	

Table 2-3 Data used for input to AT123D and soil emission and volatilization models(from Mills, 199

Cases involving 2,4-D

Scenario		*Unsaturated zone conc.*			*Vadose zone loading rate*		
		kg/ha/d	mg/kg	std. dev.	kg/ha/d	kg/yr	std. dev.
	+1 std. dev	0.45	0.025		7.50E-03	558.350793	
WAF	mean	0.33	0.01833333	0.00722934	5.50E-03	409.457248	187.353602
	-1std. dev.	0.19	0.01055556		2.50E-03	186.116931	
	+1 std. dev	0.45	0.025		8.00E-03	595.574179	
WAO	mean	0.33	0.01833333	0.00722934	5.50E-03	409.457248	205.010426
	-1std. dev.	0.19	0.01055556		2.50E-03	186.116931	
	+1 std. dev	0.78	0.04333333		0.0141	1049.69949	
WBF	mean	0.774	0.043	0.00039021	0.0139	1034.81014	14.8893545
	-1std. dev.	0.766	0.04255556		0.0137	1019.92078	
	+1 std. dev	0.78	0.04333333		0.0132	982.697396	
WBO	mean	0.774	0.043	0.00039021	0.0131	975.252718	11.3719323
	-1std. dev.	0.766	0.04255556		0.0129	960.363364	
	+1 std. dev	0.707	0.03927778		9.95E-03	740.745385	
WDF	mean	0.699	0.03883333	0.00047249	9.86E-03	734.045176	7.84345417
	-1std. dev.	0.69	0.03833333		9.74E-03	725.111563	
	+1 std. dev	0.707	0.03927778		9.65E-03	718.411354	
WDO	mean	0.699	0.03883333	0.00047249	9.56E-03	711.711144	7.45707471
	-1std. dev.	0.69	0.03833333		9.45E-03	703.521999	
	+1 std. dev	0.7	0.03888889		0.9	67002.0952	
PAF	mean	0.6	0.03333333	0.00743456	0.8	59557.4179	13008.6726
	-1std. dev.	0.435	0.02416667		0.56	41690.1925	
	+1 std. dev	0.7	0.03888889		0.9	67002.0952	
PAO	mean	0.6	0.03333333	0.00743456	0.8	59557.4179	13008.6726
	-1std. dev.	0.435	0.02416667		0.56	41690.1925	
	+1 std. dev	0.825	0.04583333		0.987	73478.9644	
PBF	mean	0.821	0.04561111	0.00022222	0.985	73330.0708	148.893545
	-1std. dev.	0.817	0.04538889		0.983	73181.1773	
	+1 std. dev	0.825	0.04583333		0.922	68639.9242	
PBO	mean	0.821	0.04561111	0.00022222	0.918	68342.1371	297.78709
	-1std. dev.	0.817	0.04538889		0.914	68044.35	
	+1 std. dev	0.681	0.03783333		0.617	45933.6586	
PDF	mean	0.68	0.03777778	3.2075E-05	0.616	45859.2118	42.9818641
	-1std. dev.	0.68	0.03777778		0.616	45859.2118	
	+1 std. dev	0.74	0.04111111		0.636	47348.1472	
PDO	mean	0.72	0.04	0.00325526	0.627	46678.1263	1353.07564
	-1std. dev.	0.63	0.035		0.601	44742.5102	

Table 2-4 Data used for input to AT123D and soil emission and volatilization models(from Mills, 1994)

Cases involving Malathion

Scenario		*Unsaturated zone conc.*			*Vadose zone loading rate*		
		kg/ha/d	mg/kg	std. dev.	kg/ha/d	kg/yr	std. dev.
	+1 std. dev.	2.50E-05	1.39E-06		0	0	
WAF	mean	0	0	8.02E-07	0	0	0
	-1 std. dev.	0	0		0	0	
	+1 std. dev.	2.50E-05	1.39E-06		0	0	
WAO	mean	0	0	8.02E-07	0	0	0
	-1 std. dev.	0	0		0	0	
	+1 std. dev.	1.48E-02	0.000822		0	0	
WBF	mean	1.30E-02	0.000722	9.18E-05	0	0	0
	-1 std. dev.	1.15E-02	0.000639		0	0	
	+1 std. dev.	1.48E-02	0.000822		0	0	
WBO	mean	1.30E-02	0.000722	9.18E-05	0	0	0
	-1 std. dev.	1.15E-02	0.000639		0	0	
	+1 std. dev.	6.50E-03	0.000361		0	0	
WDF	mean	5.60E-03	0.000311	5.28E-05	0	0	0
	-1 std. dev.	4.60E-03	0.000256		0	0	
	+1 std. dev.	6.50E-03	0.000361		0	0	
WDO	mean	5.60E-03	0.000311	5.28E-05	0	0	0
	-1 std. dev.	4.60E-03	0.000256		0	0	
	+1 std. dev.	3.00E-07	1.67E-08		4.00E-07	0.029779	
AAF	mean	6.00E-08	3.33E-09	8.82E-09	5.00E-08	0.003722	0.016225
	-1 std. dev.	0	0		0.00E+00	0	
	+1 std. dev.	3.50E-07	1.94E-08		4.00E-07	0.029779	
AAO	mean	2.00E-07	1.11E-08	9.76E-09	5.00E-08	0.003722	0.016225
	-1 std. dev.	0	0		0.00E+00	0	
	+1 std. dev.	6.00E-04	3.33E-05		6.15E-06	0.457848	
ABF	mean	5.30E-04	2.94E-05	3.89E-06	5.94E-06	0.442214	0.017144
	-1 std. dev.	4.60E-04	2.56E-05		5.69E-06	0.423602	
	+1 std. dev.	6.00E-04	3.33E-05		6.80E-06	0.506238	
ABO	mean	5.30E-04	2.94E-05	3.89E-06	6.40E-06	0.476459	0.022744
	-1 std. dev.	4.60E-04	2.56E-05		6.20E-06	0.46157	
	+1 std. dev.	2.70E-04	0.000015		1.48E-06	0.110181	
ADF	mean	2.65E-04	1.47E-05	2.78E-07	1.47E-06	0.109437	0.000744
	-1 std. dev.	2.60E-04	1.44E-05		1.46E-06	0.108692	
	+1 std. dev.	2.70E-04	0.000015		1.55E-06	0.115392	
ADO	mean	2.65E-04	1.47E-05	2.78E-07	1.54E-06	0.114648	0.000744
	-1 std. dev.	2.60E-04	1.44E-05		1.53E-06	0.113904	

Table 2-5 Data used for input to AT123D and soil emission and volatilization models(from Mills, 1994)

Cases involving Treflan

Scenario		*Unsaturated zone conc.*			*Vadose zone loading rate*	
		kg/ha/d	mg/kg	std. dev.	kg/ha/d	kg/yr
	+1 std. dev.	2.00E-08	1.11E-09		0	0
PAF	mean	0	0	6.42E-10	0	0
	-1 std. dev.	0	0		0	0
	+1 std. dev.	2.50E-08	1.39E-09		0	0
PAO	mean	0	0	8.02E-10	0	0
	-1 std. dev.	0	0		0	0
	+1 std. dev.	5.00E-09	2.78E-10		0	0
PBF	mean	2.00E-09	1.11E-10	1.27E-10	0	0
	-1 std. dev.	5.00E-10	2.78E-11		0	0
	+1 std. dev.	5.00E-09	2.78E-10		0	0
PBO	mean	2.00E-09	1.11E-10	1.27E-10	0	0
	-1 std. dev.	5.00E-10	2.78E-11		0	0
	+1 std. dev.	3.00E-05	1.67E-06		0	0
PDF	mean	2.00E-05	1.11E-06	4.75E-07	0	0
	-1 std. dev.	1.30E-05	7.22E-07		0	0
	+1 std. dev.	5.00E-05	2.78E-06		0	0
PDO	mean	2.50E-05	1.39E-06	1.12E-06	0	0
	-1 std. dev.	1.00E-05	5.56E-07		0	0
	+1 std. dev.	1.00E-05	5.56E-07		0	0
CAF	mean	0	0	3.21E-07	0	0
	-1 std. dev.	0	0		0	0
	+1 std. dev.	1.00E-05	5.56E-07		0	0
CAO	mean	0	0	3.21E-07	0	0
	-1 std. dev.	0	0		0	0
	+1 std. dev.	3.50E-05	1.94E-06		0	0
CBF	mean	2.00E-05	1.11E-06	6.99E-07	0	0
	-1 std. dev.	1.00E-05	5.56E-07		0	0
	+1 std. dev.	3.50E-05	1.94E-06		0	0
CBO	mean	2.00E-05	1.11E-06	6.99E-07	0	0
	-1 std. dev.	1.00E-05	5.56E-07		0	0
	+1 std. dev.	3.00E-13	1.67E-14		0	0
CDF	mean	0	0	9.62E-15	0	0
	-1 std. dev.	0	0		0	0
	+1 std. dev.	3.00E-13	1.67E-14		0	0
CDO	mean	0	0	9.62E-15	0	0
	-1 std. dev.	0	0		0	0

Table 2-6 Data used for input to AT123D and soil emission and volatilization models(from Mills, 1994)
Cases involving Prowl

Scenario		*Unsaturated zone conc.*			*Vadose zone loading rate*	
		kg/ha/d	mg/kg	std. dev.	kg/ha/d	kg/yr
	+1 std. dev.	5.00E-10	2.78E-11		0	0
CAF	mean	0	0	1.6E-11	0	0
	-1 std. dev.	0	0		0	0
	+1 std. dev.	5.00E-10	2.78E-11		0	0
CAO	mean	0	0	1.6E-11	0	0
	-1 std. dev.	0	0		0	0
	+1 std. dev.	5.50E-07	3.06E-08		0	0
CBF	mean	2.50E-07	1.39E-08	1.27E-08	0	0
	-1 std. dev.	1.00E-07	5.56E-09		0	0
	+1 std. dev.	5.50E-07	3.06E-08		0	0
CBO	mean	2.50E-07	1.39E-08	1.27E-08	0	0
	-1 std. dev.	1.00E-07	5.56E-09		0	0
	+1 std. dev.	3.00E-12	1.67E-13		0	0
CDF	mean	5.00E-13	2.78E-14	8.93E-14	0	0
	-1 std. dev.	0.00E+00	0		0	0
	+1 std. dev.	3.00E-12	1.67E-13		0	0
CDO	mean	5.00E-13	2.78E-14	8.93E-14	0	0
	-1 std. dev.	0.00E+00	0		0	0

Exposure Assessment

The purpose of the exposure assessment was to estimate the frequency, magnitude, and duration of potential human exposure to hazardous substances (U.S.EPA, 1989). This step included analyzing contaminant releases, identifying exposed populations, identifying exposure pathways, estimating point concentrations for each pathway, and estimating contaminant intakes by humans for specific pathways.

This step of the study was performed using the computer models included in APIDSS. The models were configured using

information gathered during the previous step (data collection) of this study. The data used to configure these models is discussed further and is listed in Chapter III.

The exposed population for this study were the "typical" farm residents of Caddo County. Caddo County farm residents were assumed to be composed of adult males and females who can be described by the statistical distributions describing typical populations provided in Gephart *et al.* (1994) and API (1994). The parameters describing the exposed population are listed in the section on configuring the models.

APIDSS is equipped to handle the following exposure routes: ingestion of contaminated water, inhalation while showering, dermal contact with contaminated water while showering, ingestion of contaminated soil, dermal contact with contaminated soil, and inhalation of air containing chemical vapors or particulates. All of these pathways were assumed to be in affect, except in cases where the pesticide did not reach the groundwater table (as specified by Mills, 1995). In these cases ingestion of water, inhalation while showering, and dermal absorption while showering were eliminated as potential pathways of exposure.

The estimation of point concentrations was performed by the models selected from those available in APIDSS. The models selected were AT123D (Yeh, 1981) for modeling

pesticide transport through the saturated zone and Farmer (Farmer et al., 1980), Cowherd (U.S.EPA, 1985), and Box (API, 1994) for modeling pesticide concentrations in the air. The configuration of these models is discussed in Chapter III. The estimation of human intake of contaminants for each pathway was also performed by the models included in APIDSS. Their configuration is also discussed in the section on configuring the models.

For estimation of contaminant concentrations in ground water APIDSS was set to run AT123D in Monte Carlo mode. It was determined that 250 runs were sufficient for the average receptor well concentrations to converge toward a single value. This behavior is shown in Figure 2-2. For estimating ambient air concentrations APIDSS was set to run the air concentration models in Monte Carlo mode. Seven hundred fifty runs were deemed sufficient to achieve convergence of the average receptor point concentrations on a single value. Figure 2-3 shows receptor point concentrations verses the number of Monte Carlo runs. For Phase 2 of this study, all of the Fate and Transport models were run in Deterministic Mode with all of the parameters set to equal their mean values.

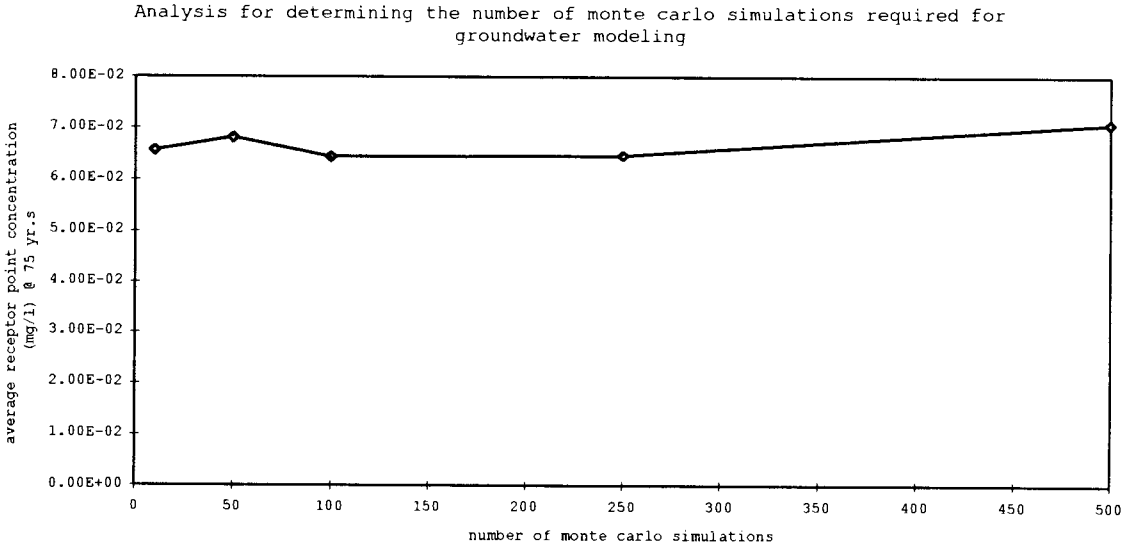


Figure 2-2

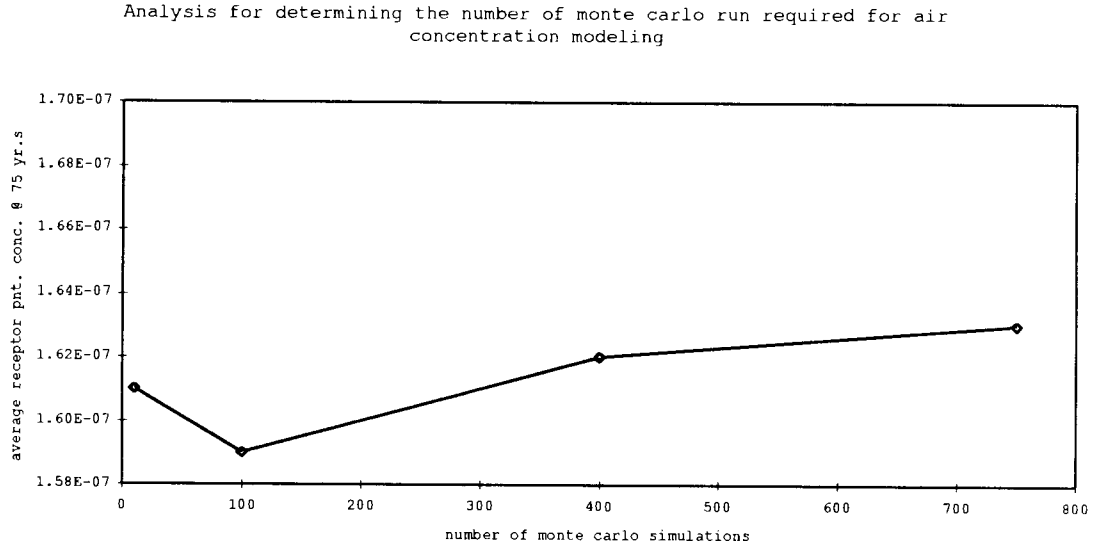


Figure 2-3

Toxicity Assessment

The toxicity assessment portion of a risk assessment should include two steps: hazard identification and dose-response assessment (U.S.EPA, 1989). The hazard identification process includes determining whether exposure to a chemical can cause an increase in the incidence of an adverse health effect and characterizing the strength of the evidence that the chemical causes the adverse effect. The dose-response evaluation involves evaluating quantitatively the toxicity information and determining the relationship between the dose of the contaminant received and the incidence of adverse health effects.

As with many similar studies, the existing information on the toxicity of the chemicals of interest to this study was rather sparse. What information was available was found in the IRIS data base maintained by the U.S.EPA (U.S.EPA, 1993). The following paragraphs summarize the critical effects and the dose-response information provided by IRIS. Because none of these pesticides were known to be carcinogenic to humans no slope factors (an estimate of the probability of developing cancer) were published in IRIS. The toxicity assessment step in this study involved compiling the information in the following paragraphs,

particularly the oral and inhalation RfDs for inclusion in the models.

The pesticide 2,4-D has been shown to have the following critical effects in oral ingestion studies done on rats: hematologic, hepatic, and renal toxicity (U.S.EPA, 1993). The oral RfD for humans was given as 0.01 mg/kg/d (U.S.EPA, 1993). This value was also used for the inhalation RfD in this study, as no value was given in IRIS.

Malathion has been shown to have the critical effect of RBC ChE depression in a subchronic human feeding study (U.S.EPA, 1993). The oral RfD was given as 0.02 mg/kg/d (U.S.EPA, 1993). For this study the inhalation RfD was assumed to be the same as the oral RfD as no value was provided in IRIS.

A twelve month feeding study in dogs showed increased liver weights and an increase in methemoglobin when Treflan (Trifluralin) was administered (U.S.EPA, 1993). The oral RfD for humans was given as 0.0075 mg/kg/d (U.S.EPA, 1993). The same number was used for the inhalation RfD in this study.

A study where Furadan (Carbofuran) was fed to dogs for one year showed red blood cell and plasma chlorinesterase inhibition, and testicular and uterine effects (U.S.EPA, 1993). The oral RfD was given to be 0.005 mg/kg/d (U.S.EPA,

1993). For this study this value was also used for the inhalation RfD as no inhalation RfD was provided in IRIS.

Gelatin capsules containing Lasso (Alachlor) were fed to dogs for a year. The study showed an increased incidence of hemosiderosis, and hemolytic anemia (U.S.EPA, 1993). The oral RfD for humans was determined to be 0.02 (U.S.EPA, 1993). This is also the value used for the inhalation RfD in this study.

Prowl (Pendimethalin) was feed to dogs for a two year period. The test dogs showed an increase in serum alkaline phosphate and liver weight (U.S.EPA, 1993). They also showed hepatic lesions (U.S.EPA, 1993). The oral RfD for humans was listed as 0.04 mg/kg/d (U.S.EPA, 1993), and this value was also used for the inhalation RfD because it was not included in IRIS.

APIDSS was designed for use with chemicals common in the petroleum industry. APIDSS has a built in data base containing variables describing many petroleum related chemicals. In order to model the pesticides in this study the data base had to be modified to include information describing them. This was done as part of completing this step of the study.

Risk Characterization

The last step in the baseline risk assessment process is risk characterization. Risk characterization involves combining the outputs of the exposure and toxicity assessments to characterize baseline risk, both quantitatively and qualitatively. This includes estimating cancer risks and the non-cancer hazard quotients as well as the uncertainty in these numbers.

APIDSS automatically uses the results from exposure modeling and combines them with the toxicity information to estimate the non-cancer hazard quotient for each route. The hazard quotients are then added to give a hazard index that is characteristic of the scenario that was modeled.

This step of the study was performed using models provided in APIDSS. The models were configured as discussed in Chapter III. The Chemical Intake and Risk Calculation module was run in Monte Carlo mode for this phase. It was run 1000 times, the maximum allowed by APIDSS. Figure 2-4 presents the hazard index verses the number of monte carlo simulations.

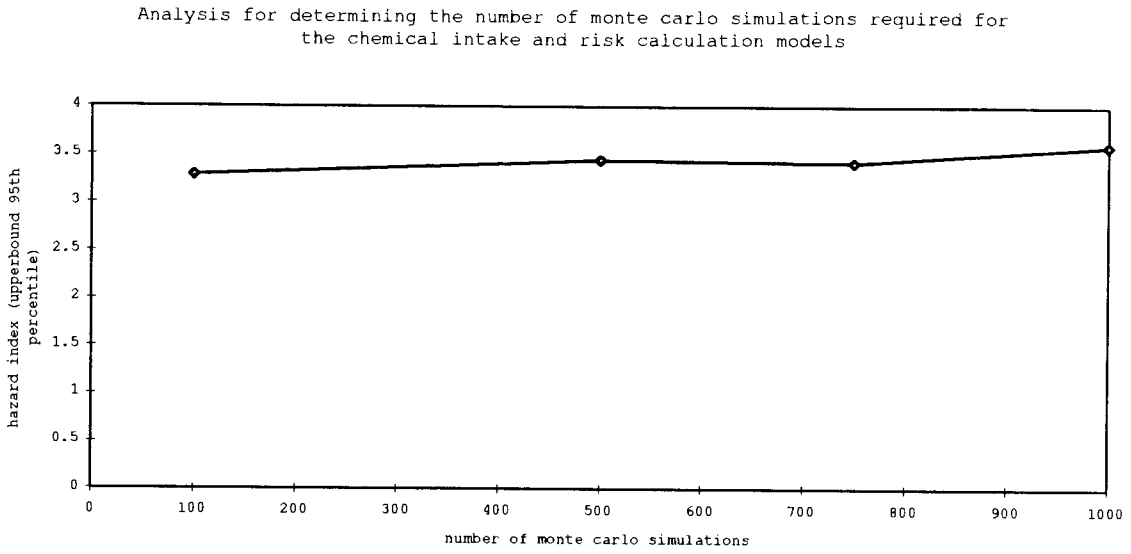

Analysis for determining the number of monte carlo simulations required for the chemical intake and risk calculation models
hazard index (upperbound 95th percentile)
4
3.5
3
2.5
2
1.5
1
0.5
0
0
100
200
300
400
500
600
700
800
900
1000
number of monte carlo simulations

Figure 2-4

Phase 2: Uncertainty Analysis

The results of a risk assessment cannot be considered complete without a corresponding estimation of the degree of uncertainty. Knowing the uncertainty of the results tells the assessor how much variability there is in the results and what can be safely concluded about the hazards presented to human health.

Estimation of Uncertainty

A quantitative approach to characterizing uncertainty in the hazard index was undertaken for the second phase of this study. The first step was to characterize the probability distributions for the key input parameters. The same probability distributions that were used for Phase 1 were used. This step is described in Chapter III in the section on configuring the Chemical Intake and Risk Calculation Models.

The second step was to determine the uncertainty due to individual parameters. To do this, all of the variables in the Chemical Intake and Risk Calculation Module were set to their mean values while the parameter of interest was represented by its probability distribution. The uncertainty in the variable represented by its probability distribution was then propagated through the Chemical Intake

and Risk Calculation models using the Monte Carlo method. For this part of the study APIDSS was set to perform 1000 Monte Carlo simulations. The Fate and Transport models were run in the Deterministic mode with all parameters set to their mean values to eliminate any variance in the receptor point concentrations.

The variance in the hazard quotient for each pathway could then be observed by examining the output of the APIDSS Risk Characterization module. When all the variables were set to their mean values there was no standard deviation in the hazard quotient for any of the exposure pathways. This meant that when only one variable was varied, all of the variance in the hazard quotient arose from variations in the variable.

This method of determining variance caused by individual exposure parameters was performed for each variable that had a probability distribution published by Gephart *et al.* (1994). These were body weight, water ingestion rate, soil ingestion rate, total skin surface area, hands and forearm skin surface area, time spent in shower, and inhalation rate. The effects of varying contaminant concentration in the soil and groundwater were also examined.

When all of these simulations were completed, the variances in the hazard quotients caused by each variable

for each exposure pathway could be compared. The variables that introduced the most uncertainty in the hazard quotients and thus the overall hazard index, were determined in this manor. The results of this analysis are presented in Chapter IV.

Summary

The following figures summarize the research structure followed during the course of this study. Figure 2-5 presents what was done for phase 1 of the study and Figure 2-6 shows what was done for phase 2.

Figure 2-5 Summary of the steps taken completing Phase 1 of this study

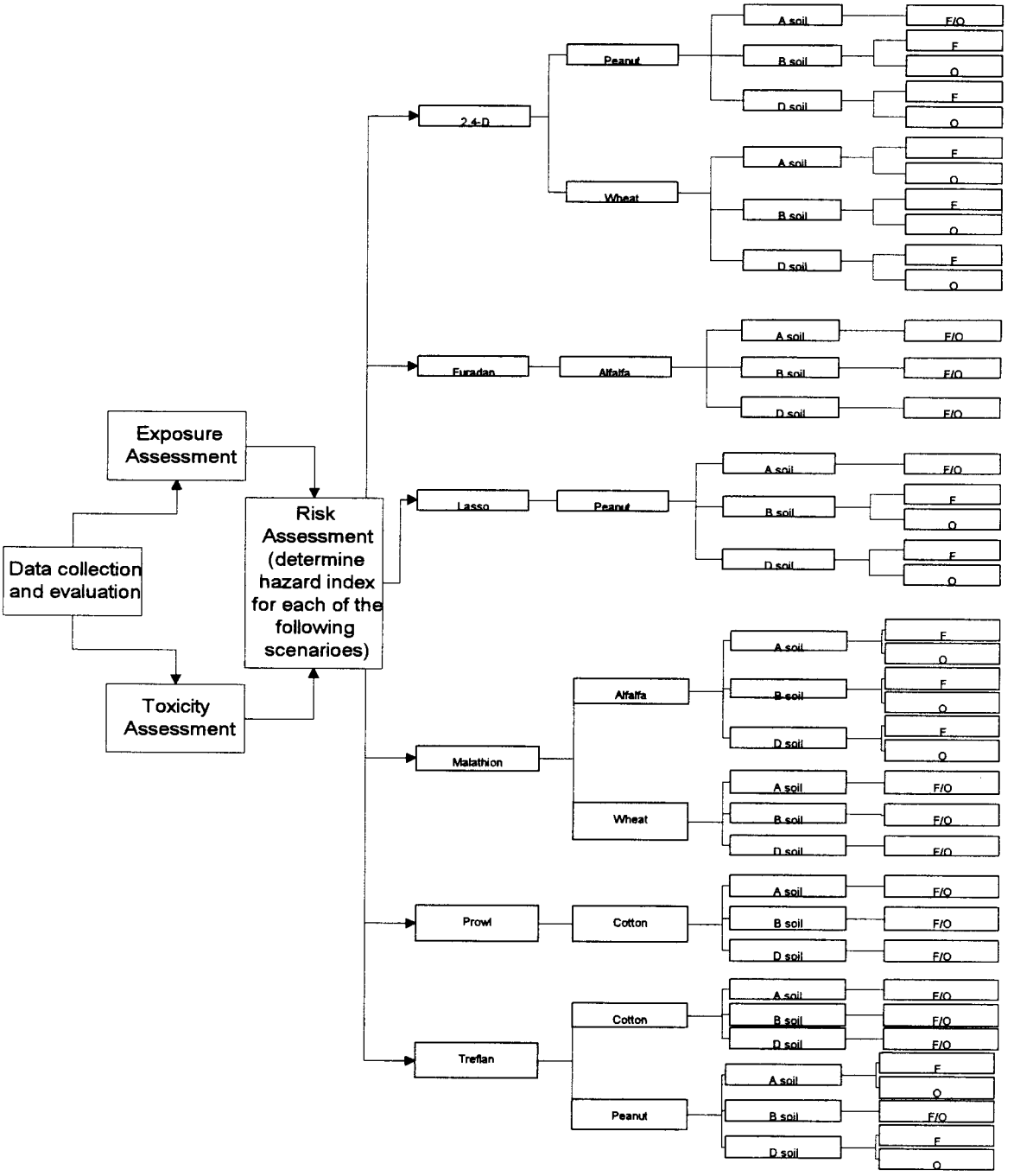
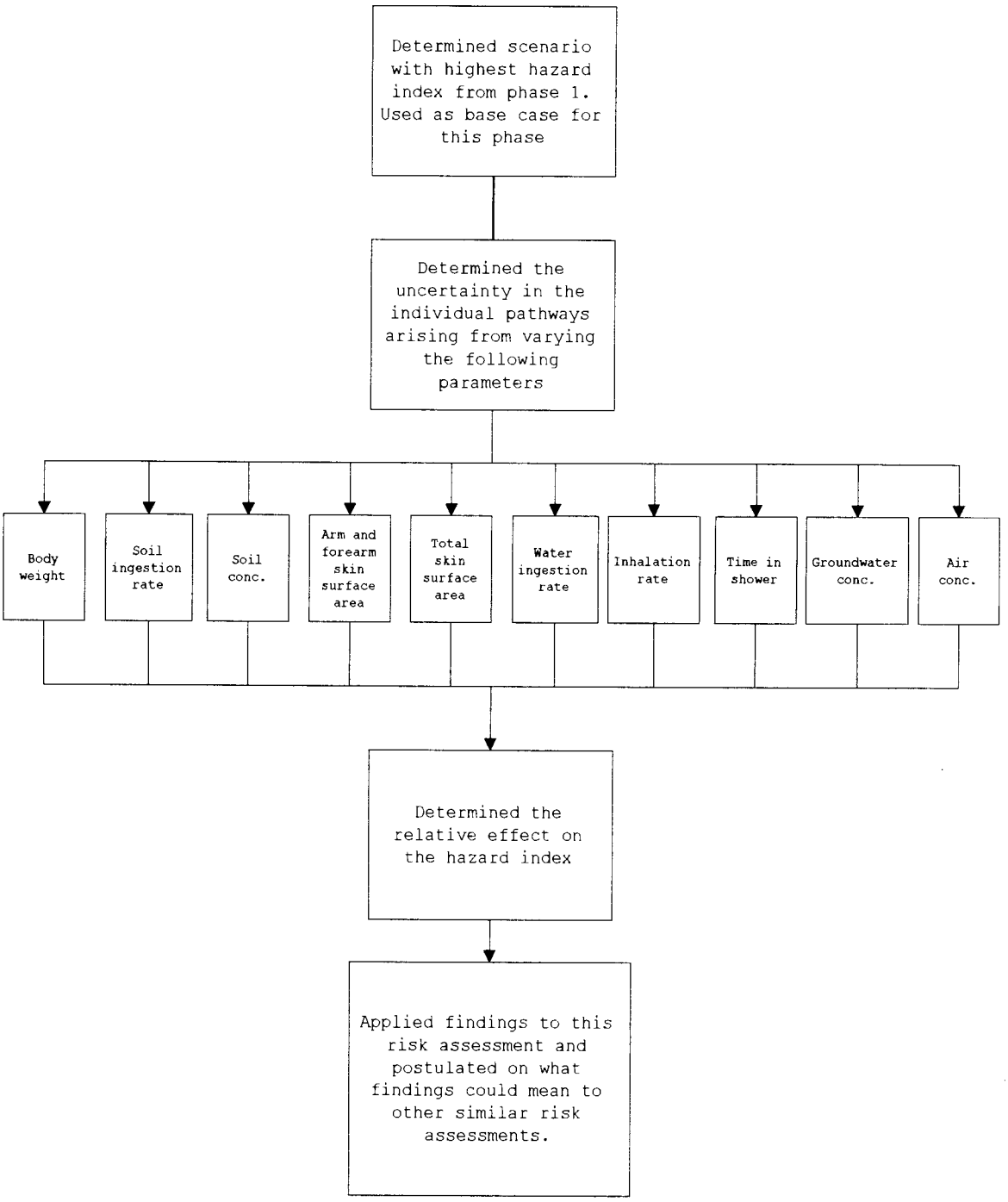


Figure 2-6 Summary of the steps taken completing Phase 2 of this study



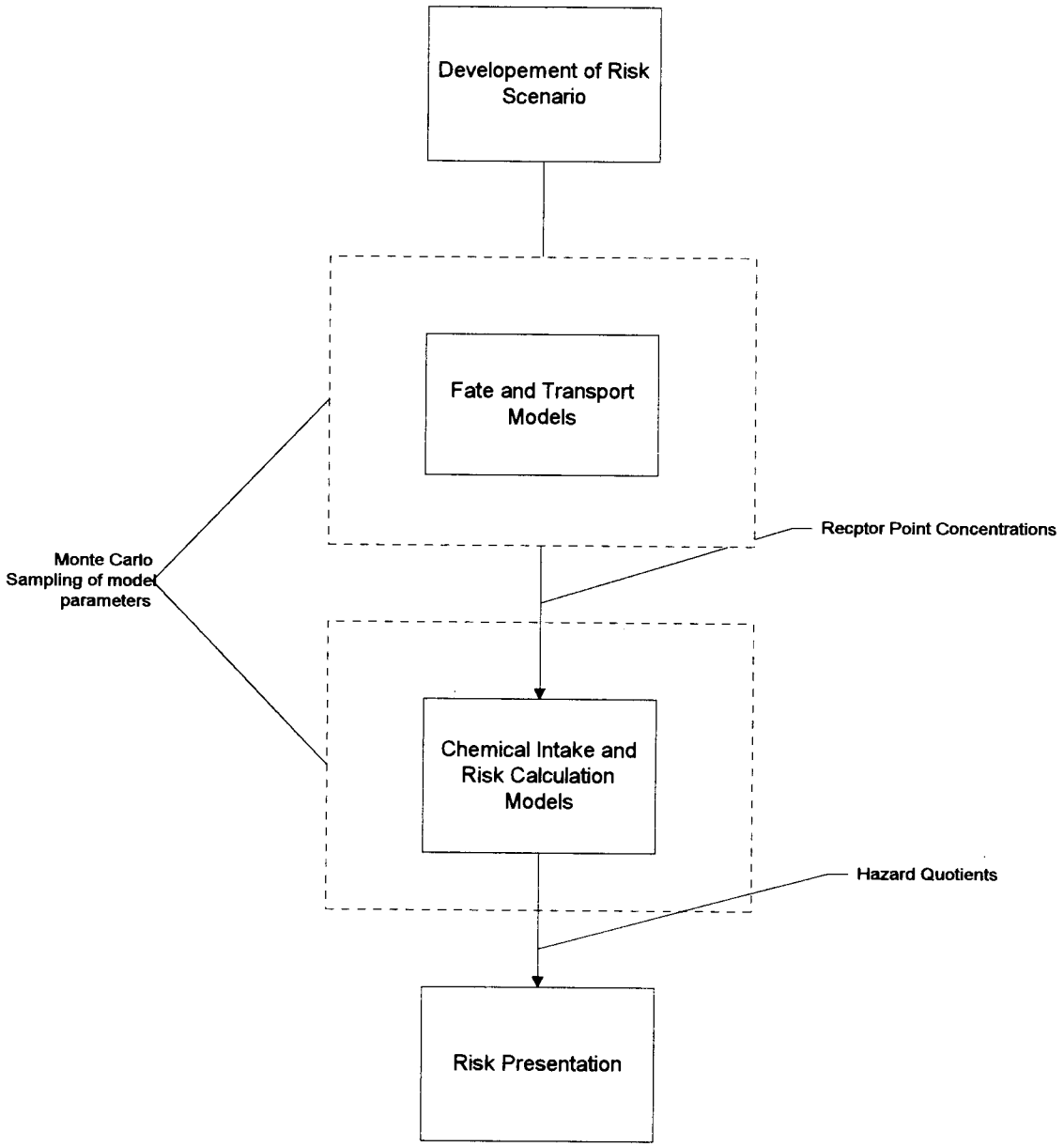
CHAPTER III

MODELING

Fundamental to this study were computer models. These models are tools for attempting to forecast events in the real world. American Petroleum Institute's Decision Support System (APIDSS) is the primary modeling tool used in this investigation (API, 1994). It is a computer software package that is meant to assist environmental professionals in estimating human exposure and risk from contaminated sites (API, 1994). This chapter discuses the basic premises behind the models included in APIDSS and how they were configured for use in this study.

APIDSS combines publicly available computer models with an easy to use user interface. The software is organized into four modules: the development of a risk scenario, fate and transport models, chemical intake and risk calculation models, and risk presentation. Each of these modules is discussed in further detail in the following paragraphs. Figure 3-1 depicts the organization of APIDSS.

Figure 3-1 The organizational structure of American Petroleum Institute's Decision Support System



Development of a Risk Scenario Module

This module allows for the development of a model of the site for the purposes of risk assessment. The user identifies the chemicals that are causing concern at the site, the relevant routes of human exposure, and the specific models to be used to estimate receptor point concentrations. This module performs elements of the data collection and analysis phase as well as the exposure assessment phase of a risk assessment which is discussed in greater detail in Chapter II.

Fate and Transport Models Module

This module consists of models that simulate the movement of contaminants from their source to a receptor. They provide receptor point concentrations as their output. Included in this module are models that simulate atmospheric emission and dispersion of contaminants and models that simulate saturated and unsaturated zone contaminant transport. The models selected for use in this study were: AT123D (Yeh, 1981) for saturated zone modeling, the Farmer soil emission model (Farmer *et al.*, 1980) for modeling contaminant volatilization to the atmosphere, the Cowherd model particulate emissions (U.S.EPA, 1985) for modeling particulate emissions, and the box model (API, 1994) for

estimating atmospheric concentrations. The models were chosen for their applicability to the scenarios being modeled for this study. The Farmer model assumes an infinite source of contaminant mass in the soil. This is acceptable since the pesticides are assumed to be applied annually. The Cowherd model (U.S.EPA, 1985) was used as it is the only model available to APIDSS for estimating particulate emissions.

The box model was used to estimate ambient air concentrations above the farm field because it is well suited to estimating air concentrations when the receptors are located on site. The alternative, the Gaussian model, (Pasquill, 1961) is better suited to estimate concentrations downwind. AT123D was used to estimate receptor point concentrations in groundwater because it is the only model available to APIDSS for doing so. The AT123D model is a standard model commonly used by groundwater modelers.

These models were configured to reflect conditions existing in Caddo County, Oklahoma with data from past studies of the area (Upthegrove, 1989; Tanaka and Davis, 1963; Shonfelt *et al.*, 1991). The configuration of the models are discussed later in this chapter.

Saturated Zone Modeling

AT123D

The AT123D model is a generalized semi-analytical transient computer model for estimating the transport of wastes in groundwater systems in one, two, or three dimensions (Yeh, 1981). AT123D was developed by Yeh to be a tool for the preliminary assessment of waste disposal sites. It provides the user with concentrations of contaminants as a function of time at any location specified by different spatial coordinates.

AT123D simulates several natural processes that contribute to the migration and transport of contaminants. These processes are advection, hydraulic dispersion, diffusion, reversible ion exchange, and chemical or biological degradation (Yeh, 1981). Advection is the movement of a solute through the soil with the same velocity as the solvent. Hydraulic dispersion is the term used to describe the meandering of a solute as it moves through the soil as a result of uneven flow around soil particles. Movement of a solute due to diffusion is a result of random Brownian motion. The effects of diffusion on contaminant plume size are usually very small (Fetter, 1993; Freeze and Cherry, 1979).

Also effecting the movement of the contaminant plume is the ion exchange process. This is the process of replacing ions in solution with other ions in the soil. The ion exchange process was not considered in this study. Biological or chemical degradation effects the spread of the plume as well. This process involves the breakdown of the contaminant into its respective components by cellular metabolism or by chemical means.

An equation that takes into account all of these processes has been developed and the solution of it is the basis of AT123D (Robertson, 1974; Yeh and Ward, 1981).

$$\frac{\partial \ n_e C}{\partial \ t} = \nabla \bullet \left(n_e \bar{\bar{D}} \nabla C \right) - \nabla \bullet C \vec{q} + \dot{M} - K n_e C - \lambda n_e C - \left(\frac{\partial \ (\rho_b C_s)}{\partial \ t} + \lambda \rho_b C_s \right)$$

(Equation 3-1)

where

$\vec{q}$ = Darcy velocity vector (LT^{-1})

$\bar{\bar{D}}$ = hydraulic dispersion coefficient tensor (L^2T^{-1})

C = dissolved concentration of the solute (ML^{-3})

C_s = absorbed concentration in the solid (MM^{-1})

ρ_b = bulk density of the media (ML^{-3})

$\dot{M}$ = rate of release of source ($ML^{-3}T^{-1}$)

n_e = effective porosity (L°)

λ = radio active decay constant (T^{-1}) (not used in this study)

K = degradation rate (T^{-1})

The first step in solving equation 3-1 is to simplify it, so AT123D makes some simplifying assumptions. Groundwater characteristics like seepage velocity, porosity, permeability, and dispersivities are assumed to be constant, even though they are known to vary in reality. Also it is assumed that the adsorption of the solute by the soil occurs quickly enough to ensure that the solute is in equilibrium with the adsorbed solute under isothermal conditions. Further, this phase transfer is assumed to be linear. These assumptions are considered "typical" and are routinely accepted by groundwater modelers (Chen and McTernan, 1992) With these assumptions equation 3-1 then becomes (Robertson, 1974):

$$\frac{\partial C}{\partial t} = \nabla \bullet \left(\overline{\overline{K}} \bullet \nabla C \right) - \nabla \bullet \vec{U} C - \left(\frac{K}{R_d} + \lambda \right) C + \frac{\dot{M}}{n_e R_d} \qquad (3\text{-}2)$$

where

R_d = Retardation factor = $(1+\rho_b K_d/n_e)$

$\overline{\overline{K}}$ = Retarded Dispersion Tensor = $\overline{\overline{D}}/R_d$

$\vec{U}$ = Retarded Seepage Velocity = $(\vec{q}/n_e)/R_d$

K_d = Distribution Coefficient

AT123D uses Green's function to solve equation 3-2. A separate solution is used for each type of source and boundary condition. The appropriate analytical solution is

chosen by AT123D depending on the source and boundary conditions input to APIDSS. As a result of solving this equation AT123D provides the user with concentrations as a function of time at any specified location within the groundwater system.

Configuration of AT123D

The majority of Caddo County, Oklahoma is situated above the Rush Springs Aquifer. Parameters representing conditions found in the Rush Springs aquifer were entered into AT123D. The values that were input and the sources they were taken from are discussed in the following paragraphs and are summarized in table 3-1.

The Rush Springs Aquifer is very fine-grained, cross-bedded sandstone, containing irregular silty lenses (Tanaka and Davis, 1963). The average depth of the aquifer is 60 meters (Tanaka and Davis, 1963) and it was taken to be infinitely wide relative to the depth.

The values of porosity and hydraulic conductivity were taken from Upthegrove (1989). This was a study of the West Cement Oil Field region of the Rush Springs Aquifer. Although this is a relatively localized area, the porosity and hydraulic conductivity values in this region are characteristic of the entire aquifer (Becker, 1994). The values for both of these parameters were fit to a log-normal

distribution for input to AT123D. This is consistent with accepted practice (Freeze *et al.*, 1987).

The hydraulic gradient was determined from water table elevation maps supplied by the Oklahoma Geological Survey. It was determined that the average hydraulic gradient was 0.003 and dipped southward.

The values for longitudinal, transverse, and vertical dispersivity were taken from the AT123D manual (Yeh, 1981). Typical values for a fine grained sand were used. The soil bulk density was given in the APIDSS manual as 1.8 g/cm^3. The fraction of organic carbon was assumed to be zero. This was a conservative estimate but was consistent with SCS data sources.

The length of the source in the X and Y directions was calculated as follows: the area of an average farm in Caddo County was found to be 504 acres (U.S. Dept. of Commerce ,1994). This is approximately 2,039,637.6 m^2 or 1428.2 meters per side. So assuming that pesticides were applied over the entire farm, the source length in the X and Y directions would be 1428.2 meters. The source was modeled as a plane in the X and Y direction so the thickness of the source was set to 0.

The receptor well was set directly in the middle of the source plane. From previous modeling efforts this location was determined to have the highest concentration of

pesticides. The coordinates were X = 714.1m and Y = 714.1m. The well was assumed to take water from the middle depth of the aquifer so it was assumed to be screened from the top of the water table to a depth of 30 meters.

The concentrations of pesticide reaching the water table were used as the input concentration to the AT123D model. These concentrations were taken from a previous modeling effort (Mills, 1994). Mills used PRZM2 (Carsel, 1987) in a Monte Carlo simulation to model the transport of pesticides from the ground surface through the unsaturated zone to the water table. Mills' effort produced annual summaries in kg/ha/day of pesticide transport to the root zone and to the top of the water table which are shown in Tables 2-1 through 2-6. These values were converted to soil concentrations and loading rate to the groundwater table. The results of this effort were fit to log-normal distributions for input to AT123D for this study. These values are also shown in Tables 2-1 through 2-6. Figure 3-2 is a schematic showing the application of AT123D in this study.

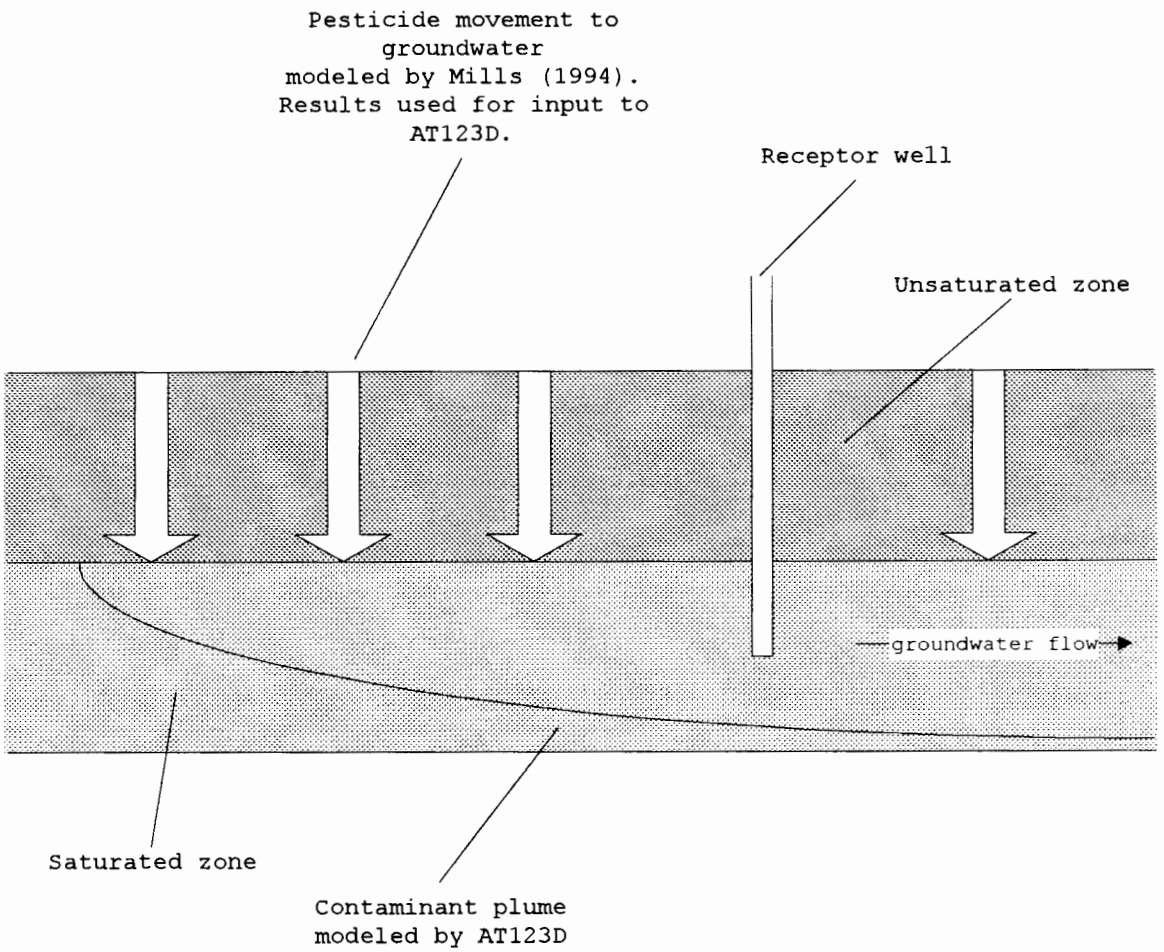


Figure 3-2 A schematic detailing the application of AT123D to this study

Table 3-1 Parameters used to configure the AT123D model.

AT123D Groundwater Transport Model *Media Specific Parameters*	*Units*	*Dist.*	*Mean*	*Std. Dev.*	*Min*	*Max*	*Source*
Effective Porosity	-	log-normal	0.331	0.032	0.294	0.434	Upthegrove, 1989
Hydraulic Conductivity	m/yr	log-normal	480.9	446.2	14.82	1482	Upthegrove, 1989
Hydraulic Gradient	-	constant	0.003	-	-	-	calculated
Longitudinal Dispersivity	m	constant	10	-	-	-	Yeh, 1981
Transverse Dispersivity	m	constant	1	-	-	-	Yeh, 1981
Vertical Dispersivity	m	constant	1	-	-	-	Yeh, 1981
Dry Wt. Soil Bulk Density	g/cm^3	constant	1.8	-	-	-	API, 1994
Fraction Organic Carbon	-	constant	0	-	-	-	estimated
Thickness of Aquifer	m	constant	60	-	-	-	Tanaka & Davis, 1963
Receptor Well Geometry							
X Coordinate of well	m	constant	714.1	-	-	-	calculated
Y Coordinate of well	m	constant	714.1	-	-	-	calculated
Top of Screen	m	constant	0	-	-	-	calculated
Bottom of Screen	m	constant	30	-	-	-	calculated
Source Geometry							
Length of Source in X dir.	m	constant	1428.2	-	-	-	calculated
Length of Source in Y dir.	m	constant	1428.2	-	-	-	calculated
Length of Source in Z dir.	m	constant	0	-	-	-	calculated

Air Concentration Modeling

Given the exposure pathways detailed in Chapter I, it is necessary to determine the concentration in air of the contaminant of concern in order to calculate intake due to inhalation. As with the groundwater section of APIDSS, actual measurements of concentrations were unavailable so APIDSS was used to provide an estimate. Contaminants can become airborne by several mechanisms including volatilization to the atmosphere from soil and shower water as well as from materials adsorbed onto soil particles.

APIDSS uses a separate model for each of these mechanisms. The results from the Farmer volatile emission model (Farmer *et al.*, 1980) were added to the results from the Cowherd particulate emission model (U.S.EPA, 1985) to give a contaminant emission rate. This contaminant emission rate is a key input to the box atmospheric dispersion model (API, 1994). Once an ambient air concentration was determined the human intake was estimated and ultimately a risk calculated.

The Farmer Model

In order to estimate the volatile emissions from contaminated soil the Farmer model was used. The Farmer equation models the loss/emission of contaminant from soil

as a diffusion controlled process (Farmer *et al.*, 1980). The process is described by using Fick's law for steady-state diffusion. The rate of emission of contaminant from the soil is described by equation 3-3 (API, 1994):

$$E = 10^2 \times A \times D_e \times \frac{C_{vs} - C_a}{d} \qquad (3\text{-}3)$$

where

E = Steady-state emission rate of chemical (g/s)
A = Area of the source (m^2)
D_e = effective diffusion coefficient of the chemical in air (cm^2/s)
C_{vs} = Vapor phase concentration for chemical in soil (g/cm^3)
C_a = air concentration of chemical at soil surface (g/cm^3)
d = depth of soil cover (m)

Equation 3-3 can be simplified if C_a is assumed to be negligible. The equation then becomes:

$$E = 10^2 \times A \times D_e \times \frac{C_{vs}}{d} \qquad (3\text{-}4)$$

If C_{vs} is unknown, APIDSS determines it from the following relationship:

$$C_{vs} = H' \times C_w \qquad (3\text{-}5)$$

where

$$C_w = C_t \frac{(\rho_b + \Theta_w \rho_w)}{(\Theta_t - \Theta_w)H' + \Theta_w + \rho_b K_d} \qquad (3\text{-}6)$$

where

H' = Henry's Law Constant [(mg/L)/(mg/L)]
C_w = the aqueous phase conc. of chemical (g/cm^3)
C_t = the total conc. of chemical in soil (g/g)
Θ_t = the total porosity of soil (cm^3/cm^3)
ρ_b = soil bulk density (g/cm^3)
ρ_w = density of water
Θ_w = the volumetric water content (cm^3/cm^3)
K_d = Soil water partition coefficient [(g/g)/(g/cm^3)]

In equation 3-6, K_d is estimated as

$$K_d = K_{oc} \times f_{oc} \qquad (3\text{-}7)$$

where

K_{oc} = organic carbon partition coefficient [(g/g)/(g/cm^3)]
f_{oc} = fractional organic carbon content [-]

Figure 3-3 is a schematic of how the Farmer equation models volatile emissions. Some of the assumptions that underlie the Farmer model and its applicability include: the model assumes that the concentration of contaminant in the soil remains constant. In other words it does not subtract the amount of contaminant that volatilizes into the atmosphere from the amount remaining in the soil (API, 1994). Also the contaminant is assumed to be fixed at a certain depth below the soil surface (API, 1994). Emissions were considered to

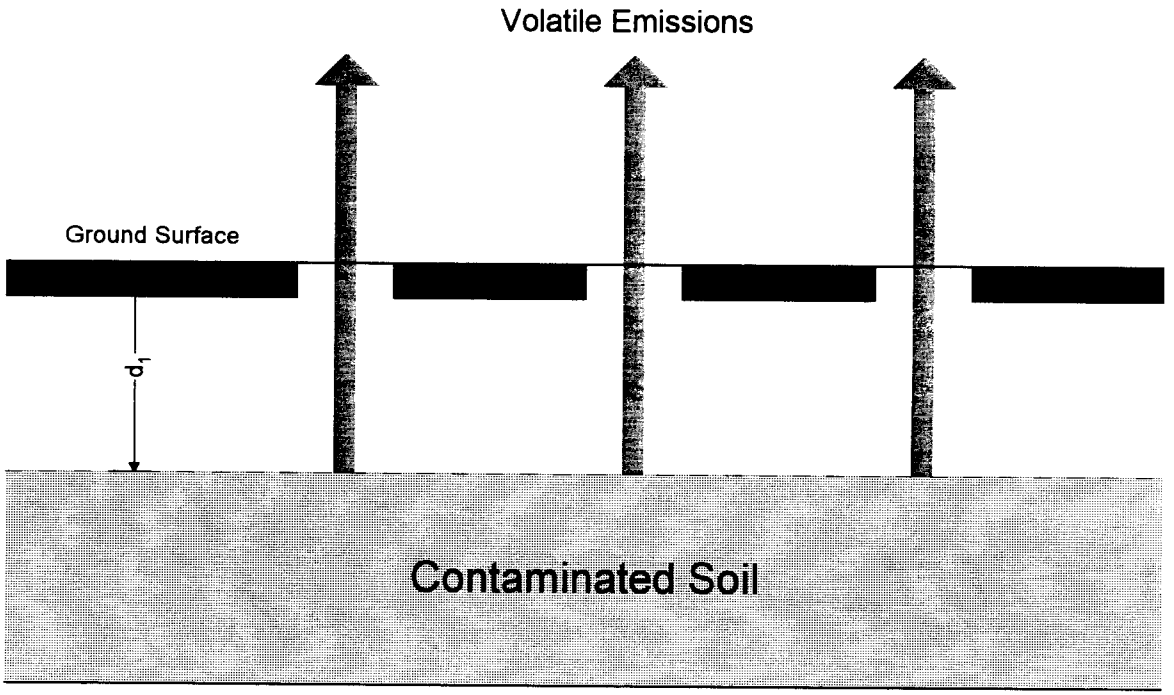


Figure 3-3 Schematic of the Farmer's Emission Model (API, 1994)

be constant and at steady state. The concentration in the air at the soil surface is insignificant compared with the concentration within the soil (API, 1994).

Configuring the Farmer model. The Farmers model requires parameters describing the contaminated soil. The area of contaminated soil was assumed to be equal to the average farm size which was listed in the 1992 Agricultural Census as 203 hectares (504 acres). The depth to contaminated soil was set at 0.01 meters. The porosity of the unsaturated zone was assumed to follow the same probability distribution as the porosity of the saturated. A typical value for the water content of soil, 0.16, was used (Das, 1985). The dry weight soil bulk density was taken from the APIDSS manual and was set at 1.8 g/cm^3. The average soil temperature was assumed to be 18° C. The fraction of organic carbon was assumed to be 0.005 (API, 1994).

The residual concentration of pesticide in the soil was different for each pesticide-soil type-irrigation practice combination. These were taken from a previous effort (Mills, 1994) as discussed in Chapter II. The soil concentrations are listed in Tables 2-1 through 2-6. Table 3-2 lists the parameters that were entered into APIDSS to configure the Farmer volatile emission model.

Farmers Volatile Emissions Model *Media Specific Parameters*	*Units*	*Dist.*	*Mean*	*Std. Dev.*	*Min*	*Max*	*Source*
Area of contaminated soil	m^2	constant	2,039,638	-	-	-	calculated
Depth to top of contaminated soil	m	constant	0.01	-	-	-	estimated
Unsaturated Zone Porosity	-	Log-Normal	0.331	0.032	0.294	0.434	Upthegrove, 1989
Water Content	-	constant	0.16	-	-	-	Das, 1990
Dry Wt. Soil Bulk Density	g/cm^3	constant	1.8	-	-	-	API, 1994
Fraction Organic Carbon	-	constant	0.005	-	-	-	API, 1994
Soil Temp	C^o	constant	18	-	-	-	Das, 1990

Table 3-2 Parameters used to configure the Farmer Model.

The Cowherd Model

APIDSS uses the Cowherd model (U.S.EPA, 1985) to estimate particulate emissions. The model was derived empirically and is based on field measurements gathered using a portable wind tunnel and mining soils. It estimates the emission rate of respirable soil particles, i.e., those with a diameter of 10μm or less (API, 1994):

$$E_{10} = 0.83 \frac{fAP\left(u^{+}\right)\left(1-V\right)}{\left(\frac{PE}{50}\right)^2} \qquad (3\text{-}8)$$

where

E_{10} = annual average emission rate of particles less than 10μm in dia. (mg/hr)

f = frequency of disturbance per month (mo^{-1})

A = area of contaminated soils (m^2)

$P(u^+) = 6.7(u^+ - u^t)$

u^+ = fastest mile wind speed (m/s)

u^t = erosion threshold wind speed at 7m (m/s)

V = fraction of vegetative cover [-]

PE = Thornwaite's Precipitation Evaporation Index [-]

This model is best suited for situations where there is a limited reservoir of soil available for erosion and situations where Thornwaite's precipitation/evaporation (PE) index is a good indicator of average surface soil moisture conditions. These were considered reasonable assumptions for this effort.

Configuring the Cowherd Model. Table 3-3 presents the data used to configure the Cowherd particulate emissions model. The monthly frequency of disturbance was set at 10/month. This was defined as an action which resulted in the exposure of fresh surface material to the erosive forces of the wind. An example would be vehicular traffic exposing fresh soil. The fastest mile wind speed was taken from data supplied in the APIDSS manual where it was listed as 24.1 m/s for the Oklahoma City area (API, 1994). The erosion threshold wind speed, also taken from the APIDSS manual was set at 1 m/s (API, 1994). Thornwaite's precipitation evaporation index

was set at 58 (API, 1994). It was assumed that the study area had a vegetative cover of 70%.

Cowherd Particulate Emissions Model *Media Specific Parameters*	*Units*	*Dist.*	*Mean*	*Std. Dev.*	*Min*	*Max*	*Source*
Monthly Frequency of Disturbance	1/mo.	constant	10	-	-	-	estimated
Fastest Mile Wind Speed	m/s	constant	24.1	-	-	-	API, 1994
Erosion Threshold Wind Speed	m/s	constant	1	-	-	-	API, 1994
Fraction of Vegetative Cover	-	constant	0.7	-	-	-	estimated
Thornwaite PE index	-	constant	58	-	-	-	API, 1994
Area of contaminated Soil	m^2	constant	2,039,638	-	-	-	calculated

Table 3-3 Parameters used to configure the Cowherd Model.

The Box Model

The box model is typically used to estimate ambient concentrations of contaminants in air when the receptors are located on or near the site (API, 1994). In order to estimate the ambient air concentration, the box model requires the contaminant emission rate which is the sum of the volatile and particulate emission rates. For this study these were obtained from the results of the Farmer and Cowherd models respectively.

The model is derived from a mass balance relationship where the boundaries for the mass balance form a 'box'. The box is bounded at the top by the mixing zone and is

ventilated by a steady flow of wind across the box. Equation 3-9 presents the general form (API ,1994).

$$C_{air} = \frac{10^3 E}{(uWH)} \qquad (3\text{-}9)$$

where

C_{air} = concentration of the chemical in air (mg/m^3)
E = average volatile chemical emission rate (g/s)
u = mean annual wind speed (m/s)
W = width of the box perpendicular to the predominant wind direction (m)
H = height of the mixing zone (m)
10^3 = conversion factor g to mg

The box model works best in applications where the steady-state contaminant emissions completely mix with the air inside the box. Some limitations to the box model are that it can only be used to estimate the average concentration within a volume of air, but this is appropriate for this study. It does not account for decreases in concentration that occur away from the source. Figure 3-4 is a graphical representation of the box model.

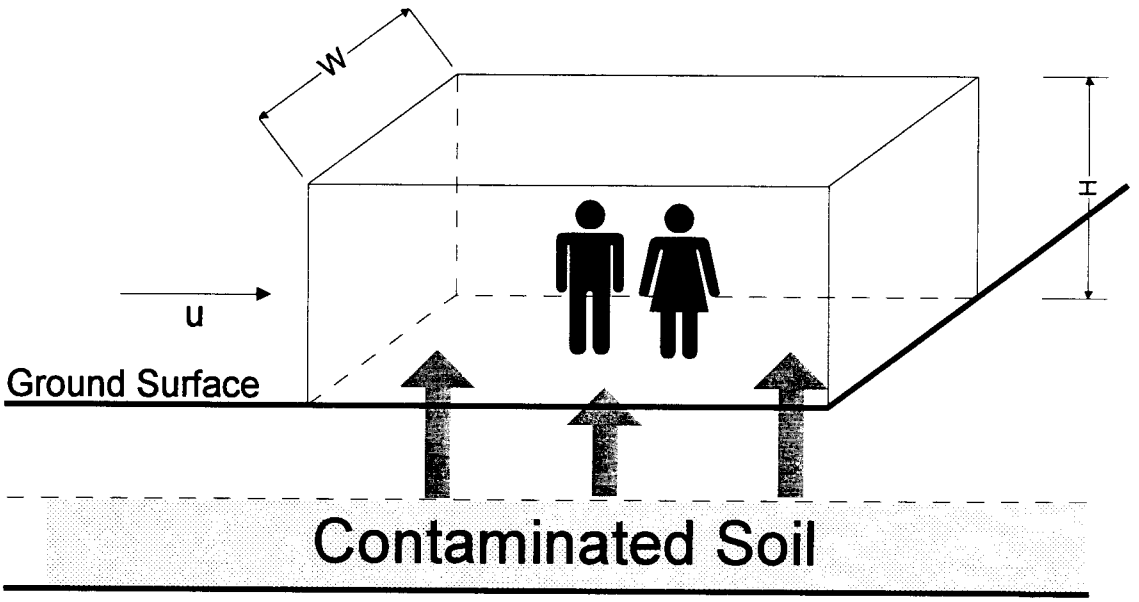


Figure 3-4 Schematic of the Box Model (API, 1994)

Configuration of the Box model. The Box model uses the volatile emissions from the Farmers model and the particulate emissions from the Cowherd model to determine an air contaminant concentration. Other requirements of the Box model are the box height, the box width, and the average wind speed. These values were set at 2 m, 1428.2 m, and 5.7 m/s respectively and are shown in table 3-4. The height of the box is determined by the average height of an adults breathing zone and is a conservative estimate. The average wind speed was taken from the APIDSS manual.

Box Dispersion Model	*Units*	*Distr.*	*Mean*	*Std. Dev.*	*Min*	*Max*	*Source*
Wind Speed	m	constant	5.7	-	-	-	API, 1994
Height of Box	m	constant	2	-	-	-	API, 1994
Width of Box	m	constant	1428.2	-	-	-	calculated

Table 3-4 Parameters used in configuring the Box Model

Shower Air Modeling

Because showering involves spraying warm water through the air, it volatilizes chemicals present in the water very effectively. If the water being used for the shower is contaminated with volatile materials, fairly high concentrations of contaminants in the shower-stall air may result, thus increasing exposure rates and possibly subsequent risks. The concentration in the shower-stall air

was required to determine the amount of contaminant inhaled while showering. The air concentrations were estimated by modeling the mass of contaminant that volatilized from the water used for showering. APIDSS estimated the fraction of the total contaminant mass that volatilized with the Foster and Chrostowski model (Foster and Chrostowski, 1986).

The Foster and Chrostowski Model

The Foster and Chrostowski Model simulates the volatilization of contaminants from shower air as a first order process (API, 1994). The fraction volatilized is given by

$$f_v = 1 - e^{\left(\frac{-K_L' t}{\left(\frac{d}{6}\right)3600}\right)} \qquad (3\text{-}10)$$

where

f_v = the efficiency of contaminant release [-]
K' = the overall mass transfer coefficient at the temperature of the shower water (cm/hr)
t = the time droplet spends in the air (sec)
d = the representative dia. of droplet (cm)

This model assumes that there is no mixing of shower air with the air in the rest of the house. It assumes that the mixing of contaminant emissions with the air in the shower-stall is instantaneous and complete. These

assumptions tend to give a conservative estimate of shower air concentrations.

Configuration of the Foster and Chrostowski Model. The variables required by this model (fraction volatilized, shower flow rate, volume of bathroom, temperature of the water, droplet diameter, droplet drop time, liquid mass trans. coeff., and gas mass trans. coeff.) were all provided by the APIDSS manual and were given as single constant variables. These values are listed in Table 3-5.

Shower Volatilization Model	*Units*	*Dist.*	*Mean*	*Std. Dev.*	*Min*	*Max*	*Source*
Fraction Volatilized	-	constant	*	-	-	-	API, 1994
Shower Flow Rate	l/min	constant	10	-	-	-	API, 1994
Volume of Bathroom	m3	constant	3	-	-	-	API, 1994
Temperature of the Water	Co	constant	45	-	-	-	API, 1994
Droplet Diameter	cm	constant	0.1	-	-	-	API, 1994
Droplet Drop Time	s	constant	2	-	-	-	API, 1994
Liquid Mass Transfer Coefficient	cm/hr	constant	20	-	-	-	API, 1994
Gas Mass Transfer Coefficient	cm/hr	constant	3000	-	-	-	API, 1994

Table 3-5 Parameters used for configuring the Foster and Chrostowski Model

Chemical Intake and Risk Calculation Module

Once the fate and transport models provided receptor point concentrations for each exposure pathway, APIDSS calculated chemical intake by human receptors. The rate of chemical intake to the body was averaged over the time of exposure and used to characterize risk. Chemical intake was calculated using the following equations for each exposure route. These equations calculated the absorbed dose, which is the mass of the substance that penetrated exchange boundaries to enter the human metabolic system (U.S.EPA, 1989).

Probability Distributions

Gephart *et al.* (1994) has compiled many probability distributions describing parameters that are useful for chemical intake and risk calculation modeling. In Monte Carlo mode many of these probability distributions can be input directly to APIDSS but some are described by a 'cumulative' distribution. APIDSS is not yet equipped to handle cumulative distributions, so it was necessary to convert these distributions to ones that were recognized by APIDSS.

This was done by calculating a mean and a standard deviation for the given cumulative distribution. Then

cumulative probability curves described by the same mean and standard deviation as the cumulative distribution were graphed with Excel® for each type of distribution that APIDSS recognized. These were normal, log-normal, exponential, uniform, and triangular distributions. The original cumulative probability curve was plotted on the same axis as the others. The distribution that fit closest the original was used to describe the parameter to APIDSS. These are included in Figures 3-4 through 3-6.

Variables that each of these models have in common

Body weight (BW) was found in all of the exposure models. It was a key variable in determining absorbed dosages. The probability distribution that was used in this study was taken from Gephart *et al.* (1994). It describes adult body weight for both males and females as a normal distribution with a mean of 64.2kg and a standard deviation of 13.19kg. Minimum and maximum values were 7kg and 107kg respectively.

The exposure duration was assumed to be the same as years spent in one residence by a typical farm family (Gephart *et al.*, 1994). This was given as cumulative function so it was converted to an exponential distribution by the method described above. This step can be seen in Figure 3-5. It had a mean of 17.73 years and standard

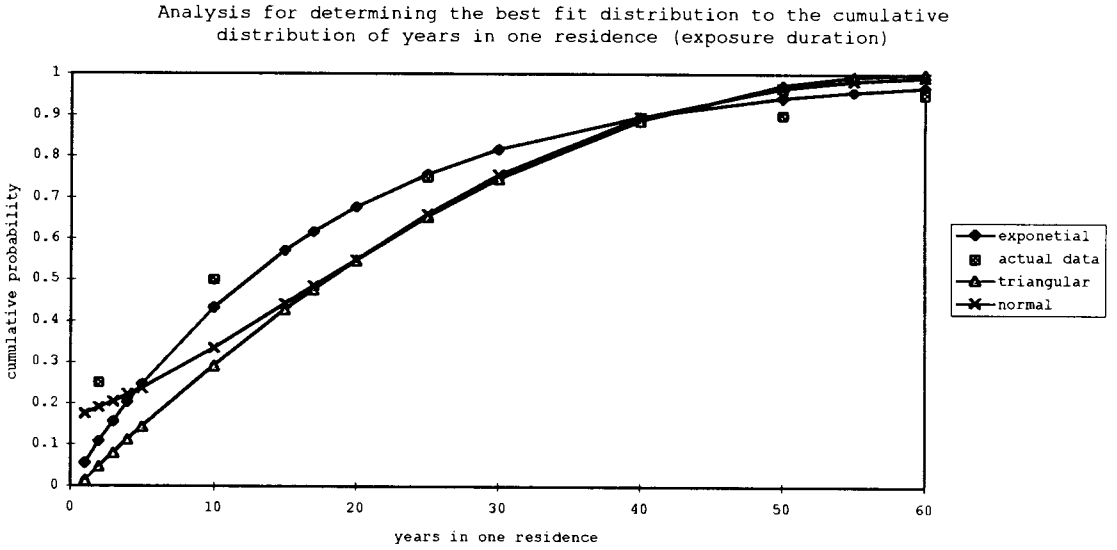


Figure 3-5

deviation of 17.79. The minimum was given as 0 years and the maximum was given as 60 years.

A typical value for the average lifespan of a person was listed as 70 years in the APIDSS manual. This was used in this effort as no additional information on statistical distributions of this variable could be found.

No information regarding the average exposure duration was available so the value listed in the APIDSS manual (350 days per year) was used. Table 3-6 lists the data that were common to all of the Chemical Intake and Risk Calculation Models.

	Units	Dist.	Mean	Std. Dev.	Min	Max	Source
Average Weight	kg	Normal	64.2	13.19	7	107	Gephart, 1994
Lifespan	yr	constant	70	-	-	-	API, 1994
Exposure Frequency	d/yr	constant	350	-	-	-	API, 1994
Exposure Duration	yr	exponential	17.73	17.79	0	60	calculated

Table 3-6 Parameters that were common to the configuration of all the Chemical Intake and Risk Calculation Models

Ingestion of Drinking Water

The mass of contaminant ingested per day from drinking contaminated water was estimated by Equation 3-11 (API, 1994):

$$DI = \frac{\beta_i \times IR \times C_w}{BW} \qquad (3\text{-}11)$$

where

DI = daily absorbed dose from drinking water (mg/kg-d)
IR = contaminated water ingestion rate (L/d)
C_w = contaminant conc. in drinking water (mg/L)
BW = body weight (kg)
β_i = chemical specific bioavailability (mg/mg)

The value for C_w was provided by AT123D. The value of DI calculated by this model was likely to be a conservative estimate because the model does not account for dilution from pumping (API, 1994).

Configuration of Drinking Water Model. The probability distribution for an adult's water ingestion rate (IR) was described in Gephart *et al.* (1994) as a normal distribution with a mean of 1.53 L/d and a standard deviation of 0.298 L/d. A minimum and maximum of 0.4 L/d and 2.2 L/d were taken from the original Gephart *et al.* data set.

The exposure frequency or the number of days spent at home was given in the APIDSS manual as a constant 350 days per year. All of the variables mentioned above are listed in Table 3-7.

Drinking Water Intake Model	*Units*	*Dist.*	*Mean*	*Std. Dev.*	*Min*	*Max*	*Source*
Exposure Frequency	d/yr	Constant	350	-	-	-	API, 1994
Exposure Duration	yr	Exponential	17.7	17.79	0	60	Gephart, 1994
Ingestion Rate	l/d	Normal	1.53	0.298	0.4	2.2	Gephart, 1994

Table 3-7 Parameters used to configure the Drinking Water Intake Model

Inhalation While Showering

If the water being used in the shower was contaminated then volatile compounds in the water could be released into the air in the shower-stall. One study has shown that the risk due to inhalation while showering can exceed risks from drinking contaminated water (McKone, 1987). The inhalation intake was computed with Equation 3-12 (API, 1994):

$$DI = \frac{\beta_{sh} \times C_{sh} \times IH \times ET}{BW} \qquad (3\text{-}12)$$

where

DI = daily absorbed dose from inhalation while showering (mg/kg-d)
C_{sh} = concentration of chemicals in shower air (mg/m^3)
IH = inhalation rate during showering (m^3/hr)
ET = shower duration (hr/day)
BW = body weight (kg)
β_{sh} = chemical-specific bioavailability (mg/mg)

The value for C_{sh} was calculated by the Foster and Chrostowski Model discussed earlier. It should be mentioned that the transport of chemical vapors from the shower to the rest of the house and the subsequent inhalation of indoor air was not taken into account in this effort.

Configuration of Inhalation Intake During Shower Model. The values used to configure this model are presented in Table 3-8. The exposure duration and frequency were the same as discussed in the section on configuring the shower inhalation model. The inhalation rate was given in Gephart *et al.* (1994) as a uniform distribution ranging from a minimum of 0.21 m^3/hr to a maximum of 0.74 m^3/hr. The time spent in the shower was given in Gephart *et al.* (1994) as a cumulative distribution. This was converted to a normal distribution with a mean of 0.15 hr/d and a standard

deviation of 0.061. (see section on probability distributions on p. 62). The distributions that were tested for curve fitting are shown in figure 3-6.

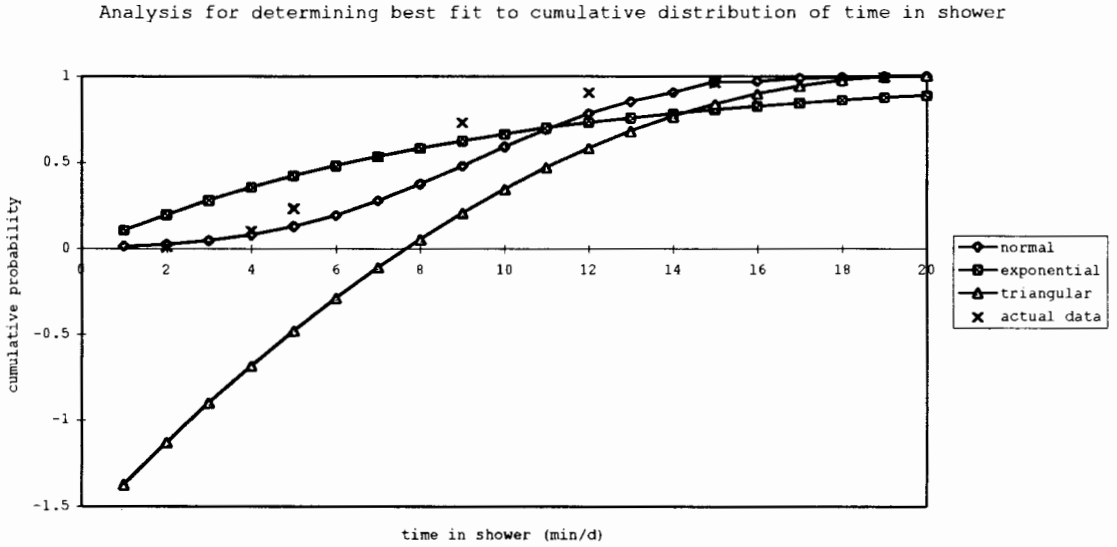


Figure 3-6

Inhalation During Shower	*Units*	*Dist.*	*Mean*	*Std. Dev.*	*Min*	*Max*	*Source*
Exposure Frequency	d/yr	constant	350	-	-	-	API, 1994
Exposure Duration	yr	exponential	17.73	17.79	0	60	Gephart, 1994
Inhalation Rate	m3/hr	uniform	0	0	0.21	0.74	Gephart, 1994
Time in Shower	hr/d	normal	0.15	0.061	0.017	0.333	Gephart, 1994
Fraction Volatilized	hr/d	constant	-	-	-	-	calculated

Table 3-8 Parameters for configuring the Inhalation During Shower Model

Dermal Absorption While Showering

Contaminants can be absorbed directly through the skin into the blood stream when people immerse themselves in contaminated water while showering. The process was described by Equation 3-13 (API, 1994):

$$D_{abs} = 10^{-3} \frac{C_w \times SA \times PC \times ET}{BW} \qquad (3\text{-}13)$$

where

D_{abs} = dermal absorbed dose (mg/kg-d)
C_w = concentration of chemicals in water (mg/L)
SA = exposed skin surface area (cm^2)
PC = chemical specific skin permeability constant (cm/hr)
ET = shower duration (hr/d)
BW = body weight (kg)

The value for C_w is taken from the results of the groundwater simulations.

Configuring the Dermal Absorption While Showering Model. The adult total skin surface area was given in Gephart *et al.* (1994) as a normal distribution with a mean of 17,000 cm^2 and a standard deviation of 1000 cm^2. The time spent in the shower was the same as in the previous model. The values entered into this model are listed in Table 3-9.

Dermal Intake During Shower	Units	Dist.	Mean	Std. Dev.	Min	Max	Source
Exposure Frequency	d/yr	constant	350	-	-	-	API, 1994
Exposure Duration	yr	exponential	17.73	17.79	0	60	Gephart, 1994
Total Skin Surface Area	cm^2	normal	17000	1000	14000	23000	Gephart, 1994
Time in Shower	hr/d	normal	0.15	0.06	0.017	0.333	Gephart, 1994

Table 3-9 Parameters used to configure the Dermal Intake During Shower Model

Ingestion of Soil

It often happens that people will incidentally ingest soil while they are outdoors. This can happen as their mouth comes into contact with their hands or clothing that may have picked up some contaminated soil. For children this can be the primary route of exposure to contaminated soils (Paustenbach, 1989a,b). Intake of contaminants through this route is estimated as follows (API, 1994):

$$DI = 10^{-6} \frac{\beta_s \times C_s \times IR \times FI}{BW} \qquad (3\text{-}14)$$

where

DI = daily absorbed dose from soil ingestion (mg/kg-d)
C_s = conc. of chemicals in contaminated soil (mg/kg)
IR = ingestion rate of soil (mg/d)
FI = the fraction of soil that is contaminated [-]
BW = body weight (kg)
β_s = chemical specific bioavailability (mg/mg)

Configuring the Soil Ingestion Model. The value for the fraction of contaminated soil for this effort was set to 1 indicating that all of the farm soils were contaminated. This was a worst-case value providing conservative risk estimates.

The amount of soil people ingest (IR) is difficult to measure and the published values are subject to a great deal of uncertainty (Gephart *et al.*, 1994). Gephart *et al.* (1994) described the soil ingestion rate with a cumulative distribution, which was converted to a normal distribution by the methods described previously. This is shown in Figure 3-7. The mean was determined to be 45.59 mg/d with a standard deviation of 68.57. The minimum value was 0 mg/d and the maximum value was 216 mg/d. The chemical-specific bioavailabilty (β_s) was determined to be 1 (a worst-case value) (API, 1994). The other variables required by this model were discussed earlier. The variables used when solving the soil ingestion equation are listed in Table 3-10.

Ingestion of Soil Model	Units	Dist.	Mean	Std. Dev.	Min	Max	Source
Exposure Frequency	d/yr	constant	350	-	-	-	API, 1994
Exposure Duration	yr	exponential	17.73	17.79	0	60	calculated
Ingestion Rate	mg/d	normal	45.59	68.57	0	216	calculated
Fraction Soil Contaminated	-	constant	1	-	-	-	API, 1994

Table 3-10 Parameters used to configure the Ingestion of Soil Model

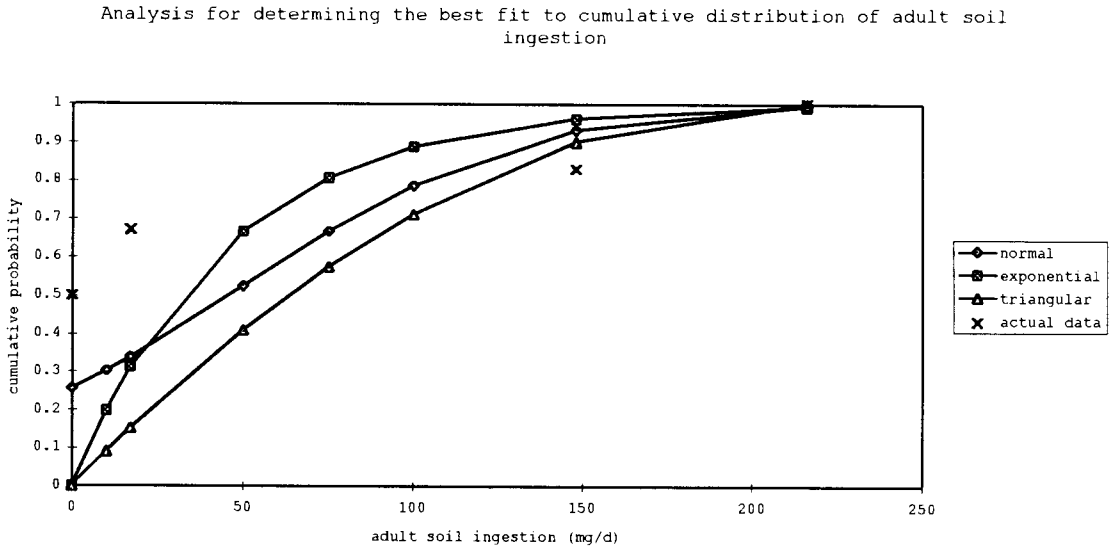


Figure 3-7

Dermal Contact With Soil

If bare skin is exposed to contaminated soil contaminants may be absorbed across the skin into the bloodstream. The absorbed dose was calculated as follows (API, 1994):

$$D_{abs} = 10^{-6} \frac{C_s \times SA \times AF \times ABS}{BW} \qquad (3\text{-}15)$$

where

D_{abs} = dermal absorbed dose (mg/kg-d)
C_s = concentration of chemicals in soil (mg/kg)
SA = skin surface area exposed to soil (cm^2/d)
AF = soil to skin adherence factor (mg/cm^2)
ABS = fraction of chemical absorbed (mg/mg)

The value for C_s was the simulated soil concentration reported in Mills (1994), and was discussed earlier.

Configuring the Dermal Contact with Soil Model. For this effort it was assumed that the hands and forearms were the only part of the body that came into direct contact with the contaminated soil. Gephart *et al.* (1994) characterized the surface area of the hands and forearms (SA) as a triangular distribution with a minimum of 3120 cm^2, a mean of 1686 cm^2 and a maximum of 4050 cm^2. The adherence factor (AF) was listed in the APIDSS manual as 0.6 mg/cm^2. The fraction of chemical absorbed (ABS) was set at 0.25 which was a typical value for organic compounds (Ryan *et al.*, 1986). These values are summarized in Table 3-11.

Dermal Contact with Soil	Units	Dist.	Mean	Std. Dev.	Min	Max	Source
Exposure Frequency	d/yr	constant	350	-	-	-	API, 1994
Exposure Duration	yr	exponential	17.73	17.79	0	60	Gephart, 1994
Skin Surface Area	cm^2	triangular	3120	68.57	0	216	Gephart, 1994
Adherence Factor	mg/cm^2	constant	0.6	-	-	-	API, 1994
Fraction of chemical absorbed	mg/mg	constant	0.25	-	-	-	Ryan et al., 1986

Table 3-11 Parameters used to configure the Dermal Contact with Soil Model

Inhalation of Soil Emissions

As emissions from contaminated soil become dispersed in the atmosphere they become available for inhalation. The emissions may spread widely endangering even people who are off-site. The soil emission inhalation intake was calculated as follows (API, 1994):

$$DI = \frac{\beta_a \times C_a \times IH \times ET}{BW} \qquad (3\text{-}16)$$

where

DI = daily absorbed dose from inhalation of soil emissions (mg/kg-d)
C_a = concentration of chemical in ambient air (mg/m^3)
IH = inhalation rate (m^3/hr)
ET = exposure time (hr/d)
BW = body weight (kg)
β_a = chemical specific bioavailability (mg/mg)

The concentration of chemical in the air (C_a) was the sum of volatile and particulate emissions as provided by the Cowherd, Farmer and box models and was discussed earlier in this section.

Configuring the Inhalation of Soil Emission Model. The inhalation rate (IH) was the same as was discussed in the configuration of the shower inhalation model. The time outdoors (ET) was taken to be 3 hours per day (API, 1994). A worst case value of 1 was used for the chemical specific

bioavailability (β_a) for all of the pesticides (API, 1994). This value is listed in Figure 3-13, which shows pesticide data. The other values used in configuring this equation are listed in Table 3-12.

Inhalation of Soil Emissions	*Units*	*Dist.*	*Mean*	*Std. Dev.*	*Min*	*Max*	*Source*
Exposure Frequency	d/yr	constant	350	-	-	-	API, 1994
Exposure Duration	yr	exponential	17.73	17.79	0	60	Gephart, 1994
Inhalation Rate	m^3/hr	uniform	0	0	0.21	0.74	Gephart, 1994
Time Outdoors	hr/d	constant	3	-	-	-	API, 1994

Table 3-12 Parameters used to configure the Inhalation of Soil Emissions Model

Chronic Daily Intake

Chronic Daily Intake (CDI) was used to evaluate the non-carcinogenic effects from chronic exposure to a chemical. The CDI is defined as the mass of substance contacted per unit body weight per unit time (U.S.EPA, 1989). A value for CDI is calculated for the daily intake from each of the above equations. The CDI was calculated as follows (API, 1994):

$$CDI = \frac{DI \times EF \times ED}{365 \times AT} \qquad (3\text{-}17)$$

where

CDI = chronic daily intake (mg/kg-d)
DI = daily intake (mg/kg-d)
EF = exposure frequency (d/yr)

ED = exposure duration (yr)
AT = averaging time (yr)

To be consistent with EPA guidance the averaging time (AT) was considered equal to the exposure duration (ED) because non-carcinogenic effects were calculated (U.S.EPA, 1989). For this study, exposure duration and averaging time canceled out. The daily intake (DI) was the absorbed dose figured previously for each intake route.

Calculation of Hazard Index

In this step the exposure information from above and the toxicity information discussed in Chapter II were integrated to form a quantitative expression of the non-cancerous risk to human health. This quantitative expression is called the hazard index (HI). The hazard index is the sum of hazard quotients (HQ) which were calculated for each exposure pathway. The equation used for determining the non-cancer hazard quotient was (API, 1994):

$$HQ_{ij} = \frac{CDI_{ij}}{RfD_{ij}} \qquad (3\text{-}18)$$

where

HQ_{ij} = hazard quotient for chemical i, exposure route j
CDI_{ij} = chronic daily intake for chemical i, exposure route j
RfD_{ij} = reference dose for chemical i, exposure route j

The hazard index is equal to the sum of the hazard quotients for each chemical and exposure route (U.S.EPA, 1989).

$$HI = \sum HQ_{ij} \qquad (3\text{-}19)$$

When evaluating non-cancerous effects it was assumed that there was a threshold level of exposure (i.e., RfD) below which it was unlikely for even sensitive populations to experience adverse health effects.

Pesticide Modeling

All of the models discussed above require parameters that are specific to each pesticide. Each time a different scenario was modeled the appropriate numbers representing the pesticide of concern were entered into each model. The values that were used for the fate and transport models are listed in Table 3-13.

Diffusion Coefficients. The values for the diffusion coefficient in air (Dair) and the diffusion coefficient in water (Dwater) for the pesticides in this study could not be found in the available sources. In order to determine the diffusion coefficients in air for the pesticides in this study, the diffusion coefficients in air for many common organic chemicals were taken from U.S.EPA (1988). It was determined that the diffusion coefficients in air had a mean

of 0.0907 cm^2/sec, a standard deviation of 0.0212, a minimum of 0.0526 cm^2/sec, and a maximum of 0.157 cm^2/sec. The cumulative distribution function describing these values was plotted and compared with exponential, normal, and triangular cumulative distribution functions described by the same mean and standard deviations. It was determined that these values best fit a normal distribution. The plot of each cumulative distribution function for diffusion in air coefficients is shown in Figure 3-8. It was then assumed that the diffusion coefficients in air for all of the pesticides in the study could be described by this normal distribution.

The same procedure was used to determine a distribution describing the diffusion coefficients in water for the pesticides in this study. The values of diffusion coefficients in water for several common organic chemicals were taken from the (API, 1994). These values were fit to a normal distribution in the same manor as described above for Dair. The distribution functions are shown in Figure 3-9. The diffusion in water (Dwater) coefficients were described by a mean of $8.96(10)^{-6}$ with a standard deviation of $2.33(10)^{-6}$, a minimum of $5.93(10)^{-6}$ and a maximum of $1.64(10)^{-5}$. These values were used for all of the pesticides in the study.

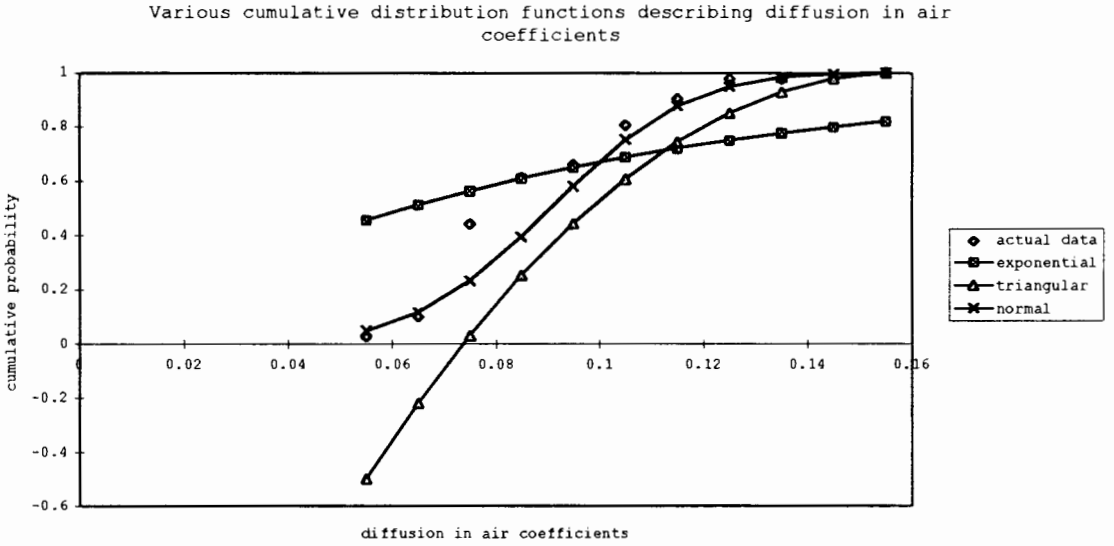


Figure 3-8

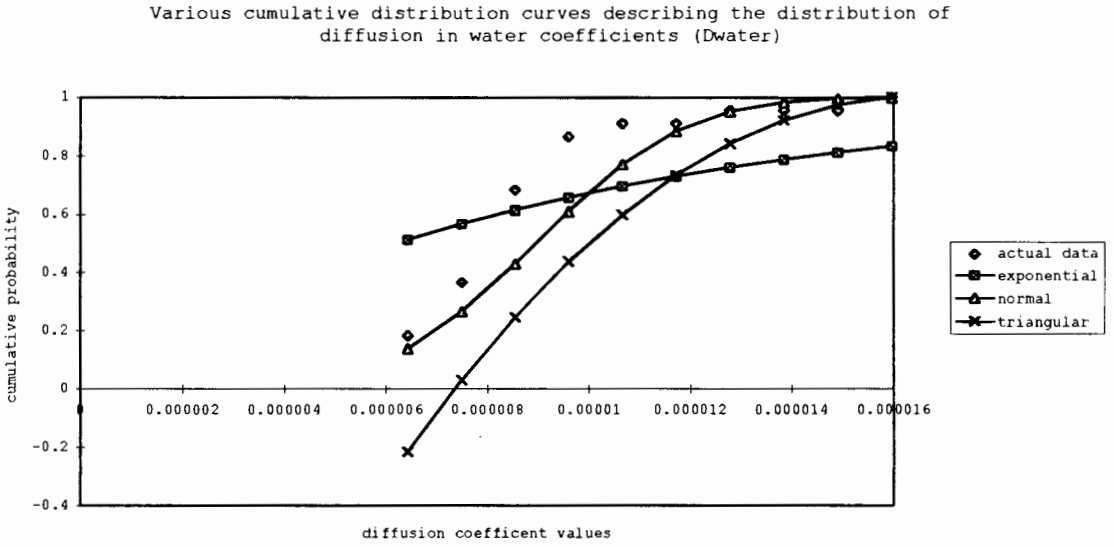


Figure 3-9

Table 3-13 Parameters describing the pesticides used in this study

Parameter	Unit	Source	(2,4-D)	Malathion	Furadan (Carbofuran)	Lasso (Alachlor)	Treflan (Trifluralin)	Prowl (Pendimethalin)
mole wt.	g/mol	1	221	330.4	221.28	269.9	335.3	281.3
vapor pressure	mmHg	3	0.4	0.00004	0.00002	0.000022	0.00011	0.00003
solubility	mg/L	1&2	620	145	700	242	24	0.5
Henry's law constant	mg/l/mg/l	7	5.6E-09	0.0000024	0.00000014	0.0000013	0.0067	9.11267E-07
log Kow		1	2.81	2.89	2.44	2.78	4.75	4.725772497
Koc	ml/g	2	20	1800	40	190	1200	5000
Dair	cm^2/s	5	*	*	*	*	*	*
Dwater	cm^2/s	5	*	*	*	*	*	*
Decay rate	1/d	1	0.0231	0.4152	0.0079	0.0384	0.0026	0
Perm Coeff	cm/hour	4	0.008452788	0.002072335	0.004598244	0.00404958	0.040473429	0.083055514
Absorb Coeff	-	6	0.25	0.25	0.25	0.25	0.25	0.25
Bioavail Inh Soil	-	4	1	1	1	1	1	1
Bioavail Inh Shower	-	4	1	1	1	1	1	1
Bioavail Soil	-	4	1	1	1	1	1	1
Bioavail Water	-	4	1	1	1	1	1	1

Sources

1. = Nash, 1980
2. = Gleams User Manual, 1990
3. = U.S.EPA, 1989
4. = API, 1994
5. = Calculated
6. = Ryan *et al.*, 1986
7. = Donigian *et al.*, 1986

Prowl. Complete data for Prowl (pendemethalin) were not available. The value's for Henry's law constant, log Kow, and decay rate could not be found in the available literature. Instead these numbers were calculated. The Henry's law constant was determined with the following equation (API, 1994):

$$H = \frac{\frac{P_v}{S}}{RT} \qquad (3\text{-}20)$$

Where

P_v = saturation vapor pressure (atm)
S = solubility (mol/m^3)
R = universal gas constant ($atm\text{-}m^3/mol\text{-}K$)
T = absolute temperature (K)
H = Henry's law constant (mg/l)/(mg/l)

The value of K_{ow} for Prowl was determined with the following equation (API, 1994):

$$\log K_{ow} = 4.5 - 0.75 \times \log S \qquad (3\text{-}21)$$

where

S = solubility of the chemical (mg/L)

Dose Response Properties. The chemical intake and risk calculation models required data describing the pesticides dose-response properties. These are listed in Table 3-14 and were discussed in Chapter II in the Toxicity Assessment section. The oral RfDs came from IRIS (1993). It was

assumed that the inhalation RfDs could be described by the same values for lack of better data.

	Inhalation RfD mg/kg*d	Oral RfD mg/kg*d
(2,4-D)	1.00E-02	1.00E-02
Malathion	2.00E-02	2.00E-02
Furadan(Carbofuran)	5.00E-03	5.00E-03
Lasso(Alachlor)	1.00E-02	1.00E-02
Treflan (Trifluralin)	7.50E-03	7.50E-03
Prowl (Pendimethalin)	4.00E-02	4.00E-02

Table 3-14 Oral and Inhalation Reference Doses for the pesticides used in this study.

CHAPTER IV

RESULTS

Phase 1: Risk Assessment

Phase 1 of this study involved performing risk assessments with computer models for conditions common in Caddo County, Oklahoma. Thirty-nine cases made up of different pesticides, soil types, crops, and irrigation practices were analyzed. An individual risk assessment was performed for each case and had a unique configuration of these four items. The results varied widely from very likely to cause adverse health effects to no hazard at all.

The APIDSS models were run completely in Monte Carlo mode for this phase of the study. This allowed APIDSS not only to provide a Hazard Index, but to provide it at any percentile specified as well as the standard deviation about the mean hazard index. The following paragraphs summarize the results by listing the median hazard index, the upperbound 95th percentile Hazard Index, and the standard deviation about the mean. The results are also shown in Figures 4-1 through 4-6. These figures show the median HI and the upperbound 95th percentile HI for each case that was modeled, in bar chart form.

2,4-D

The case involving 2,4-D applied to peanuts growing in A soil resulted in a median Hazard Index of 0.803 with a standard deviation of 0.808 and an upperbound 95th percentile of 2.47. This case was unaffected by irrigation practice (Mills, 1994). When this case was run on B soil with full irrigation the results were a median HI of 1.14 with a standard deviation of 1.11 and a upperbound 95th percentile of 3.58. This case produced the highest HI of all the cases modeled. When the same case was modeled with no irrigation the median HI became 1.03 with a standard deviation of 1.04 and a upperbound 95th percentile of 3.3. In D soil with full irrigation the median HI was 0.7 with a standard deviation of 0.67 and an upperbound 95th percentile of 2.07. With no irrigation this case resulted in a median HI 0.729 with a standard deviation of 0.839 and a upperbound 95th percentile of 2.56.

The results of modeling 2,4-D application to wheat are as follows. In A soils with full irrigation, a median HI of 0.00517 with a standard deviation of 0.00514 and an upperbound 95th percentile of 0.0151 were obtained. In A soils with no irrigation, a median HI of 0.00471 with a standard deviation of 0.00544 and an upperbound 95th

Hazard Indexes for cases involoving 2,4-D

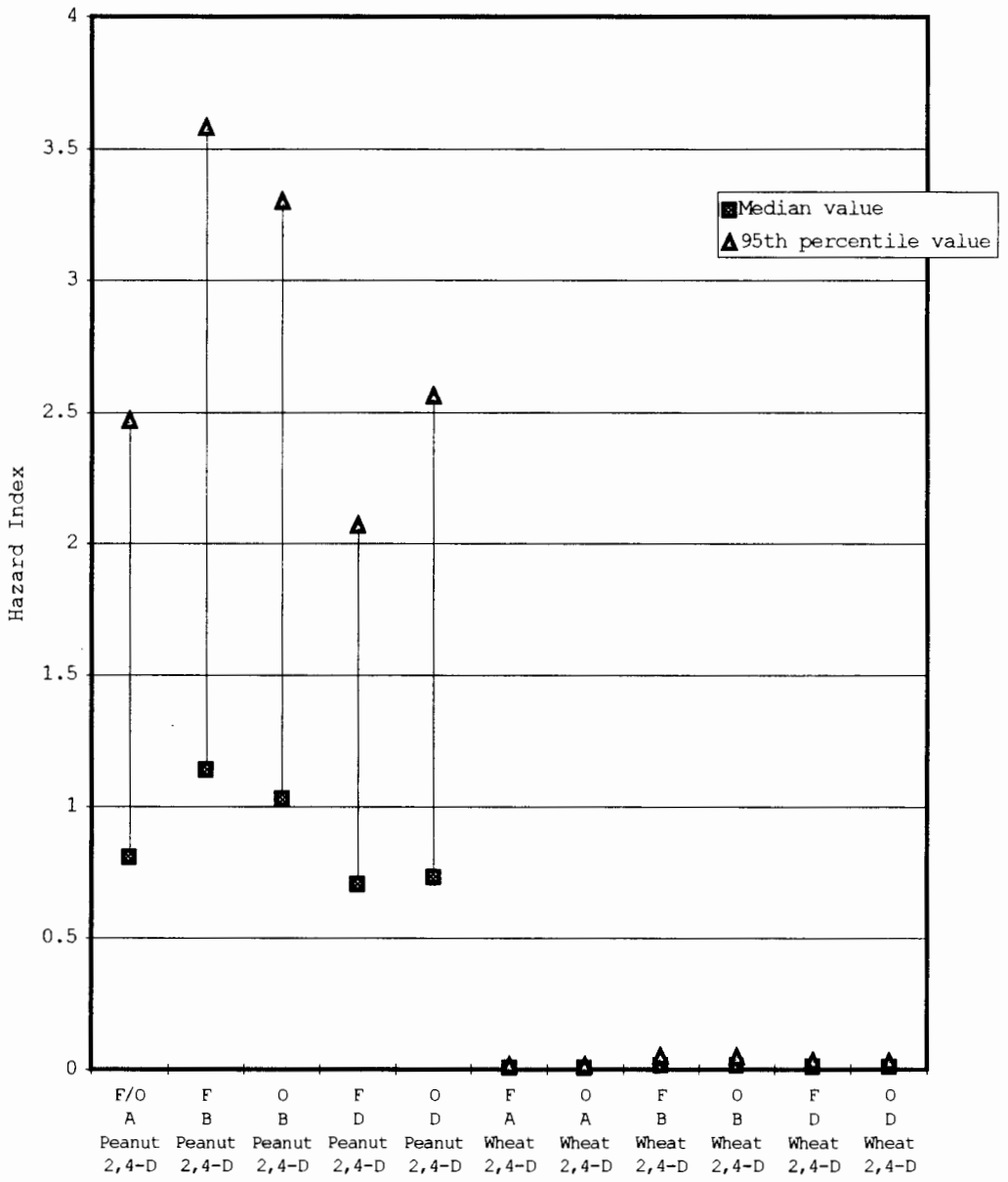


Figure 4-1

percentile of 0.0157 was obtained. In B soils with full irrigation a median HI of 0.0161 with a standard deviation of 0.0156 and an upperbound 95th percentile of 0.0506. When this was changed to no irrigation the median HI became 0.0149 with a standard deviation of 0.0147 and a upperbound 95th percentile of 0.047. When this same pesticide-crop combination was used on D soils with full irrigation, the median HI was 0.0109 with a standard deviation of 0.0111 and a upperbound 95th percentile of 0.0312. With no irrigation this scenario gave a median HI of 0.0101 with a standard deviation of 0.00102 and a upperbound 95th percentile of 0.0301. Figure 4-1 presents the results of all the cases involving 2,4-D.

Furadan

Three cases involving Furadan were modeled. In all three cases it was applied to alfalfa. The type of irrigation method modeled showed no effect in any of the cases (Mills, 1994). In A soils the models returned a median HI of 0.000306 with a standard deviation of 0.000299 and a upperbound 95th percentile of 0.00102. In B soils this scenario resulted in a median HI of 0.0382 with a standard deviation of 0.0255 and a upperbound 95th

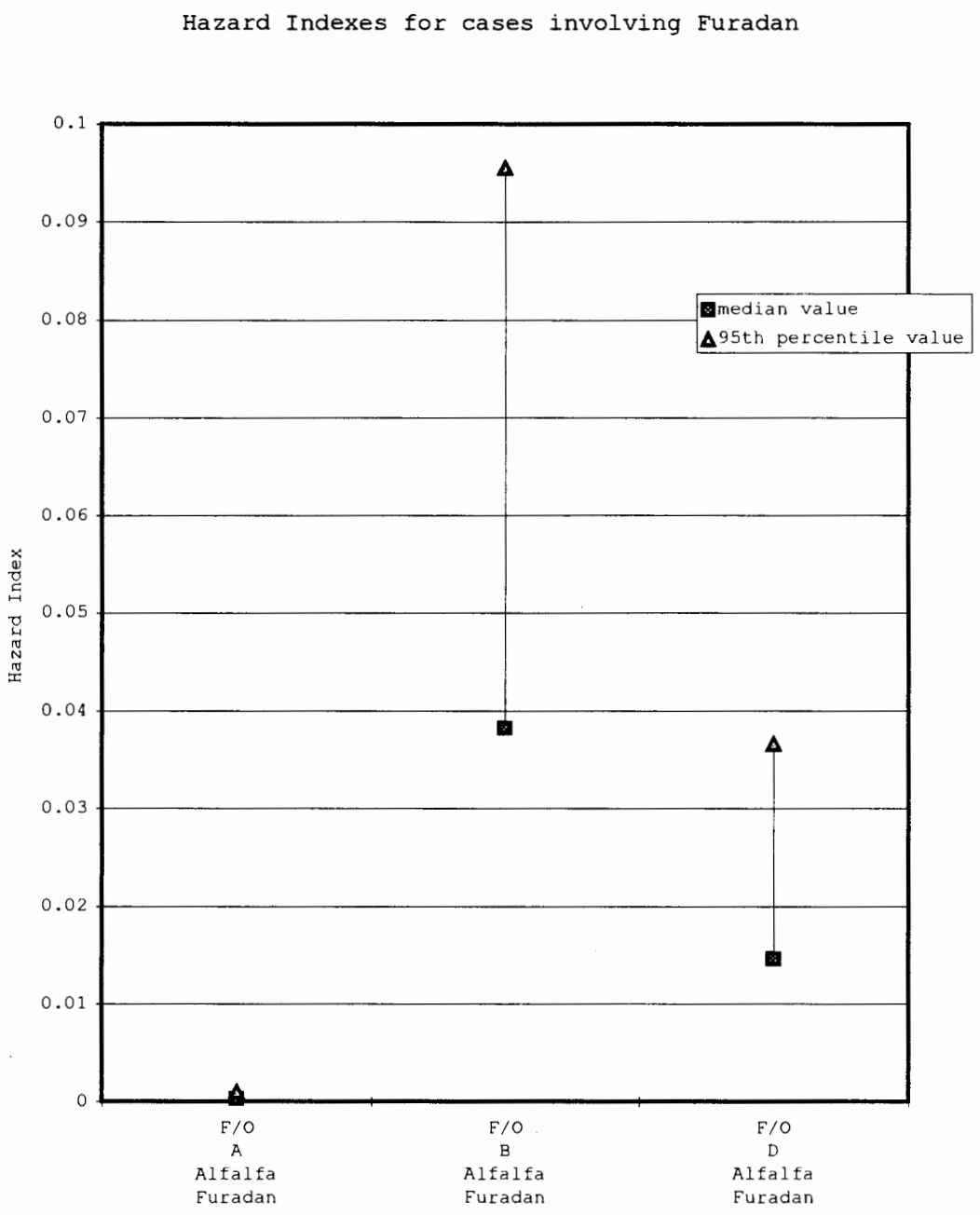

Hazard Indexes for cases involving Furadan
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
Hazard Index
median value
95th percentile value
F/O A Alfalfa Furadan
F/O B Alfalfa Furadan
F/O D Alfalfa Furadan

Figure 4-2

percentile of 0.0955. When the scenario was run with D soils the median HI was 0.0146 with a standard deviation of 0.00969 and an upperbound 95th percentile of 0.0366. The results of all the cases in which Furadan was modeled are shown in Figure 4-2.

Lasso

Lasso application to peanuts was modeled in 5 different cases. In A soil, full irrigation and no irrigation returned the same results (Mills, 1994). These results were a median HI of $4.35(10)^{-6}$ with a standard deviation of $3.2(10)^{-6}$ and an upperbound 95th percentile of $1.23(10)^{-5}$. In B soils with full irrigation the results were a median HI of $2.27(10)^{-5}$ with a standard deviation of $6.36(10)^{-6}$ and an upperbound 95th percentile of $3.88(10)^{-5}$. The case with B soils and no irrigation resulted in a median HI of $2.27(10)^{-5}$ with a standard deviation of $6.36(10)^{-5}$ and an upperbound 95th percentile of $3.88(10)^{-5}$. When the case of D soils with full irrigation was modeled, the results were a median HI of $6.64(10)^{-5}$ with a standard deviation of $1.6(10)^{-5}$ and an upperbound 95th percentile of 0.0001. This same case with no irrigation returned a median HI of $2.17(10)^{-5}$ with a standard deviation of $7.64(10)^{-6}$ and an upperbound 95th

Hazard Indexes for cases involving Lasso

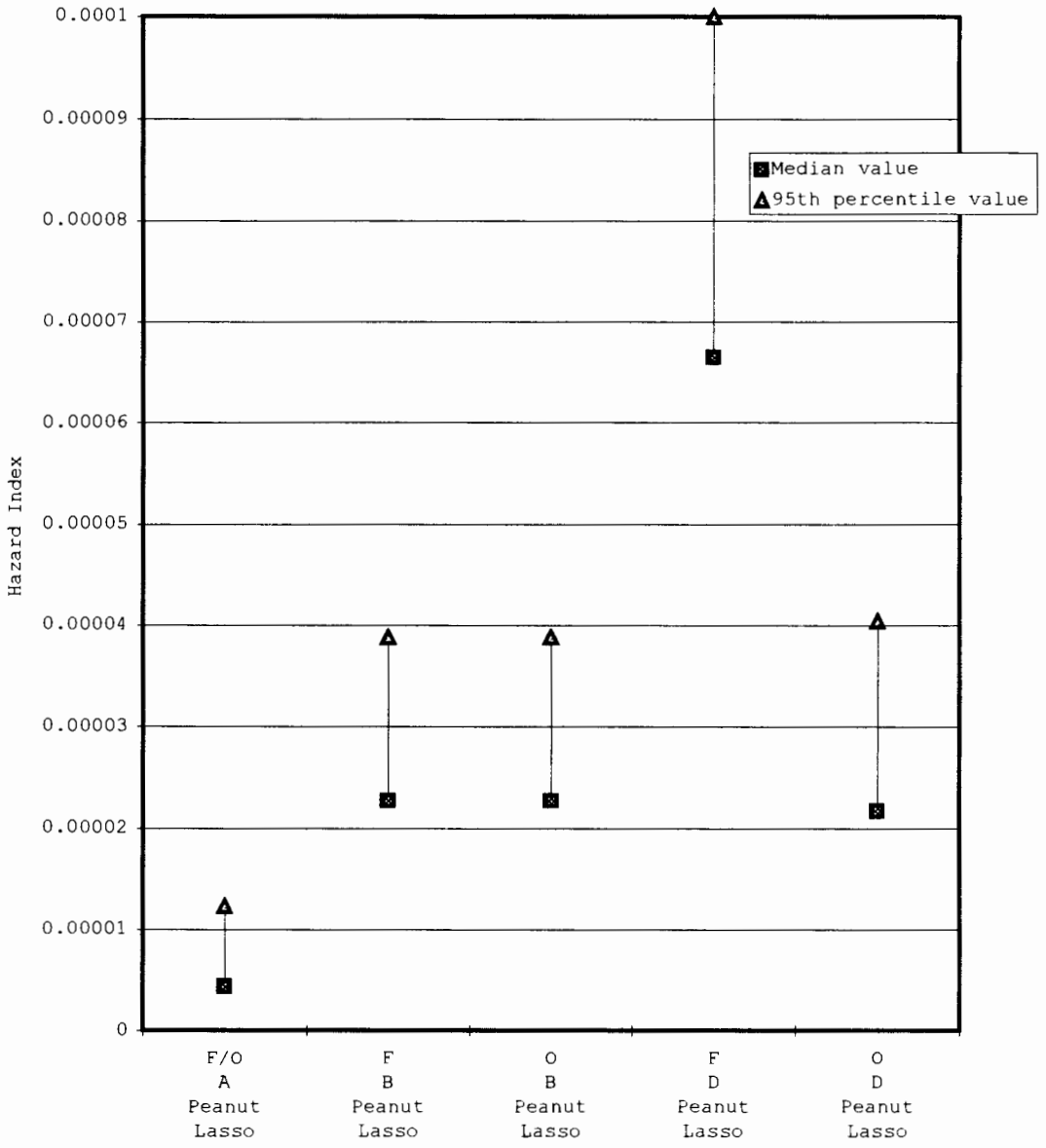


Table 4-3

percentile of $4.04(10)^{-5}$. Figure 4-3 presents the results obtained from the scenarios involving Lasso.

Malathion

Malathion was applied to alfalfa in six different sets of simulations. On A soils with full irrigation, a median HI of $1.12(10)^{-9}$ was returned with an upperbound 95th percentile of $2.17(10)^{-8}$. With no irrigation this case returned a median HI of $1.19(10)^{-9}$ with a standard deviation of $9.14(10)^{-9}$ and an upperbound 95th percentile of $2.4(10)^{-8}$. B soils with full irrigation resulted in a median HI of $7.87(10)^{-7}$ with a standard deviation of $7.99(10)^{-7}$ and an upperbound 95th percentile of $2.27(10)^{-6}$. B soils with no irrigation resulted in a median HI $8.53(10)^{-7}$ and an upperbound 95th percentile of $2.46(10)^{-6}$. The case with D soils and full irrigation resulted in a median HI of $1.88(10)^{-7}$ with a standard deviation of $2.02(10)^{-7}$ and an upperbound 95th percentile of $5.69(10)^{-7}$. With no irrigation this same case resulted in a median HI of $1.96(10)^{-7}$ with a standard deviation of $2.1(10)^{-7}$ and an upperbound 95th percentile of $5.94(10)^{-7}$.

The results of the cases where Malathion was applied to wheat were unaffected by irrigation techniques (Mills,

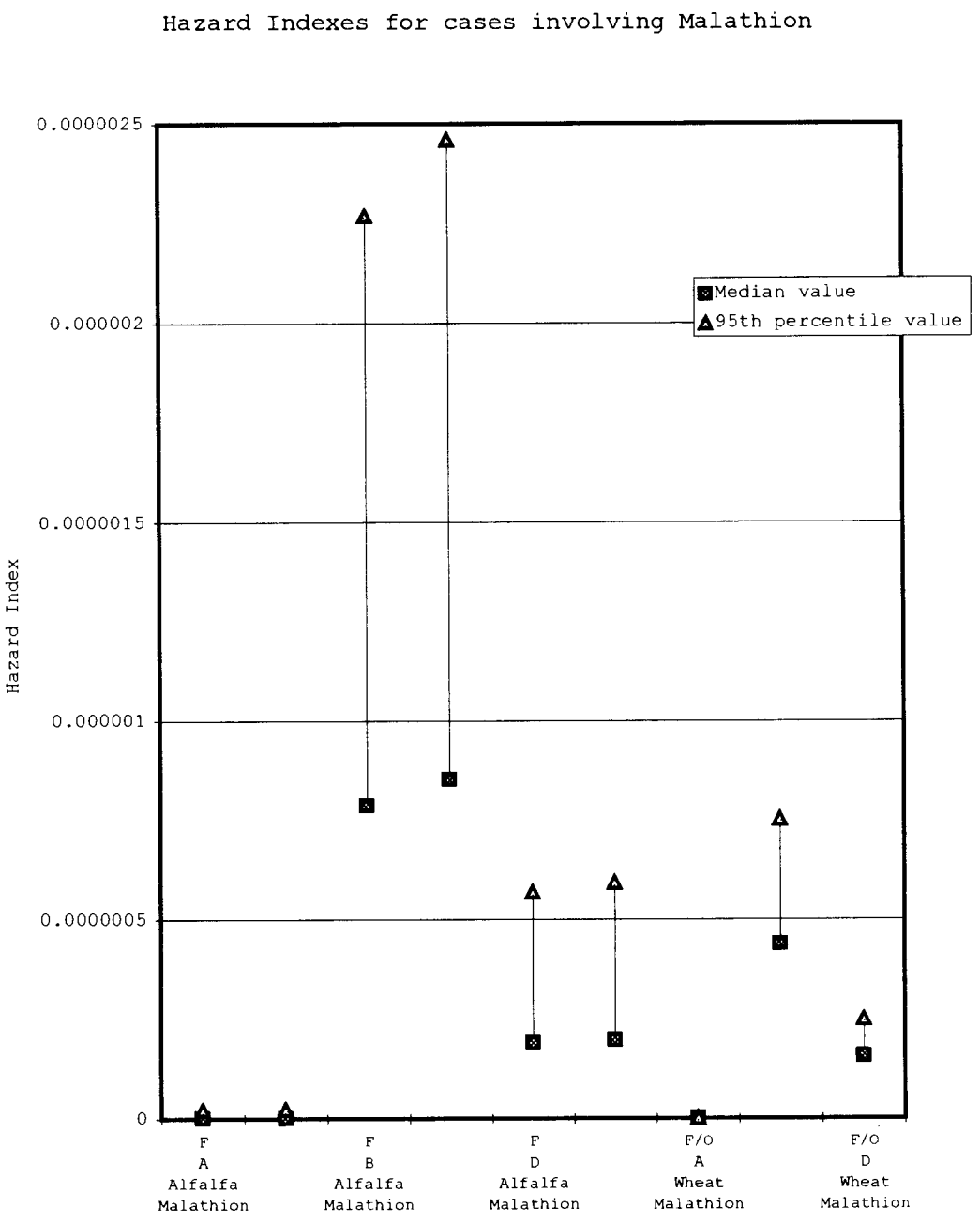

Hazard Indexes for cases involving Malathion
0.0000025
0.000002
0.0000015
0.000001
0.0000005
0
Hazard Index
Median value
95th percentile value
F A Alfalfa Malathion
F B Alfalfa Malathion
F D Alfalfa Malathion
F/O A Wheat Malathion
F/O D Wheat Malathion

Figure 4-4

1994). In A soils a median HI of $8.09(10)^{-10}$ with standard deviation of $2.25(10)^{-10}$ and an upperbound 95th percentile of $1.42(10)^{-9}$ were returned. In B soils the results were a median HI of $4.37(10)^{-7}$ with a standard deviation of $1.37(10)^{-7}$ and an upperbound 95th percentile of $7.53(10)^{-7}$. In D soils the model returned a median HI of 1.54(10)-7 with a standard deviation of 4.59(10)-8 and an upperbound 95th percentile of 2.47(10)-7. Figure 4-4 shows these results.

Prowl

The results of the cases where Prowl was applied to cotton also were unaffected by irrigation practice (Mills, 1994). In A soils the median HI was $7.4(10)^{-15}$ with a standard deviation of $1.96(10)^{-15}$ and an upperbound 95th percentile of $1.26(10)^{-14}$. In B soils the median HI was $3.21(10)^{-12}$ with a standard deviation of $1.93(10)^{-12}$ and an upperbound 95th percentile of $7.78(10)^{-12}$. Modeling this case in D soil produced a median HI $2.39(10)^{-18}$ with a standard deviation of $7.04(10)^{-18}$ and an upperbound 95th percentile of $2.09(10)^{-17}$. The results obtained from the scenarios using Prowl are shown in Figure 4-5

Hazard Indexes for cases involving Prowl

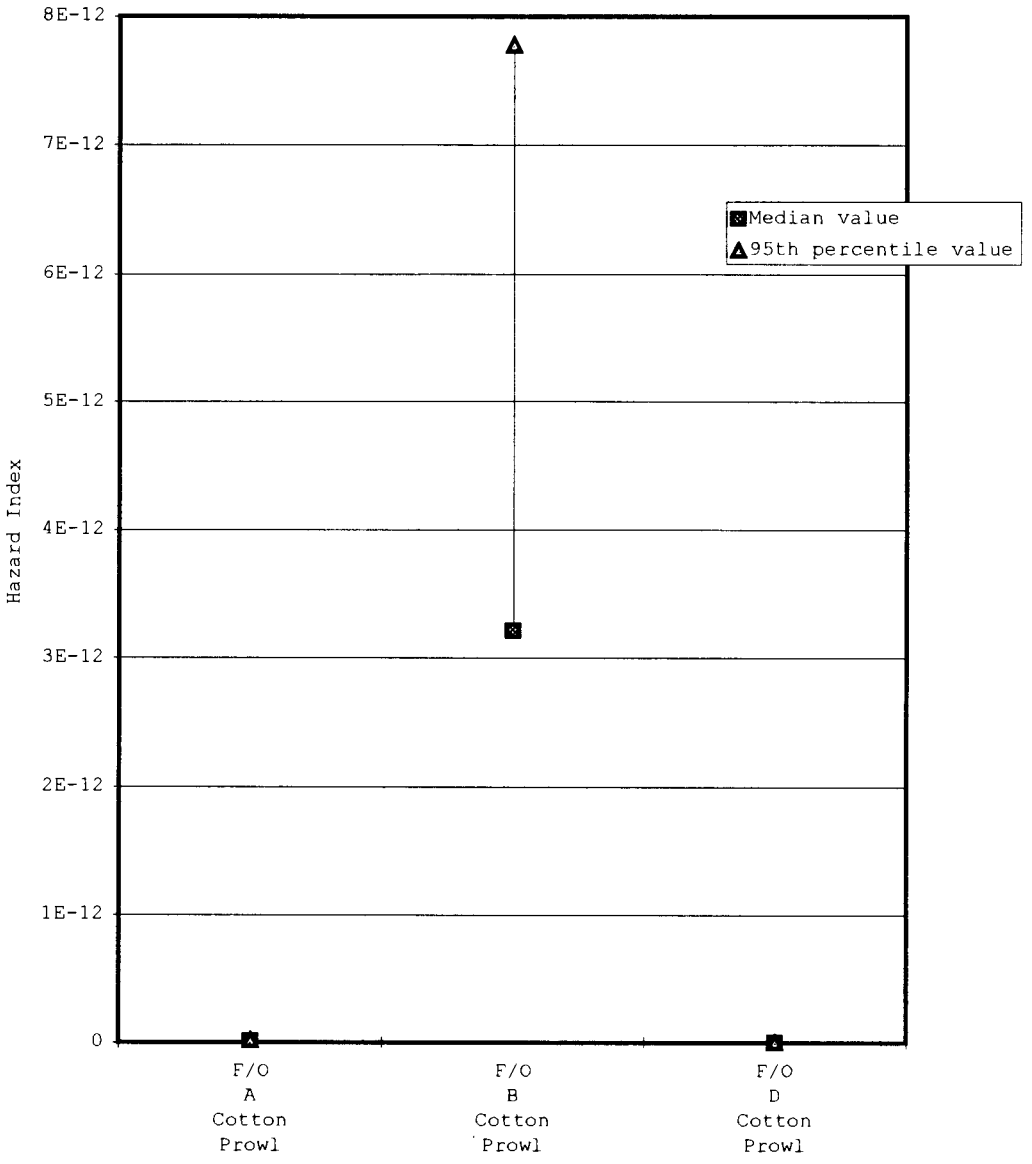


Figure 4-5

Treflan

Cases involving Treflan application to cotton were unaffected by irrigation practice (Mills, 1994). On A soils this scenario resulted in a median HI of $3.29(10)^{-7}$ with a standard deviation of $2.24(10)^{-7}$ and an upperbound 95th percentile of $8.05(10)^{-7}$. In B soils the results were median HI of $6.86(10)^{-7}$ with a standard deviation of $4.95(10)^{-7}$ and an upperbound 95th percentile of $1.71(10)^{-6}$. Modeling this scenario in D soils resulted in a median HI of $1.78(10)^{-13}$ with a standard deviation of $1.21(10)^{-13}$ and an upperbound 95th percentile of $4.35(10)^{-13}$.

Modeling the scenario where Treflan was applied to peanuts produced a median HI of $6.58(10)^{-10}$ with a standard deviation of $4.48(10)^{-10}$ and an upperbound 95th percentile of $1.6(10)^{-9}$ in A soils with full irrigation. Non-irrigated A soils resulted in a median HI of $8.24(10)^{-10}$ with a standard deviation of $5.61(10)^{-10}$ and an upperbound 95th percentile of $2.01(10)^{-9}$. When this scenario was modeled on B soils irrigation method showed no effect (Mills, 1994). The results were a median HI of $5.67(10)^{-11}$ with a standard deviation of $5.2(10)^{-11}$ and an upperbound 95th percentile of $1.67(10)^{-10}$. In D soils with full irrigation the median HI was $8.78(10)^{-7}$ with a standard deviation of $6.43(10)^{-7}$ and an

Hazard Indexes for cases involving Treflan

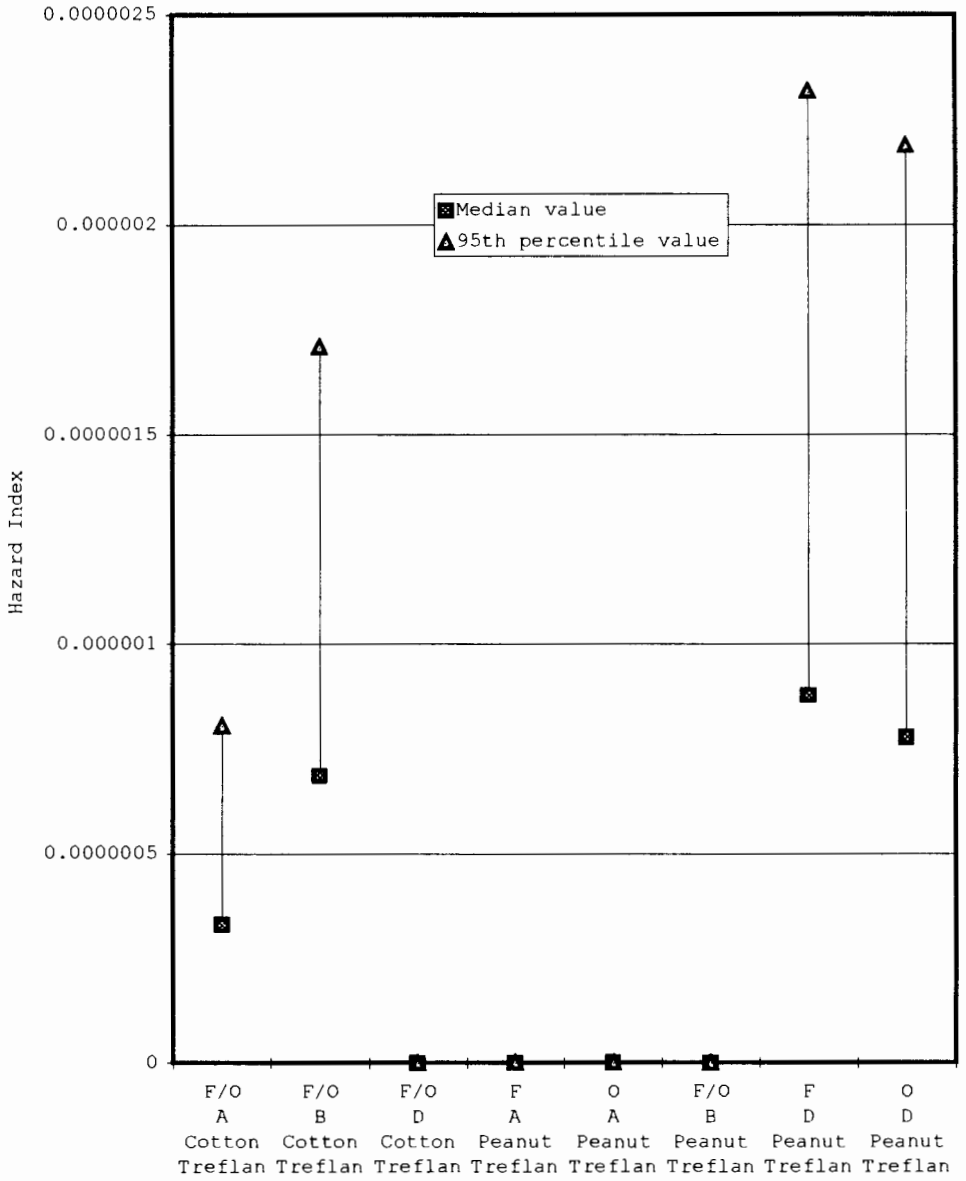


Figure 4-6

upperbound 95th percentile of $2.32(10)^{-6}$. With no irrigation this scenario resulted in a median HI of $7.78(10)^{-7}$ with a standard deviation of $6.92(10)^{-7}$ and an upperbound 95th percentile of $2.19(10)^{-7}$. The results of all of the cases involving Treflan can be seen in Figure 4-6.

Figures 4-7 and 4-8 are summaries of the results. They show which situation was modeled and the 95th percentile hazard index that resulted.

Figure 4-7 Summary of results of Phase 1

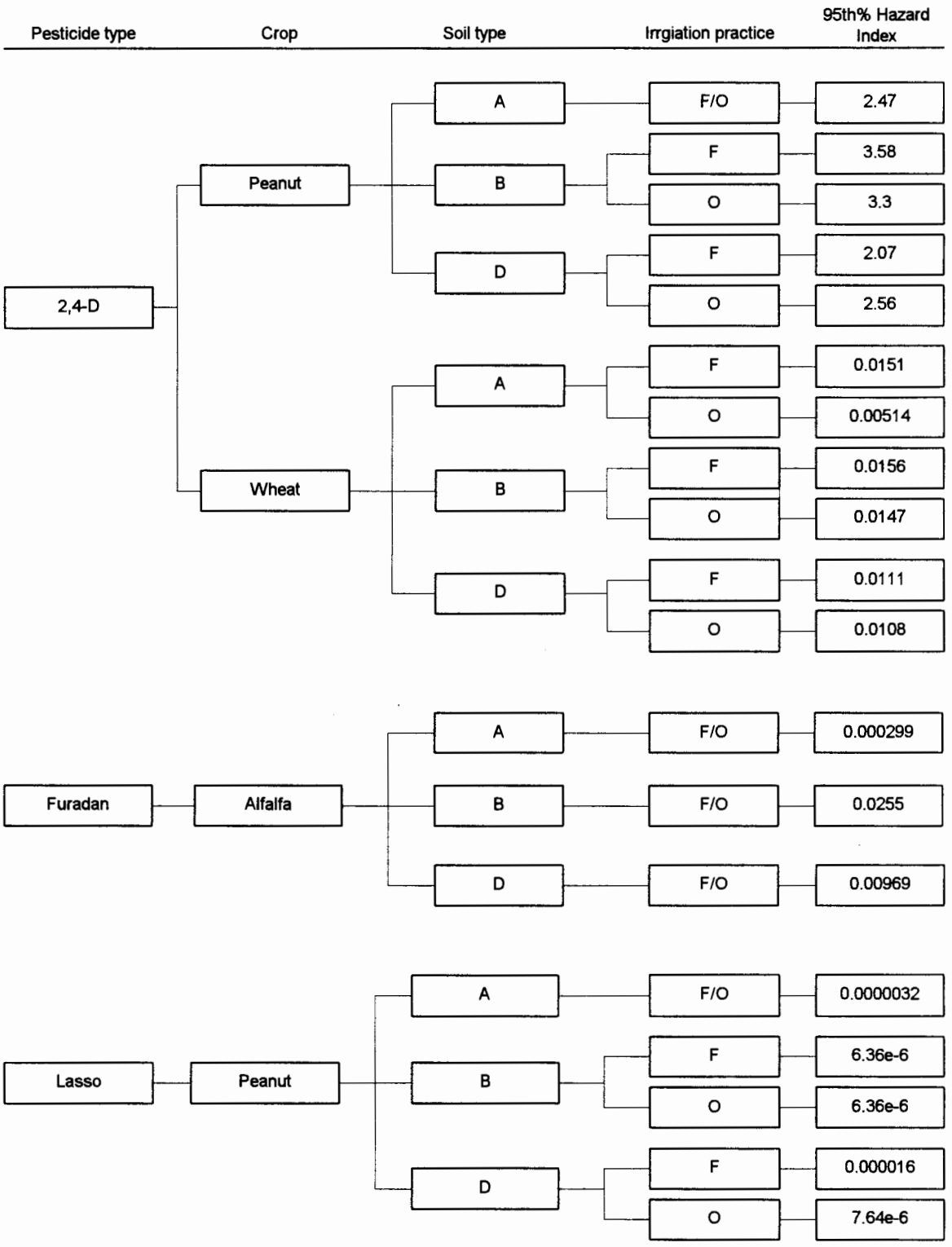
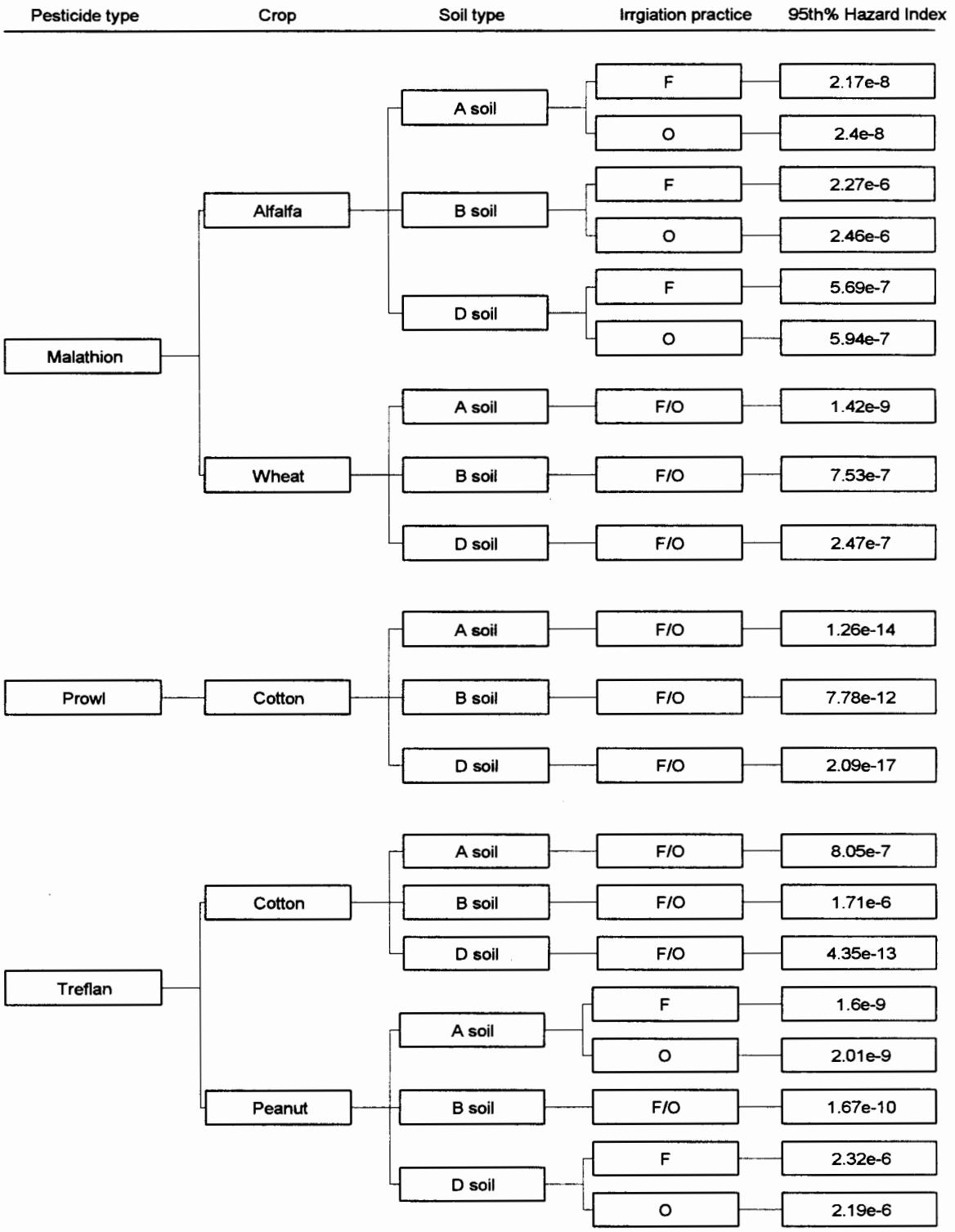


Figure 4-8 Summary of results of Phase 1 continued



Phase 2: Uncertainty Analysis

Phase 2 of this study was focused on quantifying the uncertainty in the hazard index arising from parameter selection. The purpose of this was to enable an assessor to understand how certain the results obtained from this risk assessment are. The scenario that demonstrated the highest hazard index in Phase 1 (2,4-D on peanuts in B soil with full irrigation) was used as the base case for this phase. In order to determine the uncertainty caused by each variable the variable of interest was represented by its probability distribution while all other variables were held constant. The variables that were fixed and the probability distributions they were represented by were discussed earlier. It is important to note that the variables that were studied here were variables that had published probability distributions (Gephart *et al.*, 1994). Other variables that were not tested are also capable of introducing uncertainty.

The Drinking Water Pathway

Of the variables that were studied, three demonstrated an effect on the hazard quotient for this exposure route. They were body weight, the water ingestion rate, and the pesticide concentration in groundwater. When the case with

The relative contribution of individual parameters to the uncertainty in the hazard quotient for the drinking water pathway.

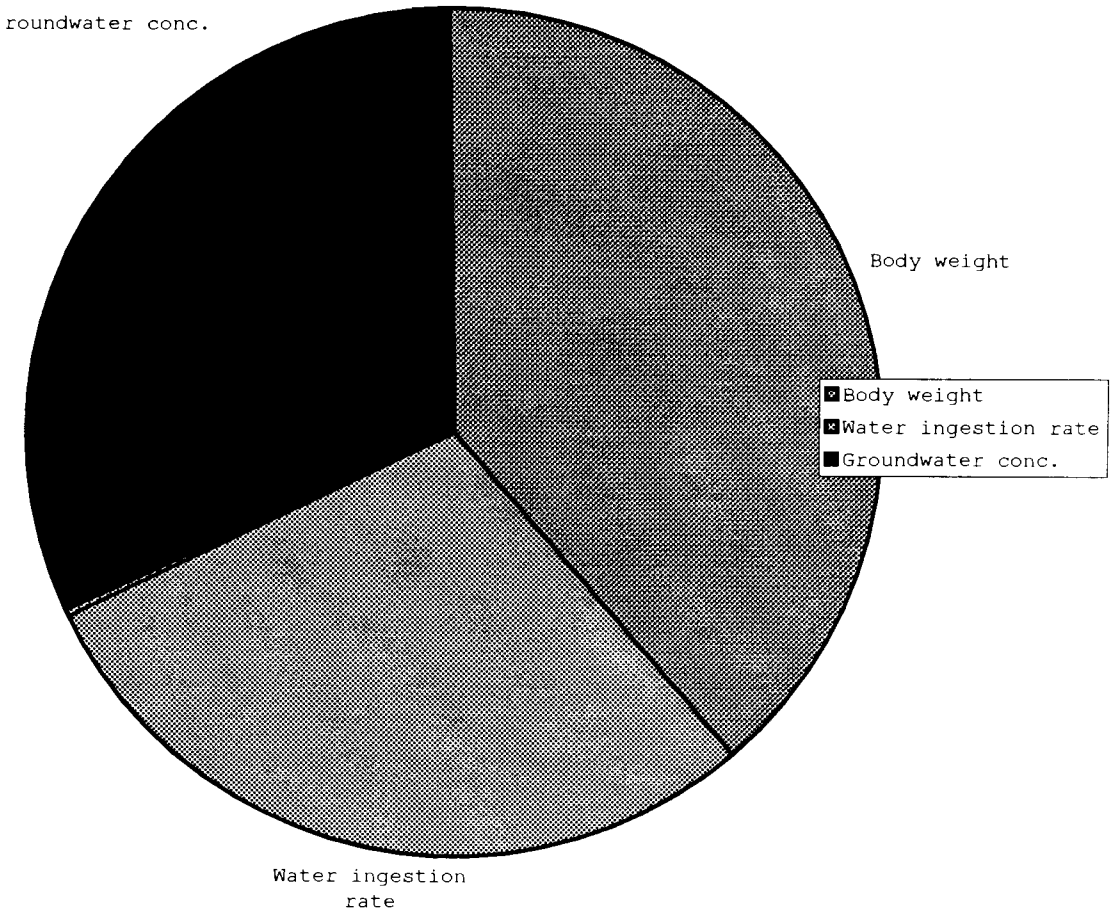


Figure 4-9

all of the variables fixed at their median values was run the hazard quotient for this route was 0.754.

When body weight was varied (set to its probability distribution) while all other parameters were fixed to their mean values and the model was run again, the median hazard quotient became 0.761. The standard deviation was 0.190 and the 95th percentile value was 1.14. When the drinking water ingestion rate was set to its probability distribution while the other parameters remained fixed the median hazard quotient became 0.747, the 95th percentile value was 0.975 and the standard deviation was 0.143. When the Fate and Transport models were left in Monte Carlo mode so that APIDSS could sample from varying groundwater concentrations the median hazard quotient became 0.763 with a standard deviation of 0.159 and a 95th percentile value of 0.831. The relative size of the standard deviations and thus the relative uncertainty are represented in Figure 4-9.

The Dermal Uptake During Shower Pathway

The variables that had an effect on increasing the uncertainty of the hazard quotient for this pathway were time spent in the shower, total body skin surface area, body weight, and pesticide concentration in groundwater. When

The relative contribution of individual parameters to the uncertainty in the hazard quotient for the dermal uptake during shower pathway.

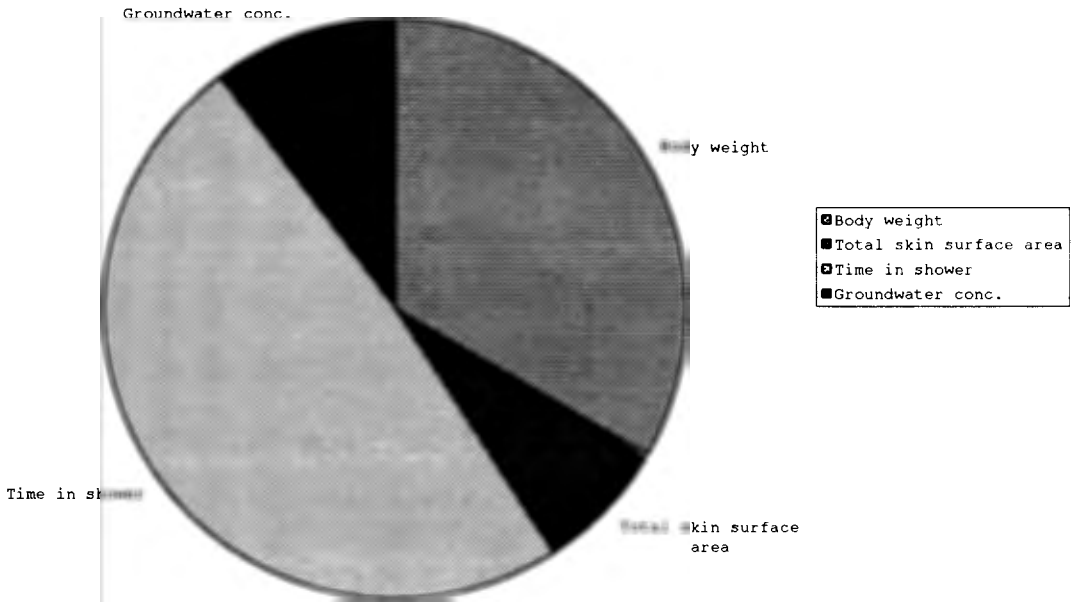


Figure 4-10

this model was run with all the variables fixed the hazard quotient was 0.0109.

When the model was run with the time spent in the shower variable represented by its probability distribution the median hazard quotient became 0.0106 with an upperbound 95th percentile value of 0.0174 and a standard deviation of 0.00404. The median hazard quotient became 0.0109 when total body skin surface area was varied while the others were held constant. This case resulted in a 95th percentile value of 0.0119 and a standard deviation of 0.000632. When body weight was varied the median HQ became 0.0110. The 95th percentile value was 0.0164 and the standard deviation. was 0.00275. When the Fate and Transport models were left in Monte Carlo mode so that APIDSS could sample from varying groundwater concentrations, the median hazard quotient became 0.0111 with a standard deviation of $8.43(10)^{-4}$ and a 95th percentile value of 0.0121. The relative magnitudes of the standard deviations in the HQ and thus the relative degree of uncertainty in the HQ caused by varying each parameter are shown in Figure 4-10.

The Inhalation During Shower Pathway

When this exposure route was examined it was shown that the variables that effect the uncertainty in the HQ were

The relative contribution of individual parameters to the uncertainty in the hazard quotient for the inhalation during shower pathway.

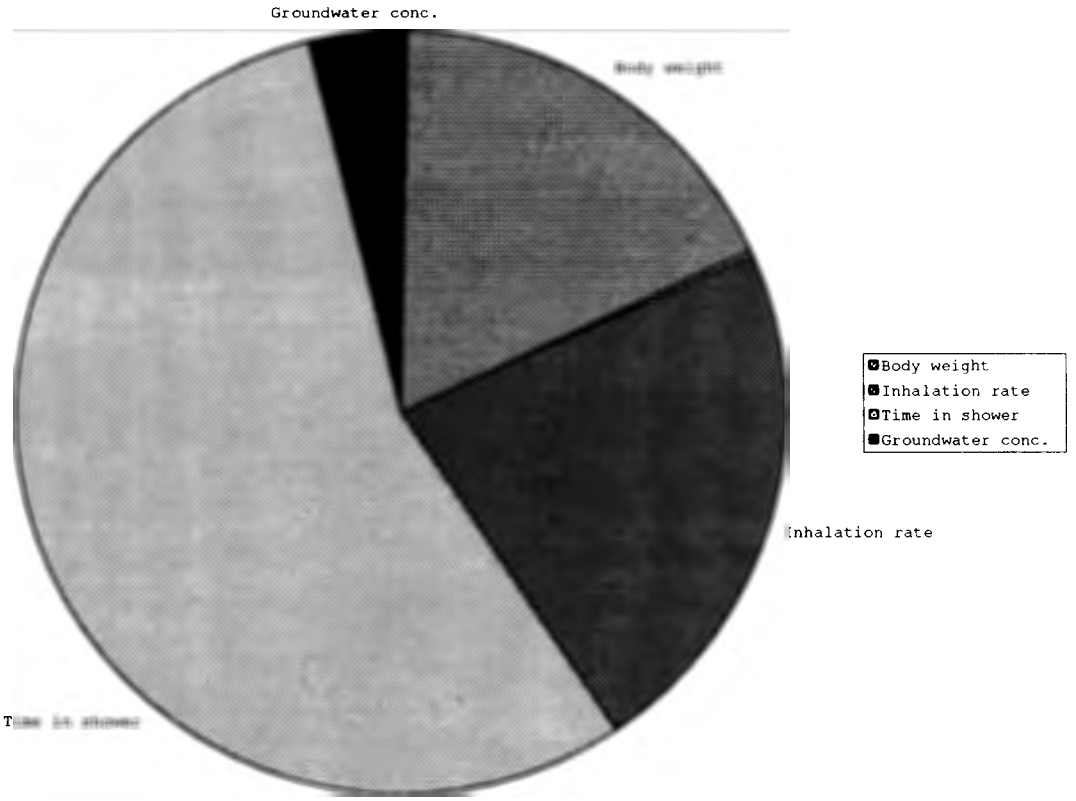


Figure 4-11

inhalation rate, body weight, time in shower, and the pesticide concentration in groundwater. When the model was run with all of the variables fixed, the HQ was $3.58(10)^{-7}$.

Varying the inhalation rate while the other parameters remained fixed resulted in a median hazard index of $2.36(10)^{-7}$, a 95^{th} percentile value of $3.53(10)^{-7}$ and a standard deviation of $7.53(10)^{-8}$. Setting body weight to its probability distribution while the other parameters remained set to their mean values resulted in a median HQ of $2.41(10)^{-7}$ with a 95^{th} percentile value of $3.61(10)^{-7}$ and a standard deviation of $6.03(10)^{-8}$. Varying the time spent in the shower parameter resulted in a median HQ of $2.27(10)^{-7}$ and a 95^{th} percentile value of $6.11(10)^{-7}$ with a standard deviation of $1.84(10)^{-7}$. When the Fate and Transport models were left in Monte Carlo mode so that APIDSS could sample from varying groundwater concentrations the median hazard quotient became 2.44(10)-7 with a standard deviation of $1.25(10)^{-8}$ and a 95^{th} percentile value of $2.63(10)^{-7}$. The relative magnitudes of the standard deviations in the HQ for this pathway and thus the relative degree of uncertainty in the HQ caused by varying each parameter are shown in Figure 4-11.

The Inhalation of Soil Emissions Pathway

The Hazard Quotient for this pathway demonstrated uncertainty from three variables, but only body weight significant. The scenario with all of the variables fixed gave an HQ of $3.4(10)^{-7}$. When body weight was varied while the other parameters were fixed the median HQ was calculated to be $3.43(10)^{-7}$. The 95^{th} percentile value was calculated to be $5.12(10)^{-7}$ and the standard deviation was calculated to be $8.57(10)^{-8}$.

Setting the inhalation rate equal to its probability distribution and fixing the other variables and rerunning the model resulted in a median *HQ* of $3.46(10)^{-7}$, a 95^{th} percentile value of $5.07(10)^{-7}$ and a standard deviation of $1.09(10)^{-7}$. The relative magnitudes of the standard deviations in the HQ for this exposure route and thus the relative degree of uncertainty in the HQ caused by varying each parameter are shown in figure 4-12.

The Dermal Contact with Soil Exposure Route

Uncertainty in the HQ for this exposure route was found to be caused by these variables: soil concentration, body weight, and the skin surface area of the arm and forearm. When all of these variable were set to their mean values the HQ was $3.19(10)^{-5}$.

The relative contribution of individual parameters to the uncertainty in the hazard quotient for the inhalation of soil emissions pathway.

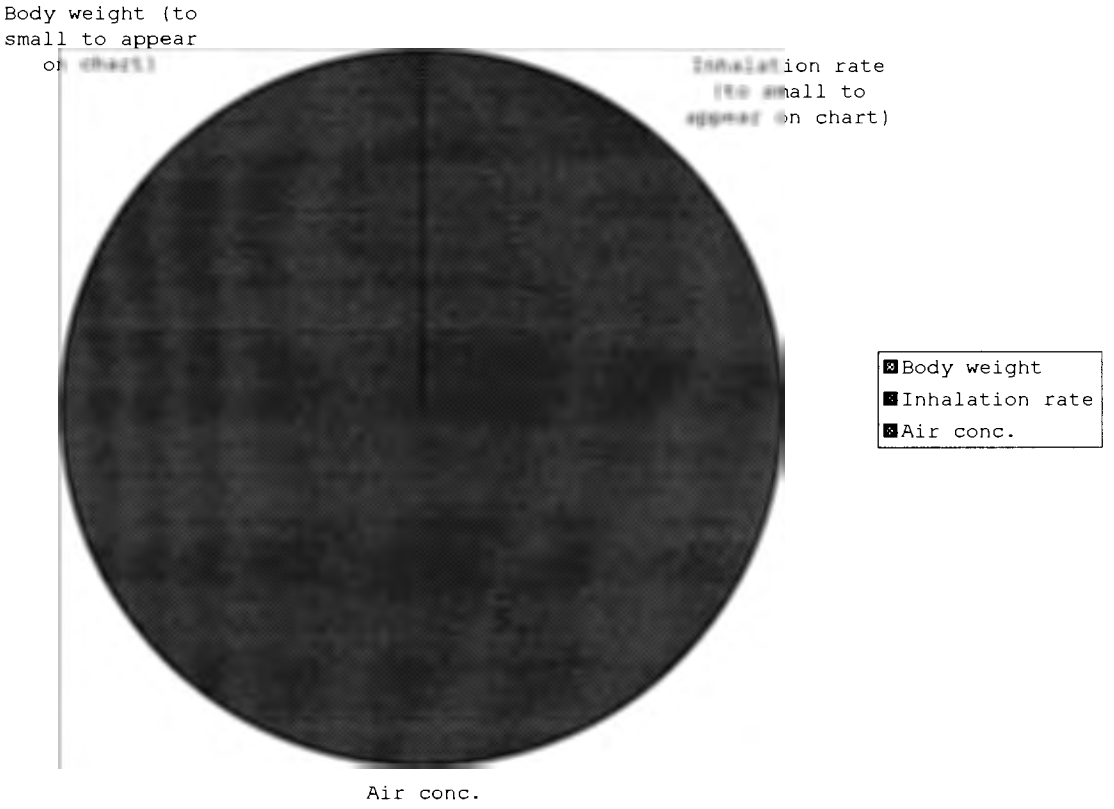


Figure 4-12

The case where pesticide concentration in soil varied yielded an HQ of $3.19(10)^{-5}$. In this case the 95th percentile value was $3.2(10)^{-5}$ and the standard deviation was $8.42(10)^{-8}$. The scenario where the skin surface area for arm and forearm was varied resulted in a median *HQ* of $4.14(10)^{-5}$, a 95th percentile value of $4.14(10)^{-5}$ and a standard deviation of $5.69(10)^{-12}$.

When body weight was varied the result was a median *HQ* of $3.22(10)^{-5}$ with a 95th percentile value of $4.81(10)^{-5}$ and a standard deviation of $8.04(10)^{-6}$. Figure 4-13 shows the relative magnitudes of the standard deviations in the HQ and thus the relative degree of uncertainty in the HQ caused by varying each parameter.

The Soil Ingestion Exposure Route

The variables that showed an effect on increasing the uncertainty in the HQ for this exposure route were: body weight, soil concentration, and soil ingestion rate. The case with all of the variables fixed resulted in an HQ of $3.11(10)^{-6}$.

The case with soil concentration varied resulted in a median HQ of $3.11(10)^{-6}$, a 95th percentile value of $3.12(10)^{-6}$, and a standard deviation of $8.53(10)^{-9}$. When the soil ingestion rate was varied with all other parameters set to

The relative contribution of individual parameters to the uncertainty in the hazard quotient for the dermal contact with soil pathway.

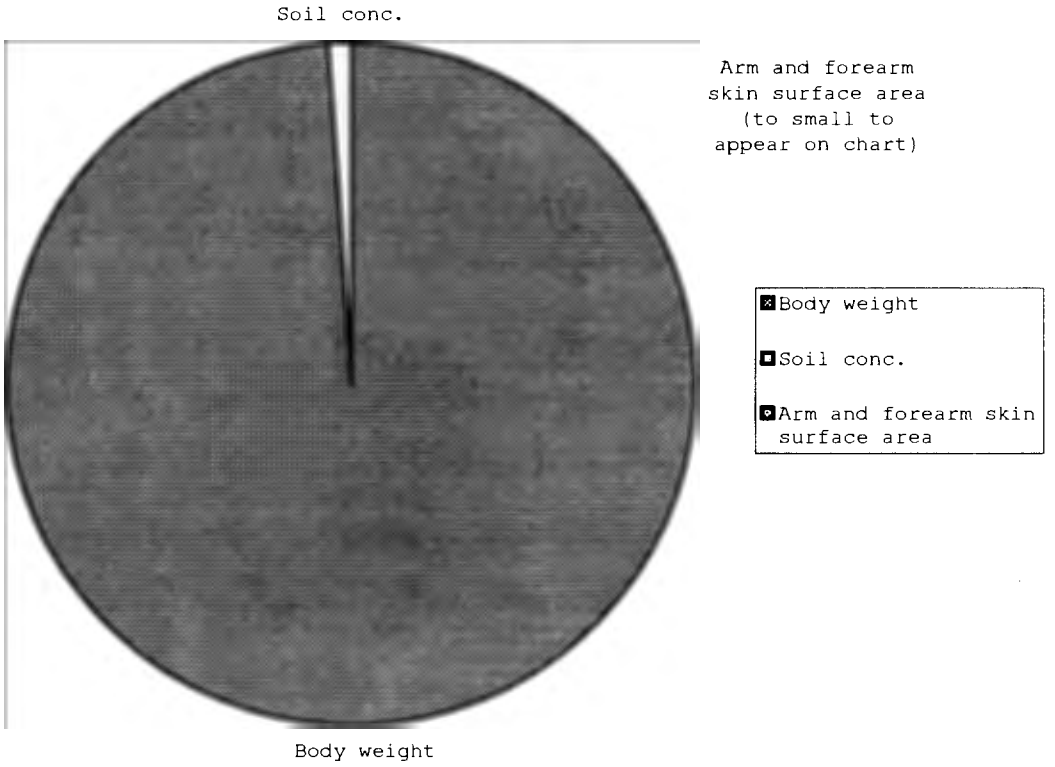


Figure 4-13

their mean values the median HQ was determined to be $4.45(10)^{-6}$, the 95^{th} percentile value was determined to be $1.11(10)^{-5}$ and the standard deviation was determined to be $3.31(10)^{-6}$. Varying the body weight provided a median HQ of $3.13(10)^{-6}$, a 95^{th} percentile value of $4.69(10)^{-6}$, and a standard deviation of $7.87(10)^{-7}$. The relative contribution of each variable to the standard deviations and thus the relative degree of uncertainty caused by that variable are shown in Figure 4-14.

Tables 4-1 and 4-2 are summaries of the results of Phase 2. Table 4-1 presents the exposure routes in decreasing order of their effect on the uncertainty in the hazard index and the individual variables that create uncertainty in the route. Table 4-2 presents the individual parameters tested in this phase of the study in decreasing order of their effect on uncertainty in the hazard index.

The relative contribution of individual parameters to the uncertainty in the hazard quotient for the soil ingestion pathway.

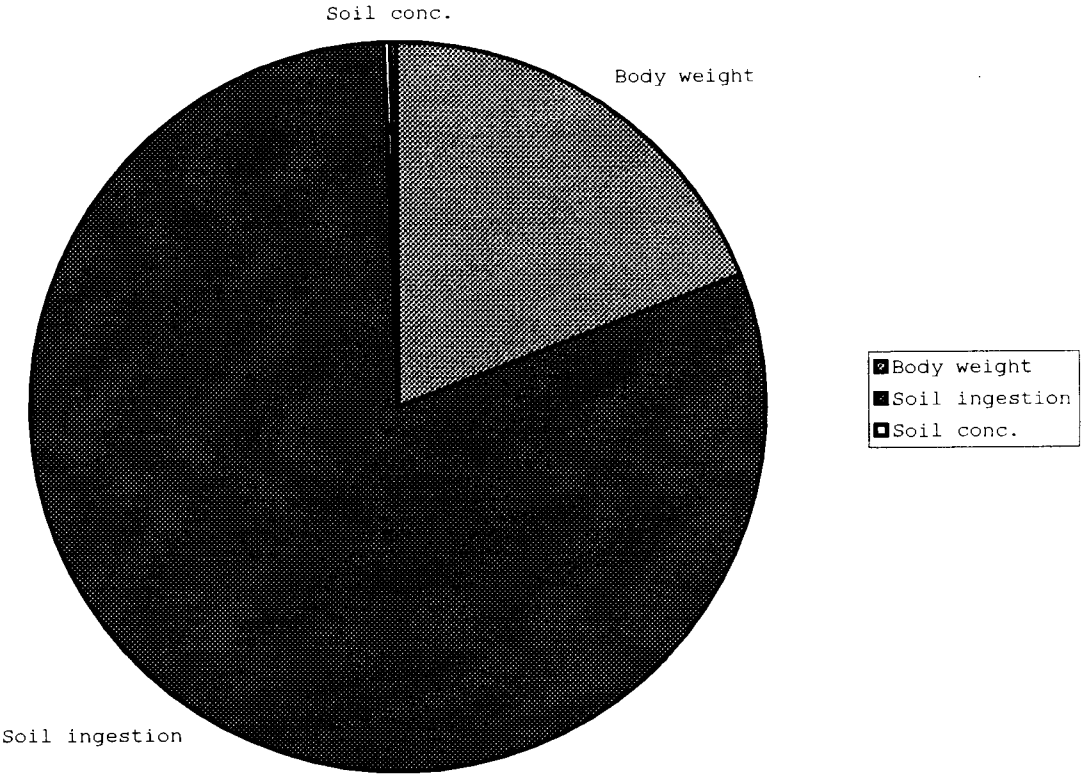


Figure 4-14

Table 4-1 Summary of results of phase 2

Exposure Routes in order of relative importance in terms of uncertainty	Hazard Quotient for exposure route	Variables tested in order of relative importance in terms of uncertainty	Standard deviation about the HQ from individual parameters
Drinking water	1.13		
		body weight	1.90E-01
		groundwater conc.	1.59E-01
		water ingestion rate	1.43E-01
Dermal uptake during shower	1.58E-02		
		time spent in shower	4.04E-03
		body weight	2.75E-03
		groundwater conc.	8.43E-04
		total skin surface area	6.32E-04
Dermal contact with soil	4.13E-05		
		body weight	8.04E-06
		soil conc.	8.42E-08
		arm and forearm skin surface area	5.69E-12
Soil ingestion	4.39E-06		
		soil ingestion rate	3.31E-06
		body weight	7.83E-07
		soil conc.	8.53E-09
Inhalation of soil emissions	3.39E-07		
		inhalation rate	1.09E-07
		body weight	8.57E-08
Inhalation during shower	2.93E-07		
		time in shower	1.84E-07
		inhalation rate	7.53E-08
		body weight	6.03E-08
		groundwater conc.	1.25E-08

Table 4-2 Summary of results of phase 2

Relative importance in terms of creating uncertainty in the HI	Sum of individual standard deviations
Body weight	1.93E-01
Groundwater conc.	1.60E-01
Water ingestion rate	1.43E-01
Time in shower	4.04E-03
Total skin surface area	6.32E-04
Soil ingestion	3.31E-06
Inhalation rate	1.84E-07
Soil conc.	9.27E-08
Arm and forearm skin surface area	5.69E-12

CHAPTER V

DISCUSSION OF RESULTS

Phase 1: Risk Assessment

This study has shown that the range of hazard indices, resulting from pesticide contamination in Caddo County, Oklahoma, can vary widely depending on the farming methods being implemented. Only a few of the cases modeled resulted in HIs greater than one. A hazard index greater that one, theoretically, means that there is potential for adverse health effects. The case with 2,4-D used on peanuts grown in a B type soil with full irrigation presented the highest hazard index: a 95^{th} percentile value of 3.58. Prowl used on cotton grown in D type soil with no irrigation presented the least hazard index; a 95^{th} percentile value of $2.09(10)^{-17}$. It should be noted that an HI of 3.58 does not mean that the hazard is 3.58 times an acceptable threshold level as the hazard does not necessarily increase linearly.

Trends in the HI due to pesticide selection

In general, cases involving 2,4-D demonstrated the highest hazard indexes particularly when peanuts were the crop grown. These were the only cases where the HI exceeded one. The next highest HI values were cases in which Furadan

was the pesticide used. The hazard index was considerably smaller for Lasso, Malathion, Treflan, and Prowl, decreasing in that order. There were no cases where Treflan or Prowl reached the water-table. This meant that exposure routes that involved contaminated ground-water were eliminated, resulting in very small hazard indexes.

Trends in the HI due to soil type

For each pesticide-crop-irrigation case the B soil type usually resulted in the highest hazard index, except for the cases involving Lasso on peanuts and Treflan on peanuts. In these cases the D soil type exhibited the highest hazard indexes. In most cases the A soil type provided the lowest HIs except for the case of 2,4-D on peanuts with no irrigation and Prowl on cotton. In these cases the D soil type resulted in the lowest HIs.

Trends in the HI due to irrigation practice

When all other things were equal irrigation practices showed mixed effects on the hazard index. In 15 of 27 different irrigation cases the irrigation practice (full or none) did not have any effect on the HI. In 7 of the 27 cases full irrigation resulted in a higher HI and in 5 of the 27 cases no irrigation resulted in a higher HI.

The minimal differences between the irrigated and non-irrigated cases may be due to the algorithm selected in the original work (Mills, 1994) to define the amount and timing of the irrigant. This algorithm used an-irrigation-on demand approach which has been shown to produce lower water use estimates than other approaches.

Trends in the HI due to crop selection

Crop selection also had mixed effects on the magnitude of the HI. In general when the same pesticide was used on more than one crop, peanuts seemed to provide the highest HIs and cotton the lowest. The low HIs resulting from cases involving cotton were due to the fact that none of the pesticides simulated reached the water table and thus eliminated those exposure routes. It was difficult to draw conclusions about the influence of crops on the hazard index. This was because there were only three cases where the same pesticide was used on different crops and even then only two different crops were involved.

What does this mean for Caddo County?

One of the questions that this study was attempting to investigate was, whether the increase in irrigation on farms

in Caddo County was likely to effect human health adversely. The results of this effort suggest that an adverse effect on humans is unlikely. However, variations in the soil type and crops grown, and pesticide used may affect the impact of pesticide use on human health depending on how they are used together in a few situations, particularly 2,4-D on peanuts.

What does this mean to other Risk Assessments?

As to what can be extrapolated from Caddo County data to other localities, if similar conditions are found (anywhere soils are well drained and similar crops with similar pesticide application rates are grown), it is probable that similar results would be noticed.

The location specific variables used in the fate and transport models, although they were attempting to reflect conditions in Caddo County and the Rush Springs aquifer, are not that different from what might be considered typical values. This is also true of the chemical intake and risk calculation variables. They could be considered typical of any location that had a "typical" cross section of the population living on the site being considered. This makes it a simple matter to see what kinds of results might be expected in other risk assessments.

Phase 2: Uncertainty Analysis

The uncertainty in the hazard index resulting from varying select exposure-related parameters is of primary interest to this phase of the study. As was mentioned earlier, the hazard index is the sum of the hazard quotients from each exposure pathway. The sources of uncertainty in the overall hazard index can be inferred by looking at sources of uncertainty in the individual hazard quotients. This is why uncertainty in the individual routes are discussed.

The Drinking Water Pathway. Examination of the outcome of the uncertainty analysis for this pathway revealed that the largest standard deviation about the hazard quotient resulted from varying body weight. This meant that body weight introduced the most uncertainty in the hazard quotient for this route. The pesticide concentration in the groundwater was the next most important variable in terms of creating uncertainty. The variable that introduced the least uncertainty for this route was the drinking water ingestion rate. These relative uncertainties can be seen in Figure 4-9.

Dermal Uptake During Shower. The analysis for uncertainty in the HQ for this pathway revealed that the time spent in the shower created the most uncertainty when it was the

parameter represented by its probability distribution found in Gephart *et al.* (1994). If it was possible to represent this variable as a fixed value the uncertainty in this pathway could be substantially reduced (from a std. dev. of 4.04(10)-3 to 2.75(10)-3 or 31.9%). The degree to which varying the other parameters effected the uncertainty in the HQ decreased in this order: body weight, groundwater concentration, and total skin surface area. The standard deviation in the HQ resulting from varying the total skin surface area was an order of magnitude less than when the time spent in shower was varied. This suggests that it was more important to narrow the range of the time spent in shower variable than the other variables affecting this route when attempting to reduce uncertainty. Figure 4-10 shows these relative uncertainties in pie chart form.

Inhalation During Shower. The variable contributing the most to the uncertainty in this pathway was again the time spent in the shower. This was apparent because it created the largest standard deviation ($1.84(10)^{-7}$) in the HQ for this pathway. The inhalation rate variable introduced the next greatest amount of uncertainty (std. dev. of $7.53(10)^{-8}$) but it was less than half of what the time spent in the shower caused. Body weight and groundwater concentration contributed substantially less to the uncertainty in the HQ

for this pathway. Figure 4-11 shows these relative uncertainties in pie chart form.

Inhalation of soil emissions. The majority of the uncertainty in the HQ for this exposure route resulted from variation in the air concentration. The standard deviation in the HQ for this route was six and seven orders of magnitude greater than inhalation rate and body weight respectively making the contribution to the uncertainty in the HQ from these two variables insignificant. To reduce the uncertainty in this route it would be necessary reduce the range of the air concentrations distribution. These results were shown in Figure 4-12

Dermal Contact with Soil. The variable that created the largest standard deviation and thus generated the most uncertainty in the HQ for this pathway was the body weight. The standard deviation arising in the hazard index when this parameter was varied was several orders of magnitude larger than when the others parameters were varied. The extremely small standard deviation created by varying the arm and forearm skin surface area ($5.69(10)^{-12}$) shows that it has almost no effect on the uncertainty of the HQ. These results were shown in Figure 4-13.

Soil Ingestion. The majority of the uncertainty in the HQ for this route came from the soil ingestion rate. This was

shown by the fact that varying this parameter resulted in the largest standard deviation about the hazard quotient. The standard deviation resulting from varying soil ingestion rate was 322.7% larger than the standard deviation resulting from varying the next largest standard deviation, which resulted from varying body weight. Varying the soil concentration resulted in the smallest standard deviation (y two orders of magnitude)which means that it introduced a relatively small amount of uncertainty. These results can be seen in Figure 4-14.

Uncertainty in the overall hazard index

By identifying the variables that create the most uncertainty in the hazard quotient it can be seen which are the most important to narrow down (measure accurately).

In this study the drinking water exposure route was the predominant source of contaminant exposure. The variable that had the largest effect on uncertainty in the drinking water route was body weight. Body weight was a factor in determining the absorbed dose for all of the exposure routes. It can therefore be reasoned that body weight is the variable that contributes the most uncertainty to the HI in this study. It is likely that any risk assessment would show substantially reduced uncertainty if the distribution

of body weights could be narrowed from the distribution published in Gephart *et al.* (1994).

Other variables in this pathway that were studied would also have a large effect on the uncertainty in the hazard index. These were groundwater concentration and groundwater ingestion rate.

The Effect of Exposure Duration on Uncertainty

It is reasonable to assume that the time one spends living or working in a contaminated area (exposure duration) would introduce some uncertainty to the HQ for each exposure route. However when dealing with non-carcinogenic compounds it is the accepted practice to set the exposure duration equal to the averaging time (U.S.EPA, 1989). This results in the cancellation of the effects of exposure duration on the chronic daily absorbed dose (CDI), thus eliminating any uncertainty that might arise from varying exposure duration. Equation 3-15 shows how the CDI was calculated for this study.

Applicability of findings to other risk assessments.

The variables that were represented by distributions taken from Gephart *et al.* (1994) should introduce a similar magnitude of uncertainty to the results of any risk

assessment depending on the exposure routes that are in effect. In another situation, where a risk assessment, is being performed, if any of the distributions can be more narrowly focused the uncertainty in the results will be reduced. For example, if another risk assessment was being performed for a job-site where only adult males were working then the distribution representing body weight could be focused to reflect the body weight of adult males. Because this study used a distribution representing the general population including women and children this would mean a substantial decrease in uncertainty.

The distributions reflecting pesticide concentrations in the groundwater and soil are specific to this study. If, in another risk assessment, the distributions are similar then that study will likely have similar uncertainties. If the range of the distributions is not as broad then it will not introduce as much uncertainty. If the distribution of concentrations is wider then more uncertainty will result.

In this study the majority of the hazard came from the drinking water route, and the other pathways had little effect in comparison. If, in other risk assessments, any pathways involving groundwater are eliminated then the other routes become more relevant and the uncertainty in them becomes more important.

One of the things that this study has shown is that the overall hazard index can go from an upperbound 95th percentile value of 3.58 for the case with all of the study variables set to their probability distributions to an upperbound 95th percentile of 0.765 when the variables were set to their mean values. This is going from a hazard index that indicates considerable potential for adverse health effects to one that shows no potential. What this says is that if the variables involved in the chemical intake modeling part of a risk assessment can be narrowed down to as close to a fixed value as possible it could be worth the extra effort. The larger the standard deviation in the hazard quotient the more sensitive the model may be to that parameter and thus the more important it is to the assessor to have accurate information when determining that particular parameter's value.

CHAPTER VI

CONCLUSIONS

Caddo County, Oklahoma has experienced an increase in irrigated agriculture as well as an increase in the use of herbicides and insecticides. This change is a result of the farmers wish for a more profitable kind of farming. Unfortunately the increased reliance on chemicals has the potential to degrade the environment and increase public health costs. A probabilistic risk assessment was conducted for "typical" farm residents in Caddo County, Oklahoma. The work was organized so as to address the effects of such farm practices as irrigation practice, soil type, and crop and pesticide selection on the amount of contaminants introduced into the unsaturated and saturated zones as well as the ambient air.

Monte Carlo simulations from a previous, related effort produced pesticide fluxes to the soils and groundwaters beneath three broad soil classifications. These classifications were based upon drainage considerations and were taken to represent all of the available soils in Caddo County. Four crops were evaluated on each of the soils selected with up to six pesticides used on the crop/soil complexes.

These data were applied in this effort as inputs to subsequent groundwater and air fate and transport models. The results from these models were applied to environmental exposure codes to define the public health risk to a typical farm family in Caddo County. As before, these analyses were completed with Monte Carlo simulation to produce probability of occurrence curves for initial contaminant concentrations at the appropriate points of exposures for these receptors and subsequently for the level of risk expected at these same locations.

Additional work was completed in order to define the relative effects of the inherent variations in the input parameters on these risk assessments. A stochastic sensitivity analysis was completed by allowing one of the critical parameters to vary over its predefined statistical range and distribution while holding the others at their mean values. In this way, the variation associated with each parameter was defined and its relative effects itemized. The following conclusions can be drawn from this effort:

Risk Assessment

- This risk assessment showed that five (5) chemical-water management- soil- crop combinations, of 39 evaluated,

proved to be potentially hazardous. Specifically, the herbicide 2,4-D when used on peanuts was found to exceed an environmental threshold level called a reference dose (RfD).

- Minimal differences were noted between the irrigated and non-irrigated systems. This may be due to the algorithm selected in the original work to define the amount and timing of the irrigant. This algorithm used an irrigation-on-demand approach which has been shown to produce lower water use estimates than other approaches.
- Conclusions about crop selection were difficult to make as the same pesticides were not always used on the same crops. However, when the same pesticides were used, peanuts usually provided the highest HQs and cotton the lowest.
- In most situations B soils resulted in higher hazard quotients than when the same case was simulated on the other soil types. D soils resulted in the lowest.

Stochastic Sensitivity Analysis

The case of 2,4-D on peanuts with full irrigation in B soils was the base case for this part of the study. The uncertainty in the HQs for individual exposure routes were examined and then their effects on the overall HI were

inferred. The exposure routes studied were: drinking water, dermal uptake during shower, inhalation during shower, inhalation of soil emissions, dermal contact with soil, and soil ingestion. · The parameters varied for this analysis included water ingestion rate, body weight, soil ingestion rate, soil concentration, inhalation rate, total skin surface area, time in shower, arm and forearm skin surface area, and groundwater concentration.

- The stochastic sensitivity analysis showed that the HI could be lowered from a 95th percentile value of 3.58 with a std. dev. of 1.11 to an HI of 0.765 when all of the variables were fixed at their mean values.
- The body weight variable had the greatest effect on uncertainty in the hazard index. This was due in part to the broad range of weights in the distribution and also because the variable occurs in the calculation of the absorbed dose for each route.
- Two of the other variables that also had a large effect on creating uncertainty were groundwater concentration and water ingestion rate.
- The least significant variable (of those tested) in terms of creating uncertainty was the arm and forearm skin surface area.

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VITA

Jon Hanson

Candidate for the Degree of

Master of Science

Thesis: A QUANTITATIVE RISK ASSESSMENT WITH ESTIMATED UNCERTAINTY FOR PESTICIDE USE IN OKLAHOMA

Major Field: Environmental Engineering

Biographical:

Personal Data: Born in Stillwater, Oklahoma, on November 21, 1969, the son of Bertil and Adelia Hanson.

Education: Graduated from Stillwater High School, Stillwater, Oklahoma in May 1988; received Bachelor of Science degree in Civil Engineering from Oklahoma State University, Stillwater, Oklahoma in December 1993. Expecting to complete the requirements for Master of Science in Environmental Engineering at Oklahoma State University, Stillwater, Oklahoma in December 1995.

Experience: Employed by Oklahoma State University as a Research Assistant to Dr. William Mcternan from October 1994 through August 1995. Acted as a Staff Engineer for HTB, inc. during summer 1993.

Professional Memberships: National Society of Professional Engineers, Oklahoma Society of Professional Engineers, American Society of Civil Engineers.