

**A QUANTITATIVE RISK ASSESSMENT WITH  
ATTENDANT UNCERTAINTY ESTIMATIONS  
FOR IRRIGATED FARMLANDS IN OKLAHOMA**

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**ABSTRACT**

Agricultural chemical use has increased dramatically in the post World War II era. Benefits to society include greater crop production and lower manpower requirements. Detriments include environmental and public health impacts. The subject research presents the results of a risk assessment which examined potential impacts of agricultural pesticide use. The two phase assessment focused in Phase 1 upon the projected risks associated with using six pesticides on four crop types within three hydrological soil groupings. Irrigation was compared with the dry land farming base case. The hypothetical target receptors were a "typical" farm family in Caddo County, Oklahoma; an area undergoing significant change from dry land farming to irrigated agriculture. Phase 2 addressed some of the uncertainties associated with the Phase 1 risk assessment. Both Phases utilized available transport and exposure codes to determine the probability of exceeding the U.S. Environmental Protection Agency's supported Reference Dose (RfD). Of the six pesticides evaluated only 2,4-D when used on peanuts presented potentially significant risk. Selection among the other variables such as other crops, the hydrologic soil groupings or the use of irrigation did not contribute consistently to this elevated risk. There was much uncertainty in these estimates. Phase 2 efforts showed that the exposure variables of receptor body weight and drinking water ingestion rate, together with the estimated pesticide concentration had the greatest impact on this uncertainty determination.

## INTRODUCTION

### Background

Increasingly the agricultural community in the United States and worldwide has become more dependent upon various chemicals to control farm pests and increase production [1]. It has been reported that over 4.5e8 kilograms of active ingredients were applied in 1991 to U.S. farms [2] representing a 100 percent increase from the previous seven years [3].

Concerns have long been expressed regarding the unintended, adverse impacts resulting from the use of these chemicals. Ecological as well as public health concerns have been cited [4]. As an example, 67,000 non-fatal pesticide poisonings were reported in 1990 [2].

Finding ways to identify and subsequently reduce the hazards associated with these chemicals has been the subject of much research [5, 6]. The problem is made more complicated by the complex interactions between these chemicals, various irrigation techniques, and other agronomic practices, different soils, and uncertainties in levels of exposure to potential human receptors. This research attempts to address some of these questions by applying fundamental risk assessment techniques to the problem of pesticide exposures at the individual farm level. In this way, the uncertainties associated with pesticide use over a range of potential environments and use practices can be addressed. A review of risk assessment in general follows.

### Risk Assessment Paradigm

As defined by the United States National Academy of Sciences and the U.S. Environmental Protection Agency, an environmental risk assessment (RA) consists of the following four elements:

- Hazard Identification;
- Dose-Response Assessment;
- Exposure Assessment; and
- Risk Characterization [7].

The Hazard Identification and Dose-Response Assessment comprise the medical or public health elements of the RA process and serve to determine if a chemical or other environmental agent is capable of inducing adverse public health effects to a potential receptor population. Chemicals can have hazardous attributes while simultaneously exhibiting minimal, adverse dose-response properties. This occurs when the chemical is poorly incorporated into the respective receptor tissues over the period of exposure. This condition results in reduced environmental risk regardless of inherent hazard or exposure to the subject chemical. These two elements combine to quantitatively identify which chemicals pose a significant hazard to exposed individuals.

The Exposure Assessment portion of a Risk Assessment involves calculation of the period of time and the types of exposures that a potential receptor population has with a chemical or other agent with adverse hazards and dose-response properties. A properly completed risk assessment includes current exposures as well as those occurring in the future. These latter calculations are much more complicated, often involving significant use of transport modeling to determine future chemical concentrations at down-gradient locations at future times.

The last element of a risk assessment is the Risk Characterization where these three elements are combined to calculate either the incremental risk of a cancer death or a comparison with a threshold concentration, which carries an inherent level of safety. These calculations are made for each chemical of concern, for each exposed population and for each potential exposure pathway.

### **Hazard Identification and Dose-Response Assessment**

As a statement of public policy in the United States chemical responses are divided into those that produce cancers and those that do not. While perhaps over-simplifying complex biomedical and pharmacological phenomena, this assumption helps establish a common basis for analysis, which in turn reduces some of the uncertainties resulting from the application of alternative and/or contradictory theories of disease causation. The agrochemicals evaluated in this effort were all considered to have non-carcinogenic effects by the U.S. Environmental Protection Agency [8]. The reference dose (RfD) and subsequently the Hazard Quotient (HQ) and the Hazard Index (HI) serve as the basis for the evaluation of these non-carcinogenic effects.

#### *Reference Doses*

The reference dose (RfD) is the U.S. EPA's preferred toxicity value for evaluating non-carcinogenic effects resulting from exposure to contaminants [7]. In order to determine a RfD value a review committee established by the agency gathers all available data examining the toxicity of a chemical. These data are evaluated for scientific merit and differences between sources are reconciled. An overall evaluation is reached and the EPA identifies the experimental exposure level representing the highest level tested at which no adverse effect is demonstrated. This highest "no-observed-adverse-effect level" (NOAEL) is the key to deriving a RfD [7]:

$$RfD = \frac{NOAEL}{UF \times MF} \quad (1)$$

where

*UF* = uncertainty factors

*MF* = modifying factor

where typical uncertainty factors (UF) include:

- Animal to human extrapolation (usually a factor of 10)
- Allowance for sensitive populations (also a factor of 10)
- Extension of subchronic data for long-term chronic exposure (also a factor of 10)
- Others as needed

Modifying Factors (MF) typically vary from 1 to 10 and reflect uncertainties in the underlying data generated during the toxicology studies.

The Reference dose is compared to the contaminant exposure by the Hazard Quotient [10]:

$$HQ_{if} = \frac{CDI_{if}}{RfD_{if}} \quad (2)$$

where

$HQ_{if}$  = hazard quotient for chemical i, exposure route j

$CDI_{if}$  = chronic daily intake for chemical i, exposure route j

$RfD_{if}$  = reference dose for chemical i, exposure route j

Finally, a Hazard Index (HI) is equal to the sum of the hazard quotients for each chemical and exposure route [7]:

$$HI = \sum HQ_{if} \quad (3)$$

Implicit in the public policy underlying the use of Reference Doses is the assumption that the HI is the threshold level of exposure below which adverse health impacts are unlikely. That is, if the calculated HI is less than 1, there is an assumed level of safety and the use of the chemical is acceptable.

## Exposure Assessment

### *Routes of Exposure*

People can be exposed to hazardous agrochemical in a variety of ways. Ingesting or bathing in contaminated water increases oral and dermal exposures. Breathing air contaminated either directly with the pesticide or indirectly with soil particles that have sorbed pesticides increases the inhalation risk. As does inhalation of pesticides volatilized from contaminated water in showers and possibly during cooking.

Pesticides that move through the environment by diffusion, mass flow, volatilization, and transport on adsorbed particles may undergo physical, chemical, and biological transformations often retain their toxic properties [6]. If these pesticides do not degrade rapidly they may come into contact with human receptors in a variety of ways. This exposure can be expressed as a Chronic Daily Intake (CDI),

which is defined as the mass of substance contacted per unit body weight per unit time [7, 9]:

$$CDI = \frac{DI \times EF \times ED}{365 \times AT} \quad (4)$$

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)

The daily intake ( $DI$ ) was the absorbed dose determined for each of the critical intake routes at the selected test site. The daily intake calculation assumes alternative functional forms depending upon the routes of exposure. Equations (5) and (6) present examples of these for oral and dermal exposures respectively.

$$DI = \frac{\beta_i \times IR \times C_w}{BW} \quad (5)$$

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)

$\beta_i$  = chemical specific bioavailability (mg/mg)

The absorbed dose was calculated as follows [9]:

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

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<sup>2</sup>/d)

$AF$  = soil to skin adherence factor (mg/cm<sup>2</sup>)

$ABS$  = fraction of chemical absorbed (mg/mg)

## Uncertainty

Environmental risk assessments inherently have significant levels of uncertainties, often as large as an order of magnitude or greater [7]. 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.

A risk assessment supplies the decision-maker not only a quantitative measure of the adverse expectation but also a determination of the variance or uncertainty in this estimate. Further, if completed properly this uncertainty estimate can supply the decision maker with a detailed description of these sources of uncertainty and their importance.

Parameter uncertainty arises from variability in the inputs used to calculate the chemical concentrations at critical receptors for current as well as for future conditions and from uncertainties in the human intake variables presented in equations such as 4-6. In order, variations in the chemical concentrations used for current use assessments result primarily from sampling and analysis errors while the corresponding variations for future conditions result from model and/or parameter uncertainties associated with the transport modeling used to predict spatially and temporally distant events.

Monte Carlo analysis and its variants have come to be the methods of choice for calculating statistical variation about an initial parameter as well as about the outputs from a stochastic model. The output from a Monte Carlo analysis results in a distribution of exposures with a corresponding probability of occurrence [8].

A Monte Carlo simulation can be described by the following:

$$C = f(x_{1..n}) \quad (7)$$

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 be defined by a statistical distribution. When equation (7) 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.

Standard deviations or other measures of statistical dispersion can be determined for the resulting cumulative density functions. Further, 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.

## RESEARCH OBJECTIVES

The objectives of the present study included the characterization and quantification of the public health risks associated with long-term exposure to select agricultural chemicals. These risk calculations were completed at the individual farm family level for a hypothetical farm in Caddo County, Oklahoma.

## SITE SELECTION

Caddo County, Oklahoma (Figure 1) was chosen for this investigation, in part, because of the significant ongoing changes seen in overall farming practices within the county. Over the last decade or longer a significant shift to an increasing use of irrigation away from dry-land winter wheat farming has been noted. While this allows for production of crops with higher profit potentials, it also offers potentially greater public health and ecological risk to affected people and ecosystems.

Over a five-year period the irrigated areas in the county have increased from about 18,000 [10] to approximately 20,000 hectares [11]. With increasing irrigation there is an increased chance of pesticides leaching to groundwater and being discharged to surface waters [5, 12]. This increased chance of ground and surface water contamination has the possibility of exposing humans to an increased risk of adverse health effects.

Caddo County is located over shallow alluvium and terrace deposits as well as the Rush Springs fresh water aquifer [13]. Within the county approximately

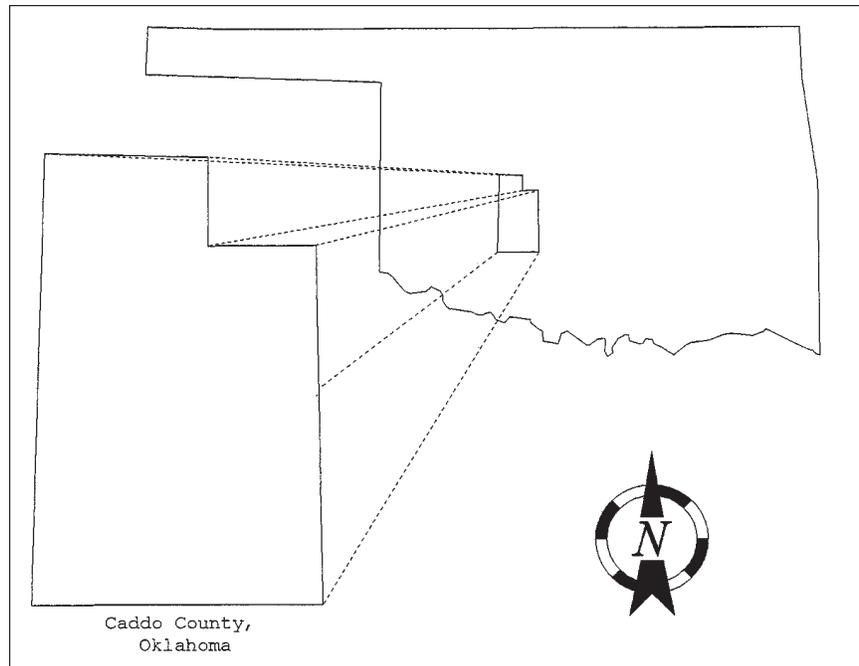


Figure 1. Research site location.

12 percent of the municipal and 91 percent of the irrigation water is derived from the groundwater reserves. Groundwater provides the majority of the water used in rural Caddo County.

Consequently the problem arises of reconciling the desire for greater profits while minimizing public health risks to those most potentially affected. Risk assessment can provide information that will lead to a more reliable understanding of the issues and uncertainties involved.

### RESEARCH STRUCTURE

A two-phase research structure was implemented in this effort where Phase 1 evaluated the risks associated with six pesticides on three soil types, for crop types and for two irrigation schemes. Figure 2 outlines this initial effort where 2,4-D, Furadan, Lasso, Malathion, Prowl, and Treflan applications onto peanuts, wheat, cotton, and alfalfa were simulated. The pesticides selected were the most frequently applied insecticide or herbicide for each crop [14] and the F or O designation in the last column of Figure 2 indicates the presence (F) or absence (O) of irrigation in the respective simulation.

Phase 2 consisted of a more detailed evaluation of the uncertainty associated with the more extreme results found during Phase 1 investigations. That is, the Phase 1 scenario that had the highest hazard index was then subjected to a detailed analysis to determine the uncertainty associated with each of the critical input variables. Figure 3 presents the general outline for the Phase 2 effort.

### METHODOLOGY

Figure 4 presents the primary routes of exposure evaluated in this effort. These included:

- drinking water;
- dermal uptake during showers;
- inhalation during showers;
- inhalation of volatile and particulate soil emissions;
- dermal contact with soil; and
- soil ingestion.

The above were chosen as they represented the primary modes of exposure found in Caddo County, Oklahoma, as well as in many mid-western U.S. farm locations.

Computer models were used to determine the chemical concentrations at each of these exposure points. The U.S. Environmental Protection Agency's PRZM-2 [15] was employed to track the pesticide from application to the top of the water table. Subsequently, the integrated codes contained in the American Petroleum Institute's Decision Support System [9] were used to route the pesticide through the aquifer to a domestic water supply well, and to quantify the various chemical

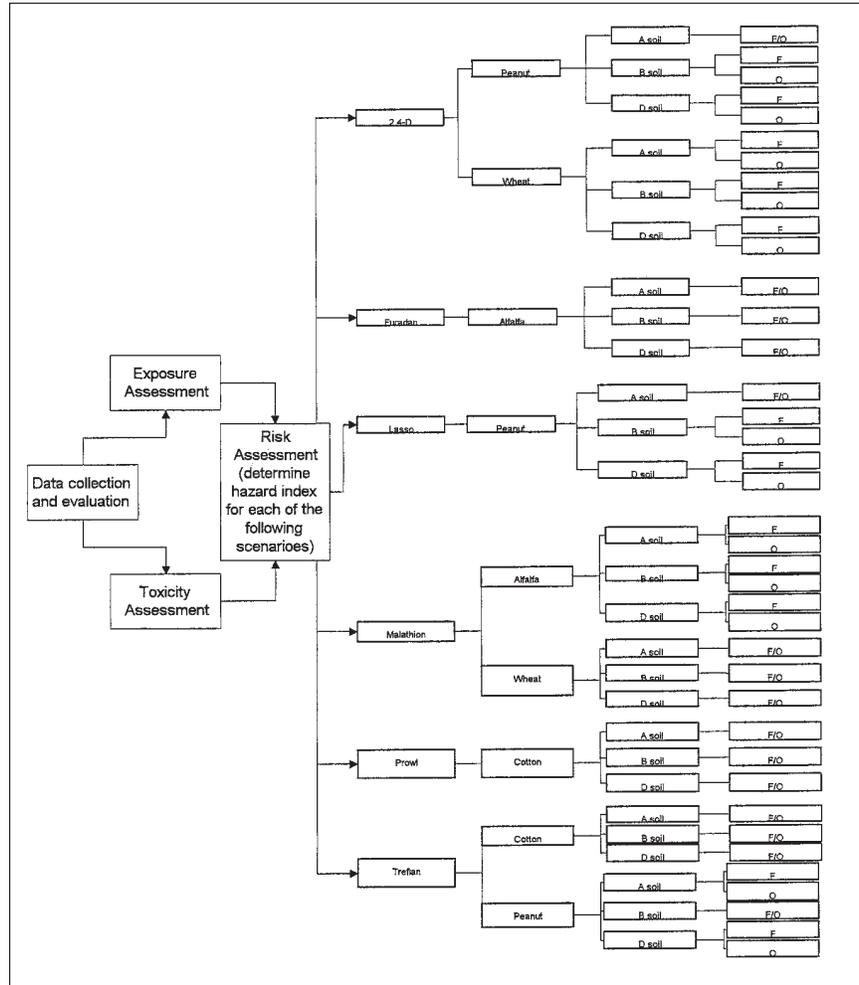


Figure 2. Summary of the steps taken completing Phase 1 of this study.

concentrations and attendant exposures associated with each of the individual pathways listed above. A brief overview of each of the models follows.

PRZM-2 is composed of extensive subroutines to model the pertinent components of the soil column; PRZM models the root zone while VADOFT simulates the vadose zone. The Monte Carlo processor allows for probabilistic estimates of pesticide loading to the top of the water table. Both PRZM and VADOFT allow simulation of multiple zones within each section. This allows PRZM-2 to

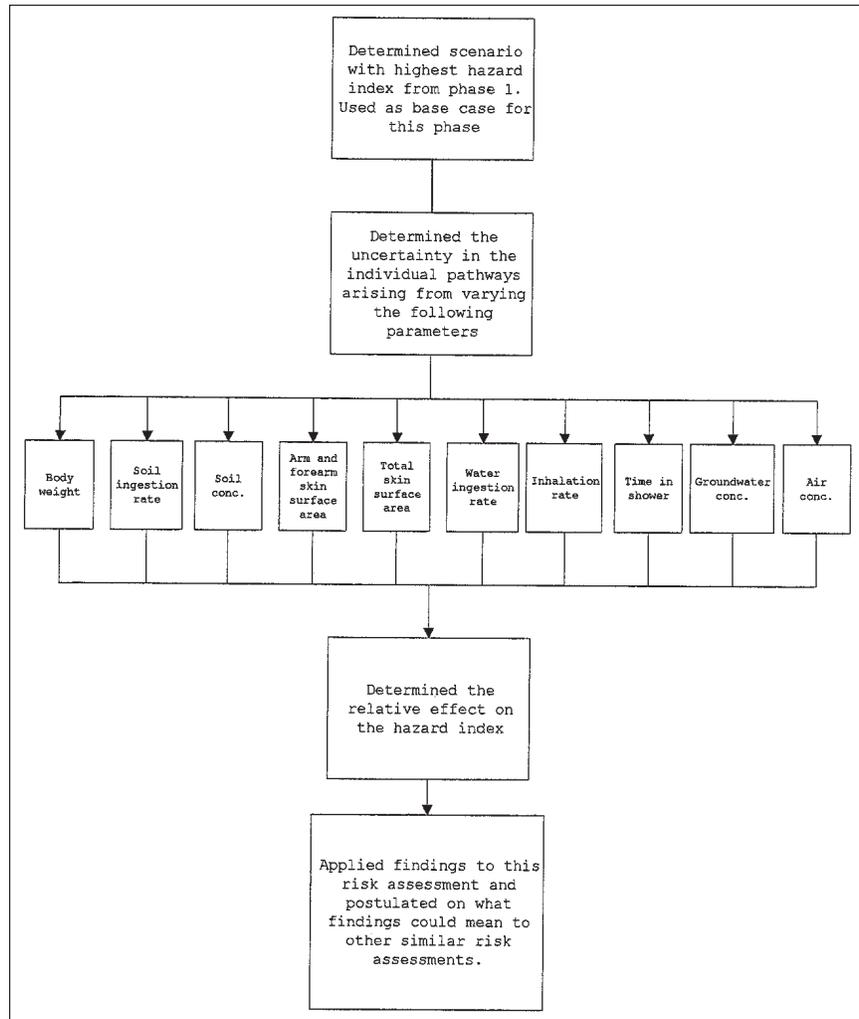


Figure 3. Summary of the steps taken completing Phase 2 of this study.

combine different root and vadose zone characteristics into a single simulation, thereby generating a more accurate representation of the complex subsurface environment encountered in an actual soil column. Equations (8) thru (10) present the generalized approach taken by PRZM-2.

Utilizing mass balance equations the surface zone expressions for the dissolved, sorbed, and vapor phases can be written as:

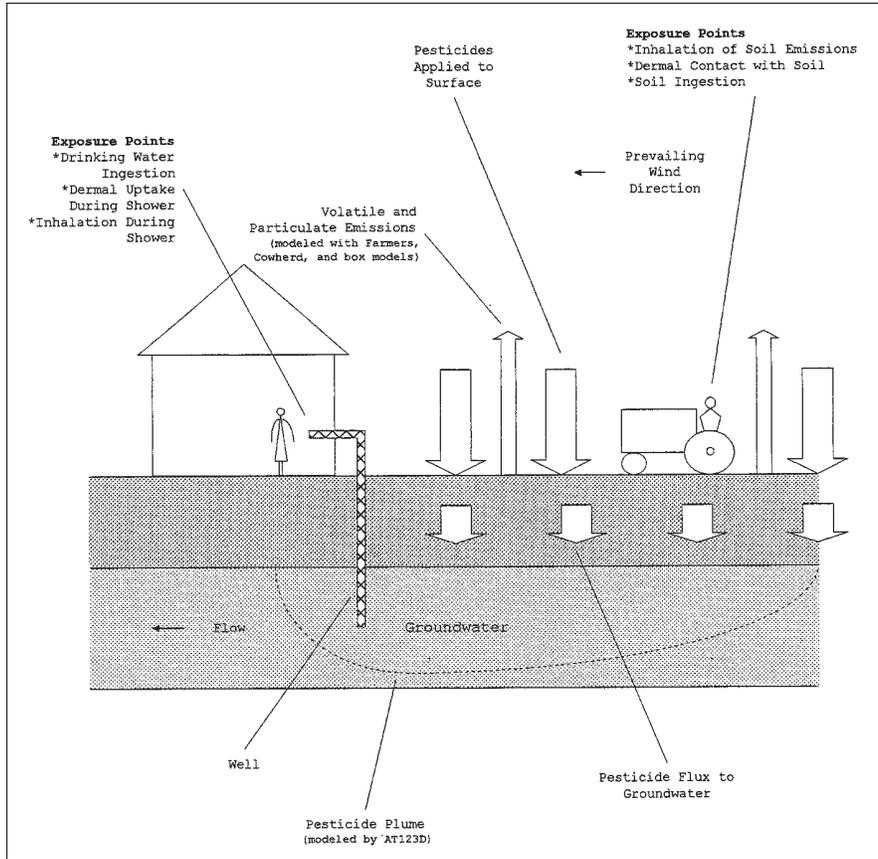


Figure 4. Pesticide exposure routes.

$$\frac{A\Delta Z\partial(C_w \Theta)}{\partial t} = J_D - J_V - J_{DW} - J_U - J_{QR} + J_{APP} + J_{FOF} + J_{TRN} \quad (8)$$

$$\frac{A\Delta Z\partial(C_s \rho_s)}{\partial t} = -J_{DS} - J_{ER} \quad (9)$$

$$\frac{A\Delta Z\partial(C_g a)}{\partial t} = -J_{GD} - J_{DG} \quad (10)$$

where:

- A = cross-sectional area of soil column (cm<sup>2</sup>)
- Δ z = depth dimension of compartment (cm)

$C_w$	=	dissolved concentration of pesticide ( $\text{g cm}^{-3}$ )
$C_s$	=	sorbed concentration of pesticide ( $\text{g g}^{-1}$ )
$C_G$	=	gaseous concentration of pesticide ( $\text{g cm}^{-3}$ )
$\theta$	=	volumetric water content of soil ( $\text{cm}^3 \text{cm}^{-3}$ )
$a$	=	volumetric air content of the soil ( $\text{cm}^3 \text{cm}^{-3}$ )
$\rho_s$	=	soil bulk density ( $\text{g cm}^{-3}$ )
$t$	=	time (d)
$J_D$	=	dissolved phase dispersion and diffusion (g/day)
$J_V$	=	dissolved phase advection in the (g/day)
$J_{GD}$	=	vapor phase dispersion and diffusion (g/day)
$J_{DW}$	=	dissolved phase degradation (g/day)
$J_{DG}$	=	vapor phase degradation (g/day)
$J_U$	=	dissolved phase plant uptake (g/day)
$J_{QR}$	=	runoff loss (g/day)
$J_{APP}$	=	soil surface deposition (g/day)
$F_{FOF}$	=	washoff from plants to soil (g/day)
$J_{DS}$	=	sorbed phase degradation (g/day)
$J_{ER}$	=	removal on eroded sediments (g/day)
$J_{TRN}$	=	gain or loss due to parent/daughter relationships (g/day)

The equations for subsurface zones are identical except for the deletion of  $J_{QR}$ ,  $J_{FOF}$ , and  $J_{ER}$ . The term  $J_{APP}$  applies to subsurface zones only when the pesticide is soil incorporated. Additionally, the term  $J_U$ , the loss rate of eroded sediments, is not utilized in subsurface layers below the root zone. A modified version of the Richard's equation is used to determine water flux from the land's surface through the various soil horizons to the top of the water table.

The soil moisture properties, field capacity, and wilting point together with bulk density and organic matter were selected as the random variables for the Monte Carlo simulation. This was consistent with previous efforts which show that the majority of the variation is expectation results from these four variables [16, 17].

Soil types included SCS hydrologic classifications A, B, and D. C type soils were excluded from analysis as very little farming was reported for these areas. Descriptive statistics for the four random variables for each of these soil types were taken from default values contained in PRZM-2, which were compiled from national data sets [15].

Pesticide flux was done by mass balance, which accounts for uptake, volatilization, leaching, and decay. The mass leached through the various soil horizons was tracked to the water table. Depth to the water table, determined from State of Oklahoma data, was found to be normally distributed with a mean and standard deviation of 13.7 and 7.8 meters respectively. The mean value was utilized for all subsequent simulations.

For this effort, the chemical fluxes simulated by PRZM-2 were used as inputs into AT123D, an analytical, saturated zone transport code described by:

$$\frac{\partial n_e C}{\partial t} = \nabla \cdot \left( n_e \bar{D} \nabla C \right) - \nabla \cdot C \bar{q} + \bar{M} - K n_e C - \lambda n_e C - \left( \frac{\partial (\rho_b C_s)}{\partial t} + \lambda \rho_b C_s \right) \quad (11)$$

where:

$\bar{q}$  = Darcy velocity vector (LT<sup>-1</sup>)

$\bar{D}$  = hydraulic dispersion coefficient tensor (L<sup>2</sup>T<sup>-1</sup>)

$C$  = dissolved concentration of the solute (ML<sup>-3</sup>)

$C_s$  = adsorbed concentration in the solid (MM<sup>-1</sup>)

$P_b$  = bulk density of the media (ML<sup>-3</sup>)

$\bar{M}$  = rate of release of source (ML<sup>-3</sup>T<sup>-1</sup>)

$n_e$  = effective porosity (L<sup>0</sup>)

$\lambda$  = radioactive decay constant (T<sup>-1</sup>) (not used)

$K$  = degradation rate (T<sup>-1</sup>) [19, 20].

AT123D, a generalized semi-analytical transient computer model for estimating the transport of wastes in groundwater systems in one, two, or three dimensions [20] was developed as 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. In all cases the data employed in this effort were either taken from existing sources or generated from typical field geometries.

### Air Concentration Modeling

Given the exposure pathways detailed in Figure 2, it was necessary to determine the contaminant concentration in the air affecting potential receptors. As before, actual measurements of these concentrations were unavailable so a modeling effort provided 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. Four approaches were used to make these estimates:

- Farmers model
- Cowherd model
- Box model
- Foster and Chrostowski Shower model

The Farmer equation models the loss/emission of contaminant from soil as a diffusion controlled process [21]. 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 (12) [9]:

$$E = 10^2 \times A \times D_e \times \frac{C_{vs} - C_a}{d} \quad (12)$$

where:

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

Similarly, the Cowherd model was employed to estimate particulate emissions [22]. The model was derived empirically and is based on field measurements gathered using a portable wind tunnel with mining soils. It estimates the emission rate of respirable soil particles, i.e., those with a diameter of 10 μm or less [9]:

$$E_{10} = 0.83 \frac{fAP(u^+)(1-V)}{\left(\frac{PE}{50}\right)^2} \quad (13)$$

where:

- $E_{10}$  = annual average emission rate of particles less than 10 μm in dia. (mg/hr)
- $f$  = frequency of disturbance per month (mo<sup>-1</sup>)
- $A$  = area of contaminated soils (m<sup>2</sup>)
- $P(u^+) = 6.7 (u^+ - u^t)$
- $u^+$  = 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 [-]

The Box model is typically used to estimate ambient concentrations of contaminants in air when the receptors are located at or near the site [9]. In order to estimate the ambient air concentration, the box model requires a contaminant emission rate that is the sum of the volatile and particulate emission rates 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 (14) presents the general form [9]:

$$C_{air} = \frac{10^3 E}{(uWH)} \quad (14)$$

where:

- $C_{air}$  = concentration of the chemical in air (mg/m<sup>3</sup>)
- $E$  = 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

Because showering involves spraying warm water through the air, volatilization of soluble chemicals can be significant. 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 Foster and Chrostowski Model simulates the volatilization of contaminants from shower air as a first order process. The fraction volatilized is given by:

$$f_v = 1 - e^{\left(\frac{-k' t}{\left(\frac{d}{6}\right)^3 3600}\right)} \tag{15}$$

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)

**Uncertainty Concerns for Exposure Assessment**

Once the fate and transport models provided point concentrations for each exposure pathway, uptake by human receptors was calculated for each pesticide. The rate of chemical intake to the body was averaged over the time of exposure and used to characterize risk. Probability distributions taken primarily from Gephart et al. were used for chemical intake and risk calculation modeling [24]. Table 6 presents the variables common to all of the analyses together with their distributions and related parameter values while Tables 1 through 7 present similar information for each of the exposure pathways selected.

Table 1. Parameters that were Common to the Configuration of All the Chemical Intake and Risk Calculation Models

Variables common to all exposure models	Units	Dist.	Mean	Std. Dev.	Min	Max	Source
Average weight	kg	Normal	64.2	13.19	7	107	[24]
Lifespan	yr	Constant	70	—	—	—	[9]
Exposure frequency	d/hr	Constant	350	—	—	—	[9]
Exposure duration	yr	Exponential	17.73	17.79	0	60	Calculated

Table 2. Parameters Used to Configure the Drinking Water Intake Model

Drinking Water Intake Model	Units	Dist.	Mean	Std. Dev.	Min	Max	Source
Exposure frequency	d/yr	Constant	350	—	—	—	[9]
Exposure duration	yr	Exponential	17.7	17.79	0	60	[24]
Ingestion rate	l/d	Normal	1.53	0.298	0.4	2.2	[24]

Table 3. Parameters for Configuring the Inhalation During Shower Model

Inhalation During Shower Model	Units	Dist.	Mean	Std. Dev.	Min	Max	Source
Exposure frequency	d/yr	Constant	350	—	—	—	[9]
Exposure duration	yr	Exponential	17.73	17.79	0	60	[24]
Inhalation rate	m <sup>3</sup> /hr	Uniform	0	0	0.21	0.74	[24]
Time in shower	hr/d	Normal	0.15	0.061	0.017	0.333	[24]
Fraction volatilized	hr/d	Constant	—	—	—	—	Calculated

Table 4. Parameters Used to Configure the Dermal Intake During Shower Model

Dermal Intake During Shower Model	Units	Dist.	Mean	Std. Dev.	Min	Max	Source
Exposure frequency	d/yr	Constant	350	—	—	—	[9]
Exposure duration	yr	Exponential	17.73	17.79	0	60	[24]
Total skin surface area	cm <sup>2</sup>	Normal	17000	1000	14000	23000	[24]
Time in shower	hr/d	Normal	0.15	0.06	0.017	0.333	[24]

Table 5. Parameters Used to Configure the Ingestion of Soil Model

Ingestion of Soil Model	Units	Dist.	Mean	Std. Dev.	Min	Max	Source
Exposure frequency	d/yr	Constant	350	—	—	—	[9]
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	—	—	—	—	[9]

Table 6. Parameters Used to Configure the Dermal Contact with Soil Model

Dermal Contact with Soil Model	Units	Dist.	Mean	Std. Dev.	Min	Max	Source
Exposure frequency	d/yr	Constant	350	—	—	—	[9]
Exposure duration	yr	Exponential	17.73	17.79	0	60	[24]
Skin surface area	cm <sup>2</sup>	Triangular	3120	68.57	0	216	[24]
Adherence factor	mg/cm <sup>2</sup>	Constant	0.6	—	—	—	[9]
Fraction of chemical absorbed	mg/mg	Constant	0.25	—	—	—	[26]

Table 7. Parameters Used to Configure the Inhalation of Soil Emissions Model

Inhalation of Soil Emissions	Units	Dist.	Mean	Std. Dev.	Min	Max	Source
Exposure frequency	d/yr	Constant	350	—	—	—	[9]
Exposure duration	yr	Exponential	17.73	17.79	0	60	[24]
Inhalation rate	m <sup>3</sup> /hr	Uniform	0	0	0.21	0.74	[24]
Time outdoors	hr/d	Constant	3	—	—	—	[9]

## RESULTS

### Phase 1 Modeling

With the exception of 2,4-D, none of the pesticides simulated produced adverse public health concerns. The Hazard Indexes (HI) for each of the other five pesticides were considerably under 1, indicating a measure of safety for the exposed populations. 2,4-D however, exhibited more toxic behavior when used on B soils, for peanuts and was selected for Phase 2 uncertainty analyses. Figures 5 and 6 summarize these Phase 1 results. When used on other crops or when other chemicals were used on peanuts, little toxic concern was modeled. Similarly, irrigation appeared to add no additional risk when evaluated for all of the chemicals, crops, and soils. On the basis of this study, the shift to irrigated agriculture in Caddo County, Oklahoma, should have little relative impact on the incremental risk associated with pesticide use when viewed at the local farm level.

### Phase 2 Modeling

Figure 7 presents the simulation results for the 2,4-D application scenarios. This figure presents the median as well as the 95 percent upper bound response for each condition modeled. Significant variation or uncertainty exists in these data where median response for the peanut crop lies around the critical 1.0 value. The 95%UB however, varies from about 2.1 to over 3.5. Additional investigation was warranted to identify the source or sources of this uncertainty. This evaluation was completed for each exposure pathway where the variable of interest was represented by its probability distribution while other model inputs were held constant. It is important to note that the variables that were studied here were variables that had published probability distributions [24]. Other variables that were not tested are also capable of introducing uncertainty.

Table 8 presents the Phase 2 results for the following exposure pathways in order of decreasing relative importance to overall uncertainty:

- Drinking water ingestion
- Dermal uptake during showering
- Dermal contact with soil
- Soil ingestion
- Inhalation of soil emissions
- Inhalation during showering

This table includes the HQ, which would result solely from the respective exposure route, the variables that impacted the HQ calculation, and the standard deviation introduced by variations in the individual parameter.

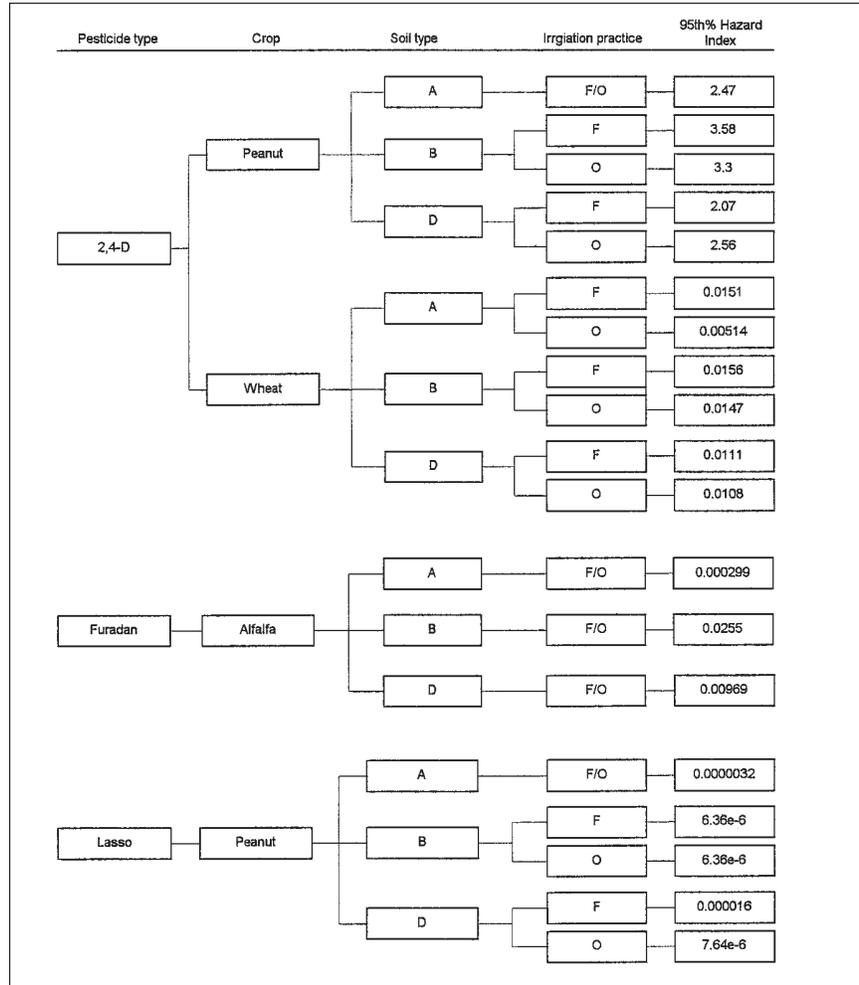


Figure 5. Summary of results of Phase 1.

The relative importance of each of these variables to the entire HQ is included in Table 9. These data show that variations in receptor body weight, the pesticide concentration in the groundwater, and the ingestion rate contribute the most uncertainty to the assessment. In terms of improving the quality of our Risk Assessments, this is relatively positive in that both body weight and ingestion rate can be measured precisely which should lower uncertainty. Concentrations in the groundwater, particularly for future conditions for which no measurements are possible, would remain a significant source of uncertainty, however.

Pesticide type	Crop	Soil type	Irrigation practice	95th% Hazard Index
Malathion	Alfalfa	A soil	F	2.17e-8
			O	2.4e-8
		B soil	F	2.27e-6
			O	2.46e-6
		D soil	F	5.69e-7
			O	5.94e-7
	Wheat	A soil	F/O	1.42e-9
		B soil	F/O	7.53e-7
		D soil	F/O	2.47e-7
Prowl	Cotton	A soil	F/O	1.26e-14
		B soil	F/O	7.78e-12
		D soil	F/O	2.09e-17
Treflan	Cotton	A soil	F/O	8.05e-7
		B soil	F/O	1.71e-6
		D soil	F/O	4.35e-13
	Peanut	A soil	F	1.6e-9
			O	2.01e-9
		B soil	F/O	1.67e-10
		D soil	F	2.32e-6
			O	2.19e-6

Figure 6. Summary of results of Phase 1 (continued).

## DISCUSSION

### 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 than one, theoretically, means that there is potential for adverse health effects. The case with 2,4-D used on peanuts

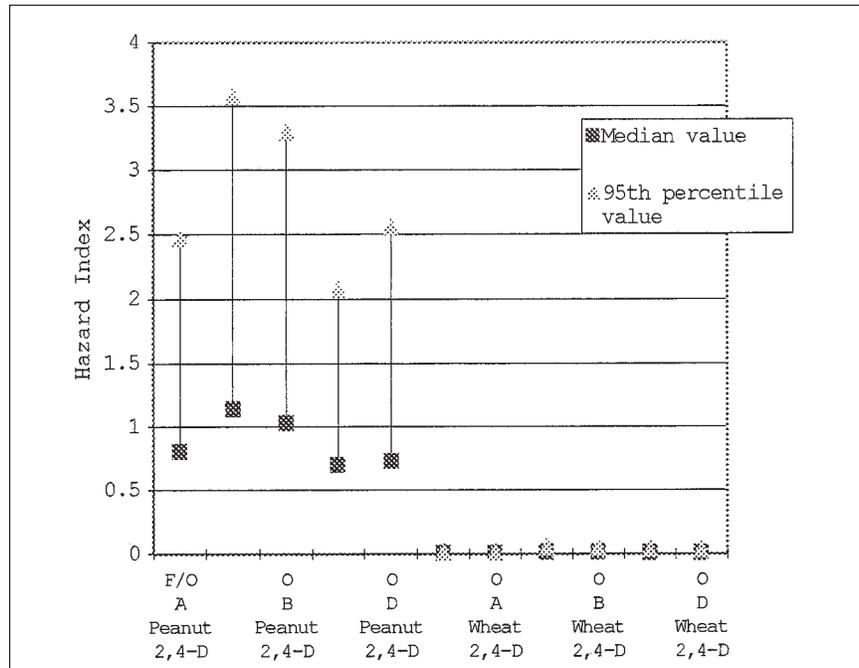


Figure 7. Hazard indexes for cases involving 2,4-D.

grown in a B type soil with full irrigation presented the highest hazard index: a 95th percentile value of 3.58. All other pesticides simulated displayed HIs far less than 1.0. It should be noted that a 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 Soil Type*

Generally the B soil type resulted in the highest hazard index, except for the cases involving Lasso 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*

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

Table 8. Summary of Results of Phase 2 Modeling

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 concentration	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 concentration	8.43E-04
		Total skin surface area	6.32E-04
Dermal contact with soil	4.13E-05	Body weight	8.04E-06
		Soil concentration	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 concentration	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 concentration	1.25E-08

effect on the HI. In seven of the 27 cases full irrigation resulted in a higher HI and in five 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 to define the amount and timing of this irrigant [25]. 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

Table 9. 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 concentration	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 concentration	9.27E-08
Arm and forearm skin surface area	5.69E-12

provide the highest HIs and cotton the lowest where the pesticides seldom reached the water table and thus eliminated those exposure routes.

## Phase 2: Uncertainty Analysis

The uncertainty in the hazard index resulting from varying select exposure-related parameters is of primary interest to this study. 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 was presented.

In general, variables that create the most uncertainty in the hazard quotient are the most important to 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, which was employed 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 [24]. Similarly better estimates of groundwater concentration and drinking water ingestion rate could also have a significant impact in reducing uncertainty.

## CONCLUSIONS

The following conclusions can be drawn from this effort:

### Risk Assessment

- This risk assessment showed that five 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 irritant.
- Conclusions regarding 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. This was expected as B soils are characterized by higher sand fractions than are the others which should allow greater pesticide leaching rates than would the soils high in clay with low permeability.

### Stochastic Sensitivity Analysis

The case of 2,4-D on peanuts with full irrigation in B soils was the base case for this phase of the study. The uncertainties in the HQs for individual exposure routes were examined and then the 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 following conclusions were drawn:

- The stochastic sensitivity analysis showed that the HI could be lowered from a 95th percentile value of 3.58 with a standard deviation 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 exposure route.
- Two of the other variables that also had a large effect on creating uncertainty were groundwater concentration and drinking 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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