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## Development and Evaluation of State-Specific Landscape Data Sets for Multimedia Source-to-Dose Models

Thomas E. McKone, Agnes B. Bodnar,  
and Edgar G. Hertwich

**Environmental Energy  
Technologies Division**

July 2001



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# Development and Evaluation of State-Specific Landscape Data Sets for Multimedia Source-to-Dose Models

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## ABSTRACT

The specific aims of this study are (i) to develop for the CalTOX multimedia exposure model landscape data sets for each state in and several regions of the US and (ii) use these data sets to explore the regional variation of risk screening calculations. We develop and evaluate forty-eight state-specific and nine region-specific landscape data sets for use in calculating toxic equivalency potentials (TEPs). TEPs address the information needs of risk management actions that require the comparison and aggregation of releases of several chemicals to a number of environmental compartments. We use state- and region-specific landscape data sets to calculate TEPs for releases to both air and water among a large set of chemically hazardous agents. We compare the TEPs calculated among states having significantly different landscape properties. The purpose of this exercise is to evaluate the extent to which TEPs will vary when applied in different US states or geographic regions. This exercise is also used to explore the premise that a single default US landscape data set is sufficient for making many kinds of LCIA classification. 278 chemicals are used in the analysis. Of these, 230 are on the TRI list, 123 have carcinogen potencies, and 244 have non-cancer allowable daily intakes. The results of the comparison suggest that TEPs can be reliably derived with a single default US landscape data set. As a result, state-specific TEP values may not be needed for assessments within the conterminous US.

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## 1.0 Introduction

The purpose of this report is to develop and evaluate forty-eight state-specific and nine region-specific landscape data sets for use in calculating toxic equivalency potentials (TEPs). TEPs address the information needs of risk management actions that require the comparison and aggregation of releases of several chemicals to a number of environmental compartments (Hertwich et al., 1998). These releases require assessments that are intermediate between simple hazard ranking and a detailed, site-specific chemical risk assessment. Whereas simple hazard ranking is used to prioritize between environmental chemicals or hazardous waste sites and usually produces an ordinal evaluation (Davis et al. 1994), risk assessments often involve highly detailed site-specific analyses. The main uses for equivalency potentials are in the evaluation of the US Environmental Protection Agency's (EPA) Toxics Release Inventory (TRI), in Design-For-Environment (DfE), and in Life-Cycle Impact Assessment (LCIA). They require cardinal measures of hazard to weight mass releases but do not allow for a full-scale risk assessment because a site-specific evaluation is either too expensive or a characterization of the release sites is not available.

### 1.1. Life-Cycle Impact Assessment and Exposure Modeling

LCIA practice involves development of cumulative impact indicators of that are derived using mass release data and chemical-specific "equivalency factors." Equivalency factors normalize a chemical's hazard by comparison with a benchmark carcinogen or non-carcinogen chemical. Until recently, these factors have generally been based primarily on toxicity measures (e.g., weighting releases by relative carcinogenic potency) and have not incorporated chemical-specific variations in exposure potential attributable to differences in fate and transport in the environment. Hertwich et al. (1998) and Pease et al. (1998) have shown the importance of including both toxicity factors and exposure potential in the LCIA analysis.

Pease et al. (1998) have developed human toxicity potentials for 278 chemicals including 230 compounds or groups of compounds contained in the TRI. These TEPs have been used in *The Chemical Scorecard* (hereafter referred to as *Scorecard*) calculations (EDF, 1998) and a revised and expanded set of TEPs of this sort are being considered for use in the EPA TRACI program (Bare, et al., 1998). Currently, TEP calculations carried out at UC Berkeley rely on the proposal for a human toxicity potential (HTP) by Guinee and Heijungs (1993). But in contrast to Guinee and Heijungs, we distinguish between cancer and non-cancer effects (Hertwich et al., 1998; Pease et al., 1998). The human toxicity potential presents evaluations of hazard based on the toxic potency of a substance and the exposure in a so-called unit world. The toxic potency is expressed by cancer potency factors  $q1^*$  or the inverse of the allowable daily intake or reference dose. The exposure potential is calculated using CalTOX (McKone 1993a, 1993b, 1993c; Maddalena et al. 1995), a multimedia risk assessment



model that integrates a multimedia environmental fate model with a multiple pathway exposure model. This type of HTP comes significantly closer to an actual risk assessment than alternative approaches without requiring site-specific input data (Hertwich, al. 1998).

TEPs developed by Hertwich et al. (1998) and Pease et al. (1998) were based on a set of landscape data developed for the state of California to be used as default values in the CalTOX model (Schwalen et al., 1995). A mean value and coefficient of variation (CV) were characterized for each landscape parameter based on geographical variations of these parameters within California. This raises the question whether TEP values are sensitive to selection of California as the default landscape. It also raises the additional question of how TEPs would change if some other state were used as the default state for the landscape parameters. Moreover, there is the further issue of whether a national default set of landscape parameters should be used for TEP calculations. Insight on the sensitivity of CalTOX to landscape data has been reported by Eisenberg and McKone (1998) who carried out simulations with CalTOX for 75 chemicals placed in soil. Their simulation studies suggest that chemical properties define the broad structure of the potential for chemical exposure. The variance of the landscape and exposure properties in most cases did not alter exposure rankings among chemicals. Nevertheless, the extent to which the Eisenberg and McKone (1998) observations applies the LCIA for air and water emissions has not been explored.

### 1.2 The Aims of This Study

The purpose of this document is to report collect, summarize, and evaluate landscape data from derived from multiple data references. This is done to provide regional-scale information for use in characterizing landscapes in multiple regions of the United States. The specific aims of this study are to develop for the CalTOX multimedia exposure model landscape data sets for each state in the US. With these landscape data sets, we calculate TEPs for releases to both air and water among a large set of chemically hazardous agents. We compare the TEPs calculated among states having significantly different landscape properties. The purpose of this exercise is to evaluate the extent to which TEPs will vary when applied in different US states or geographic regions. This exercise is also used to explore the premise that a single default US landscape data set is sufficient for making many kinds of LCIA classifications. We used 278 chemicals in this analysis. Of these, 230 are on the TRI list, 123 have carcinogen potencies, and 244 have non-cancer allowable daily intakes.

### 1.3 Overview of this Report

The remainder of this report is organized into four section. In Section 2, we provide a brief overview of and key citations for the CalTOX model, summarize the types of landscape data used by CalTOX, and describe how CalTOX is applied to LCIA. In

Section 3, we explain the databases and data sources we obtained for our analysis and how the data sets were used to develop state- and region-specific landscape parameters. In Section 4, we present the results of the data collection process and an evaluation of the state and regional variations observed in these new data sets. Finally, in Section 5, we provide an evaluation of how the state- and region-specific data is likely to alter existing rankings for the chemicals in the *Scorecard* system.

## 2.0 The CalTOX Model

The modeling components of CalTOX include a multimedia transport and transformation model, exposure scenario models, and add-ins to quantify uncertainty and variability (McKone, 1993a). CalTOX facilitates examining the impact of chemical and landscape properties on both the dominant routes of exposure and the total potential dose of a toxicant (McKone, 1993, Hertwich, et al., 1998). The equations of the CalTOX model contain over one hundred variables. Developing values for these variables in the CalTOX model requires three sets of data—chemical properties data, landscape data, and exposure factors data. The types of landscape data needed include meteorological data (average annual wind speed, deposition velocities, air temperature, and depth of the mixing layer), hydrological data (annual rainfall, runoff, soil infiltration, ground-water recharge, surface water depth and sediment loads), and soil properties (bulk density, porosity, water content, and root-zone depth). Table 1 lists the landscape parameters for which input values are needed to run CalTOX. Both a mean value and coefficient of variation (CV) are required for each input. These are required to be yearly-averaged data over a relatively large region. Uncertainty and sensitivity analyses have shown that the CalTOX risk calculations are less sensitive to landscape properties than chemical properties (Maddalena et al. 1995; Eisenberg and McKone, 1998).

The CalTOX model computes a risk factor by relating the concentration of a chemical in environmental media with the daily dose a person would receive through inhalation, ingestion and dermal exposure routes (McKone, 1993c). CalTOX is a spreadsheet-based model used to assist in health-risk assessments and soil remediation clean-up goals. The model includes three components--a multimedia transport and transformation model, an exposure scenario model, an output uncertainty and sensitivity analyses component. The multimedia transport and transformation model is a dynamic model that can be used to assess time-varying concentrations of contaminants. Source terms are constructed as either previously contaminated soil layers or as continuous releases to air, surface soil, or water. This model assists the user in examining how chemical and landscape properties impact both the ultimate route and quantity of human contact.

Table 1. Summary of the Landscape Parameters Used in the CalTOX Model.

Landscape properties	Symbol
Contaminated area in m <sup>2</sup>	Area
Annual average precipitation (m/d)	rain
Flux: surface water into landscape (m/d)	inflow
Land surface runoff (m/d)	runoff
Atmospheric dust load (kg/m <sup>3</sup> )	rhob_a
Deposition velocity of air particles (m/d)	v_d
Plant dry mass inventory (kg[DM]/m <sup>2</sup> )	bio_inv
Plant dry-mass fraction	bio_dm
Plant fresh-mass density kg/m <sup>3</sup>	rho_p
Ground-water recharge (m/d)	recharge
Evaporation of water from surface water (m/d)	evaporate
Thickness of the ground soil layer (m)	d_g
Soil particle density (kg/m <sup>3</sup> )	rhos_s
Water content in surface soil (volume fraction)	beta_g
Air content in the surface soil (volume fraction)	alpha_g
Erosion of surface soil (kg/m <sup>2</sup> -d)	erosion_g
Thickness of the root-zone soil (m)	d_s
Water content of root-zone soil (volume fraction)	beta_s
Air content of root-zone soil (volume fraction)	alpha_s
Thickness of the vadose-zone soil (m)	d_v
Water content: vadose-zone soil (volume fraction.)	beta_v
Air content of vadose-zone soil (volume fraction.)	alpha_v
Thickness of the aquifer layer (m)	d_q
Solid material density in aquifer (kg/m <sup>3</sup> )	rhos_q
Porosity of the aquifer zone	beta_q
Fraction of land area in surface water	f_arw
Average depth of surface waters (m)	d_w
Suspended sediment in surface water (kg/m <sup>3</sup> )	rhob_w
Suspended sediment deposition (kg/m <sup>2</sup> /d)	deposit
Thickness of the sediment layer (m)	d_d
Solid material density in sediment (kg/m <sup>3</sup> )	rhos_d
Porosity of the sediment zone	beta_d
Sediment burial rate (m/d)	bury_d
Ambient environmental temperature (K)	Temp
Surface water current in m/d	current_w
Organic carbon fraction in upper soil zone	foc_s
Organic carbon fraction in vadose-zone	foc_v
Organic carbon fraction in aquifer zone	foc_q
Organic carbon fraction in sediments	foc_d
Boundary layer thickness in air above soil (m)	del_ag
Yearly average wind speed (m/d)	v_w

Multimedia, multiple pathway exposure calculations are used in CalTOX to estimate average daily doses to a human population accruing from twenty-three exposure pathways. The exposure assessment process consists of relating contaminant concentrations in the multimedia model compartments to contaminant concentrations in the media with which a human population has contact (e.g., personal air, tap water, foods). Figure 1 provides a schematic diagram of the CalTOX calculations. Exposure models and model parameters used in CalTOX are based on those described by the U.S. EPA (USEPA, 1989, 1992, 1997) and by the California Department of Toxic Substances Control (DTSC; 1992a, 1992b). The model algorithms in CalTOX have been reviewed extensively by reviewers inside and outside of Cal-EPA for consistency with current scientific literature and with values used by other regulatory agencies such as the U.S. EPA.

CalTOX has been selected for calculation of TEPs because it is the only currently available multimedia fate model that is fully linked with a multipathway exposure assessment and has the capability for carrying out extensive sensitivity analyses and uncertainty analyses. CalTOX has been reviewed by the Science Advisory Board Integrated Human Exposure Committee and was described as “potentially the most advanced of all of the models reviewed” (USEPA SAB, 1997).

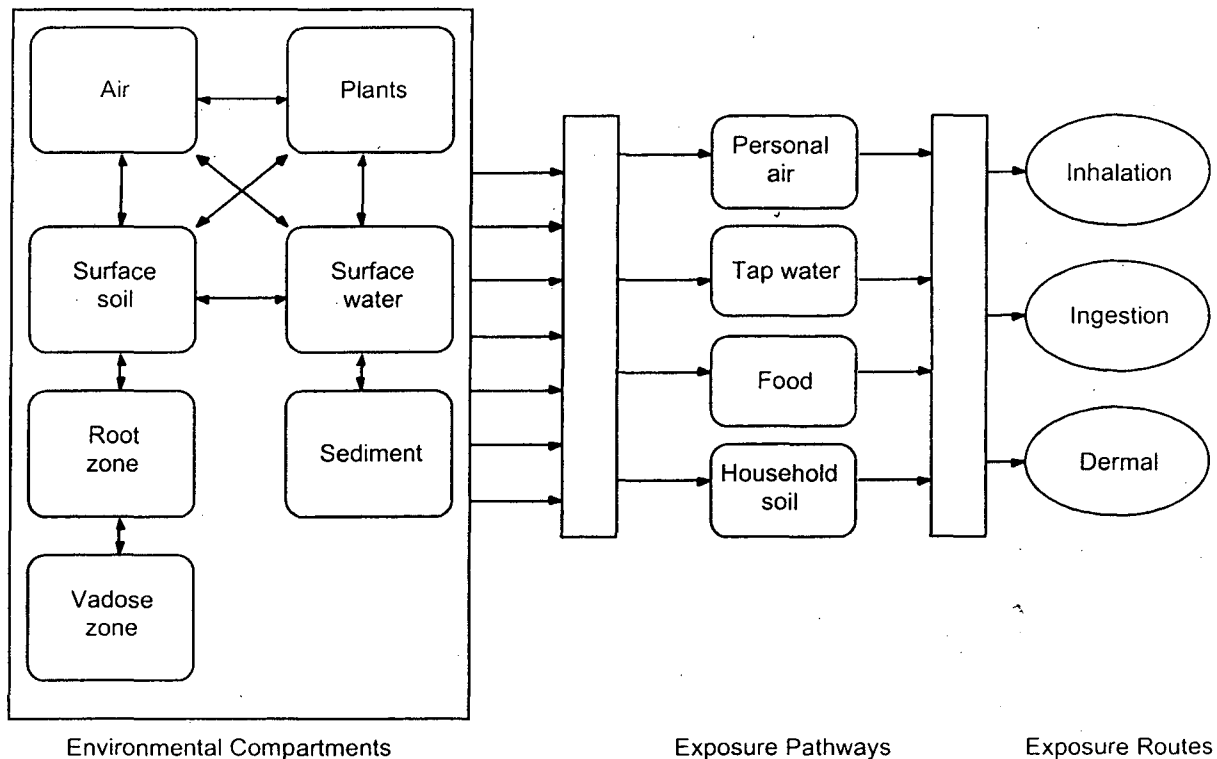


Figure 1. Schematic diagram of the CalTOX exposure/risk calculation framework.

## 3.0 Approach and Methods

Two techniques were used to generate region and state-specific value ranges for landscape variables in CalTOX. The first technique utilizes existing tabular data from a variety of printed reports to develop the mean and CV for those variables. The second technique utilizes data from existing geographic information systems (GIS) to develop a mean and CV for some variables. The criteria for selecting one method over the other was based on the availability of suitable data. If no GIS database was readily available, then the tabular method was used.

### 3.1 Available Data Sources

Landscape summary data sets for the conterminous United States were generated from several sources. The principal data sources include the US Statistical Abstract (US Bureau of Census, 1997), National Climate Data Center- National Oceanic and Atmospheric Administration (NCDC-NOAA) Internet resources (NOAA, 1998), the US EPA Pesticide Assessment Tool for Rating Investigations of Transport (PATRIOT) system (Imhoff, et al, 1994), the US Department of Agriculture Agricultural Resource Service (USDA/ARS) soil properties assessment tools on the Internet (USDA, 1998), and the *Water Encyclopedia* (van der Leeden, 1991).

Table 2 provides a list of the CalTOX parameters from Table 1 for which region- and state-specific landscape parameters are developed in this report. Also listed in Table 2 are the primary data set reference use to determine a value range for the parameters. Table 3 lists the landscape parameters in CalTOX as listed in Table 1 for which existing default parameter value ranges are retained. There are no new values considered here for these parameters and the mean and coefficient of variation (CV) listed in Table 3 for these parameters are those developed for the CalTOX 2.2 and CalTOX 2.3 data files. These value ranges have been developed either by Schwalen et al (1995) or were developed for the original CalTOX documentation (McKone, 1993b). In order to obtain state- and region-specific values for parameters in Table 2, the forty-eight conterminous states of the United States were grouped into 9 regions as shown in Table 4. These groupings are also illustrated in Figure 2. These groupings follow those used in the US Statistical Abstract (US Bureau of Census, 1997).

Table 2. Landscape Parameters in CalTOX (Table 1) for which State and Region-Specific Values have been Developed in this Report.

Landscape Variable	Symbol	Primary Reference
Landscape area in m <sup>2</sup>	<i>Area</i>	Statistical Abstracts of the US, Bureau of Census (1997)
Annual average precipitation (m/d)	<i>rain</i>	NOAA (1998)
Land surface runoff (m/d)	<i>runoff</i>	van der Leeden (1991, p 70, Table 2-18)
Plant dry mass inventory (kg[DM]/m <sup>2</sup> )	<i>bio_inv</i>	Layton, et al. (1986)
Ground-water recharge (m/d)	<i>recharge</i>	Layton, et al. (1986)
Evaporation of water from surface water (m/d)	<i>evaporate</i>	van der Leeden (1991, p 94, Table 2-48)
Water content in surface soil (volume fraction)	<i>beta_g</i>	PATRIOT (Imhoff, et al, 1994) USDA (1998)
Air content in the surface soil (volume fraction)	<i>alpha_g</i>	PATRIOT (Imhoff, et al, 1994) USDA (1998)
Erosion of surface soil (kg/m <sup>2</sup> -d)	<i>erosion_g</i>	van der Leeden (1991, p. 83 and p.86, Table 2-39)]
Thickness of the root-zone soil (m)	<i>d_s</i>	PATRIOT (Imhoff, et al, 1994) USDA (1998)
Water content of root-zone soil (volume fraction)	<i>beta_s</i>	PATRIOT (Imhoff, et al, 1994) USDA (1998)
Air content of root-zone soil (volume fraction)	<i>alpha_s</i>	PATRIOT (Imhoff, et al, 1994) USDA (1998)
Thickness of the vadose-zone soil (m)	<i>d_v</i>	PATRIOT (Imhoff, et al, 1994)
Water content; vadose-zone soil (volume fraction)	<i>beta_v</i>	PATRIOT (Imhoff, et al, 1994) USDA (1998)
Air content of vadose-zone soil (volume fraction)	<i>alpha_v</i>	PATRIOT (Imhoff, et al, 1994) USDA (1998)
Fraction of land area in surface water	<i>f_arw</i>	Statistical Abstracts of the US, Bureau of Census (1997)
Ambient environmental temperature (kelvins)	<i>Temp</i>	NOAA (1998)
Organic carbon fraction in upper soil zone	<i>foc_s</i>	PATRIOT (Imhoff, et al, 1994)
Organic carbon fraction in vadose zone	<i>foc_v</i>	PATRIOT (Imhoff, et al, 1994)
Organic carbon fraction in aquifer zone	<i>foc_q</i>	PATRIOT (Imhoff, et al, 1994)
Yearly average wind speed (m/d)	<i>v_w</i>	NOAA (1998)

Table 3. Landscape Parameters in CalTOX as listed in Table 1 for which Existing Default Values are Retained.

Landscape Variable	Symbol	Mean Value	CV
Flux; surface water into landscape (m/d)	<i>inflow</i>	0	0
Atmospheric dust load (kg/m <sup>3</sup> )	<i>rhob_a</i>	$6.15 \times 10^{-8}$	0.2
Deposition velocity of air particles (m/d)	<i>v_d</i>	500	0.3
Plant dry-mass fraction	<i>bio_dm</i>	0.2	0.2
Plant fresh-mass density kg/m <sup>3</sup>	<i>rho_p</i>	1,000	0.2
Thickness of the ground-surface soil layer (m)	<i>d_g</i>	0.01	1
Soil particle density (kg/m <sup>3</sup> )	<i>rhos_s</i>	2,600	0.05
Thickness of the aquifer layer (m)	<i>d_q</i>	3	0.3
Solid material density in aquifer (kg/m <sup>2</sup> )	<i>rhos_q</i>	2,600	0.05
Porosity of the aquifer zone	<i>beta_q</i>	0.20	0.2
Average depth of surface waters (m)	<i>d_w</i>	5.0	1
Suspended sediment load in surface water (kg/m <sup>3</sup> )	<i>rhob_w</i>	0.8	1
Suspended sediment deposition (kg/m <sup>2</sup> /d)	<i>deposit</i>	10.5	0.3
Thickness of the sediment layer (m)	<i>d_d</i>	0.05	1
Solid material density in sediment (kg/m <sup>2</sup> )	<i>rhos_d</i>	2,600	0.05
Porosity of the sediment zone	<i>beta_d</i>	0.2	0.2
Sediment burial rate (m/d)	<i>bury_d</i>	$1.0 \times 10^{-6}$	5
Surface water current in m/d	<i>current_w</i>	0	0
Organic carbon fraction in sediments	<i>foc_d</i>	0.02	1
Boundary layer thickness in air above soil (m)	<i>del_ag</i>	0.005	0.2

Table 4. List of the Nine Landscape Regions and the States Included in the Regions.

Middle Atlantic	New England	East North Central	West North Central	South Atlantic
New Jersey New York Pennsylvania	Connecticut Maine Massachusetts New Hampshire Rhode Island Vermont	Illinois Indiana Michigan Ohio Wisconsin	Iowa Kansas Minnesota Missouri Nebraska North Dakota South Dakota	Delaware Florida Georgia Maryland North Carolina South Carolina Virginia West Virginia
East South Central	West South Central	Mountain	Pacific	
Alabama Kentucky Mississippi Tennessee	Arkansas Louisiana Oklahoma Texas	Arizona Colorado Idaho Montana Nevada New Mexico Utah Wyoming	California Oregon Washington	



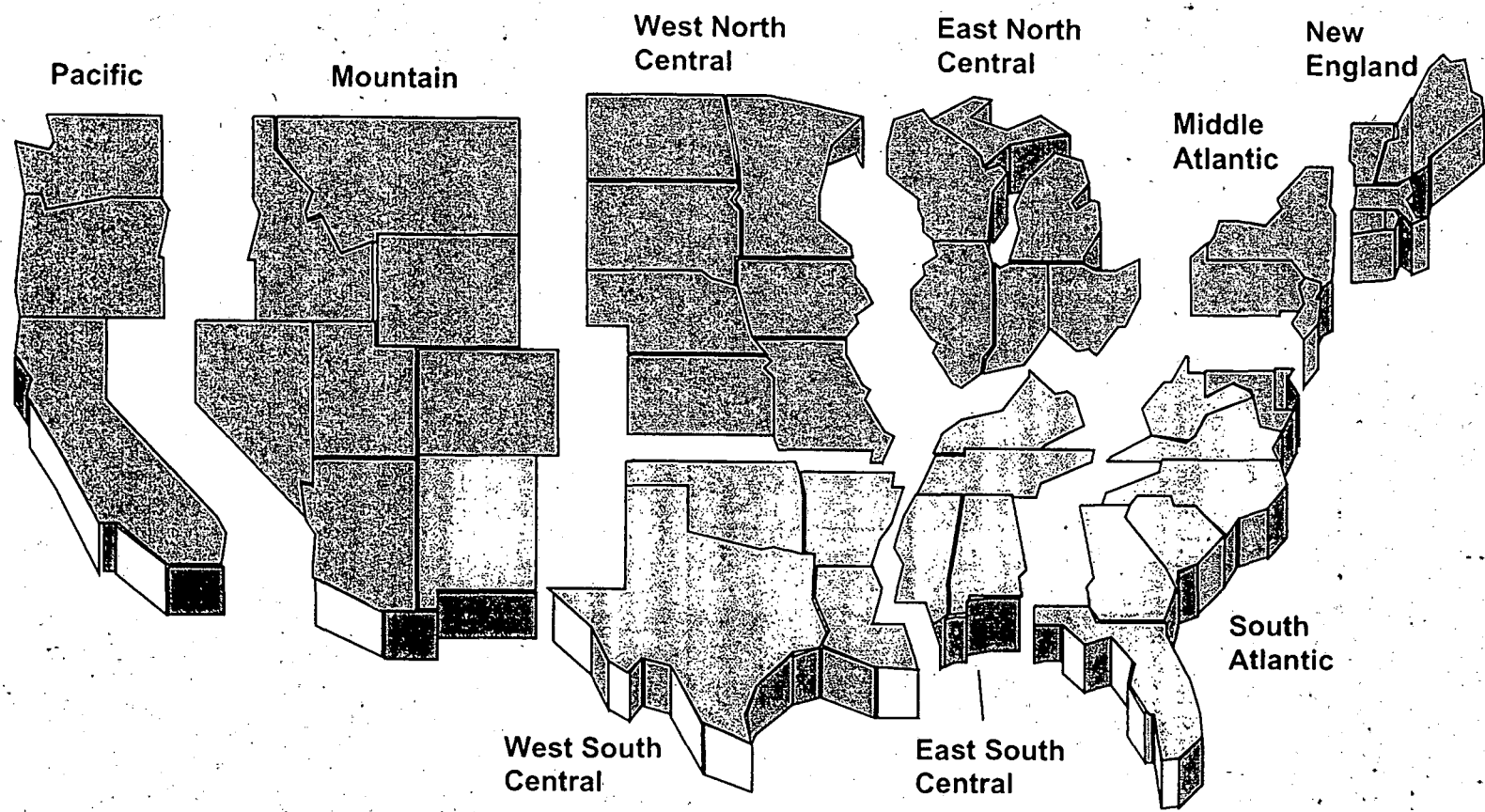


Figure 2. The division of the U.S. into nine regions for consideration of landscape properties variation.

### 3.2 Calculation Methods

For each of approximately 130 input parameters, CalTOX requires a minimum of two inputs to describe the range of values associated with the parameter. These descriptive factors are an arithmetic mean value for the parameter and the coefficient of variation (CV) that reflects the spread in the parameter range associated with variability and uncertainty. Two techniques were used to generate region and state-specific value ranges for landscape variables in CalTOX. The first technique develops a mean and CV from tabular data for landscape properties that have been compiled for the states. The second technique uses data from existing geographic information systems (GIS) to develop a mean and CV for some variables. In these data sets, the states are divided into an area-based set. Then for each defined area we develop a mean value of the parameter.

#### 3.2.1 Mean and CV for Tabular Data

The tubular data collected for a given state or region was assumed to represent multiple samples that have variability within the region, but not a strong dependence on geographical location. A simple arithmetic mean ( $\bar{x}$ ), standard deviation, and coefficient of variation was calculated from the multiple reported values from a state/region.

$$\text{Arithmetic mean } (\bar{x}) = \left( \sum_{i=1}^n x_i \right) / n \quad (1)$$

where  $\sum_{i=1}^n x_i$  is the sum of the observed values and  $n$  is the number of observations.

The coefficient of variation (CV) is computed by dividing the arithmetic standard deviation ( $\sigma$ ) by the mean.

$$\text{standard deviation } (\sigma) = \sqrt{\frac{\sum_{i=1}^n (x_i - \bar{x})^2}{n}} \quad (2)$$

$$\text{coefficient of variation (CV)} = \frac{\sigma}{\bar{x}} \quad (3)$$

It should be noted, that based on the central limit theorem of statistics, the confidence associated with the estimate of  $(\bar{x})$  becomes large as the number of samples used to estimate  $(\bar{x})$  also becomes large. Therefore, the reliability of the mean and CV estimates of a parameter are low when the sample size is small. An estimate of the error associated with estimating a mean from a small sample size is the standard error of the mean [S.E.  $(\bar{x})$ ].

$$\text{Standard error of the mean, S.E. } (\bar{x}) = \sqrt{\frac{\sum_{i=1}^n (x_i - \bar{x})^2}{n(n-1)}} \quad (4)$$

### 3.2.1 Mean and CV of Area-Based Landscape Properties

Properties associated with soils and the subsurface environment, such as void fraction, organic carbon content, and moisture content, can have large variations with a given geographic/political region, such as a state or county. Moreover, similar soil types occur with different frequencies within any defined area. Because of the strong geographic variation in soil-related properties, we use area-weighting within a defined region such as a state to determine the range, mean value, and CV of soil characteristics parameters. The area-weighted mean and CV of landscape parameters within each state are calculated as follows:

$$\text{area-weighted mean, } \bar{x}_j = \frac{\sum_{i=1}^n (x_{i,j} \times \text{Area}_i)}{\sum_{i=1}^n \text{Area}_i} = \sum_{i=1}^n (x_{i,j} \times f_i) \quad (5)$$

$$\text{area-weighted standard deviation, } \sigma_j = \sqrt{\frac{\sum_{i=1}^n [(\bar{x}_j - x_{i,j})^2 \times \text{Area}_i]}{\sum_{i=1}^n \text{Area}_i}} \quad (6)$$

$$\text{area-weighted CV, } CV_j = \frac{\text{area-weighted mean}}{\text{area-weighted-standard deviation}} = \sqrt{\sum_{i=1}^n (CV_{ij}^2 \times f_i)} \quad (7)$$

where,

$\bar{x}_j$  = area-weighted arithmetic mean value of the parameter  $x$  in region  $j$  (such as a state or group of states), which is made of  $n$  sub-areas with both a defined area,  $\text{Area}_i$  and a defined value  $x_{i,j}$  of parameter  $x$ ;

- $x_{i,j}$  = the value of parameter  $x$  in sub-region  $i$  of the region  $j$ ;
- $Area_i$  = area of sub-region  $i$  of region  $j$ ,  $m^2$ ;
- $f_i$  = the fraction of the area of region  $j$ ,  $Area_j$ , occupied by sub-region  $i$ ;
- $n$  = the total number of sub-regions  $i$  in the region  $j$ ;
- $\sigma_j$  = standard deviation of the parameter  $x$  in region  $j$ ;
- $CV_j$  = coefficient of variation of parameter  $x$  in region  $j$ ; and
- $CV_{ij}$  = coefficient of variation of parameter  $x$  in region  $i$  that is within region  $j$ .

## 4.0 Data Compilation Results and Evaluation

In this section we describe how the mean and coefficient of variation for each individual parameter were derived from the designated data sources. We begin with the parameters derived from state-based tabular data using simple averaging. We next give results for parameters derived from the PATRIOT system using area-weighting.

### 4.1 Data Compiled from State-Based Tabular Data

Data compiled from state-based tabular references include:

- areas of states and regions of the US,
- variations in yearly average precipitation in states and regions,
- surface water runoff,
- biomass inventory,
- ground water recharge,
- evaporation from surface water,
- soil erosion, fraction of total area that is surface water,
- the annual ambient environmental temperature, and
- the yearly average wind speed.

#### 4.1.1 Areas of States and Regions

Areas of states and regions were obtained from the Statistical Abstracts of the United States (US Bureau of the Census, 1997) and are listed in Table 5.

Table 5. Total Area, Land Area, and Surface Water Area of States and Regions.

Region	State	State number	total area [km <sup>2</sup> ]	land area [km <sup>2</sup> ]	Surface water area [km <sup>2</sup> ]
Middle Atlantic	New Jersey	1	21,277	19,215	2,062
	New York	2	139,833	122,310	17,523
	Pennsylvania	3	119,291	116,083	3,208
	TOTAL		280,401	257,608	22,793
New England	Connecticut	4	14,358	12,550	1,808
	Maine	5	87,388	79,939	7,449
	Massachusetts	6	29,934	20,300	3,634
	New Hampshire	7	24,044	23,231	813
	Rhode Island	8	3,189	2,707	482
	Vermont	9	24,903	23,956	947
	TOTAL		183,816	162,683	15,133
East North Central	Illinois	10	150,007	143,987	6,021
	Indiana	11	94,328	92,904	1,424
	Michigan	12	250,465	147,136	103,329
	Ohio	13	116,103	106,067	10,036
	Wisconsin	14	169,643	140,672	28,971
	TOTAL		780,546	630,766	149,781
West North Central	Iowa	15	145,754	144,716	1,038
	Kansas	16	213,110	211,922	1,189
	Minnesota	17	225,182	206,207	18,975
	Missouri	18	180,546	178,446	2,100
	Nebraska	19	200,358	199,113	1,245
	North Dakota	20	183,123	178,695	4,428
	South Dakota	21	199,744	196,571	3,174
	TOTAL		1,347,817	1,315,670	32,149
	South Atlantic	Delaware	22	6,206	5,062
Florida		23	155,214	139,697	15,517
Georgia		24	152,750	150,010	2,740
Maryland		25	31,849	25,316	6,533
North Carolina		26	136,421	126,180	10,241
South Carolina		27	80,779	77,988	2,791
Virginia		28	109,625	102,558	7,067
West Virginia		29	62,759	62,384	375
TOTAL			735,603	689,195	46,408
East South Central	Alabama	30	135,293	131,443	3,850
	Kentucky	31	104,665	102,907	1,759
	Mississippi	32	125,060	121,506	3,553
	Tennessee	33	109,158	106,758	2,400
	TOTAL		474,176	462,614	11,562

Table 5. (continued)

Region	State	State number	total area [km <sup>2</sup> ]	land area [km <sup>2</sup> ]	Surface water area [km <sup>2</sup> ]
West South Central	Arkansas	34	137,742	134,875	2,867
	Louisiana	35	128,595	112,836	15,759
	Oklahoma	36	181,048	177,877	3,171
	Texas	37	692,248	678,358	13,890
	TOTAL		1,139,633	1,103,946	35,687
Mountain	Arizona	38	295,276	294,333	943
	Colorado	39	269,618	268,658	960
	Idaho	40	216,456	214,325	2,131
	Montana	41	380,849	376,991	3,859
	Nevada	42	286,367	284,396	1,971
	New Mexico	43	314,939	314,334	605
	Utah	44	219,902	212,815	7,086
	Wyoming	45	253,349	251,501	1,848
	TOTAL		2,236,756	2,217,353	19,403
Pacific	California	46	411,470	403,971	7,499
	Oregon	47	251,571	248,646	2,925
	Washington	48	182,949	172,445	10,503
	TOTAL		845,990	825,062	20,927
US TOTAL			8,024,738	7,664,897	353,843

#### 4.1.2 Annual Average Precipitation

The annual average precipitation [m/d] was calculated for each of the 48 contiguous United States from NCDC-NOAA data sets located on the web (NOAA, 1998). This data set provides precipitation information for 261 sites throughout the US. The annual average precipitation (*rain*), [m/d], was calculated from the annual-average values of normal monthly precipitation [inches] given in the NCDC-NOAA (1998) database. The normal monthly precipitation is expressed as the arithmetic mean for each month over the 30-year period and includes the liquid water equivalent of snowfall. The mean and CV of precipitation were calculated from the annual cumulative precipitation values given in the NOAA (1998) data. The arithmetic mean and CV for a state were based on the direct use of all values for the precipitation collection sites within that state (no weighting factor was applied). The mean value and CV for regionally-averaged annual average precipitation was based on area weighting using the states in that region. Figure 3 displays the annual average precipitation of the 48 United States grouped by region. We also calculated seasonal variation in the reported normal monthly precipitation. In order to compare precipitation among the seasons, we calculated the CV of precipitation among summer, fall, winter and spring averages. The largest seasonal CV was 0.59 in the Pacific region and the lowest was in the New England region, 0.053. Other states have seasonal variations with a CV in the range 0.1 to 0.4. A value of precipitation (*rain*) [m/d] was developed separately for each of the 48 states. Individual state values for

annual average precipitation are given in Table A-1 in Appendix A. Regional average values of precipitation are provided in Table A-5 of Appendix A and summarized in Table 6 and Figure 3.

Table 6 Summary by Region of Precipitation Data Compiled from NOAA (1998) Data Files on the Internet.

Region	precipitation [m/d]	CV
Middle Atlantic	0.0028	0.094
New England	0.0031	0.28
East North Central	0.0032	0.069
West North Central	0.0031	0.15
South Atlantic	0.0031	0.085
East South Central	0.0037	0.088
West South Central	0.0024	0.24
Mountain	0.00084	0.47
Pacific	0.0019	0.67
All regions combined	0.0023	0.29

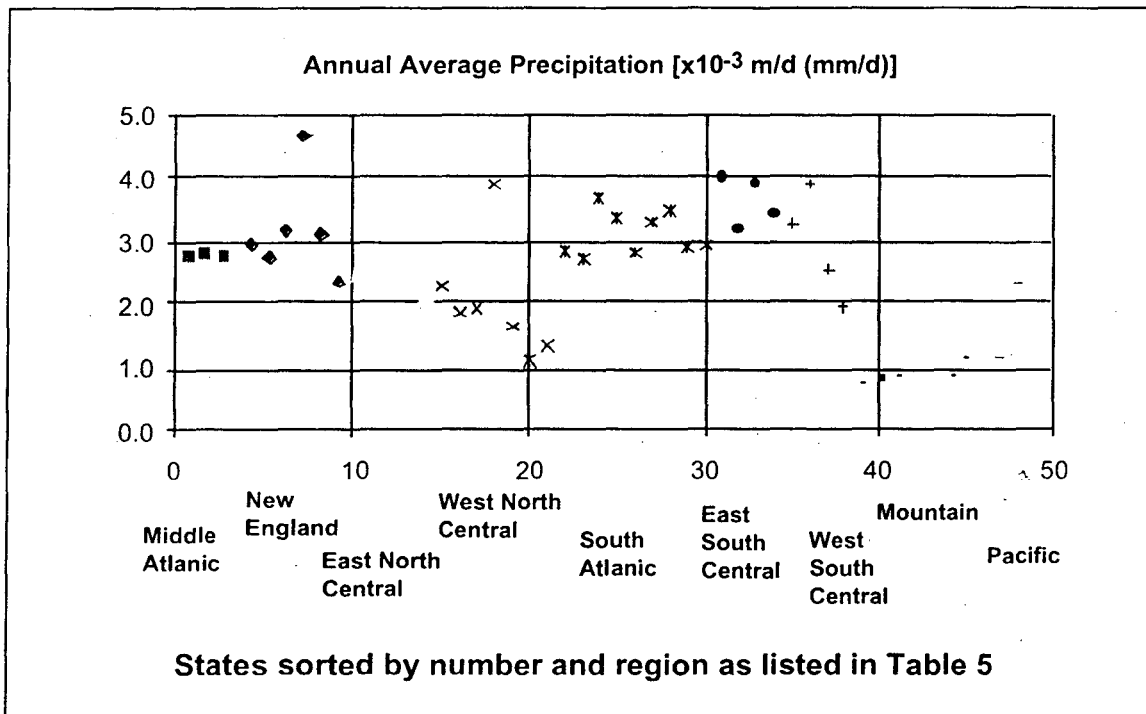


Figure 3. Annual average precipitation calculated from NOAA (1997) data for 48 contiguous United States.

### 4.1.3 Land Surface Runoff:

Data for land surface runoff is collected by Water Resource Region (WRR) (van der Leeden, 1991) and is not available on a state-by-state basis. We used the WRR data to develop a runoff value for the nine US regions. The runoff values assigned to each state is based on its region. Table 7 summarizes runoff data (and erosion data) compiled by van der Leeden et al. (1991). Based on the area of the states associated with the WRR, these WRR runoff values in gallons/d were converted to [ $\text{m}^3/\text{day}/\text{land area}$ ] to obtain runoff in units of [ $\text{m}/\text{d}$ ]. A default value of  $\text{CV} = 1$  is used. Table 8 summarizes the mean and CV of runoff developed for each of the nine US regions.

Table 7. Summary of US Runoff and Erosion Rates in the Major Water Resource Regions (van der Leeden et al., 1991)

Water Resource Region	States included in Water Resource Region	Mean Runoff in $10^9$ gal/day	Erosion based on sediment yield, tons/sq mi/yr	Erosion based on sediment load tons/sq mi/yr
Arkansas-White-Red:	Arkansas, Oklahoma	95.8	2200	
California	California	65.1	1300	190
Columbia-North Pacific	Idaho, Oregon, Washington	210	400	
Great Basin	Nevada, Utah	5.89	400	530, 808
Great Lakes	Michigan	63.2	100	
Lower Colorado	Arizona, New Mexico	3.19	600	199
Lower Mississippi	Mississippi	48.4	5200	
Missouri	Kansas, Missouri, Montana, Nebraska, South Dakota, Wyoming	54.1	1500	114
North Atlantic	Connecticut, Delaware, D.C., Maine, Maryland, Massachusetts, New Hampshire, New Jersey, New York, Pennsylvania, Rhode Island, Vermont, Virginia, West Virginia	163	250	265, 270
Ohio	Indiana, Kentucky, Ohio	125	850	
Rio Grande	Half of Texas (other half is part of Texas-Gulf)	4.9	1300	336, 105
South Atlantic-Gulf	Alabama, Florida, Georgia, North Carolina, South Carolina	197	800	183
Tennessee	Tennessee	41.5	700	
Texas-Gulf	Louisiana and half of Texas (other half part of Rio Grande)	39.1	1800	336, 105, 337
Upper Colorado	Colorado	13.45	1800	
Upper Mississippi	Iowa, Illinois, Minnesota, Wisconsin	64.6	800	510



Table 8. Calculated Land Surface Runoff [m/d] for Nine US Regions and the US Regional Area-Weighted Average.

Region	runoff [m/d]	CV
Middle Atlantic	0.0010	1.0
New England	0.0010	1.0
East North Central	0.0011	1.0
West North Central	0.00021	1.0
South Atlantic	0.0011	1.0
East South Central	0.0014	1.0
West South Central	0.00048	1.0
Mountain	0.00020	1.0
Pacific	0.00095	1.0
US Average	0.00061	1.0

4.1.4 Plant Dry Mass Inventory:

US variations in the reported plant dry mass inventory were obtained from Layton, et al. (1986) who divided the US into three geographical regions with similar landscape attributes. These regions are the Western Interior region with a plant dry mass inventory of 0.7 kg/m<sup>2</sup>, the Central-Northeastern region with a plant dry-mass inventory of 30 kg/m<sup>2</sup>, and the Southeastern region also with a plant dry-mass inventory of 30 kg/m<sup>2</sup>. These values were applied the respective states within a region. A default CV of 1 was assumed and used. Table 9 summarizes the vegetation inventory value used in each region. In the Layton et al. (1986) scheme,

the Central-Northeastern region includes the states:

New Jersey	New York	Pennsylvania	Connecticut
Maine	Massachusetts	New Hampshire	Rhode Island
Vermont	Delaware	Maryland	Virginia
West Virginia	Kentucky	Tennessee	Illinois
Indiana	Michigan	Ohio	Wisconsin
Iowa	Minnesota	Missouri	

the Southeastern region includes the states:

Florida	Georgia	North Carolina	South Carolina
Alabama	Mississippi	Louisiana	Arkansas

and the Western-Interior region includes the states:

Oklahoma	Texas	Kansas	Nebraska
North Dakota	South Dakota	Arizona	Colorado
Idaho	Montana	Nevada	New Mexico
Utah	Wyoming	California	Oregon
Washington			

Table 9. Plant Dry-Mass Inventory [kg/m<sup>2</sup>] Used for the Nine US Regions and the US Regional Area-Weighted Average.

Region	Plant Dry-Mass Inventory, kg/m <sup>2</sup>	CV
Middle Atlantic	30	1.0
New England	30	1.0
East North Central	30	1.0
West North Central	18	1.0
South Atlantic	30	1.0
East South Central	30	1.0
West South Central	30	1.0
Mountain	0.7	1.0
Pacific	0.7	1.0
US Average	17	1.0

#### 4.1.5 Ground Water Recharge

Based on an assumption used by Layton et al. (1986), which is consistent with the regional hydrology data reported in van der Leeden et al. (1991), the rate at which ground water is recharged in the US is assumed to be 5 per cent of total annual precipitation. Because of uncertainty in this assumption, ground-water recharge rates are developed only for specific regions, but not for specific states. In addition, a CV of 1 is assumed and used as a default for the recharge parameter. Table 10 lists the ground water recharge values for the nine US regions along with the default CV.

Table 10. Ground Water Recharge Rates for Nine US Regions and the Total US Based on Regional Area-Weighted Averages.

Region	recharge [m/d]	CV
Middle Atlantic	$1.4 \times 10^{-4}$	1.00
New England	$1.6 \times 10^{-4}$	1.00
East North Central	$1.6 \times 10^{-4}$	1.00
West North Central	$1.5 \times 10^{-4}$	1.00
South Atlantic	$1.7 \times 10^{-4}$	1.00
East South Central	$1.8 \times 10^{-4}$	1.00
West South Central	$1.2 \times 10^{-4}$	1.00
Mountain	$4.3 \times 10^{-5}$	1.00
Pacific	$9.5 \times 10^{-5}$	1.00
US	$1.2 \times 10^{-4}$	1.00

#### 4.1.6 Evaporation of Water from Surface Water

Currently available literature and data bases do not provide information on the rate of evaporation of water from the surface waters on a state or regional basis. Thus, to develop a representative value of the rate of evaporation from surface waters, we used the annual reservoir evaporation at selected stations in the US. This evaporation rate is reported in the *Water Encyclopedia* (van der Leeden, 1991) and has been use previously to calculate the evaporation of water from surface water in CalTOX (McKone, 1993b). In the *Water Encyclopedia*, the annual reservoir evaporation is reported as the sum of the mean monthly computed values [inches] at select stations (one station per given state, except for Texas with two annual reported values that were averaged). Table 11 summarizes the measurements from the states with stations reporting evaporation measurements.

Table 11. States with Stations Reporting Evaporation Measurements, and Their Annual Reservoir Evaporation, [m/d].

Reporting States	Non reporting states (estimated from reporting states)	annual reservoir evaporation [m/d]
Arizona		0.0070
California		0.0038
Colorado		0.0038
Florida		0.0036
Georgia		0.0034
Maine	New Hampshire	0.0011
Minnesota	Iowa	0.0022
Mississippi	Alabama	0.0032
Missouri	Arkansas, Kansas	0.0033
Montana	Wyoming	0.0030
Nebraska		0.0036
New Mexico		0.0049
New York	Connecticut, Massachusetts, New Jersey, Pennsylvania, Rhode Island, Vermont	0.0021
North Dakota	South Dakota	0.0027
Ohio	Michigan	0.0023
Oklahoma		0.0046
Oregon	Idaho	0.0026
South Carolina	North Carolina	0.0036
Tennessee	Indiana, Kentucky	0.0027
Texas*	Louisiana	0.0030 0.0048
Utah	Nevada	0.0038
Virginia	Delaware, Maryland, West Virginia	0.0027
Washington		0.0017
Wisconsin	Illinois	0.0020

\* two values are reported for Texas

These values represent the evaporation rate over the reservoir. These values were used to estimate the evaporation rates for non reporting states. Table 12 displays the calculated evaporation rates for the nine US Regions and US regional area weighted averages. These values are converted to a total land area basis and thus include the fraction of the state that is surface water in the calculation. Because this data is applied only on a regional basis and is based on a proxy parameter, a default CV of 1 was assumed and used.

Table 12. The Evaporation of Water From Surface Water Calculated for Nine US Regions

Region	evaporate [m/d]	CV
Middle Atlantic	$1.7 \times 10^{-4}$	1.0
New England	$1.3 \times 10^{-4}$	1.0
East North Central	$4.3 \times 10^{-4}$	1.0
West North Central	$6.0 \times 10^{-5}$	1.0
South Atlantic	$2.1 \times 10^{-4}$	1.0
East South Central	$7.4 \times 10^{-5}$	1.0
West South Central	$1.2 \times 10^{-4}$	1.0
Mountain	$3.2 \times 10^{-5}$	1.0
Pacific	$6.3 \times 10^{-5}$	1.0
<b>US Average</b>	<b><math>1.2 \times 10^{-4}</math></b>	<b>1.0</b>

#### 4.1.7 Erosion of Surface Soil

Regional variations in soil run-off erosion are based on the net transfer of suspended sediment by surface water in various regions of the US. Data on runoff surface erosion are collected and reported by Water Resource Region (WRR) (van der Leeden, 1991) and are not available on a state-by-state basis. We used the WRR data to develop surface-soil erosion values for the nine US regions. The erosion values assigned to each state is based on its region. Two relevant measures of run-off erosion are reported by van der Leeden (1991)—(1) the average sediment yield (tons/square-mile/year) in the major rivers draining the various regions and (2) the total average sediment load/drainage area (tons/square-mile/year). The sediment yield is for US drainage areas of less than 100 square miles, whereas the total average sediment load per drainage area applies to the entire drainage area of a large river system. Table 7 summarizes the values of both of these parameters for each of the WRR of the US based on data in van der Leeden et al. (1991). Among these two parameters, we selected the second, the total average sediment load per drainage area, as more appropriate for constructing erosion values for CalTOX. However, for a WRR without a reported sediment load value, the sediment yield was used to assess erosion. The sediment loads in tons/square mile/year were multiplied by  $9.6 \times 10^{-7}$  to convert from tons/(square mile)/year to  $\text{kg}/\text{m}^2/\text{d}$ . A default value of  $\text{CV} = 1$  is used. Table 13 summarizes the regional (state area weighted average) and US (region area weighted average) erosion rate and CV.

Table 13. Estimated Soil Erosion Rates by Region in the US.

Region	erosion [kg/m <sup>2</sup> -d]	CV
Middle Atlantic	$2.9 \times 10^{-4}$	1.0
New England	$2.9 \times 10^{-4}$	1.0
East North Central	$5.5 \times 10^{-4}$	1.0
West North Central	$4.6 \times 10^{-4}$	1.0
South Atlantic	$2.2 \times 10^{-4}$	1.0
East South Central	$3.2 \times 10^{-4}$	1.0
West South Central	$2.8 \times 10^{-4}$	1.0
Mountain	$3.5 \times 10^{-4}$	1.0
Pacific	$1.6 \times 10^{-4}$	1.0
US Average	$3.6 \times 10^{-4}$	1.0

#### 4.1.8 Fraction of Land Area that is Surface Water

The fraction area in each state that is covered by surface water ( $f_{arw}$ ) is obtained from the Statistical Abstract of the US (US Bureau of the Census, 1997). Values of the parameter  $f_{arw}$  for each state are presented in Table A-1 of Appendix A. Table 14 summarizes the area-weighted average of  $f_{arw}$  for each of the nine US regions and for the area of the 48 states considered. A CV of 0.2 is used for this parameter based on prior use in CalTOX (McKone, 1993b).

Table 14. Summary by Region of Fraction of Land Area that is Surface Water  
Compiled from US Bureau of the Census (1997).

Region	f_arw	CV
Middle Atlantic	0.081	0.20
New England	0.086	0.20
East North Central	0.19	0.20
West North Central	0.024	0.20
South Atlantic	0.063	0.20
East South Central	0.024	0.20
West South Central	0.031	0.20
Mountain	0.0087	0.20
Pacific	0.025	0.20
<b>All regions combined</b>	<b>0.044</b>	<b>0.20</b>

#### 4.1.9 Ambient Environmental Temperature

The annual average ambient environmental temperature (in kelvins) was calculated for each of the 48 contiguous United States from NCDC-NOAA data sets located on the web (NOAA, 1998). This data set provides temperature information for 261 sites throughout the US. The annual average ambient temperature ( $Temp$ ), [K], was calculated from the annual values of normal monthly temperature [ $^{\circ}$ F] given in the NCDC-NOAA (1998) database. The normal monthly temperature is expressed as the arithmetic mean for each month over the 30-year period. For each state, the mean and CV of temperature were calculated from the annual cumulative average temperature values for that state given in the NOAA (1998) data. The arithmetic mean and CV for a state were based on the direct use of all values for the temperature collection sites within that state (no weighting factor was applied). The mean value and CV for regionally-averaged annual average ambient temperature was based on area weighting using the states in that region. Figure 4 displays the annual average ambient temperature of the 48 contiguous United States grouped by region. We also calculated seasonal variations in the reported normal monthly temperatures. In order to compare temperature among the seasons, we calculated the CV of temperature among summer, fall, winter and spring averages. The largest seasonal CV was 0.04 in the West North Central region and the lowest was in the Pacific region, 0.019. A value of ambient temperature ( $Temp$ ) [K] was developed separately for each of the 48 states. Individual state values for annual average ambient temperature are given in Table A-1 in Appendix A. Regional average values of ambient environmental temperature are provided in Table A-5 of Appendix A.

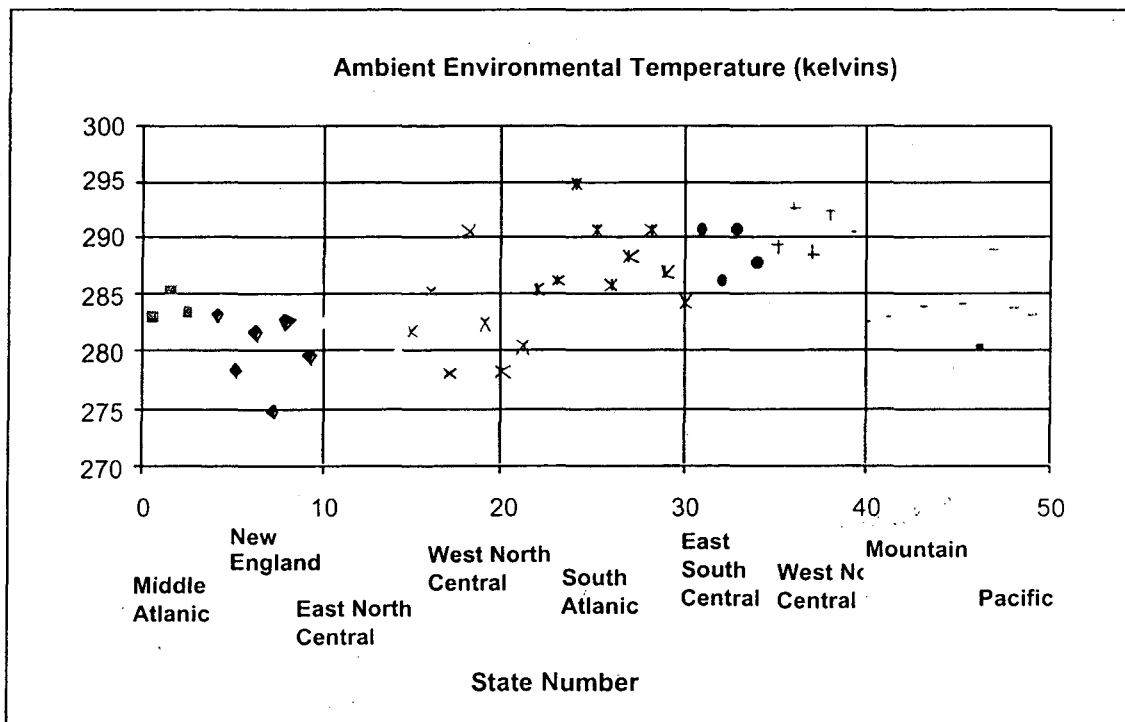


Figure 4. Ambient environmental temperature (in kelvins) displayed for 48 contiguous United States from NOAA (1997) data.

#### 4.1.10 Yearly Average Wind Speed

The annual average wind speed (in m/d) was calculated for each of the 48 contiguous United States from NCDC-NOAA data sets located on the web (NOAA, 1998). This data set provides wind-speed information for 261 sites throughout the US. The average wind speed is based on the speed of the wind regardless of direction. The annual average wind speed ( $v_w$ ), [m/d], was calculated from the annual average values of normal monthly wind speed [mph] given in the NCDC-NOAA (1998) database. The normal monthly wind speed is expressed as the arithmetic mean for each month over the 30-year period. For each state, the mean and CV of wind speed were calculated from the annual cumulative average wind-speed values for that state given in the NOAA (1998) data. The arithmetic mean and CV for a state were based on the direct use of all values for the wind-speed collection sites within that state (no weighting factor was applied). The mean value and CV for regionally-averaged annual average wind speed was based on area weighting using the states in that region. Figure 5 displays the resulting annual average wind speed of the 48 contiguous United States grouped by region. We also calculated seasonal variations in the reported normal monthly wind speed. In order to compare wind speed among the seasons, we calculated the CV of wind speed among summer, fall, winter and spring averages. The largest seasonal CV was 0.13 in the New England region and the lowest was in the Pacific region, 0.09. A value of wind speed was developed separately for each of the 48



states. Individual state values for annual average wind speed are given in Table A-1 in Appendix A. Regional average values of ambient environmental temperature are provided in Table A-5 of Appendix A.

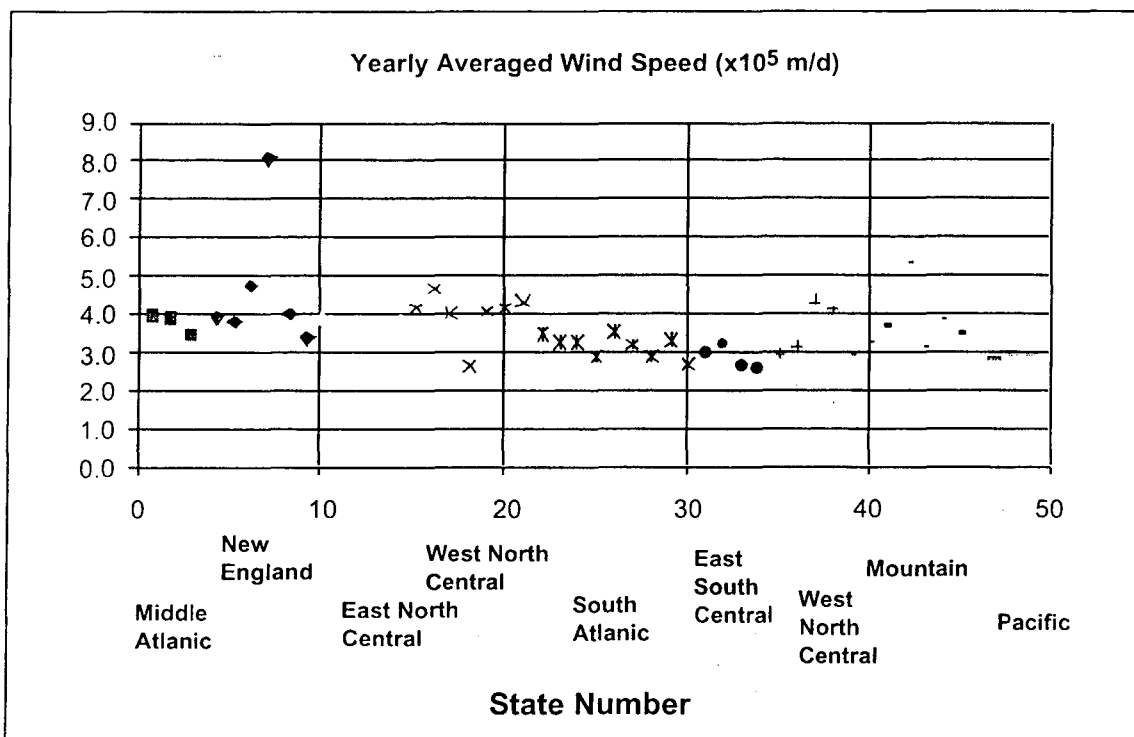


Figure 5. Yearly averaged wind speed calculated from NOAA (1997) data for 48 contiguous United States.

#### 4.1.11 Summary of Data Compiled from State-Based Tabular Data

Data collected from tabular data sources were compiled as state-specific data for the parameters representing yearly average precipitation, fraction of total area that is surface water, the annual ambient temperature, and the yearly average wind speed. State-specific values for these parameters are provided in Table A-1 in Appendix A.

Data collected from tabular data sources were compiled as region-specific data for parameters representing surface water runoff, biomass inventory, ground water recharge, evaporation from surface water, and soil erosion. State-specific values for these parameters are obtained by assigning the region-specific value to all states in the region. State-specific values for these and all other parameters are provided in Table A-5 in Appendix A.

## 4.2 Data Compiled from the PATRIOT System

The US EPA PATRIOT system version 1.2 was designed for area-specific analyses of soil transport in the conterminous US (Imhoff, et al., 1994). Among the components of PATRIOT are comprehensive databases of soil properties and an interface that allows the user to explore the databases and build up sets of soil properties for any local environment within the US. The NRI/SOILS5 database, made up of data from 229,000 agricultural land use sample sites in the conterminous US, constitutes the soils database in PATRIOT. These capabilities of PATRIOT were used here to develop state and region-specific soil-properties data. In particular, PATRIOT was used to develop surface soil, upper soil zone and vadose zone properties—including the depth of various soil layers, the fraction of organic carbon in defined soil layers, and water and air content (volume fraction) of the soil layers.

### 4.2.1 Soil Data In the PATRIOT System

In the PATRIOT system, soil properties are given for four soil layers, including (1) what is referred to in PATRIOT as the "surface soil" (SUR) and defined as the A, E, EB and AB horizons of the soil column, (2) the subsoil (SUB), or the part of the soil column below the plow depth but above the C Horizon (i.e., the B Horizon), (3) the stratified substratum (STR), or the part of the soil below the A and B horizons, and (4) the layer beneath substratum layer (SST), which is the non-soil materials and often consists of weathered/unweathered bedrock or stratified rock. The ground-surface soil layer and the upper soil layer (or root-zone soil) layers in CalTOX correspond to the "surface-soil" in PATRIOT, but some of the upper-soil layer in CalTOX includes the subsoil layer in PATRIOT. The surface-soil properties in CalTOX were calculated based on surface layer data from PATRIOT. The properties of the upper soil compartment from CalTOX are calculated from a combination of surface-soil- and subsoil-layer properties from PATRIOT. The substratum and beneath-substratum layer properties from PATRIOT were used to calculate vadose zone soil compartment properties for the CalTOX input.

The PATRIOT databases include high and low data values for the soil layer depth [cm], percent of organic matter in the soil layer, the available water content (volume fraction), bulk density, percent clay and percent sand for the four soil layers. Within each state, PATRIOT provides a large number of soil-properties and soil-occurrence data. The soil-occurrence data define the areas of each state having a set of soil properties. For each soil property, the methods described in Section 3.2.1 of this report are used to develop area-weighted averages based on the sample areas and properties provided in PATRIOT for a given state.

In the paragraphs below, we provide a brief description of how individual soil parameters (including fraction of organic carbon, water content, air content) were compiled for each area within a state.

4.2.1.1 *Thickness of the Upper Soil and Vadose Zone Soil Compartments*

The thickness of the CalTOX upper soil layer, with the properties of the surface (SUR) and subsurface (SUB) soil given in PATRIOT, is taken as the SUB depth. The CalTOX vadose soil includes both the stratified (STR) and beneath stratified (SST) layer in PATRIOT. The thickness of the vadose-zone soil, is taken as the SST depth minus the calculated upper soil depth. In cases where this procedure results in a very low state average vadose-soil-zone thickness, a default vadose-zone thickness of 5 m can be used based on the observation of Pankow et al. (1997) that 5 m is the depth to shallow ground water typical of many US urban areas.

4.2.1.2 *Determination of Soil Properties from Vertical Averaging*

All calculated soil properties (i.e., water content, air content, organic-carbon fraction) set-up for the CalTOX upper-soil and vadose-zone soil compartments were vertically averaged from the PATRIOT system. We did this using a combination of properties weighted with the thickness of the layers in the zone (e.g., the thickness of the SUR and SUB layer in the upper soil compartment and the thickness of the STR and SST in the vadose-zone compartment). Thus, the upper-soil-zone and vadose-zone soil properties mean and CV's were calculated using the formulae:

$$x_{i,k} = \frac{\sum y_j x_{ij}}{y_k} \quad (8)$$

$$CV_{i,k} = \sqrt{\frac{\sum (y_j \times CV_{ij}^2)}{y_k}} \quad (9)$$

For example the property,  $x_i$ , in the upper soil layer is calculated from the PATRIOT data as:

$$x_{i,usz} = \frac{y_{sur} \times x_{i sur} + y_{sub} \times x_{i sub}}{y_{usz}} \quad (10)$$

$$CV_{i,usz} = \sqrt{\frac{y_{sur} \times CV_{i sur}^2 + y_{sub} \times CV_{i sub}^2}{y_{usz}}} \quad (11)$$

$x_{i,k}$  = mean value of soil property,  $i$ , in CalTOX soil zone  $k$  (i.e., usz or vadose zone)

$y_j$  = thickness of soil layer,  $j$  (i.e., SUR, SUB, STR, or SST)

$x_{i,j}$  = mean value of soil property  $i$  in soil layer,  $j$ .

$y_k$  = thickness of soil zone k

$CV_{i,k}$  = coefficient of variation of soil property i in CalTOX soil zone k

$CV_{i,j}$  = coefficient of variation of soil property i in PATRIOT v1.20 soil layer, j.

#### 4.2.1.3 Fraction of Organic Carbon

PATRIOT reports the % organic matter (OM) for each sublayer, SUR, SUB, STR, and SST. The area-weighted average fraction of organic carbon, with respect to the soil sample area, was calculated for each of the four PATRIOT layers. The % OM was converted to fraction organic carbon,  $f_{oc}$  using,

$$f_{oc} = \frac{\%OM/100}{1.72} \quad (12)$$

The weighted average  $f_{oc}$ 's for each layer were then averaged, with respect to the thickness of the PATRIOT layers, to give the upper-soil-layer (SUR and SUB layer in PATRIOT) and vadose zone (STR and SST layer in PATRIOT) organic carbon fraction. The surface soil organic carbon fraction in CalTOX was taken as that calculated from the PATRIOT SUR layer. By default, the mean and CV of the vadose zone  $f_{oc}$  was used for the aquifer zone.

#### 4.2.1.4 Soil Water and Air Content

The water and air content [both as volume fraction] of the soil reported in CalTOX input fields were derived from % sand and % clay and the bulk-density parameters given in PATRIOT. The water content was found from the permanent wilting point (WP) and field capacity (FC)

$$water\_content = \left( \frac{WP + FC}{2} \right) \quad (13)$$

The WP is approximately equivalent to the lower limit of the Available Water, expressed as volume water/volume soil, which is also the water content at a matric potential of -1,500 kPa (-15 bars). Field capacity (FC, expressed as volume-water/volume soil) is the water content at the upper limit of the Available Water (AW) or drained upper limit. In soil terms, FC roughly corresponds to a matric potential of -30 kPa (-0.3 bars) in most soils and to -10 kPa (-0.1 bars) in sandy soils. FC and WP are given by:

$$FC = \left( \frac{0333}{a} \right)^{\frac{1}{b}} \quad (14)$$

$$WP = \left(\frac{15}{a}\right)^{\frac{1}{b}} \quad (15)$$

where a and b are defined as:

$$a = \exp\left[-4396 - (0.0715 \times C) - 0.000488S^2 - 0.11114285CS^2\right]$$

$$b = -3.14 - 0.00222C^2 - 0.00003484CS^2$$

and

C = % clay in soil layer

S = % sand in soil layer

The defining equations for WP, FC and water content are taken from the “soil triangle” developed by Saxton et al. (1986).

The air content of the upper-soil and vadose-soil zones was calculated from the bulk density (blkd) reported in PATRIOT and the water content of the soil, obtained from Equation 13, using the formula:

$$air\_content = 1 - \left(\frac{blkd}{2.6}\right) - water\_content \quad (16)$$

#### 4.2.2 Surface Soil Parameters Derived from PATRIOT

The ground-surface-soil compartment properties for each state were derived from the surface (SUR) layer data given in the PATRIOT databases. Table 15 provides a summary of the water content, beta\_g, and air content, alpha\_g, parameters for each US region and their associated CVs. Specific state values for these parameters are provided in Table A-2 of Appendix A. A default soil thickness of 0.01 m is used as the ground-surface-soil-compartment thickness in CalTOX.

Table 15 Calculated Water Content (beta\_g) and Air Content (alpha\_g) for the 9 US Regions.

Region	beta_g	CV	alpha_g	CV
Middle Atlantic	0.17	0.34	0.34	0.14
New England	0.15	0.31	0.43	0.17
East North Central	0.19	0.60	0.28	0.17
West North Central	0.21	0.57	0.26	0.17
South Atlantic	0.15	0.36	0.30	0.13
East South Central	0.19	0.51	0.26	0.19
West South Central	0.21	0.63	0.23	0.28
Mountain	0.19	0.46	0.30	0.20
Pacific	0.19	0.48	0.31	0.24
US Average	0.19	0.46	0.28	0.19

#### 4.2.3 Upper-Soil-Zone Parameters Derived from PATRIOT

Using methods described in Section 4.2.1, the mean and CV of upper-soil-zone (or root-zone soil) properties are determined for the 48 conterminous US states and the 9 US regions. Table 16 provides a summary of these root-zone soil properties. For the parameters soil depth, organic-carbon content, soil-air content, and soil-water content, respectively, Figures 6 through 9 present the variation among the 48 contiguous United States in the area-weighted average values of these parameters in root zone soil. Specific state values for these parameters are provided in Table A-3 of Appendix A.

Table 16 Summary by Region of the Mean and CV of the Upper-Soil-Zone Parameters Calculated Using PATRIOT.

Region	d <sub>s</sub> [m]	CV	beta <sub>s</sub>	CV	alpha <sub>s</sub>	CV	foc <sub>s</sub>	CV
Middle Atlantic	0.69	0.37	0.18	0.38	0.30	0.21	0.009	1.8
New England	0.56	0.40	0.15	0.34	0.36	0.20	0.017	1.7
East North Central	0.79	0.41	0.20	0.61	0.24	0.31	0.008	1.6
West North Central	0.70	0.44	0.19	0.58	0.23	0.24	0.011	1.3
South Atlantic	0.93	0.44	0.18	0.40	0.26	0.24	0.006	1.8
East South Central	0.89	0.49	0.23	0.52	0.21	0.31	0.005	1.4
West South Central	0.91	0.51	0.23	0.60	0.19	0.21	0.007	1.2
Mountain	0.72	0.60	0.21	0.50	0.26	0.25	0.006	1.4
Pacific	0.77	0.50	0.20	0.50	0.28	0.29	0.010	1.7
US	0.79	0.47	0.21	0.48	0.25	0.25	0.008	1.6

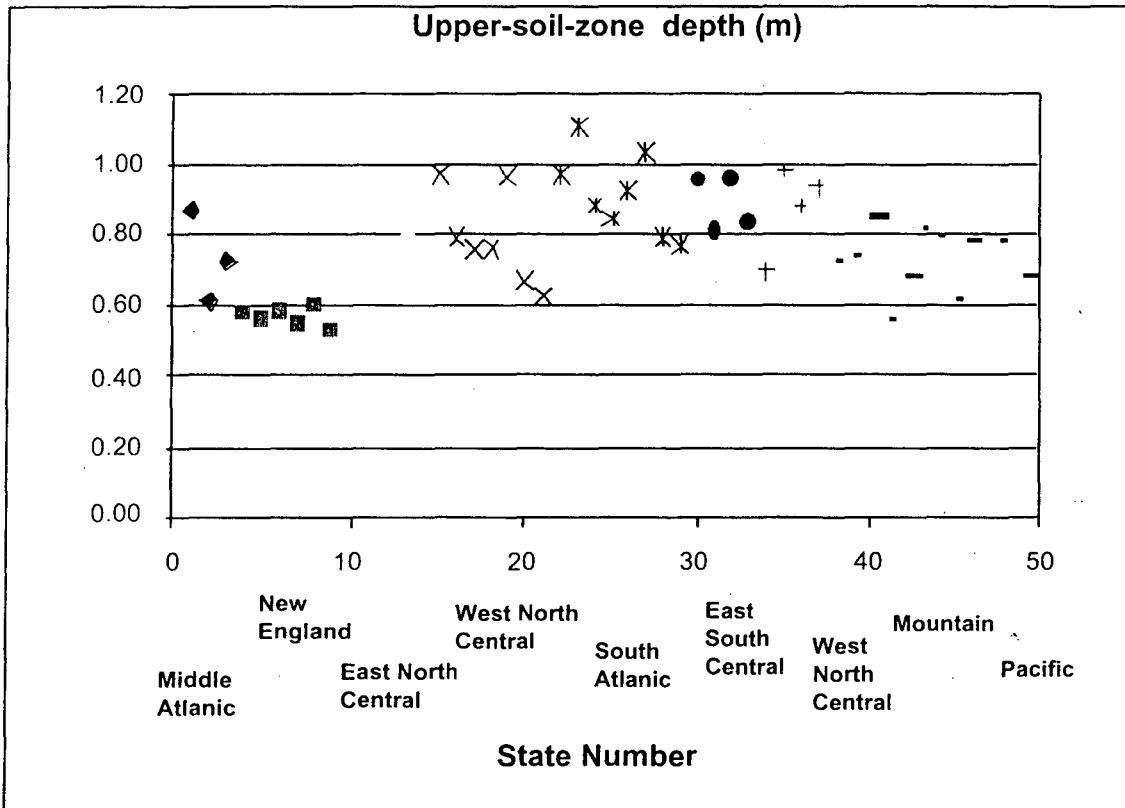


Figure 6. Variation among the 48 contiguous United States in the area-weighted average upper-soil-zone depth as derived from PATRIOT system.

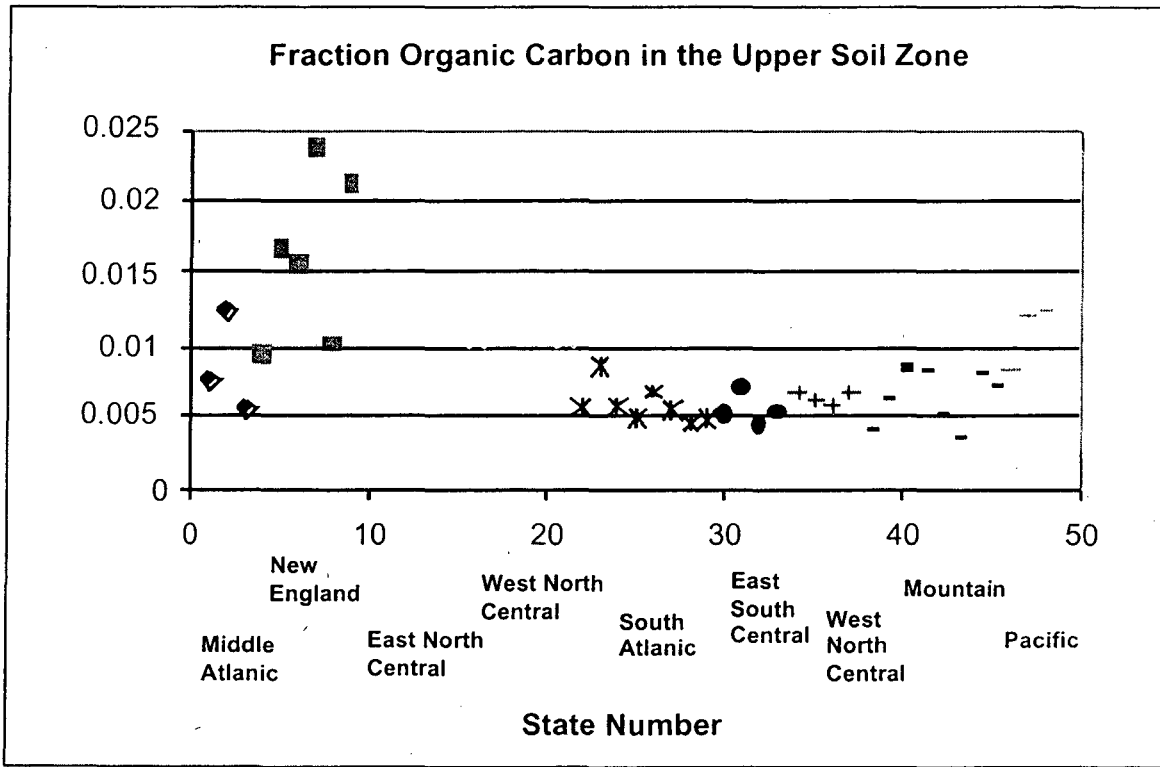


Figure 7. Variation among the 48 United States in the area-weighted average organic-carbon content in the root-zone soil as derived from PATRIOT.



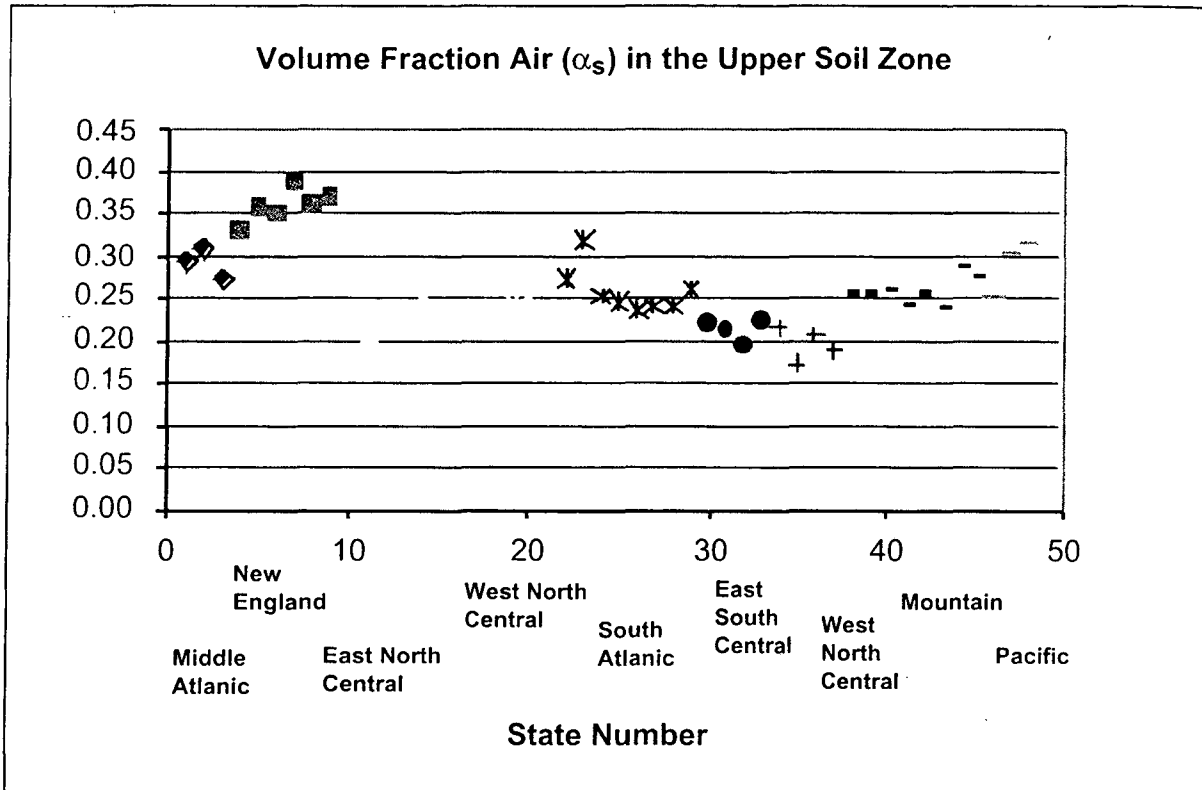


Figure 8. Variation among the 48 contiguous United States in the area-weighted average air content in the root-zone soil as derived from PATRIOT.

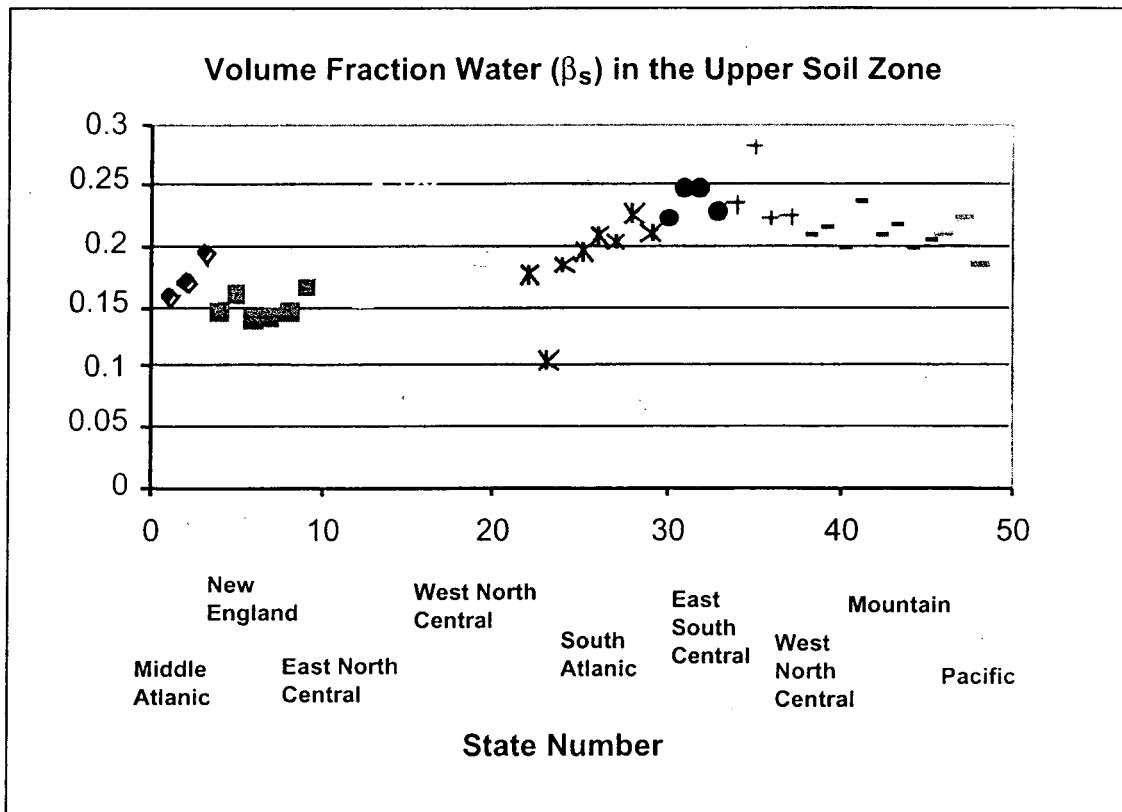


Figure 9. Variation among the 48 contiguous United States in the area-weighted average water content in the root-zone soil as derived from PATRIOT.

#### 4.2.4 Vadose-Zone Soil Parameters Derived from PATRIOT

Using methods described in Section 4.2.1, the mean and CV of vadose-zone soil properties are determined for the 48 conterminous US states and the 9 US regions. Table 17 provides a summary of these root-zone soil properties by region. For the parameters soil depth, organic carbon content, soil-air content, and soil-water content, respectively, Figures 10 through 13 present the variation among the 48 contiguous United States in the area-weighted average values of these parameters in vadose soil. Specific state values for these parameters are provided in Table A-4 of Appendix A.

Table 17 Summary by Region of the Mean and CV of the Upper-Soil-Zone Parameters Calculated Using PATRIOT.

Region	d_v [m]	CV	beta_v	CV	alpha_v	CV	foc_v	CV
Middle Atlantic	1.4	0.40	0.17	0.39	0.22	0.35	0.003	0.23
New England	1.3	0.42	0.14	0.39	0.25	0.40	0.005	0.57
East North Central	1.5	0.28	0.19	0.56	0.20	0.41	0.002	0.15
West North Central	1.5	0.25	0.23	0.59	0.21	0.28	0.003	0.24
South Atlantic	1.7	0.29	0.19	0.37	0.24	0.29	0.003	0.17
East South Central	1.5	0.35	0.24	0.48	0.19	0.38	0.002	0.18
West South Central	1.7	0.34	0.26	0.53	0.16	0.47	0.004	0.31
Mountain	1.3	0.46	0.19	0.50	0.26	0.24	0.003	0.33
Pacific	1.3	0.39	0.20	0.51	0.26	0.29	0.003	0.64
US	1.4	0.37	0.21	0.47	0.22	0.35	0.003	0.37

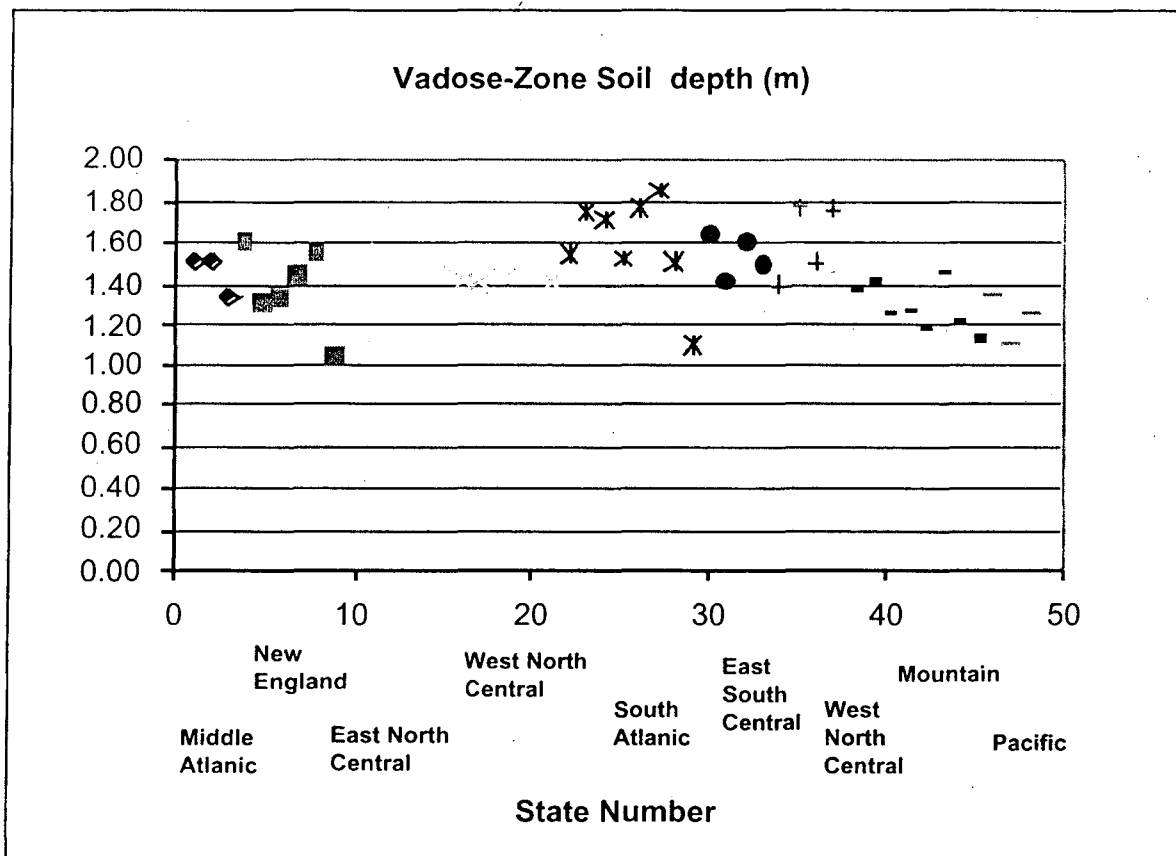


Figure 10. Variation among the 48 contiguous United States in the area-weighted average vadose-zone soil depth as derived from PATRIOT.

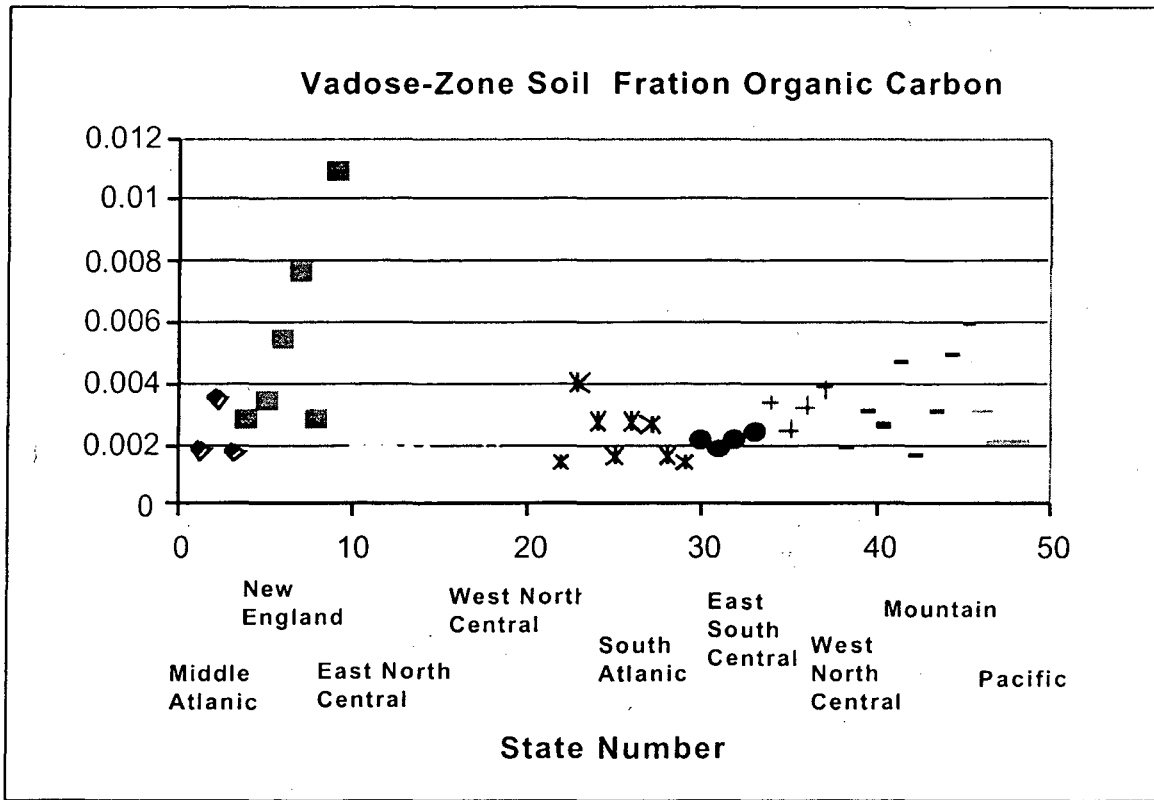


Figure 11. Variation among the 48 contiguous United States in the area-weighted average vadose-zone soil organic carbon fraction as derived from PATRIOT.

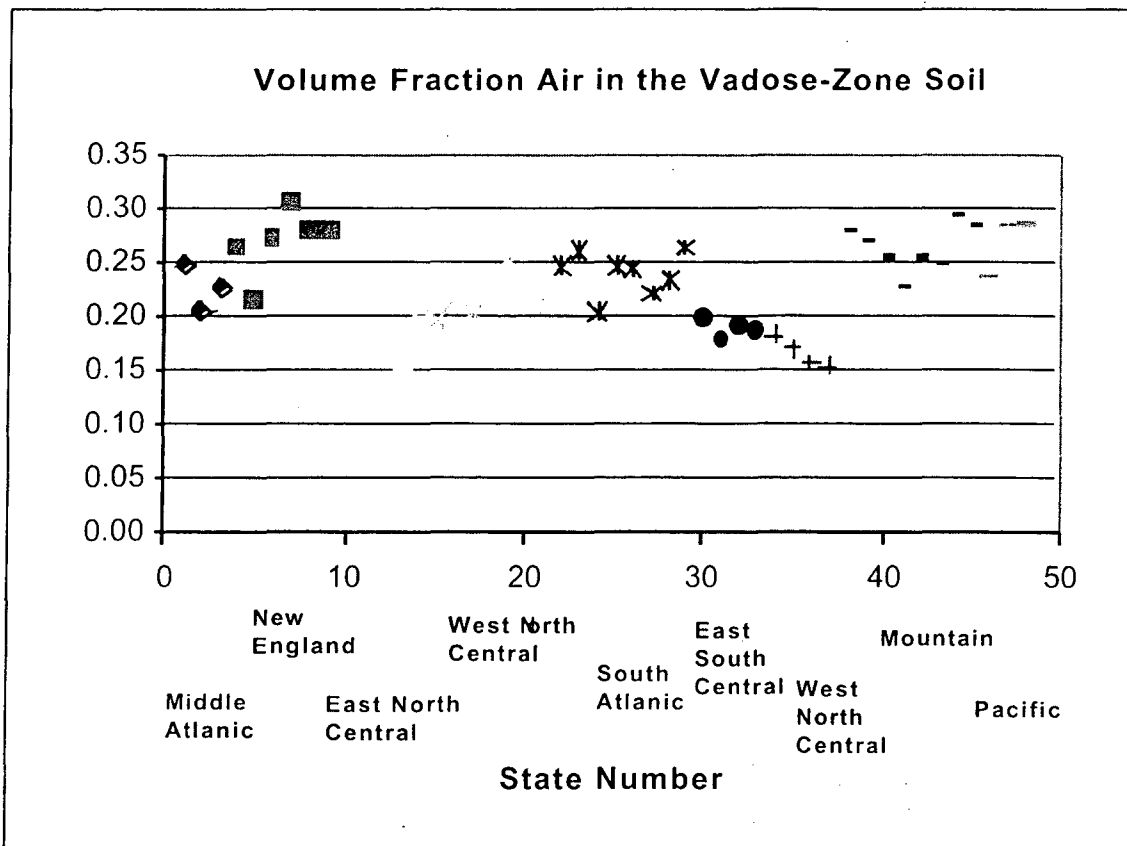


Figure 12. Variation among the 48 contiguous United States in the area-weighted average vadose-zone soil volumetric air content as derived from PATRIOT.

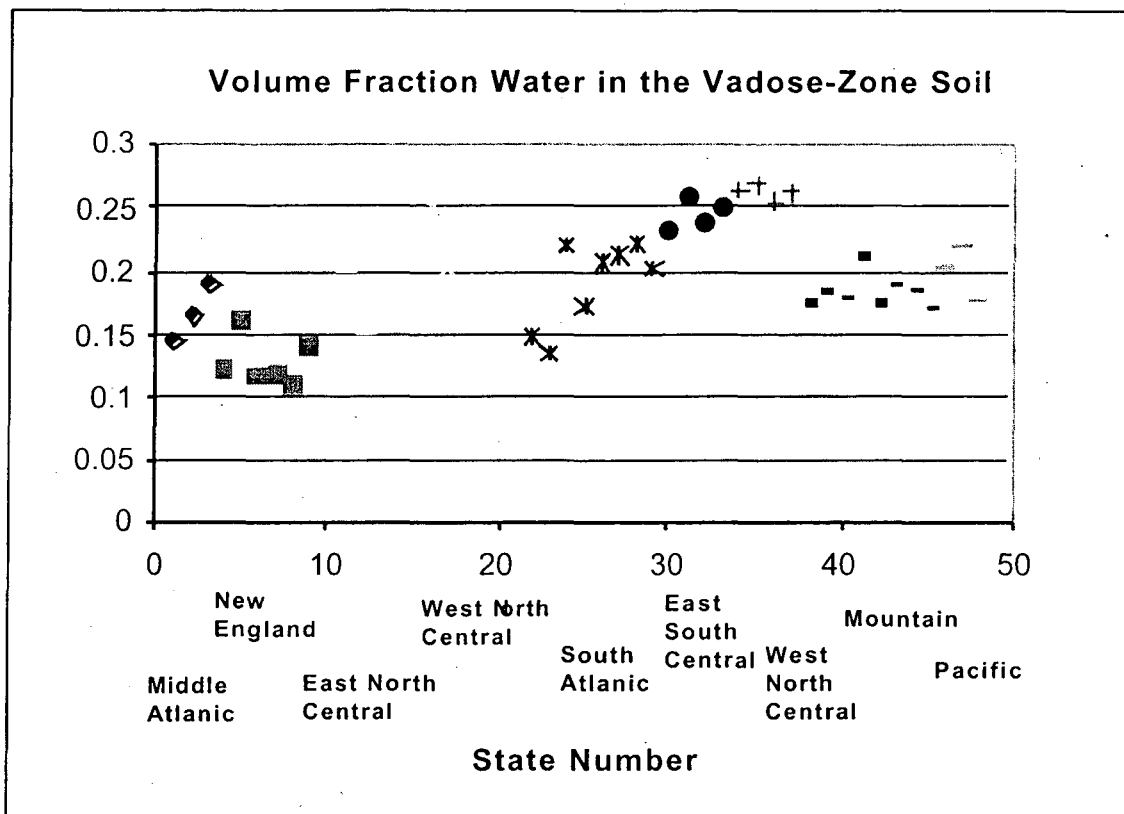


Figure 13. Variation among the 48 contiguous United States in the area-weighted average vadose-zone soil volumetric water content as derived from PATRIOT.

## 5.0 Discussion and Evaluation of Results: Comparison of TEP's for Selected US States

In order to evaluate the impact and value of the multiple-state, multiple region landscape data, TEPs for 278 chemicals in the Scorecard/CalTOX database were developed for six states within different regions of the US. These states have significantly different landscape characteristics. The six states used in this analysis include Maine (New England), California (Pacific), Florida (South Atlantic), Iowa (West North Central), Maine (New England), New Jersey (Middle Atlantic), and Texas (West South Central). TEPs were developed for both carcinogenic and non-carcinogenic effects and for emissions to air and emissions to surface water. Carcinogenic TEP's are in benzene equivalent units (i.e., normalized with respect to benzene). Non carcinogenic TEP's are in toluene equivalent units (i.e., normalized with respect to toluene). The results of this analysis are presented graphically in Figures 14 through 23 (a) and (b).

Figures 14 through 18 are for 1 mol/day air emissions. Figures 19 through 23 are for 1 mol/day surface water emissions. On each page, the "(a)" figure provides a comparison of carcinogen TEPs in benzene equivalents for Florida, Iowa, Maine, New Jersey, and Texas versus California. Also on each page, the "(b)" figure provides a comparison of non-carcinogen TEPs in toluene equivalents for Florida, Iowa, Maine, New Jersey, and Texas versus California non-carcinogen TEPs.

In each figure the x's on the plot correspond to the plot of the logarithm of the TEP in a given state versus the logarithm of the TEP in California. The solid black line is the line that corresponds to no difference in TEP between California and the given state (i.e.  $y=x$ ). The dashed line is the best linear fit of the x's on the plot. A formula for this line is given in each figure. Also on each figure is the  $R^2$ , which is the coefficient of determination that tells us what proportion of variance in the spread of logarithm of TEP observed for each state can be explained when California data is substituted for the landscape data of that state. In all cases, the linear distribution had a  $R^2$  greater than 0.95, suggesting that California or other state's landscape data could be substituted for another state's landscape data with very little impact on the TEP scores obtained for that state.

These results suggest that state-specific TEP values may not be needed for assessments within the conterminous US. Instead TEPs can be reliably derived with a single default US landscape data set. However, there can be situations in which regional and seasonal variations in landscape properties can be important to the LCIA process and these situations should continue to be explored in the development of LCIA measures.

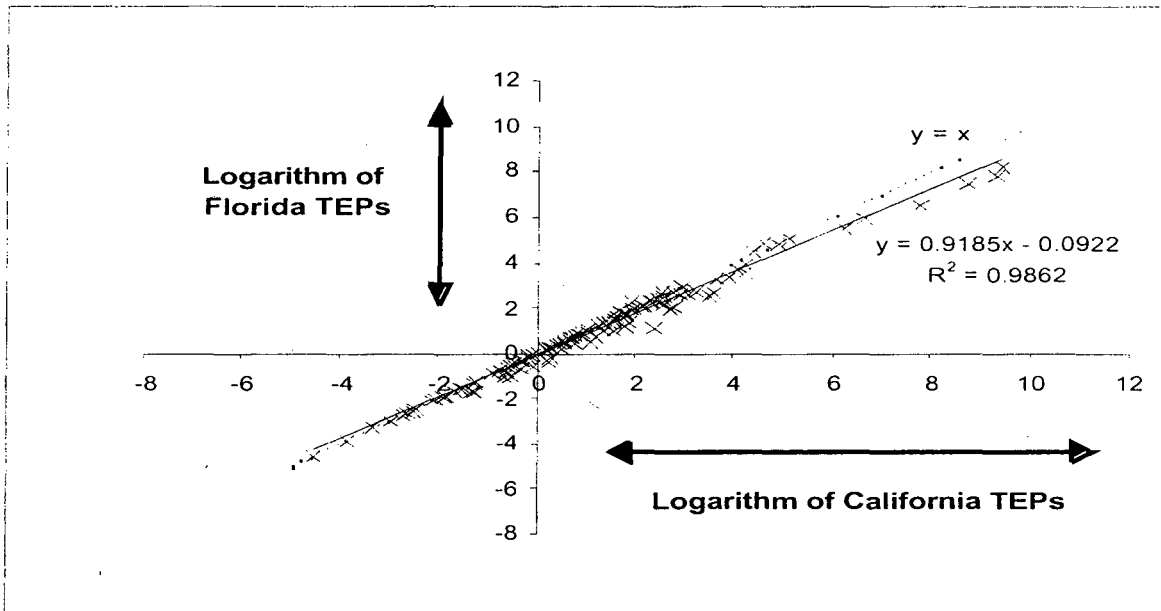


Figure 14(a) Logarithm of Florida carcinogen TEP's (in benzene equivalents) vs. logarithm of California carcinogen TEP's for 1 mol/d air emissions.

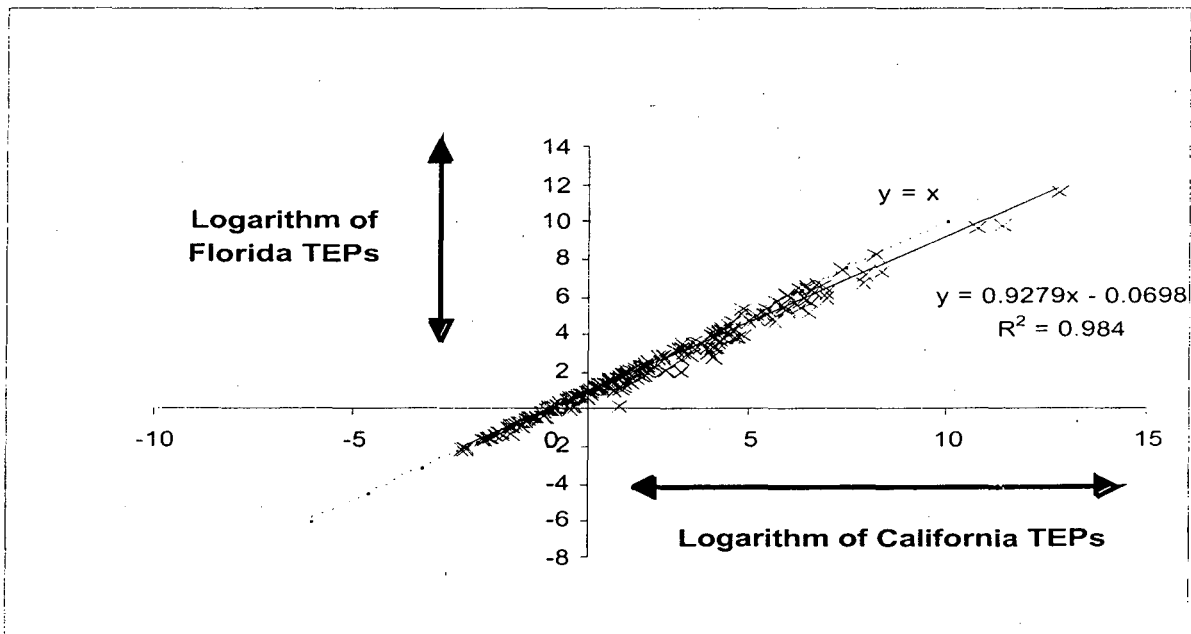


Figure 14(b) Logarithm of Florida non-carcinogen TEP's (in toluene equivalents) vs. logarithm of California non-carcinogen TEP's for 1 mol/d air emissions.



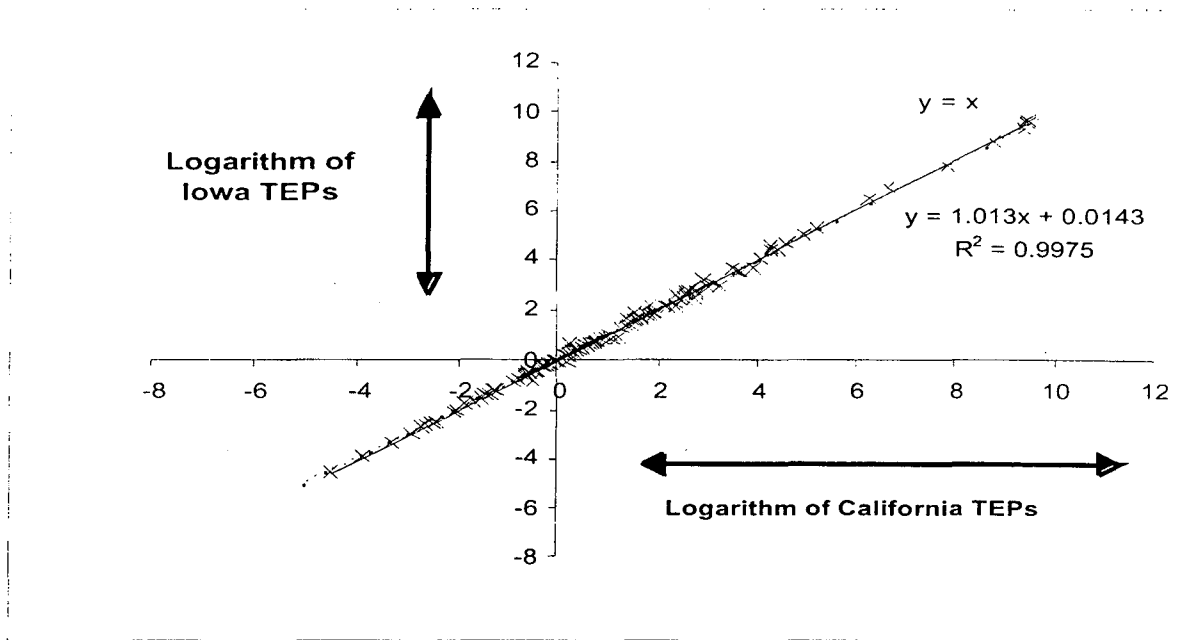


Figure 15(a) Logarithm of Iowa carcinogen TEP's (in benzene equivalents) vs. logarithm of California carcinogen TEP's for 1 mol/d air emissions.

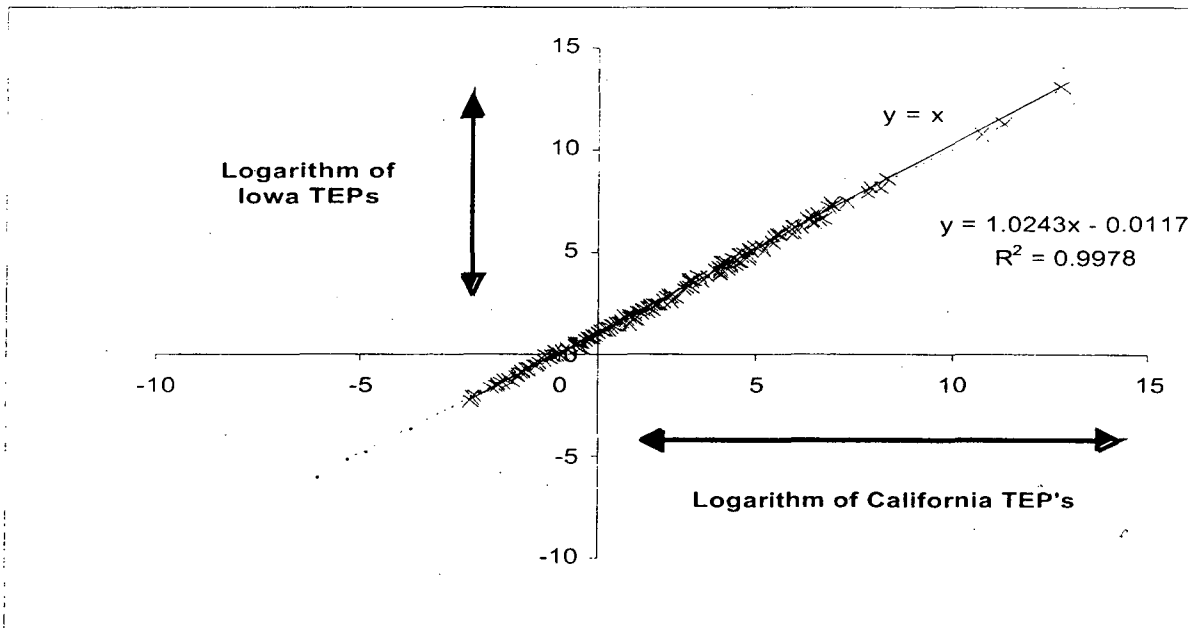


Figure 15(b) Logarithm of Iowa non-carcinogen TEP's (in toluene equivalents) vs. logarithm of California non-carcinogen TEP's for 1 mol/d air emissions.

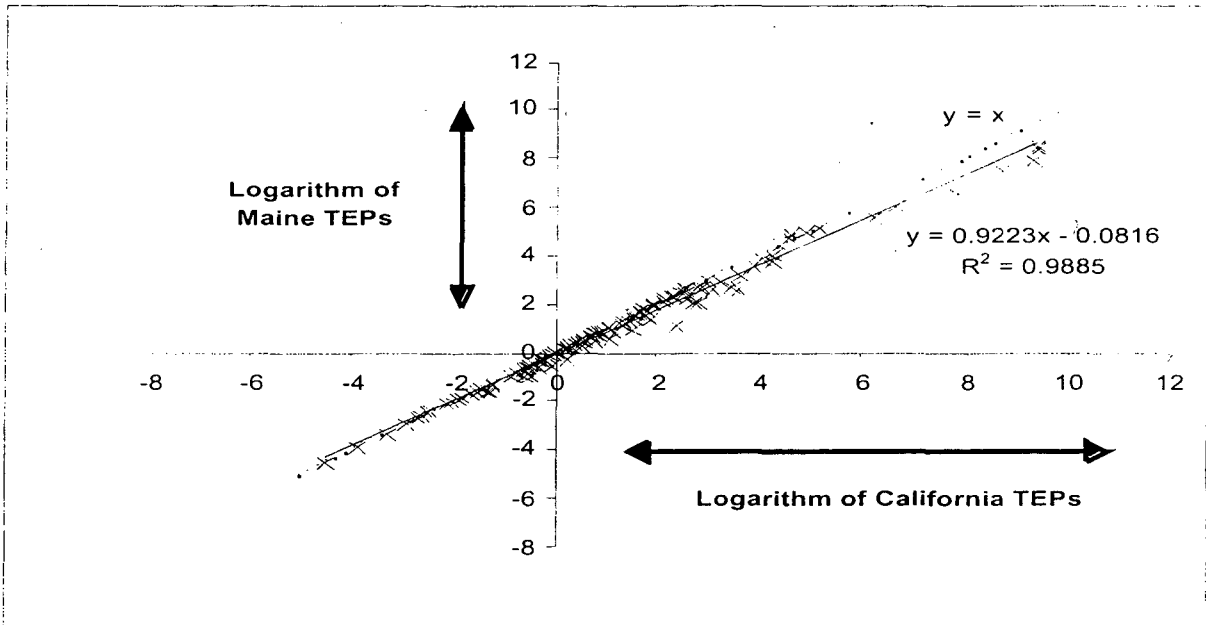


Figure 16(a) Logarithm of Maine carcinogen TEP's (in benzene equivalents) vs. logarithm of California carcinogen TEP's for 1 mol/d air emissions.

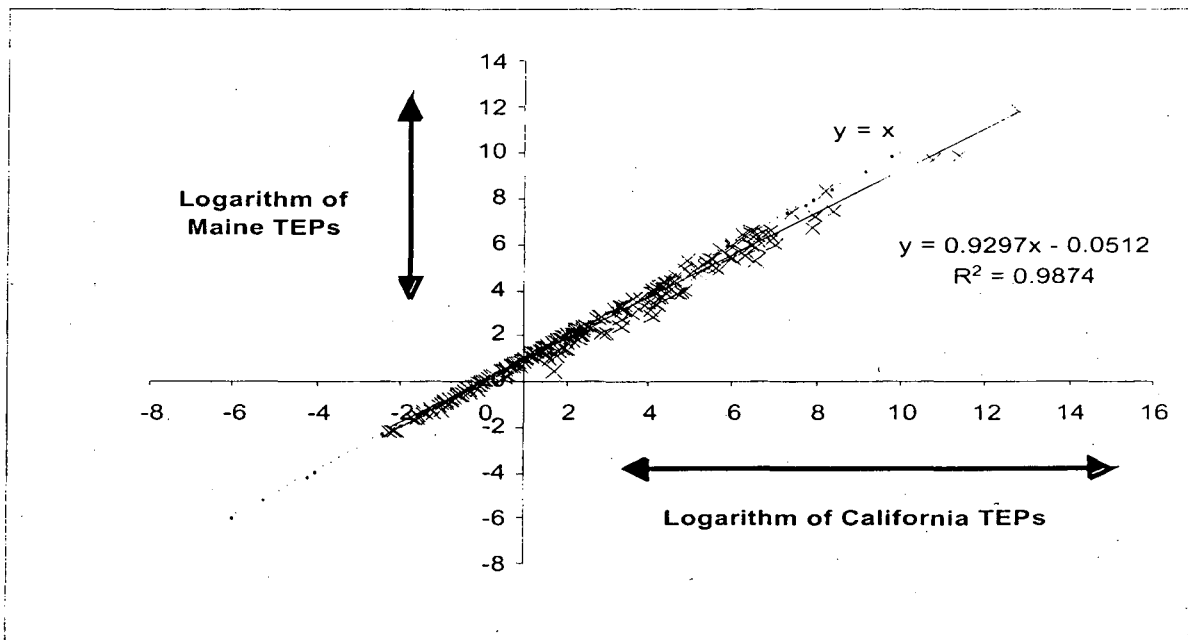


Figure 16(b) Logarithm of Maine non-carcinogen TEP's (in toluene equivalents) vs. logarithm of California non-carcinogen TEP's for 1 mol/d air emissions.

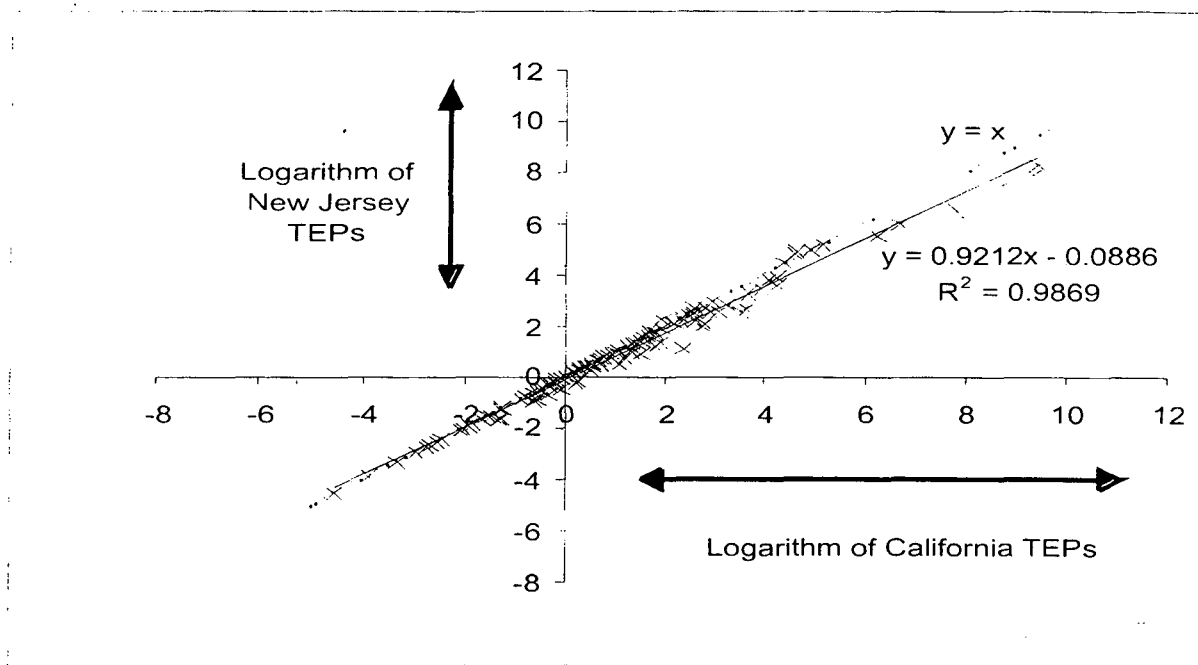


Figure 17(a) Logarithm of New Jersey carcinogen TEP's (in benzene equivalents) vs. logarithm of California carcinogen TEP's for 1 mol/d air emissions.

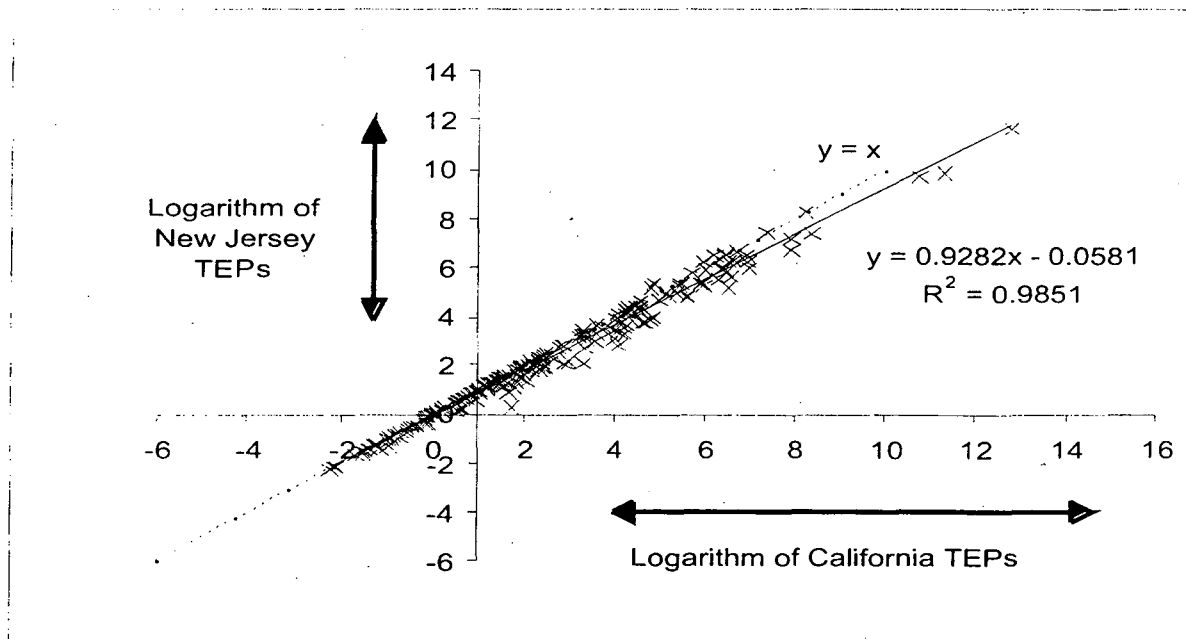


Figure 17(b) Logarithm of New Jersey non-carcinogen TEP's (in toluene equivalents) vs. logarithm of California non-carcinogen TEP's for 1 μmol/d air emissions.

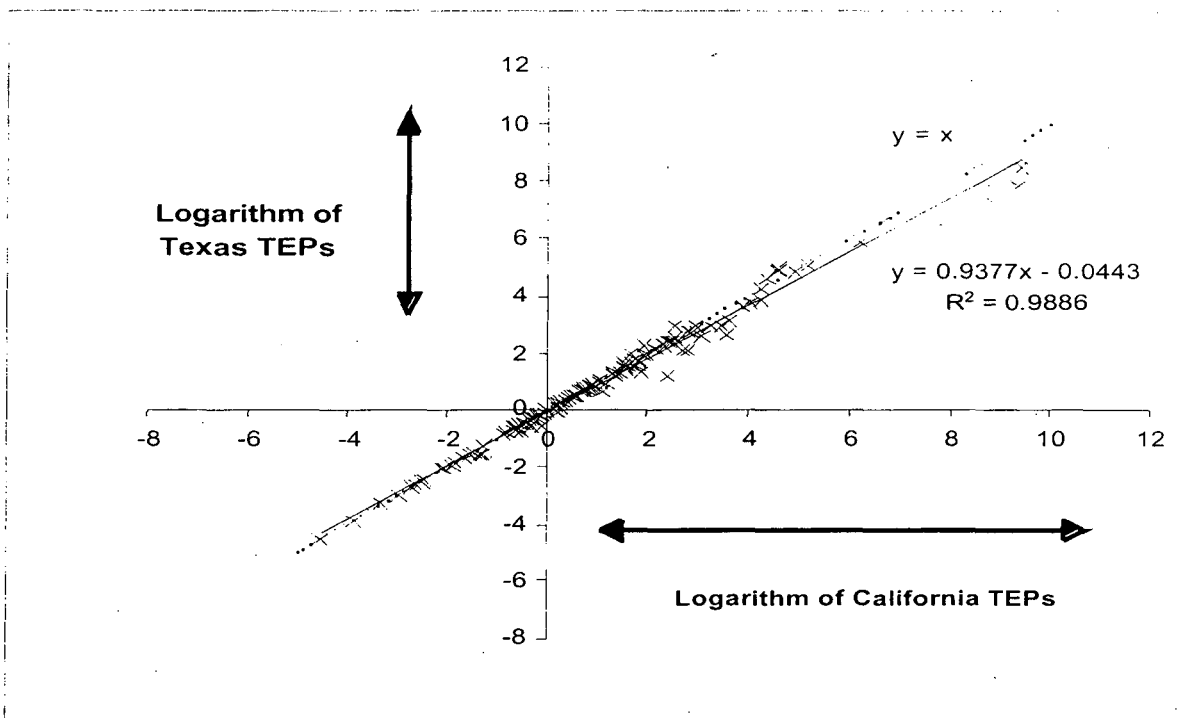


Figure 18(a) Logarithm of Texas carcinogen TEP's (in benzene equivalents) vs. logarithm of California carcinogen TEP's for 1 mol/d air emissions.

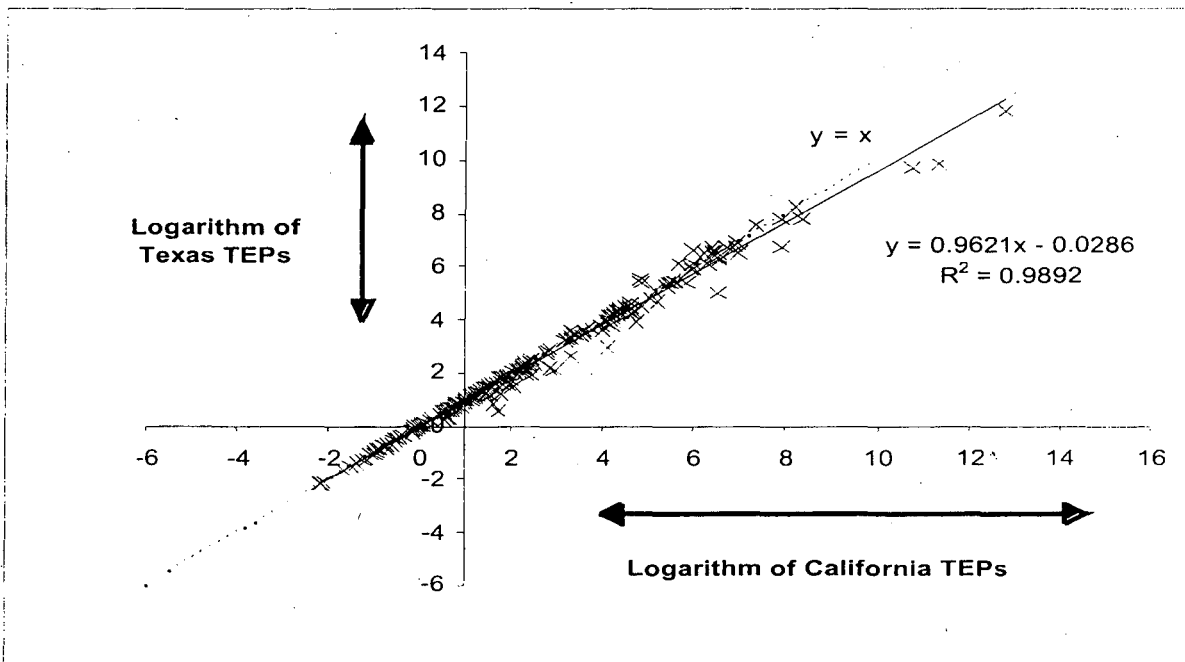


Figure 18(b) Logarithm of Texas non-carcinogen TEP's (in toluene equivalents) vs. logarithm of California non-carcinogen TEP's for 1 mol/d air emissions.

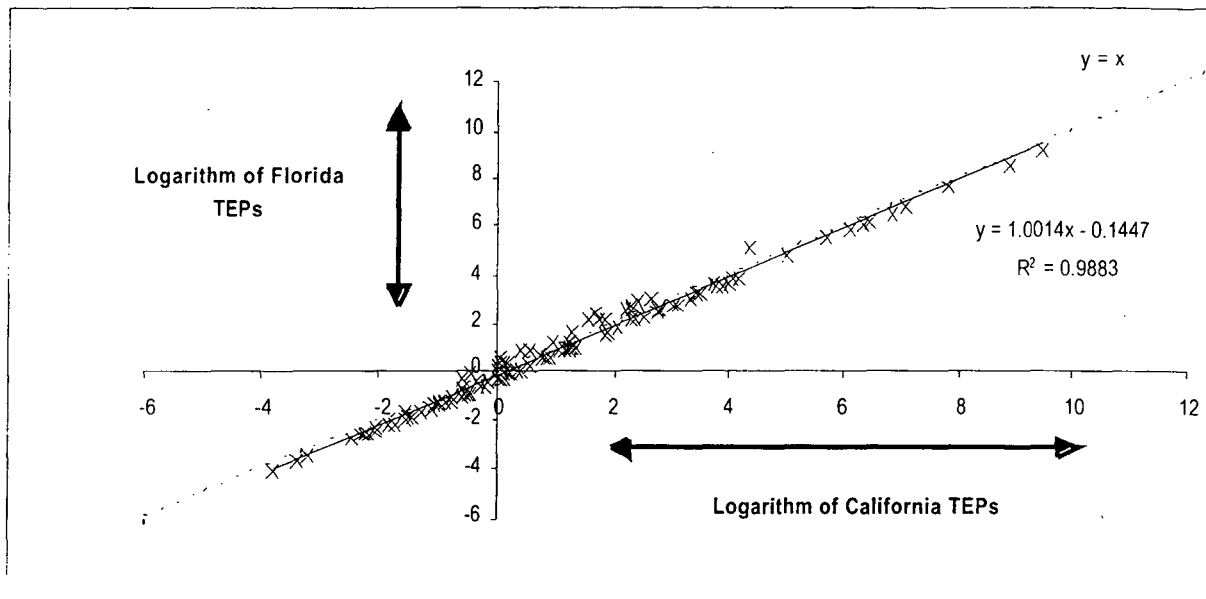


Figure 19(a) Logarithm of Florida carcinogen TEP's (in benzene equivalents) vs. logarithm of California carcinogen TEP's for 1 mol/d surface-water emissions.

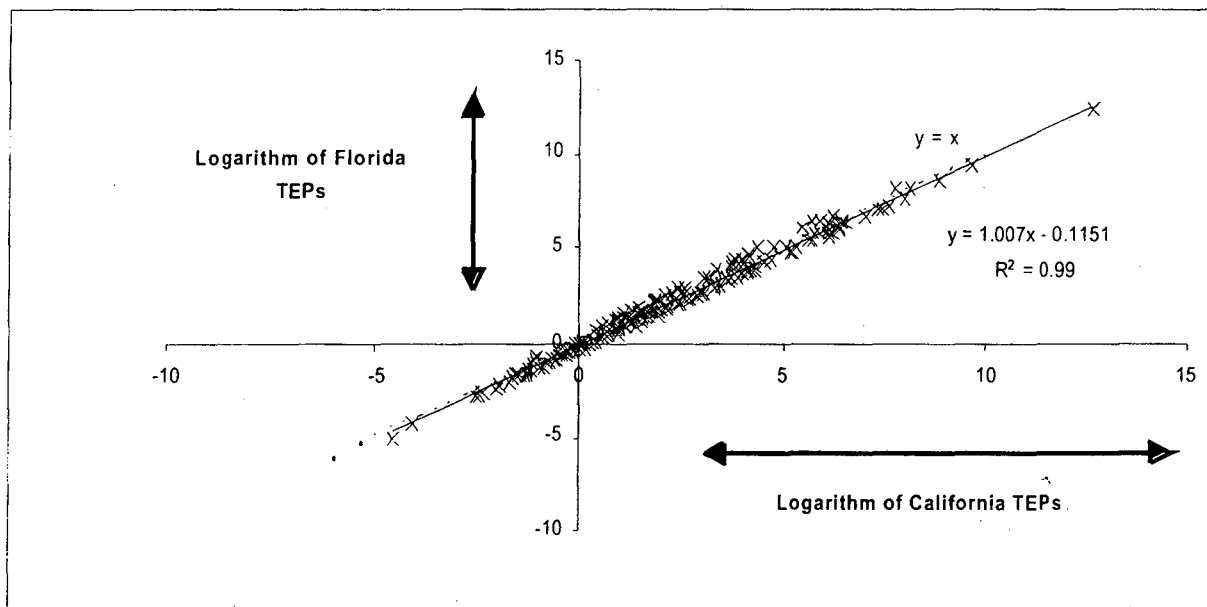


Figure 19(b) Logarithm of Florida non-carcinogen TEP's (in toluene equivalents) vs. logarithm of California non-carcinogen TEP's for 1 mol/d surface-water emissions.

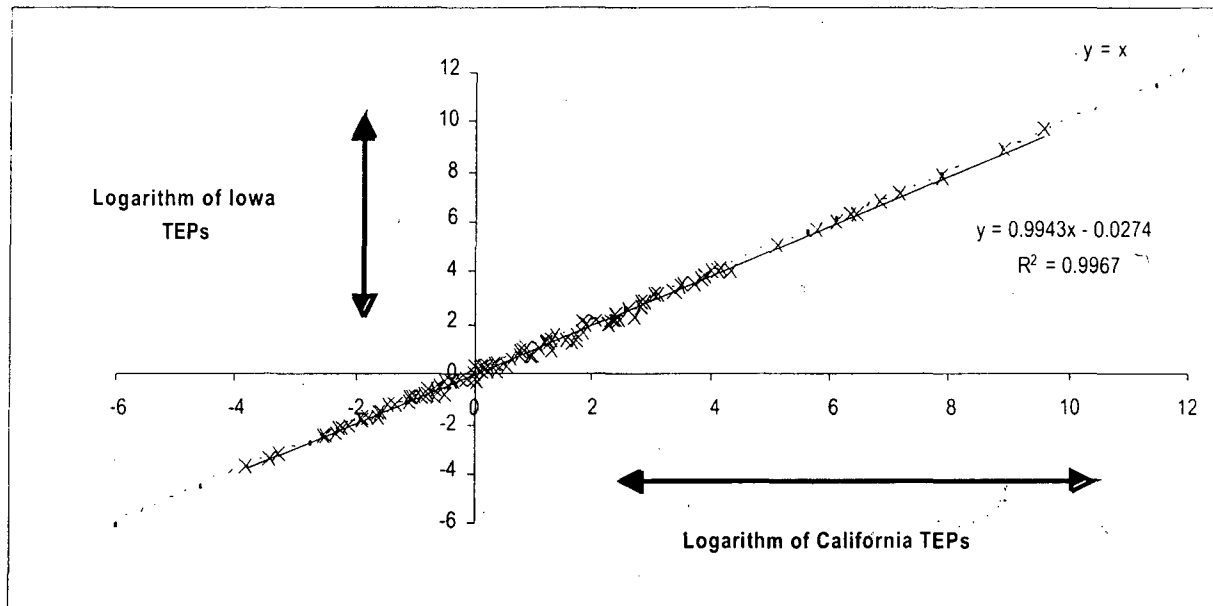


Figure 20(a) Logarithm of Iowa carcinogen TEP's (in benzene equivalents) vs. logarithm of California carcinogen TEP's for 1 mol/d surface-water emissions.

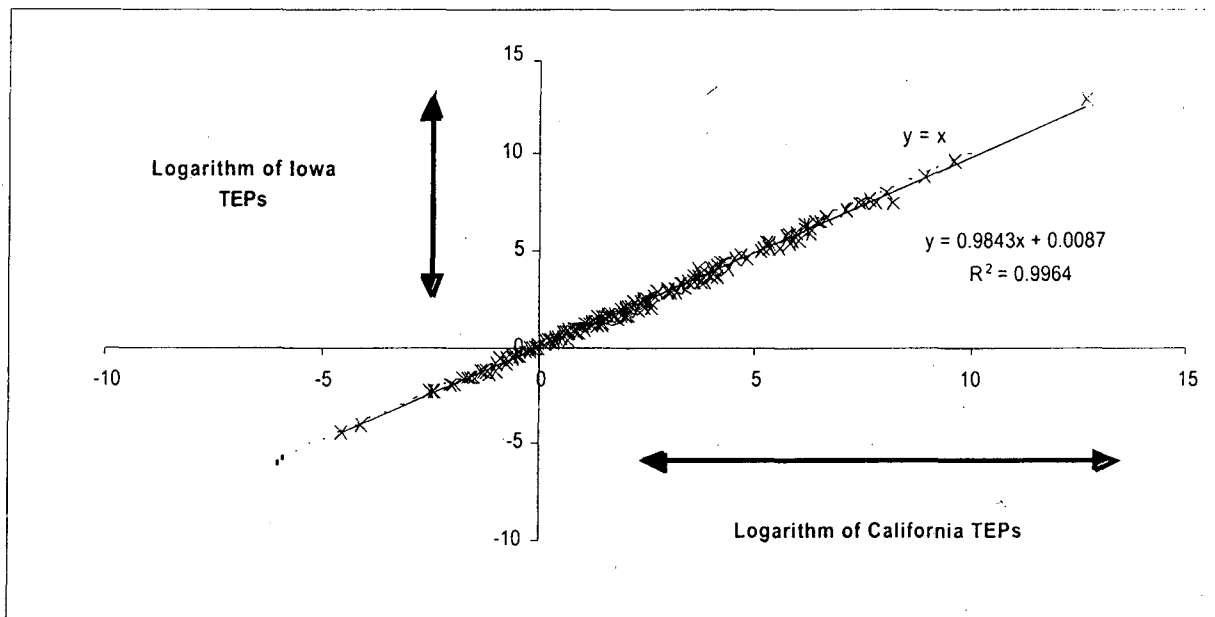


Figure 20(b) Logarithm of Iowa non-carcinogen TEP's (in toluene equivalents) vs. logarithm of California non-carcinogen TEP's for 1 mol/d surface-water emissions.

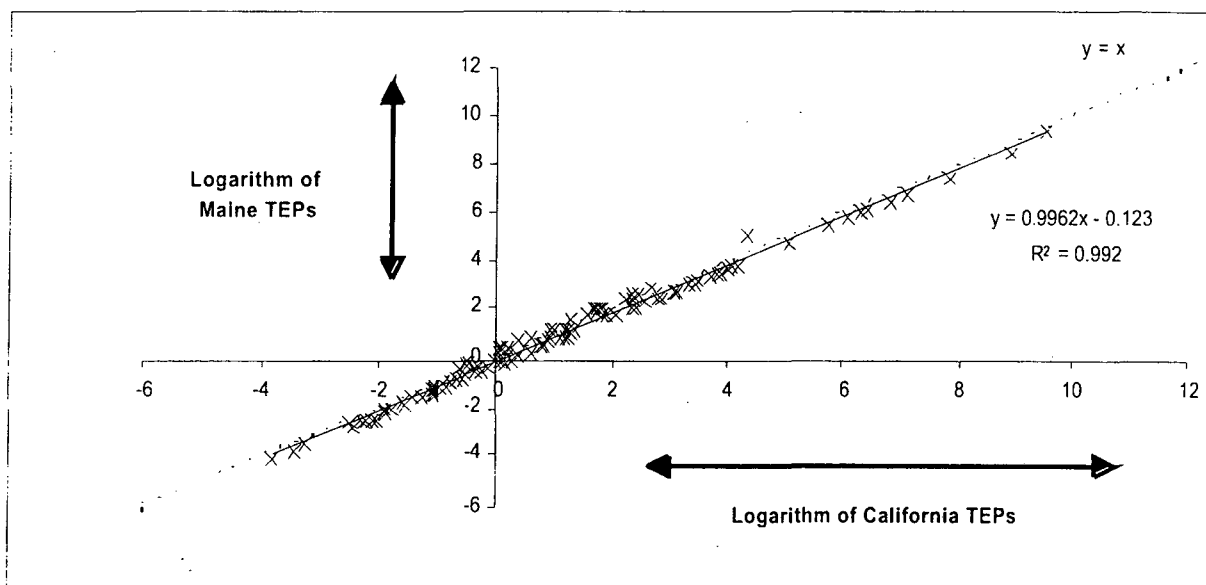


Figure 21(a) Logarithm of Maine carcinogen TEP's (in benzene equivalents) vs. logarithm of California carcinogen TEP's for 1 mol/d surface-water emissions.

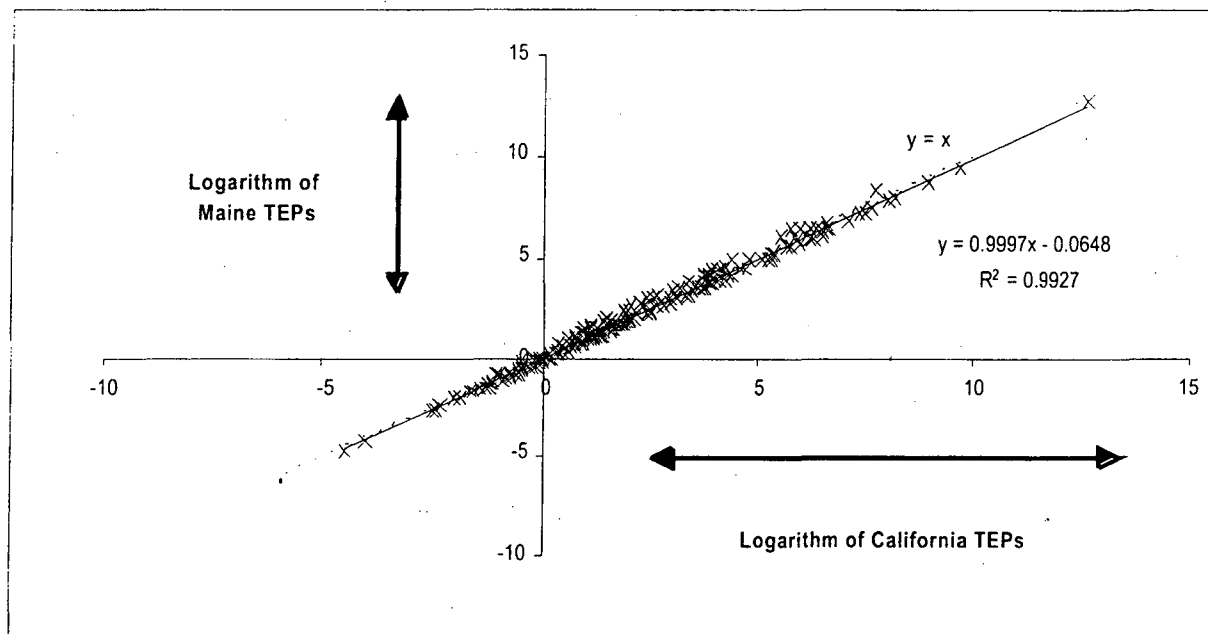


Figure 21(b) Logarithm of Maine non-carcinogen TEP's (in toluene equivalents) vs. logarithm of California non-carcinogen TEP's for 1 mol/d surface-water emissions.

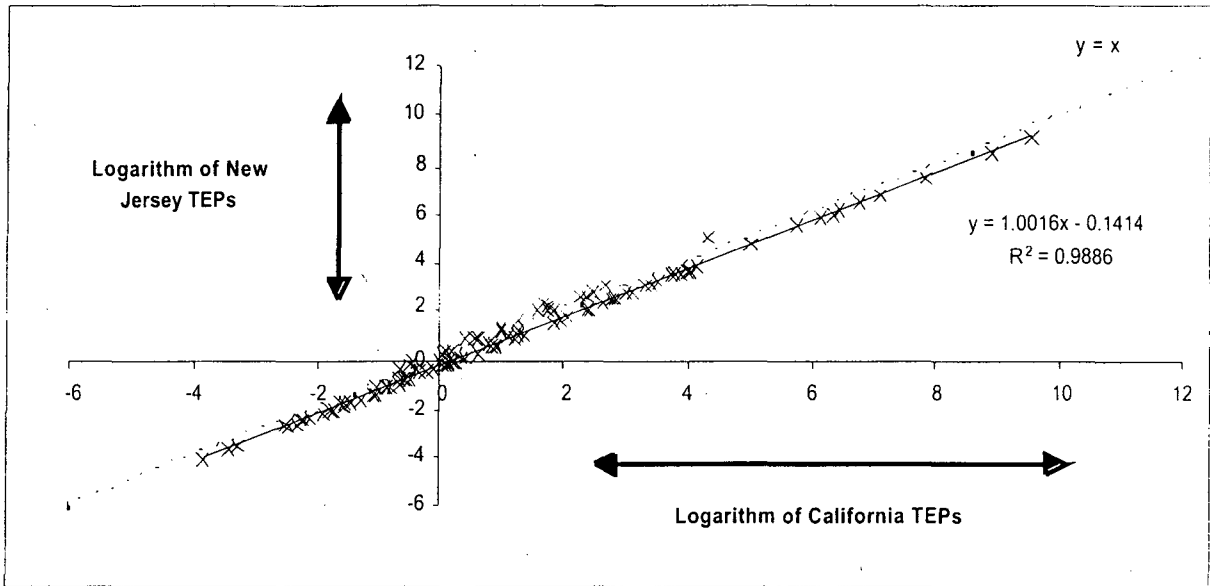


Figure 22(a) Logarithm of New Jersey carcinogen TEP's (in benzene equivalents) vs. logarithm of California carcinogen TEP's for 1 mol/d surface-water emissions.

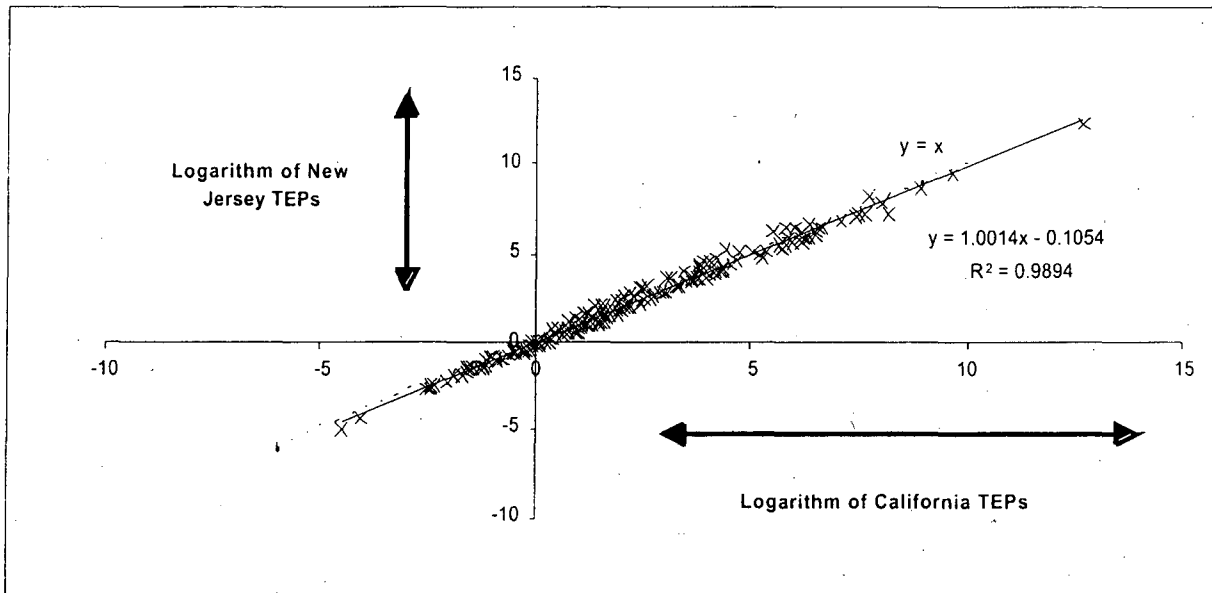


Figure 22(b) Logarithm of New Jersey non-carcinogen TEP's (in toluene equivalents) vs. logarithm of California non-carcinogen TEP's for 1 mol/d surface-water emissions.



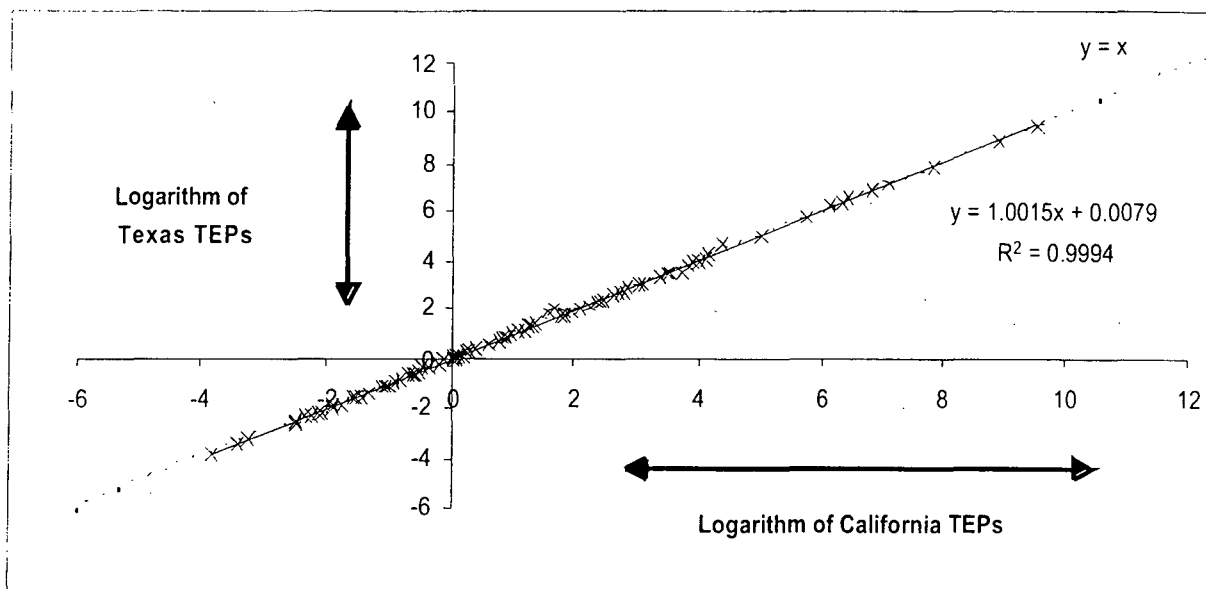


Figure 23(a) Logarithm of Texas carcinogen TEP's (in benzene equivalents) vs. logarithm of California carcinogen TEP's for 1 mol/d surface-water emissions.

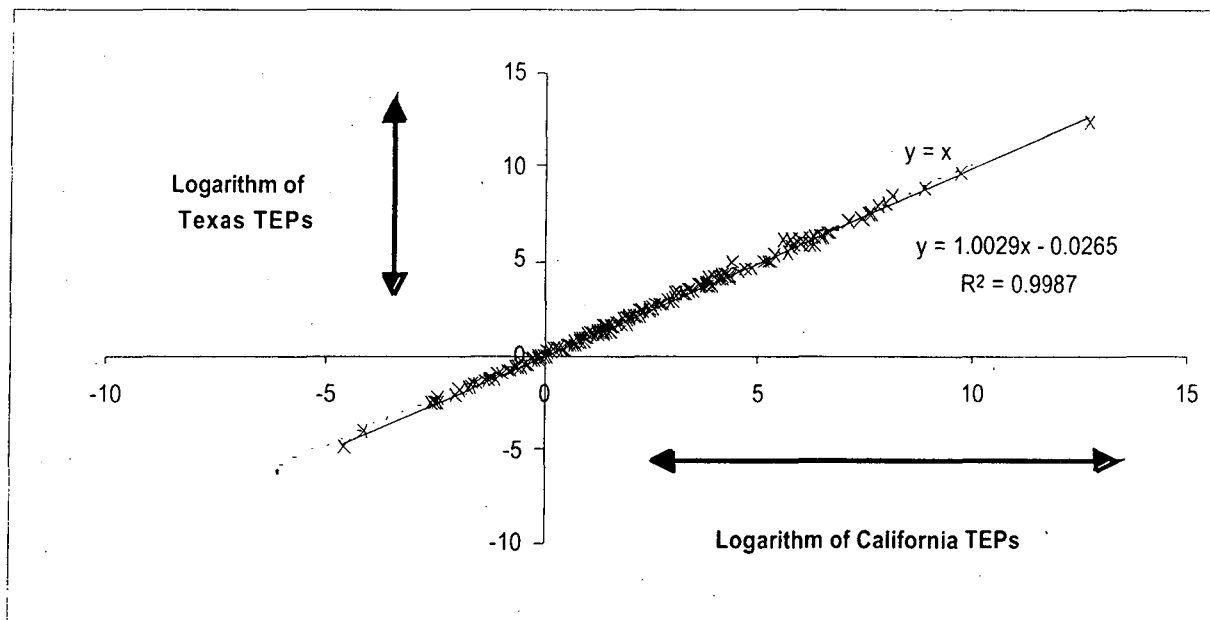


Figure 23(b) Logarithm of Texas non-carcinogen TEP's (in toluene equivalents) vs. logarithm of California non-carcinogen TEP's for 1 mol/d surface-water emissions.

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## Appendix A Summary Tables of State Tabular and PATRIOT-Derived Data for CalTOX

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Table A-1 Summary by State and by Region of Landscape Data Compiled from Tabular Data Sets and Compiled Both by State and by Region for the CalTOX Data Files.

Region	State	state #	f_arw	Temp [K]	CV	Wind Speed [10 <sup>-5</sup> m/d]	CV	Precipitation [10 <sup>-3</sup> m/d]	CV
<b>New England</b>	Connecticut	1	0.126	283	0.05	3.94	0.250	2.99	0.041
	Maine	2	0.085	279	0.11	3.84	0.178	2.82	0.135
	Massachusetts	3	0.152	282	0.05	4.89	0.210	3.21	0.087
	New Hampshire	4	0.038	275	0.37	8.11	0.963	4.71	0.654
	Rhode Island	5	0.151	283	0.00	4.05	0.000	3.17	0.000
	Vermont	6	0.038	280	0.00	3.48	0.000	2.40	0.000
<b>Middle Atlantic</b>	New York	7	0.125	283	0.07	3.96	0.133	2.78	0.121
	New Jersey	8	0.097	285	0.02	3.88	0.021	2.82	0.085
	Pennsylvania	9	0.027	284	0.04	3.46	0.133	2.79	0.066
<b>East North Central</b>	Illinois	10	0.040	283	0.04	3.95	0.048	2.54	0.041
	Indiana	11	0.015	284	0.06	3.64	0.104	2.73	0.088
	Michigan	12	0.413	280	0.08	3.81	0.065	2.23	0.087
	Ohio	13	0.086	283	0.03	3.78	0.087	2.57	0.055
	Wisconsin	14	0.171	280	0.03	3.86	0.112	2.14	0.055
<b>West North Central</b>	Iowa	15	0.007	282	0.04	4.16	0.019	2.28	0.158
	Kansas	16	0.006	285	0.04	4.68	0.122	1.85	0.254
	Minnesota	17	0.084	278	0.08	3.99	0.189	1.95	0.081
	Missouri	18	0.012	290	0.02	2.63	0.082	3.90	0.012
	Nebraska	19	0.006	283	0.03	4.03	0.085	1.66	0.233
	North Dakota	20	0.024	278	0.01	4.18	0.118	1.13	0.183
	South Dakota	21	0.016	280	0.03	4.33	0.017	1.38	0.155

Table A-1 (continued)

Region	State	state #	f_arw	Temp [K]	CV	Wind Speed [10 <sup>-5</sup> m/d]	CV	Precipitation [10 <sup>-3</sup> m/d]	CV
South Atlantic	Delaware	22	0.184	285	0.00	3.48	0.000	2.84	0.000
	District of Columbia	23	0.102	286	0.05	3.24	0.168	2.74	0.029
	Florida	24	0.100	295	0.05	3.23	0.146	3.68	0.138
	Georgia	25	0.018	291	0.03	2.89	0.128	3.36	0.061
	Maryland	26	0.205	286	0.00	3.51	0.000	2.84	0.000
	North Carolina	27	0.075	288	0.05	3.22	0.172	3.31	0.133
	South Carolina	28	0.035	291	0.04	2.88	0.132	3.50	0.028
	Virginia	29	0.064	287	0.03	3.28	0.166	2.92	0.046
	West Virginia	30	0.006	284	0.06	2.68	0.190	2.96	0.040
	East South Central	Alabama	31	0.028	291	0.05	2.96	0.134	3.99
Kentucky		32	0.017	286	0.03	3.21	0.105	3.19	0.078
Mississippi		33	0.028	290	0.02	2.63	0.082	3.90	0.012
Tennessee		34	0.022	288	0.04	2.55	0.247	3.42	0.000
West South Central	Arkansas	35	0.021	289	0.01	2.97	0.018	3.27	0.114
	Louisiana	36	0.123	293	0.02	3.15	0.052	3.89	0.130
	Oklahoma	37	0.021	289	0.00	4.34	0.132	2.57	0.138
	Texas	38	0.020	292	0.06	4.10	0.137	1.96	2.403
Mountain	Arizona	39	0.003	290	0.19	2.90	0.157	0.75	0.693
	Colorado	40	0.004	283	0.10	3.26	0.131	0.82	0.331
	Idaho	41	0.010	283	0.06	3.63	0.105	0.85	0.014
	Montana	42	0.010	280	0.04	5.33	2.191	0.96	0.159
	Nevada	43	0.007	284	0.17	3.10	0.228	0.56	0.303
	New Mexico	44	0.002	287	0.07	3.77	0.181	0.85	0.256
	Utah	45	0.032	284	0.00	3.40	0.000	1.13	0.000
	Wyoming	46	0.007	280	0.01	3.91	0.315	0.95	0.073
Pacific	California	47	0.018	289	0.06	2.80	0.166	1.12	0.560
	Oregon	48	0.012	284	0.07	2.86	0.190	2.31	0.628
	Washington	49	0.057	283	0.04	2.91	0.179	2.96	0.808



Table A-2. Summary by State of the Area-Weighted Mean Value and CV of Ground-Surface-Soil Parameter Value Ranges Derived from the PATRIOT System.

Regions	State	beta_g	CV	alpha-g	CV
Middle Atlantic	New Jersey	0.15	0.29	0.34	0.14
	New York	0.17	0.23	0.36	0.18
	Pennsylvania	0.19	0.12	0.32	0.10
New England	Connecticut	0.15	0.11	0.41	0.08
	Maine	0.16	0.17	0.44	0.13
	Massachusetts	0.14	0.15	0.42	0.10
	New Hampshire	0.14	0.16	0.44	0.11
	Rhode Island	0.15	0.14	0.46	0.26
	Vermont	0.17	0.35	0.43	0.25
East North Central	Illinois	0.23	0.14	0.26	0.15
	Indiana	0.21	0.19	0.25	0.19
	Michigan	0.14	0.32	0.31	0.19
	Ohio	0.22	0.17	0.25	0.19
	Wisconsin	0.18	0.26	0.28	0.15
West North Central	Iowa	0.23	0.14	0.25	0.15
	Kansas	0.22	0.19	0.26	0.19
	Minnesota	0.20	0.32	0.27	0.21
	Missouri	0.21	0.17	0.27	0.20
	Nebraska	0.18	0.38	0.26	0.18
	North Dakota	0.21	0.21	0.28	0.15
	South Dakota	0.25	0.34	0.27	0.26

Table A-2 (continued)

Regions	State	beta_g	CV	alpha-g	CV
South Atlantic	Delaware	0.14	0.27	0.36	0.11
	Florida	0.09	0.36	0.36	0.14
	Georgia	0.15	0.29	0.29	0.15
	Maryland	0.18	0.17	0.27	0.16
	North Carolina	0.16	0.22	0.28	0.13
	South Carolina	0.15	0.30	0.29	0.14
	Virginia	0.18	0.18	0.30	0.14
	West Virginia	0.20	0.19	0.30	0.15
	East South Central	Alabama	0.17	0.29	0.27
Kentucky		0.22	0.18	0.27	0.23
Mississippi		0.20	0.33	0.24	0.25
Tennessee		0.20	0.18	0.26	0.16
West South Central	Arkansas	0.20	0.34	0.25	0.28
	Louisiana	0.23	0.35	0.22	0.30
	Oklahoma	0.20	0.26	0.25	0.21
	Texas	0.22	0.36	0.23	0.31
Mountain	Arizona	0.18	0.30	0.29	0.31
	Colorado	0.19	0.26	0.29	0.13
	Idaho	0.19	0.17	0.29	0.26
	Montana	0.22	0.24	0.29	0.22
	Nevada	0.18	0.25	0.29	0.16
	New Mexico	0.18	0.23	0.29	0.16
	Utah	0.19	0.19	0.31	0.12
Pacific	Wyoming	0.19	0.27	0.31	0.16
	California	0.19	0.33	0.27	0.29
	Oregon	0.20	0.21	0.34	0.25
	Washington	0.18	0.20	0.35	0.17

Table A-3. Summary by State of the Area-Weighted Mean Value and CV of All Root-Zone-Soil Parameter Value Ranges Derived from the PATRIOT System.

Region	State	root-zone soil depth [m]	CV	$f_{oc-s}$	CV	Bulk density kg/L	CV	beta_s	CV	alpha_s	CV
New England	Connecticut	0.58	0.291	0.009	0.806	1.35	0.097	0.14	0.116	0.33	0.127
	Maine	0.55	0.470	0.017	1.615	1.19	0.231	0.16	0.417	0.36	0.211
	Massachusetts	0.59	0.425	0.016	2.784	1.27	0.221	0.14	0.210	0.35	0.157
	New Hampshire	0.54	0.392	0.023	0.996	1.19	0.197	0.14	0.218	0.39	0.191
	Rhode Island	0.59	0.389	0.010	0.774	1.30	0.138	0.14	0.285	0.36	0.213
	Vermont	0.53	0.359	0.021	0.929	1.19	0.172	0.16	0.318	0.37	0.278
Middle Atlantic	New Jersey	0.88	0.351	0.008	2.336	1.39	0.122	0.16	0.443	0.30	0.207
	New York	0.62	0.378	0.013	1.691	1.32	0.136	0.17	0.446	0.31	0.232
	Pennsylvania	0.73	0.380	0.006	1.193	1.37	0.057	0.19	0.353	0.28	0.202
East North Central	Illinois	0.93	0.381	0.009	1.544	1.39	0.067	0.24	0.991	0.23	0.222
	Indiana	0.87	0.347	0.007	1.469	1.46	0.074	0.23	0.673	0.21	0.309
	Michigan	0.72	0.437	0.009	1.787	1.40	0.227	0.16	0.400	0.27	0.290
	Ohio	0.81	0.344	0.007	1.268	1.46	0.060	0.24	0.558	0.19	0.421
	Wisconsin	0.73	0.502	0.008	2.042	1.41	0.207	0.18	0.677	0.25	0.273
West North Central	Iowa	0.97	0.297	0.014	1.425	1.38	0.077	0.24	0.651	0.22	0.214
	Kansas	0.80	0.469	0.010	1.005	1.39	0.071	0.24	0.709	0.22	0.321
	Minnesota	0.76	0.495	0.014	1.804	1.33	0.258	0.20	0.642	0.24	0.298
	Missouri	0.77	0.517	0.007	1.318	1.38	0.067	0.24	0.647	0.23	0.313
	Nebraska	0.96	0.449	0.006	1.504	1.47	0.148	0.19	0.846	0.25	0.202
	North Dakota	0.67	0.510	0.014	1.087	1.37	0.055	0.21	0.498	0.25	0.202
	South Dakota	0.63	0.518	0.010	1.138	1.31	0.092	0.26	0.612	0.23	0.306

Table A-3. (continued)

Region	State	root-zone soil depth [m]	CV	$f_{oc-s}$	CV	Bulk density kg/L	CV	beta_s	CV	alpha_s	CV
<b>South Atlantic</b>	Delaware	0.97	0.289	0.006	1.293	1.43	0.066	0.17	0.407	0.27	0.274
	Florida	1.11	0.501	0.009	2.330	1.43	0.185	0.11	0.354	0.32	0.183
	Georgia	0.88	0.599	0.006	1.815	1.46	0.076	0.18	0.406	0.25	0.219
	Maryland	0.85	0.372	0.005	1.106	1.40	0.076	0.19	0.440	0.25	0.214
	North Carolina	0.93	0.516	0.007	2.748	1.41	0.127	0.20	0.424	0.24	0.252
	South Carolina	1.03	0.535	0.006	2.131	1.45	0.071	0.20	0.452	0.24	0.274
	Virginia	0.79	0.475	0.005	2.379	1.39	0.065	0.22	0.406	0.24	0.310
	West Virginia	0.77	0.343	0.005	0.929	1.36	0.044	0.21	0.405	0.26	0.252
<b>East South Central</b>	Alabama	0.96	0.554	0.005	1.544	1.46	0.068	0.21	0.471	0.22	0.289
	Kentucky	0.81	0.376	0.007	1.123	1.40	0.055	0.24	0.529	0.21	0.368
	Mississippi	0.96	0.378	0.004	1.321	1.45	0.070	0.23	0.721	0.19	0.452
	Tennessee	0.83	0.507	0.005	1.310	1.43	0.046	0.22	0.556	0.23	0.260
<b>West South Central</b>	Arkansas	0.70	0.584	0.007	1.146	1.43	0.055	0.22	0.671	0.22	0.227
	Louisiana	0.99	0.387	0.006	1.179	1.39	0.164	0.27	0.739	0.17	0.207
	Oklahoma	0.89	0.545	0.006	1.368	1.48	0.040	0.21	0.566	0.21	0.191
	Texas	0.94	0.477	0.007	1.238	1.45	0.060	0.25	0.548	0.19	0.225
<b>Mountain</b>	Arizona	0.73	0.604	0.004	1.848	1.40	0.117	0.20	0.436	0.26	0.342
	Colorado	0.74	0.566	0.006	1.268	1.38	0.075	0.21	0.550	0.26	0.196
	Idaho	0.85	0.490	0.009	1.184	1.38	0.147	0.19	0.624	0.26	0.292
	Montana	0.56	0.624	0.008	1.285	1.35	0.078	0.23	0.509	0.25	0.288
	Nevada	0.68	0.626	0.005	1.398	1.40	0.077	0.20	0.494	0.26	0.219
	New Mexico	0.83	0.553	0.004	1.335	1.42	0.064	0.21	0.452	0.24	0.241
	Utah	0.81	0.572	0.008	1.488	1.33	0.076	0.19	0.445	0.29	0.158
	Wyoming	0.62	0.659	0.008	0.841	1.35	0.089	0.20	0.444	0.28	0.183
<b>Pacific</b>	California	0.79	0.470	0.008	1.979	1.41	0.124	0.20	0.479	0.25	0.313
	Oregon	0.79	0.522	0.012	1.505	1.22	0.143	0.22	0.525	0.31	0.318
	Washington	0.69	0.502	0.012	1.615	1.20	0.203	0.18	0.598	0.32	0.212

Table A-4. Summary by State of the Area-Weighted Mean Value and CV of All Vadose-Zone-Soil Parameter Value Ranges Derived from the PATRIOT System.

Region	State	vadose depth [m]	CV	$f_{oc-v}$	CV	bulk density	CV	beta_v	CV	alpha_v	CV
<b>New England</b>	Connecticut	1.60	0.340	0.003	2.903	1.60	0.110	0.12	0.342	0.26	0.348
	Maine	1.31	0.359	0.003	0.766	1.62	0.140	0.16	0.337	0.22	0.516
	Massachusetts	1.33	0.371	0.006	1.491	1.34	0.240	0.12	0.716	0.27	0.367
	New Hampshire	1.44	0.686	0.008	0.875	1.50	0.145	0.12	0.440	0.30	0.364
	Rhode Island	1.55	0.149	0.003	0.712	1.59	0.122	0.11	0.275	0.28	0.364
	Vermont	1.05	0.442	0.011	1.152	1.52	0.151	0.14	0.454	0.28	0.411
<b>Middle Atlantic</b>	New Jersey	1.52	0.261	0.002	1.406	1.56	0.074	0.15	0.320	0.25	0.243
	New York	1.52	0.351	0.004	1.474	1.62	0.120	0.17	0.393	0.21	0.422
	Pennsylvania	1.35	0.528	0.002	1.079	1.37	0.165	0.19	0.237	0.23	0.364
<b>East North Central</b>	Illinois	1.51	0.220	0.002	1.911	1.51	0.066	0.23	0.198	0.19	0.296
	Indiana	1.57	0.264	0.002	1.742	1.59	0.083	0.21	0.273	0.18	0.410
	Michigan	1.54	0.291	0.002	1.156	1.55	0.138	0.16	0.443	0.23	0.393
	Ohio	1.53	0.259	0.002	1.157	1.58	0.083	0.23	0.260	0.16	0.546
	Wisconsin	1.35	0.352	0.002	2.020	1.60	0.087	0.17	0.454	0.21	0.382
<b>West North Central</b>	Iowa	1.48	0.198	0.003	2.018	1.50	0.079	0.23	0.214	0.20	0.251
	Kansas	1.42	0.274	0.005	1.234	1.39	0.082	0.25	0.242	0.22	0.311
	Minnesota	1.41	0.256	0.003	2.431	1.40	0.141	0.20	0.410	0.20	0.361
	Missouri	1.50	0.363	0.002	1.339	1.43	0.097	0.28	0.252	0.17	0.428
	Nebraska	1.49	0.220	0.003	1.257	1.44	0.115	0.19	0.360	0.25	0.169
	North Dakota	1.48	0.266	0.003	1.074	1.45	0.055	0.22	0.245	0.22	0.220
	South Dakota	1.41	0.298	0.003	1.273	1.42	0.087	0.24	0.285	0.21	0.302

Table A-4 (continued)

Region	State	vadose depth [m]	CV	$f_{oc-v}$	CV	bulk density	CV	beta_v	CV	alpha_v	CV
<b>South Atlantic</b>	Delaware	1.54	0.169	0.001	0.746	1.57	0.075	0.15	0.245	0.25	0.297
	Florida	1.76	0.364	0.004	2.001	1.57	0.055	0.13	0.447	0.26	0.283
	Georgia	1.72	0.338	0.003	2.087	1.50	0.086	0.22	0.299	0.20	0.381
	Maryland	1.52	0.250	0.002	1.681	1.51	0.093	0.17	0.275	0.25	0.288
	North Carolina	1.78	0.277	0.003	2.218	1.42	0.077	0.21	0.309	0.24	0.284
	South Carolina	1.85	0.258	0.003	1.872	1.47	0.091	0.21	0.293	0.22	0.345
	Virginia	1.50	0.318	0.002	1.594	1.41	0.062	0.22	0.377	0.23	0.350
	West Virginia	1.10	0.393	0.001	0.790	1.39	0.048	0.20	0.262	0.26	0.251
<b>East South Central</b>	Alabama	1.65	0.356	0.002	1.584	1.48	0.072	0.23	0.284	0.20	0.312
	Kentucky	1.41	0.348	0.002	1.232	1.46	0.063	0.26	0.282	0.18	0.450
	Mississippi	1.60	0.260	0.002	1.216	1.49	0.061	0.24	0.342	0.19	0.442
	Tennessee	1.49	0.352	0.002	1.698	1.46	0.057	0.25	0.255	0.19	0.369
<b>West South Central</b>	Arkansas	1.40	0.410	0.003	1.316	1.44	0.030	0.26	0.318	0.18	0.407
	Louisiana	1.77	0.222	0.002	1.292	1.46	0.084	0.27	0.338	0.17	0.438
	Oklahoma	1.51	0.375	0.003	1.247	1.53	0.068	0.25	0.311	0.16	0.557
	Texas	1.76	0.336	0.004	0.952	1.51	0.066	0.26	0.267	0.16	0.479
<b>Mountain</b>	Arizona	1.36	0.461	0.002	1.221	1.46	0.164	0.18	0.317	0.28	0.282
	Colorado	1.41	0.390	0.003	1.223	1.43	0.073	0.18	0.315	0.27	0.151
	Idaho	1.25	0.367	0.003	1.323	1.48	0.118	0.18	0.371	0.25	0.324
	Montana	1.27	0.405	0.005	1.145	1.46	0.095	0.21	0.289	0.22	0.314
	Nevada	1.19	0.460	0.002	0.961	1.49	0.077	0.18	0.382	0.25	0.215
	New Mexico	1.46	0.608	0.003	1.090	1.47	0.057	0.19	0.310	0.25	0.247
	Utah	1.22	0.442	0.005	1.696	1.36	0.085	0.19	0.292	0.29	0.154
	Wyoming	1.13	0.492	0.006	0.500	1.42	0.076	0.17	0.313	0.28	0.151
<b>Pacific</b>	California	1.34	0.373	0.003	0.957	1.46	0.122	0.20	0.317	0.24	0.300
	Oregon	1.11	0.434	0.002	0.788	1.29	0.114	0.22	0.309	0.28	0.297
	Washington	1.25	0.364	0.002	1.563	1.35	0.154	0.18	0.414	0.28	0.265

Table A-5. Summary by Region of All Calculated CalTOX Inputs as Mean Values and CVs.

Calculated CalTOX values		Middle Atlantic		New England		East North Central		West North Central		South Atlantic	
		mean	CV	mean	CV	mean	CV	mean	CV	mean	CV
Regional area in m <sup>2</sup>	<i>Area</i>	2.80E+11	0.300	1.78E+11	1.254	7.71E+11	0.500	1.35E+12	0.700	7.36E+11	0.900
annual average precipitation (m/d)	<i>rain</i>	2.79E-03	0.094	3.09E-03	0.281	3.15E-03	0.069	2.88E-03	0.163	3.31E-03	0.085
land surface runoff (m/d)	<i>runoff</i>	1.01E-03	1.000	1.01E-03	1.000	1.12E-03	1.000	1.85E-04	0.926	1.14E-03	1.000
plant dry mass inventory (kg[DM]/m <sup>2</sup> )	<i>bio_inv</i>	3.00E+01	1.000	3.00E+01	1.000	3.00E+01	1.000	1.78E+01	0.926	3.00E+01	1.000
ground-water recharge (m/d)	<i>recharge</i>	1.41E-04	1.000	1.56E-04	1.000	1.59E-04	1.000	1.45E-04	0.926	1.65E-04	1.000
evaporation of water from surface water (m/d)	<i>evaporate</i>	1.70E-04	1.000	1.33E-04	0.913	4.32E-04	1.000	5.35E-05	0.926	2.06E-04	1.000
water content in surface soil (volume fraction)	<i>beta_g</i>	1.74E-01	0.344	1.54E-01	0.306	1.86E-01	0.595	1.76E-01	0.568	1.49E-01	0.363
air content in the surface soil (volume fraction)	<i>alpha_g</i>	3.41E-01	0.145	4.34E-01	0.169	2.79E-01	0.173	2.25E-01	0.167	3.05E-01	0.132
erosion of surface soil (kg/m <sup>2</sup> -d)	<i>erosion_g</i>	2.89E-04	1.000	2.89E-04	1.000	5.46E-04	1.000	4.65E-04	1.000	2.22E-04	1.000
thickness of the root-zone soil (m)	<i>d_s</i>	6.86E-01	0.375	5.55E-01	0.396	7.94E-01	0.411	6.96E-01	0.437	9.32E-01	0.442
water content of root-zone soil (vol. fraction)	<i>beta_s</i>	1.79E-01	0.377	1.53E-01	0.337	2.00E-01	0.609	1.87E-01	0.576	1.79E-01	0.401
air content of root-zone soil (vol. fraction)	<i>alpha_s</i>	2.97E-01	0.214	3.62E-01	0.202	2.38E-01	0.310	2.00E-01	0.244	2.63E-01	0.236
thickness of the vadose-zone soil (m)	<i>d_v</i>	1.45E+00	0.396	1.32E+00	0.422	1.50E+00	0.280	1.45E+00	0.248	1.66E+00	0.286
water content; vadose-zone soil (vol. fraction)	<i>beta_v</i>	1.74E-01	0.388	1.43E-01	0.392	1.94E-01	0.562	1.93E-01	0.589	1.93E-01	0.370
air content of vadose-zone soil (vol. fraction)	<i>alpha_v</i>	2.20E-01	0.351	2.49E-01	0.397	2.01E-01	0.414	1.80E-01	0.280	2.37E-01	0.295
fraction of land area in surface water	<i>f_arw</i>	8.13E-02	0.200	8.57E-02	0.200	1.93E-01	0.200	2.15E-02	0.185	6.31E-02	0.200
ambient environmental temperature (K)	<i>Temp</i>	2.83E+02	0.000	2.81E+02	0.000	2.82E+02	0.000	2.41E+02	0.000	2.90E+02	0.000

Table A-5 (continued). Summary by US Region of All Calculated CalTOX Input Mean Values and CV's.

Calculated CalTOX values		East South Central		West South Central		Mountain		Pacific	
		mean	CV	mean	CV	mean	CV	mean	CV
contaminated area in m <sup>2</sup>	<i>Area</i>	4.74E+11	0.300	1.14E+12	0.400	2.24E+12	0.800	8.46E+11	0.300
annual average precipitation (m/d)	<i>rain</i>	3.66E-03	0.088	2.44E-03	0.236	8.52E-04	0.471	1.87E-03	0.674
land surface runoff (m/d)	<i>runoff</i>	1.42E-03	1.000	4.78E-04	1.000	1.99E-04	1.000	9.45E-04	1.000
plant dry mass inventory (kg[DM]/m <sup>2</sup> )	<i>bio_inv</i>	3.00E+01	1.000	3.00E+01	1.000	7.00E-01	1.000	7.00E-01	1.000
ground-water recharge (m/d)	<i>recharge</i>	1.82E-04	1.000	1.21E-04	1.000	4.26E-05	1.000	9.35E-05	0.816
evaporation of water from surface water (m/d)	<i>evaporate</i>	7.38E-05	1.000	1.19E-04	1.000	3.15E-05	1.000	6.29E-05	1.000
water content in surface soil (volume fraction)	<i>beta_g</i>	1.92E-01	0.507	2.14E-01	0.630	1.87E-01	0.457	1.90E-01	0.480
air content in the surface soil (volume fraction)	<i>alpha_g</i>	2.59E-01	0.194	2.34E-01	0.277	2.96E-01	0.200	3.07E-01	0.243
erosion of surface soil (kg/m <sup>2</sup> -d)	<i>erosion_g</i>	3.17E-04	1.000	2.85E-04	1.000	3.53E-04	1.000	1.62E-04	1.000
thickness of the root-zone soil (m)	<i>d_s</i>	8.94E-01	0.486	9.07E-01	0.509	7.16E-01	0.604	7.65E-01	0.501
water content of root-zone soil (vol. fraction)	<i>beta_s</i>	2.25E-01	0.520	2.27E-01	0.604	2.06E-01	0.498	2.03E-01	0.499
air content of root-zone soil (vol. fraction)	<i>alpha_s</i>	2.13E-01	0.309	1.95E-01	0.213	2.58E-01	0.247	2.83E-01	0.285
thickness of the vadose-zone soil (m)	<i>d_v</i>	1.55E+00	0.352	1.68E+00	0.343	1.29E+00	0.459	1.25E+00	0.391
water content; vadose-zone soil (vol. fraction)	<i>beta_v</i>	2.37E-01	0.478	2.60E-01	0.533	1.86E-01	0.500	1.99E-01	0.510
air content of vadose-zone soil (vol. fraction)	<i>alpha_v</i>	1.89E-01	0.381	1.61E-01	0.474	2.59E-01	0.240	2.60E-01	0.288
fraction of land area in surface water	<i>f_arw</i>	2.44E-02	0.200	3.13E-02	0.200	8.67E-03	0.200	2.47E-02	0.200
ambient environmental temperature (K)	<i>Temp</i>	2.89E+02	0.000	2.91E+02	0.000	2.81E+02	0.000	2.86E+02	0.000



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