LBNL - 43722

ERNEST ORLANDO LAWRENCE
BERKELEY NATIONAL LABORATORY

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

School of Public Health
University of California, Berkeley

Environmental Energy
Technologies Division

July 2001

Research Supported by:
The U.S. Environmental Protection Agency
  Sustainable Technology Division
    National Risk Management Research Laboratory
  National Exposure Research Laboratory
The Environmental Defense Fund

LBNL - 43722

Development and Evaluation of State-Specific Landscape Data Sets for Life-Cycle Impact Assessment

Thomas E. McKone[1,2], Agnes B. Bodnar[1,2], and Edgar G. Hertwich[3]

[1]Environmental Energy Technologies Divisions
Lawrence Berkeley National Laboratory
Berkeley, CA 94720

[2]School of Public Health
University of California
Berkeley, CA 94720

[3]Life Cycle Assessment Laboratory
Institute for Product Design
Norwegian University of Science and Technology
Kolbjørn Hejes vei 2b
7491 Trondheim, Norway

September 2000

This work was supported by the U.S. Environmental Protection Agency (EPA) and Environmental Defense and carried out in part at the Lawrence Berkeley National Laboratory (LBNL) through U.S. Department of Energy under Contract Grant No. DE-AC03-765F00098. Work was also carried out at the University of California-Berkeley (UCB). Work at UCB was support by the EPA, National Risk Management Laboratory, Sustainable Technology Division through Cooperative Research Agreement No. CR-826925-01-0. Work at UCB was also supported by an Environmental Defense Minigrant. Work at LBNL was supported by the EPA National Exposure Research Laboratory through Interagency Agreement No. DW-988-38190-01-0.

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.

TABLE OF CONTENTS

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^2	*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^3)	*rhob_a*
Deposition velocity of air particles (m / d)	*v_d*
Plant dry mass inventory (kg[DM] / m^2)	*bio_inv*
Plant dry-mass fraction	*bio_dm*
Plant fresh-mass density kg / m^3	*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^3)	*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^2-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^3)	*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^3)	*rhob_w*
Suspended sediment deposition (kg / m^2 / d)	*deposit*
Thickness of the sediment layer (m)	*d_d*
Solid material density in sediment (kg / m^3)	*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).

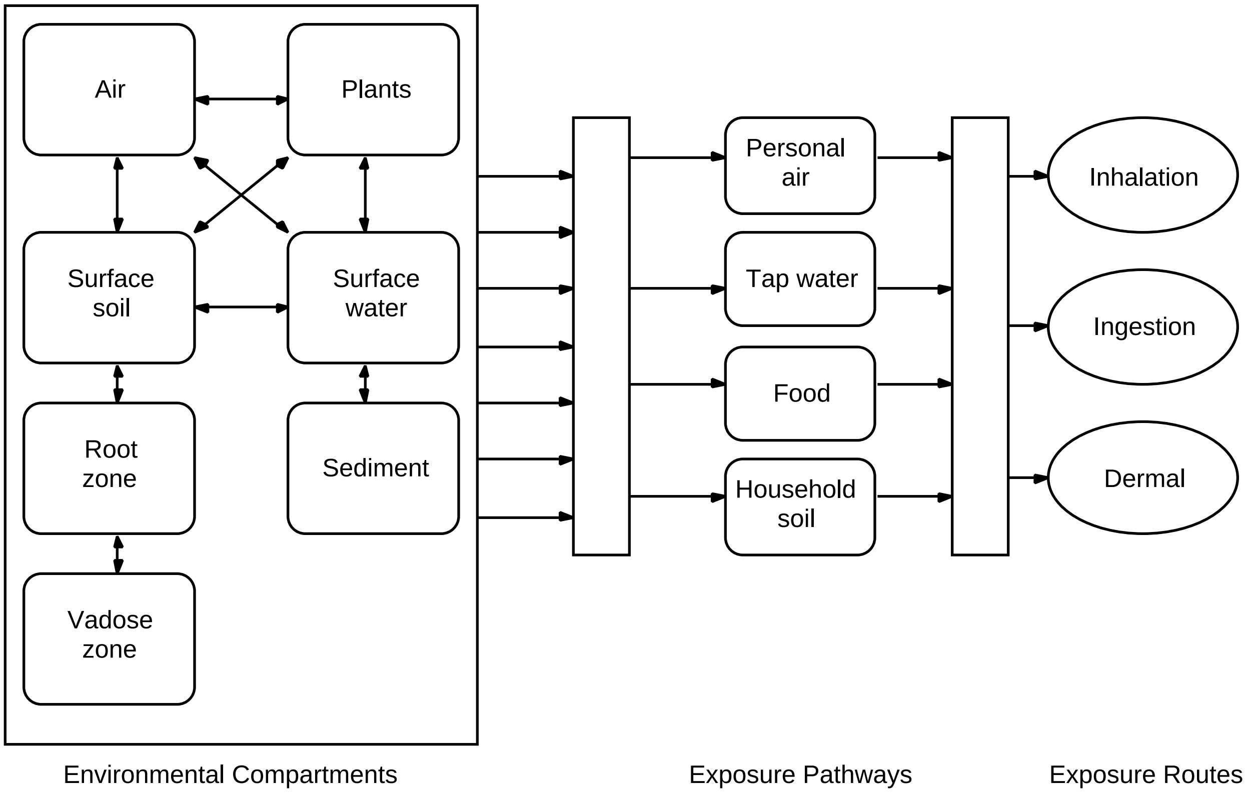

Figure 1. Schematic diagram of the CalTOX exposure/risk calculation framework.

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^2	*Area*	Statistical Abstracts of the US, Bureau of Census (1997)
Annual average precipitation (m/d)	*rain*	NOAA (1998)
Land surface runoff (m/d)	*runoff*	van der Leeden (1991, p 70, Table 2-18)
Plant dry mass inventory (kg[DM]/m^2)	*bio_inv*	Layton, et al. (1986)
Ground-water recharge (m/d)	*recharge*	Layton, et al. (1986)
Evaporation of water from surface water (m/d)	*evaporate*	van der Leeden (1991, p 94, Table 2-48)
Water content in surface soil (volume fraction)	*beta_g*	PATRIOT (Imhoff, et al, 1994) USDA (1998)
Air content in the surface soil (volume fraction)	*alpha_g*	PATRIOT (Imhoff, et al, 1994) USDA (1998)
Erosion of surface soil (kg/m^2-d)	*erosion_g*	van der Leeden (1991, p. 83 and p.86, Table 2-39)]
Thickness of the root-zone soil (m)	*d_s*	PATRIOT (Imhoff, et al, 1994) USDA (1998)
Water content of root-zone soil (volume fraction)	*beta_s*	PATRIOT (Imhoff, et al, 1994) USDA (1998)
Air content of root-zone soil (volume fraction)	*alpha_s*	PATRIOT (Imhoff, et al, 1994) USDA (1998)
Thickness of the vadose-zone soil (m)	*d_v*	PATRIOT (Imhoff, et al, 1994)
Water content; vadose-zone soil (volume fraction)	*beta_v*	PATRIOT (Imhoff, et al, 1994) USDA (1998)
Air content of vadose-zone soil (volume fraction)	*alpha_v*	PATRIOT (Imhoff, et al, 1994) USDA (1998)
Fraction of land area in surface water	*f_arw*	Statistical Abstracts of the US, Bureau of Census (1997)
Ambient environmental temperature (kelvins)	*Temp*	NOAA (1998)
Organic carbon fraction in upper soil zone	*foc_s*	PATRIOT (Imhoff, et al, 1994)
Organic carbon fraction in vadose zone	*foc_v*	PATRIOT (Imhoff, et al, 1994)
Organic carbon fraction in aquifer zone	*foc_q*	PATRIOT (Imhoff, et al, 1994)
Yearly average wind speed (m/d)	*v_w*	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)	*inflow*	0	0
Atmospheric dust load (kg / m^3)	*rhob_a*	6.15×10^{-8}	0.2
Deposition velocity of air particles (m / d)	*v_d*	500	0.3
Plant dry-mass fraction	*bio_dm*	0.2	0.2
Plant fresh-mass density kg / m^3	*rho_p*	1,000	0.2
Thickness of the ground-surface soil layer (m)	*d_g*	0.01	1
Soil particle density (kg / m^3)	*rhos_s*	2,600	0.05
Thickness of the aquifer layer (m)	*d_q*	3	0.3
Solid material density in aquifer (kg / m^2)	*rhos_q*	2,600	0.05
Porosity of the aquifer zone	*beta_q*	0.20	0.2
Average depth of surface waters (m)	*d_w*	5.0	1
Suspended sediment load in surface water (kg / m^3)	*rhob_w*	0.8	1
Suspended sediment deposition (kg / m^2 / d)	*deposit*	10.5	0.3
Thickness of the sediment layer (m)	*d_d*	0.05	1
Solid material density in sediment (kg / m^2)	*rhos_d*	2,600	0.05
Porosity of the sediment zone	*beta_d*	0.2	0.2
Sediment burial rate (m / d)	*bury_d*	1.0×10^{-6}	5
Surface water current in m / d	*current_w*	0	0
Organic carbon fraction in sediments	*foc_d*	0.02	1
Boundary layer thickness in air above soil (m)	*del_ag*	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	Connecticut	Illinois	Iowa	Delaware
New York	Maine	Indiana	Kansas	Florida
Pennsylvania	Massachusetts	Michigan	Minnesota	Georgia
	New Hampshire	Ohio	Missouri	Maryland
	Rhode Island	Wisconsin	Nebraska	North Carolina
	Vermont		North Dakota	South Carolina
			South Dakota	Virginia
				West Virginia

East South Central	**West South Central**	**Mountain**	**Pacific**
Alabama	Arkansas	Arizona	California
Kentucky	Louisiana	Colorado	Oregon
Mississippi	Oklahoma	Idaho	Washington
Tennessee	Texas	Montana	
		Nevada	
		New Mexico	
		Utah	
		Wyoming	

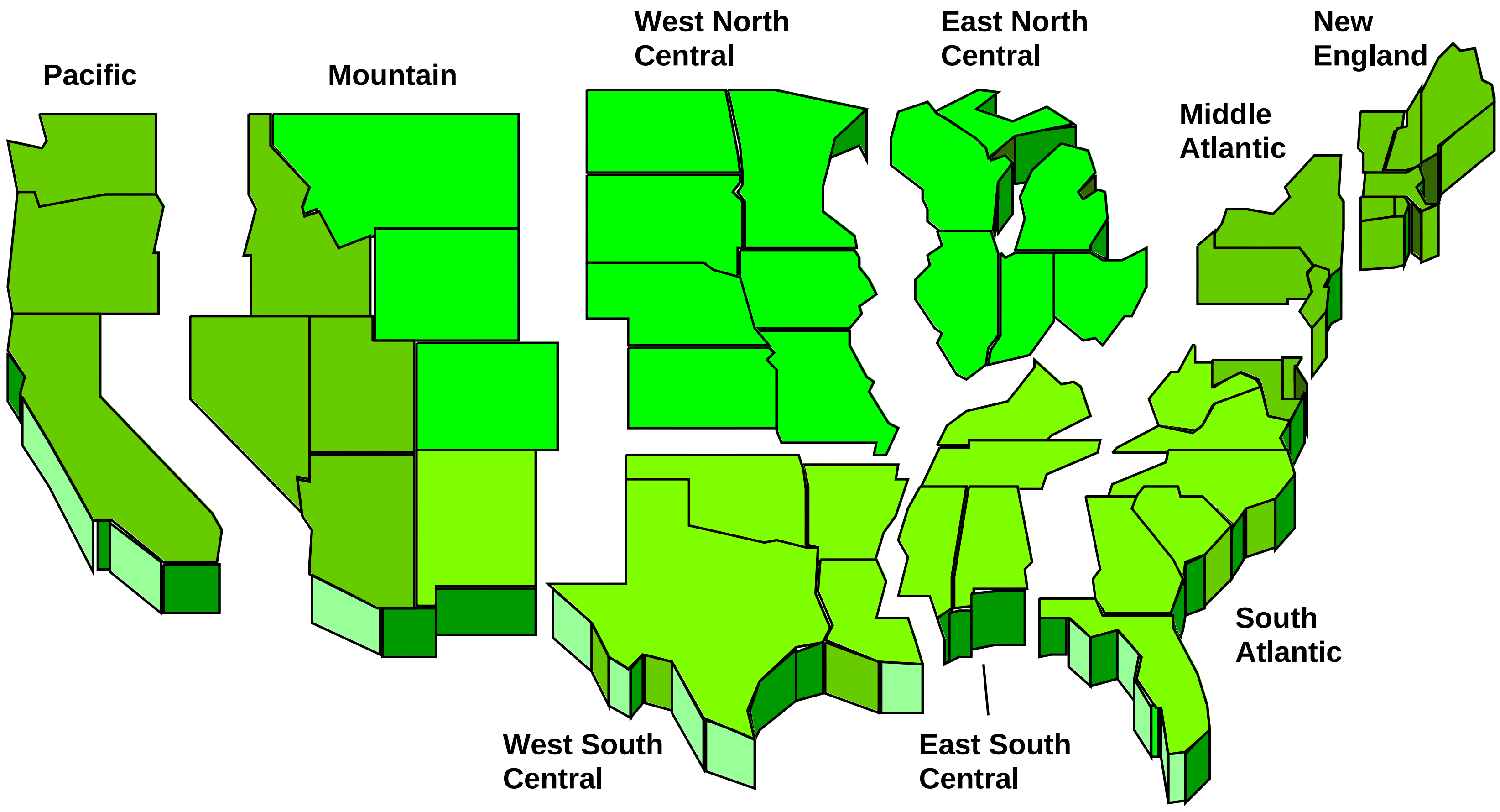

Figure 2. The division of the U.S. into nine regions for consideration of landscape properties variation.

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 ($\bar{\mathrm{x}}$), standard deviation, and coefficient of variation was calculated from the multiple reported values from a state/region.

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

where $\sum_{\mathrm{i=1}}^{\mathrm{n}} \mathrm{x_i}$ 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 (σ) by the mean.

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

$$\textit{coefficient of variation}\ (\mathrm{CV}) = \frac{\sigma}{\bar{\mathrm{x}}} \qquad (3)$$

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. ($\bar{x}$)].

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

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:

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

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

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

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, $Area_i$ 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;

σ_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^2]**	**land area [km^2]**	**Surface water area [km^2]**
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	1,144
	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^2]	land area [km^2]	Surface water area [km^2]
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**

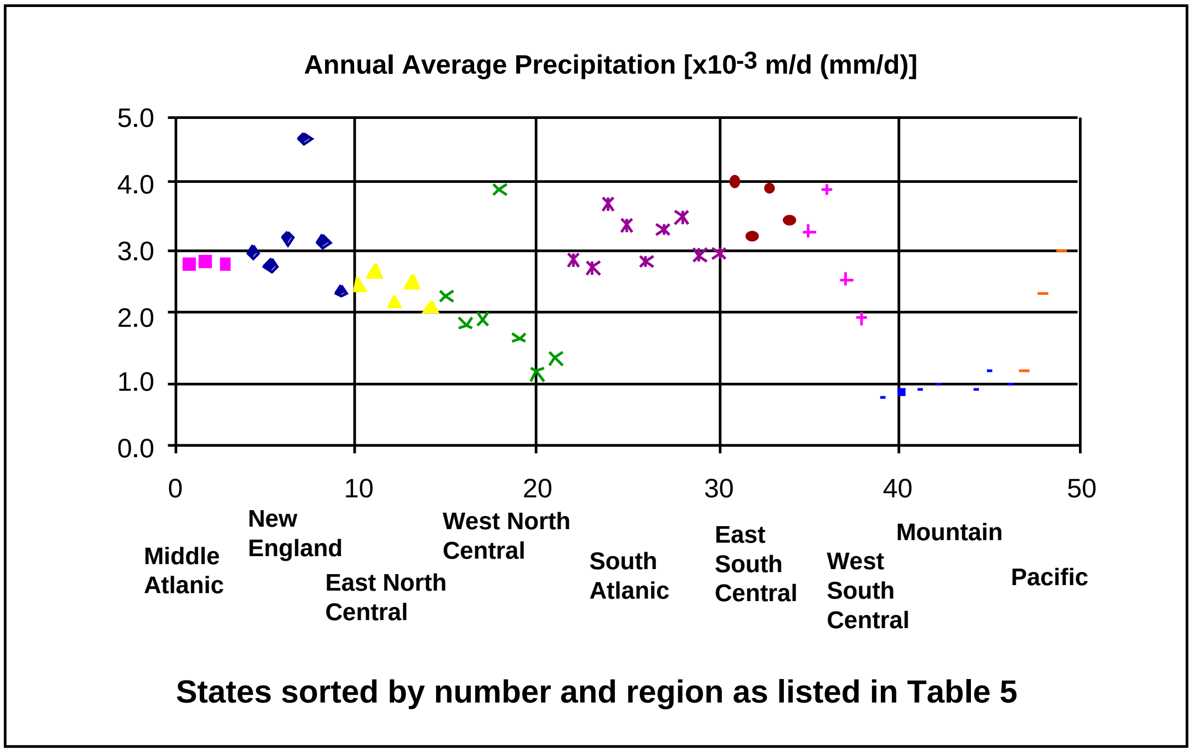

Figure 3. Annual average precipitation calculated from NOAA (1997) data for 48 contiguous United States.

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 [m^3/day/land area] to obtain runoff in units of [m/d]. A default value of 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^2, the Central-Northeastern region with a plant dry-mass inventory of 30 kg / m^2, and the Southeastern region also with a plant dry-mass inventory of 30 kg / m^2. 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
Maine
Vermont
West Virginia
Indiana
Iowa
New York
Massachusetts
Delaware
Kentucky
Michigan
Minnesota
Pennsylvania
New Hampshire
Maryland
Tennessee
Ohio
Missouri
Connecticut
Rhode Island
Virginia
Illinois
Wisconsin

the Southeastern region includes the states:

Florida
Alabama
Georgia
Mississippi
North Carolina
Louisiana
South Carolina
Arkansas

and the Western-Interior region includes the states:

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

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

Region	Plant Dry-Mass Inventory, kg/m^2	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	1.4×10^{-4}	1.00
New England	1.6×10^{-4}	1.00
East North Central	1.6×10^{-4}	1.00
West North Central	1.5×10^{-4}	1.00
South Atlantic	1.7×10^{-4}	1.00
East South Central	1.8×10^{-4}	1.00
West South Central	1.2×10^{-4}	1.00
Mountain	4.3×10^{-5}	1.00
Pacific	9.5×10^{-5}	1.00
US	$\mathbf{1.2 \times 10^{-4}}$	**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	1.7×10^{-4}	1.0
New England	1.3×10^{-4}	1.0
East North Central	4.3×10^{-4}	1.0
West North Central	6.0×10^{-5}	1.0
South Atlantic	2.1×10^{-4}	1.0
East South Central	7.4×10^{-5}	1.0
West South Central	1.2×10^{-4}	1.0
Mountain	3.2×10^{-5}	1.0
Pacific	6.3×10^{-5}	1.0
US Average	$\mathbf{1.2 \times 10^{-4}}$	**1.0**

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 to 9.6×10^{-7} to convert from tons/(square mile)/year to kg/m^2/d. A default value of 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^2-d]**	**CV**
Middle Atlantic	2.9×10^{-4}	1.0
New England	2.9×10^{-4}	1.0
East North Central	5.5×10^{-4}	1.0
West North Central	4.6×10^{-4}	1.0
South Atlantic	2.2×10^{-4}	1.0
East South Central	3.2×10^{-4}	1.0
West South Central	2.8×10^{-4}	1.0
Mountain	3.5×10^{-4}	1.0
Pacific	1.6×10^{-4}	1.0
US Average	$\mathbf{3.6 \times 10^{-4}}$	**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
All regions combined	**0.044**	**0.20**

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 [°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.

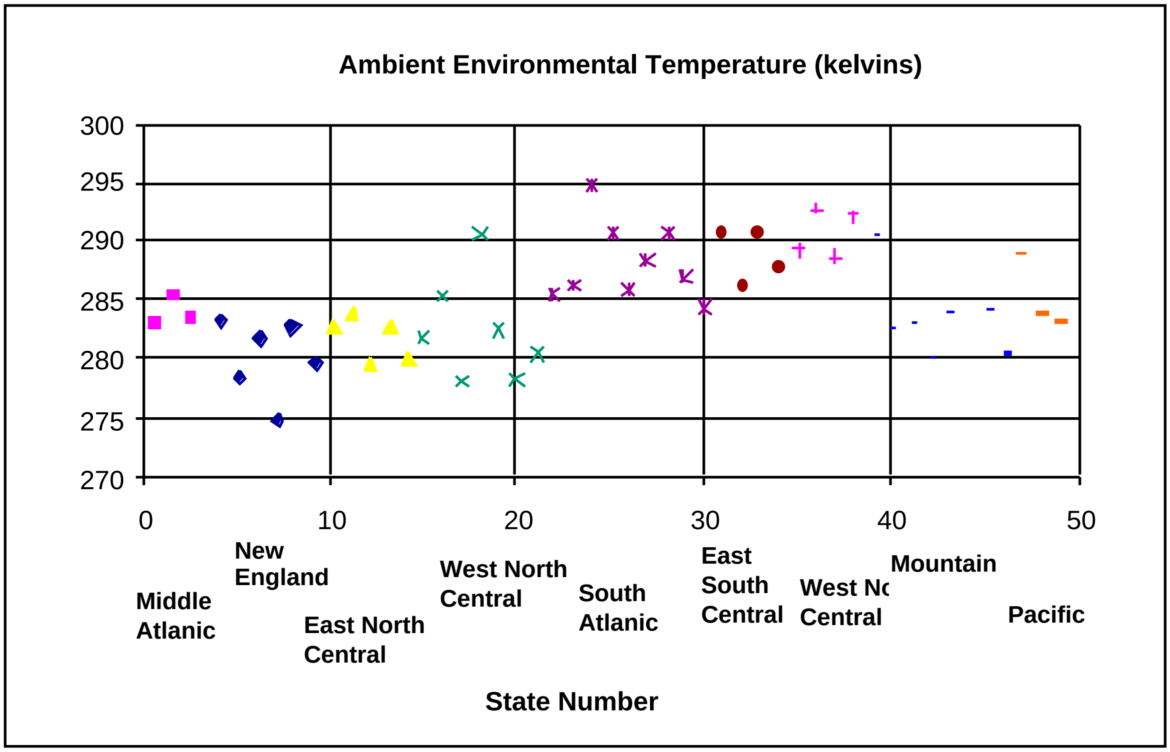

Figure 4. Ambient environmental temperature (in kelvins) displayed for 48 contiguous United States from NOAA (1997) data.

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.

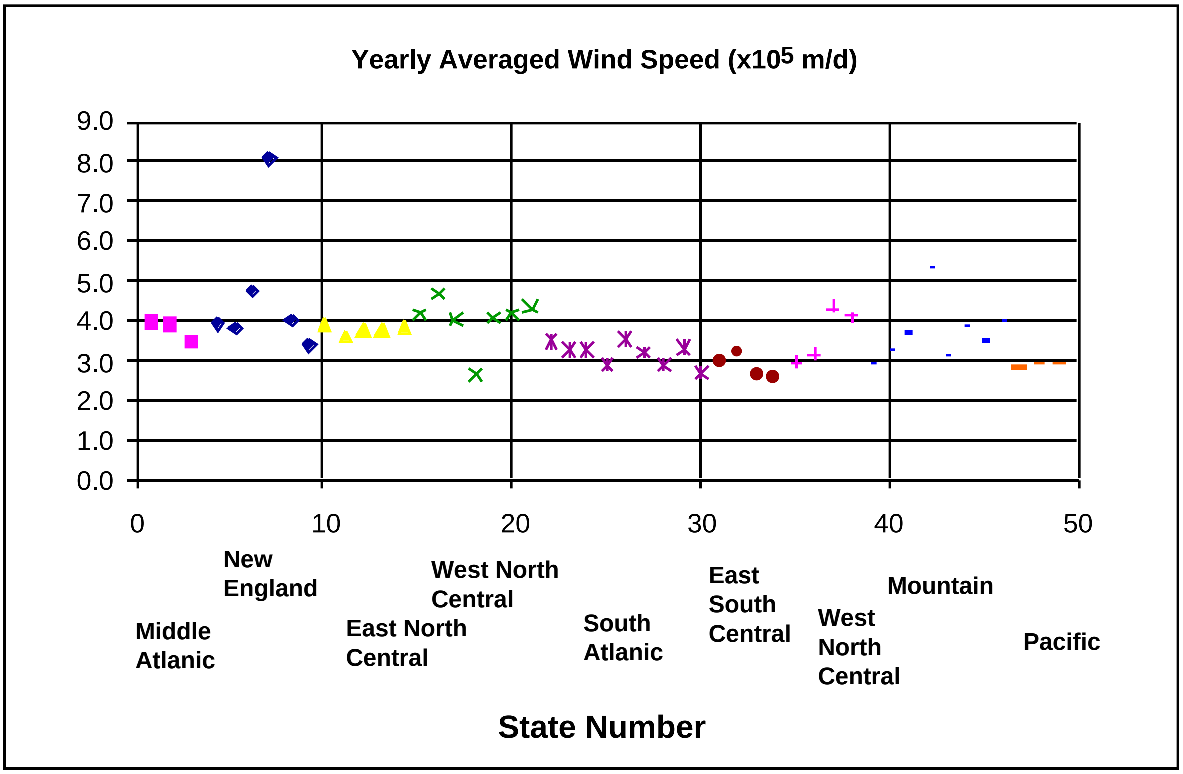

Figure 5. Yearly averaged wind speed calculated from NOAA (1997) data for 48 contiguous United States.

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:

$$x_{i,k} = \frac{\sum y_j \, x_{ij}}{y_k} \tag{8}$$

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

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

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

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

$x_{i,k}$ = 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,

$$f_{oc} = \frac{\%OM/100}{1.72} \tag{12}$$

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)

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

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:

$$FC = \left(\frac{0.333}{a} \right)^{\frac{1}{b}} \tag{14}$$

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

where a and b are defined as:

$$a = \exp\left[-4.396 - (0.0715 \times C) - 0.000488 S^2 - 0.11114285 CS^2\right]$$

$$b = -3.14 - .00222 C^2 - 0.00003484 CS^2$$

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:

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

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_s [m]**	**CV**	**beta_s**	**CV**	**alpha_s**	**CV**	**foc_s**	**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**

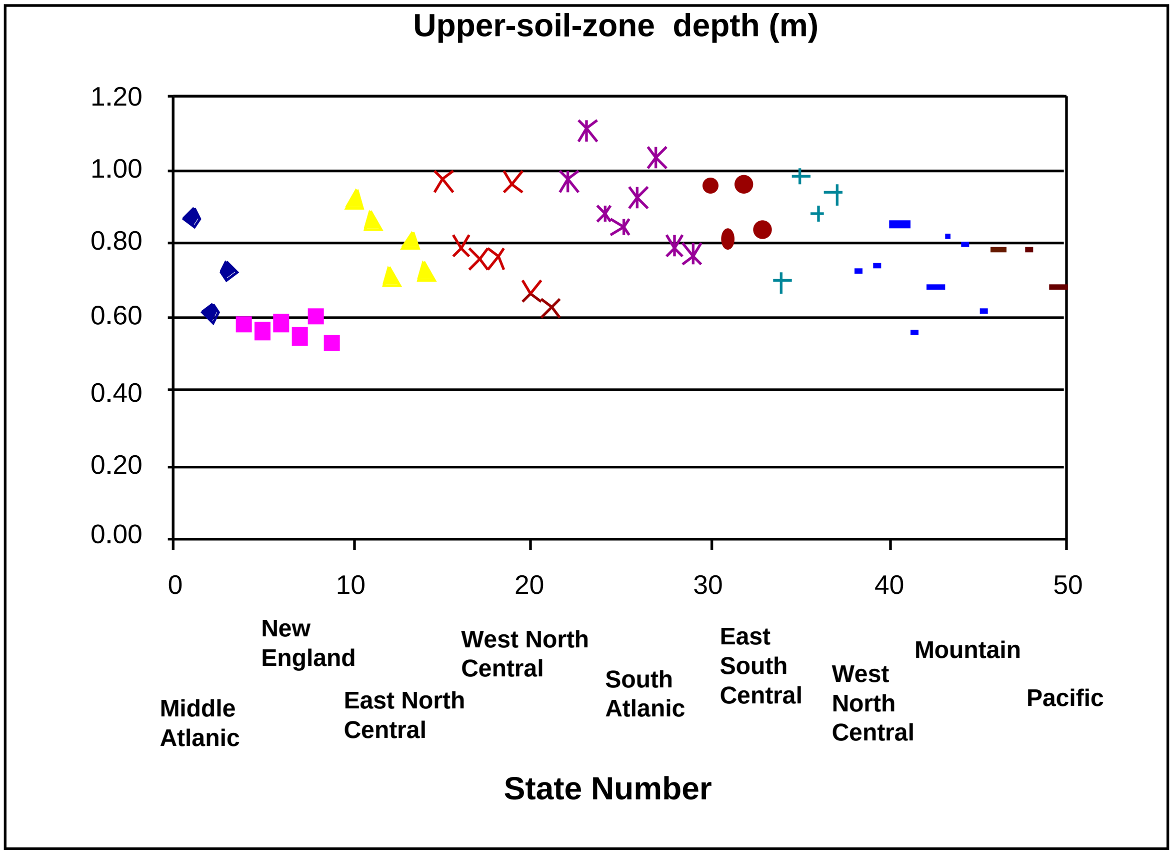

Figure 6. Variation among the 48 contiguous United States in the area-weighted average upper-soil-zone depth as derived from PATRIOT system.

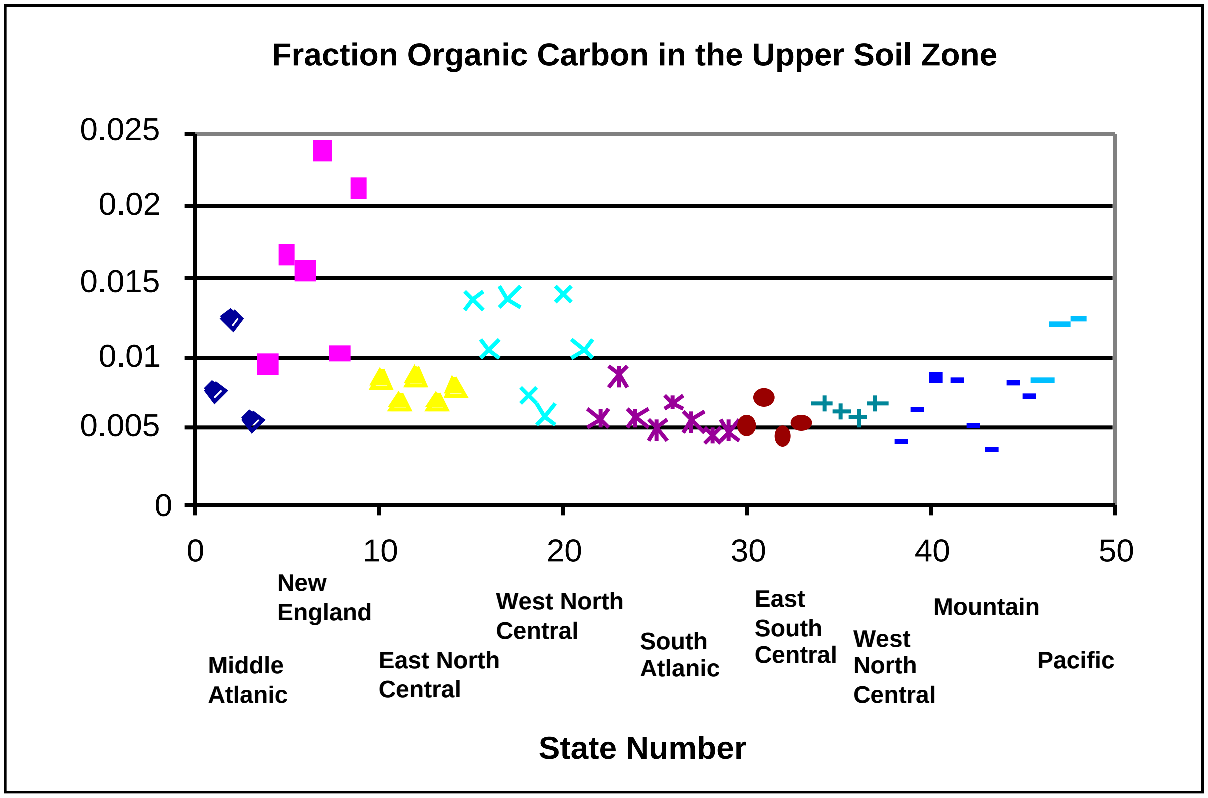

Figure 7. Variation among the 48 United States in the area-weighted average organic-carbon content in the root-zone soil as derived from PATRIOT.

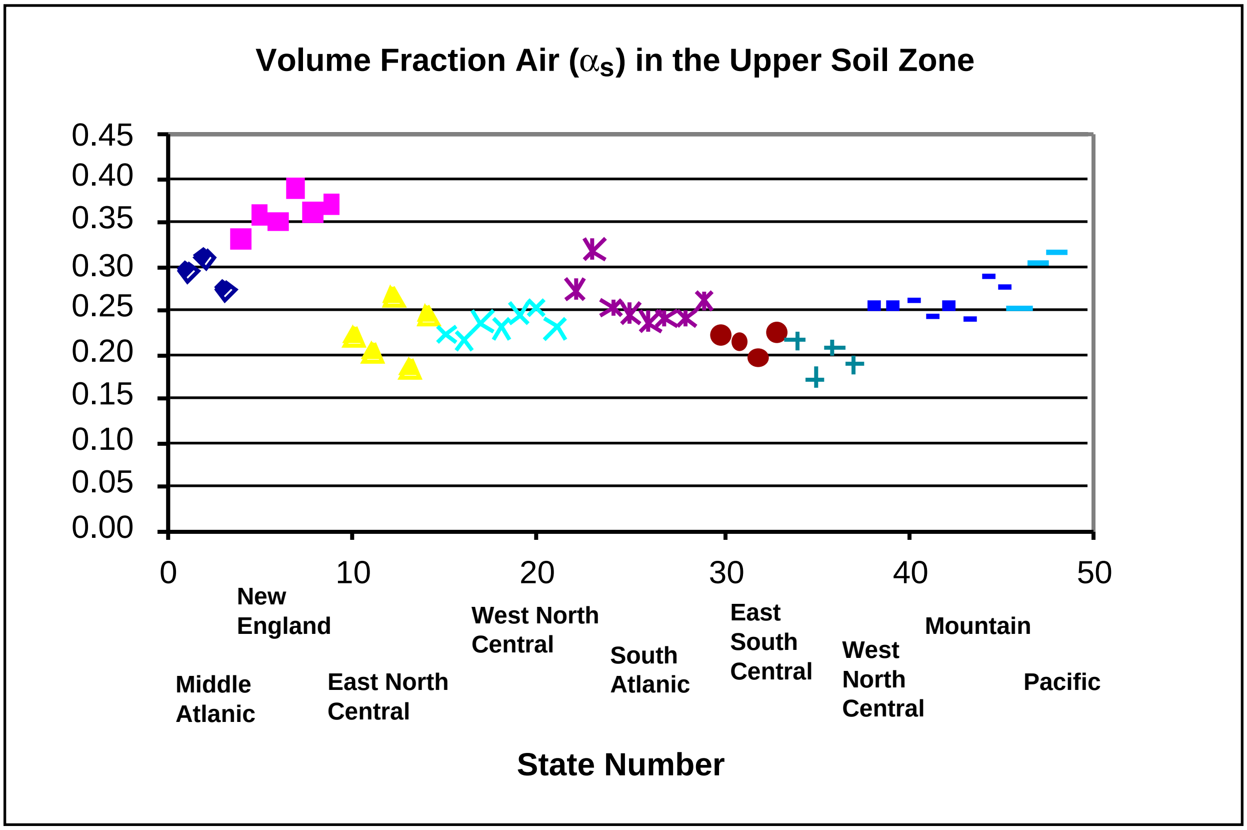

Figure 8. Variation among the 48 contiguous United States in the area-weighted average air content in the root-zone soil as derived from PATRIOT.

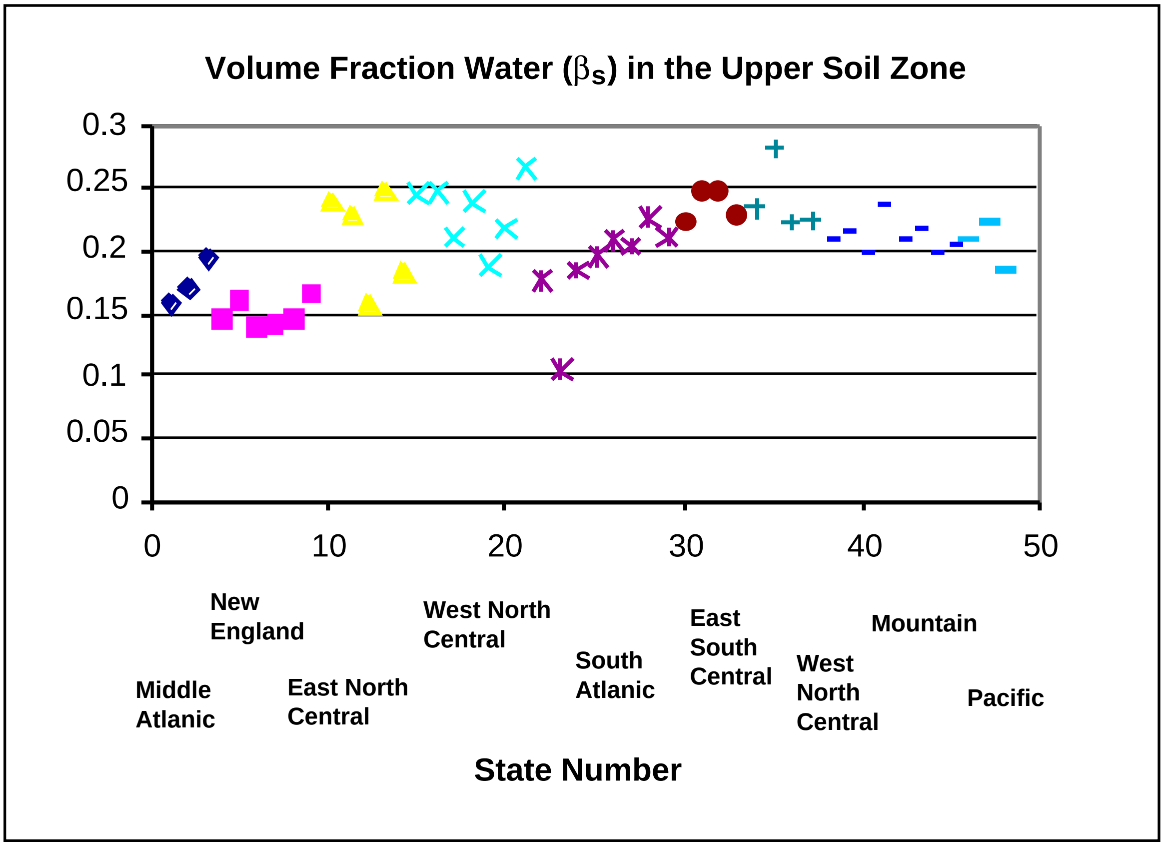

Figure 9. Variation among the 48 contiguous United States in the area-weighted average water content in the root-zone soil as derived from PATRIOT.

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**

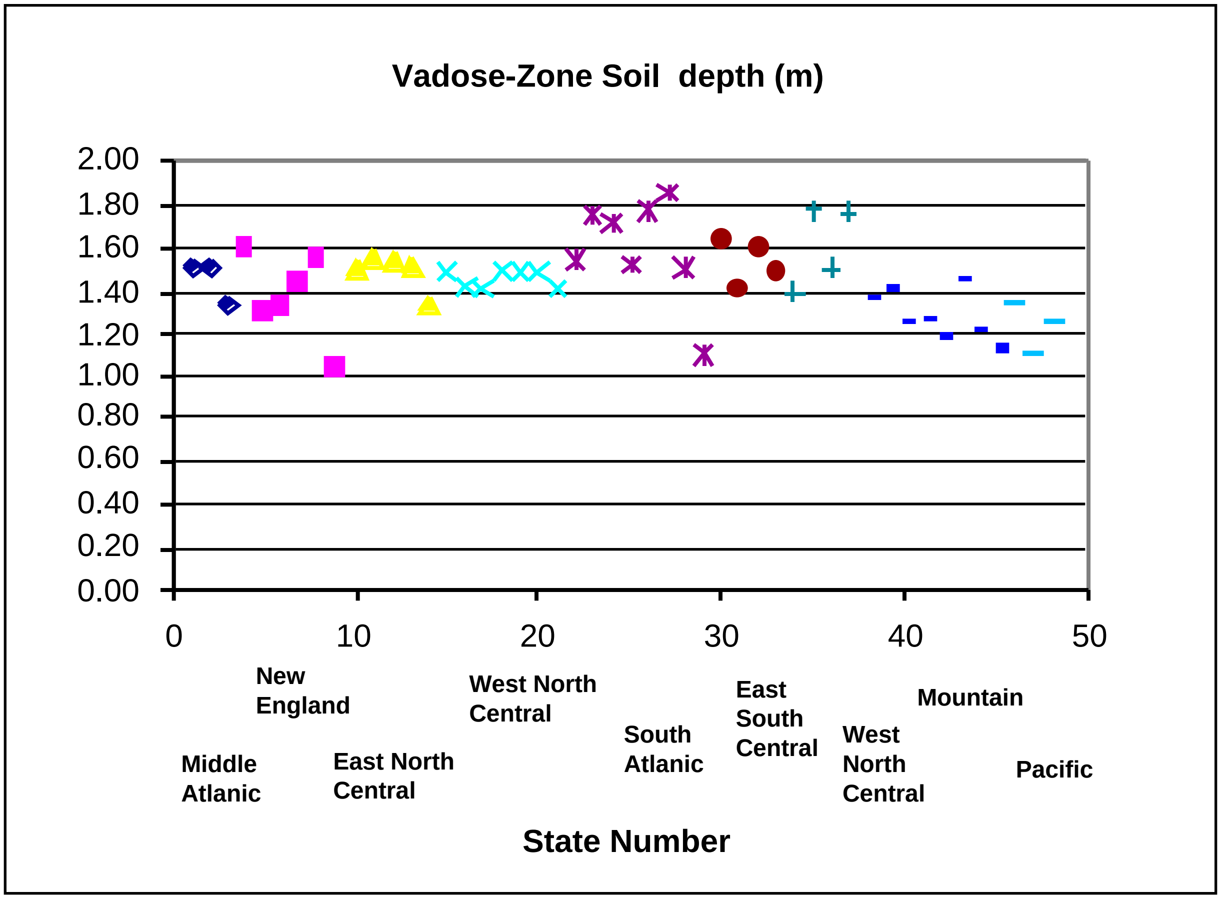

Figure 10. Variation among the 48 contiguous United States in the area-weighted average vadose-zone soil depth as derived from PATRIOT.

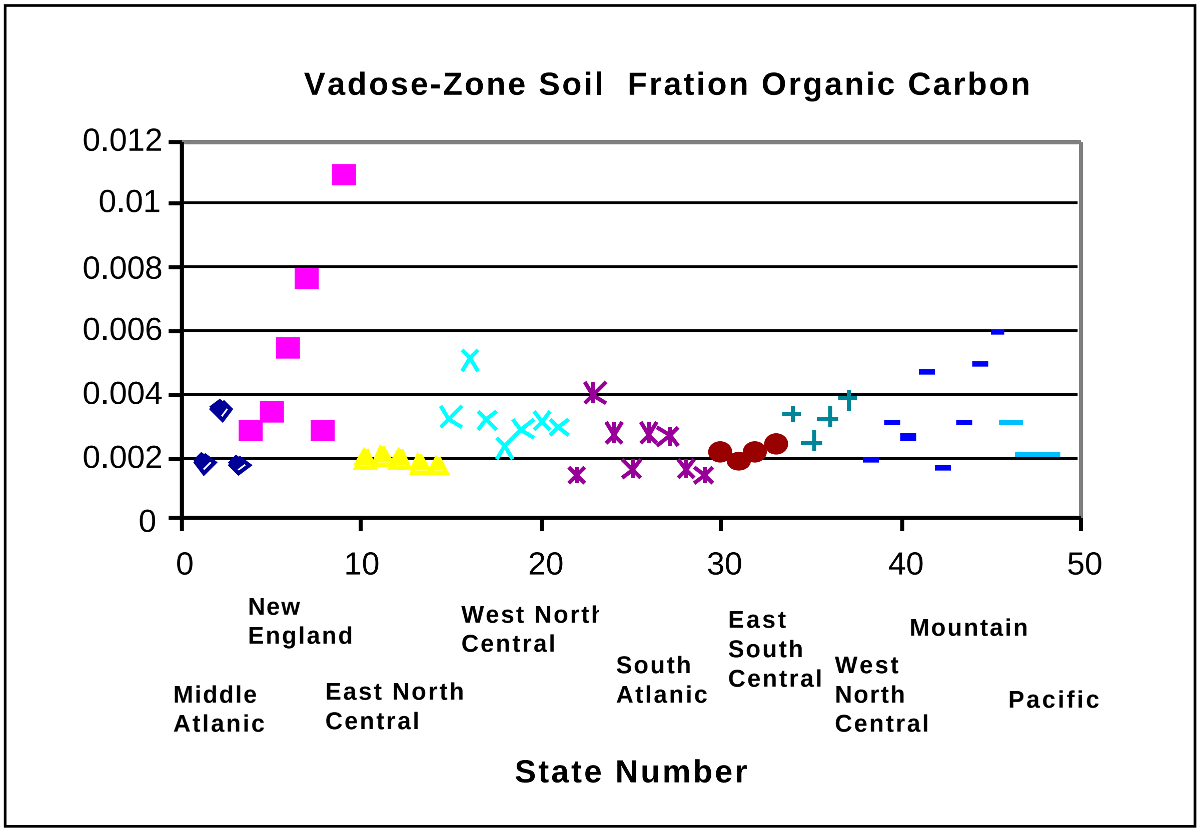

Figure 11. Variation among the 48 contiguous United States in the area-weighted average vadose-zone soil organic carbon fraction as derived from PATRIOT.

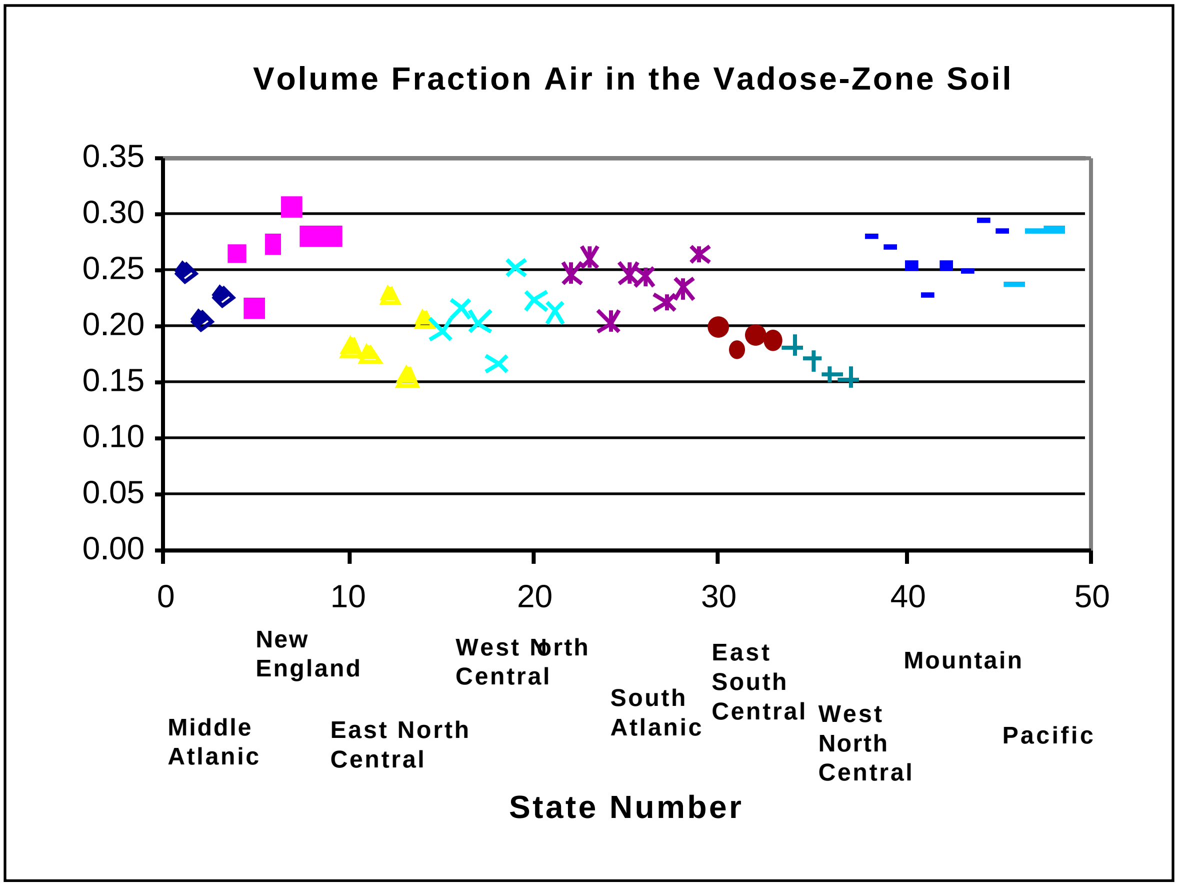

Figure 12. Variation among the 48 contiguous United States in the area-weighted average vadose-zone soil volumetric air content as derived from PATRIOT.

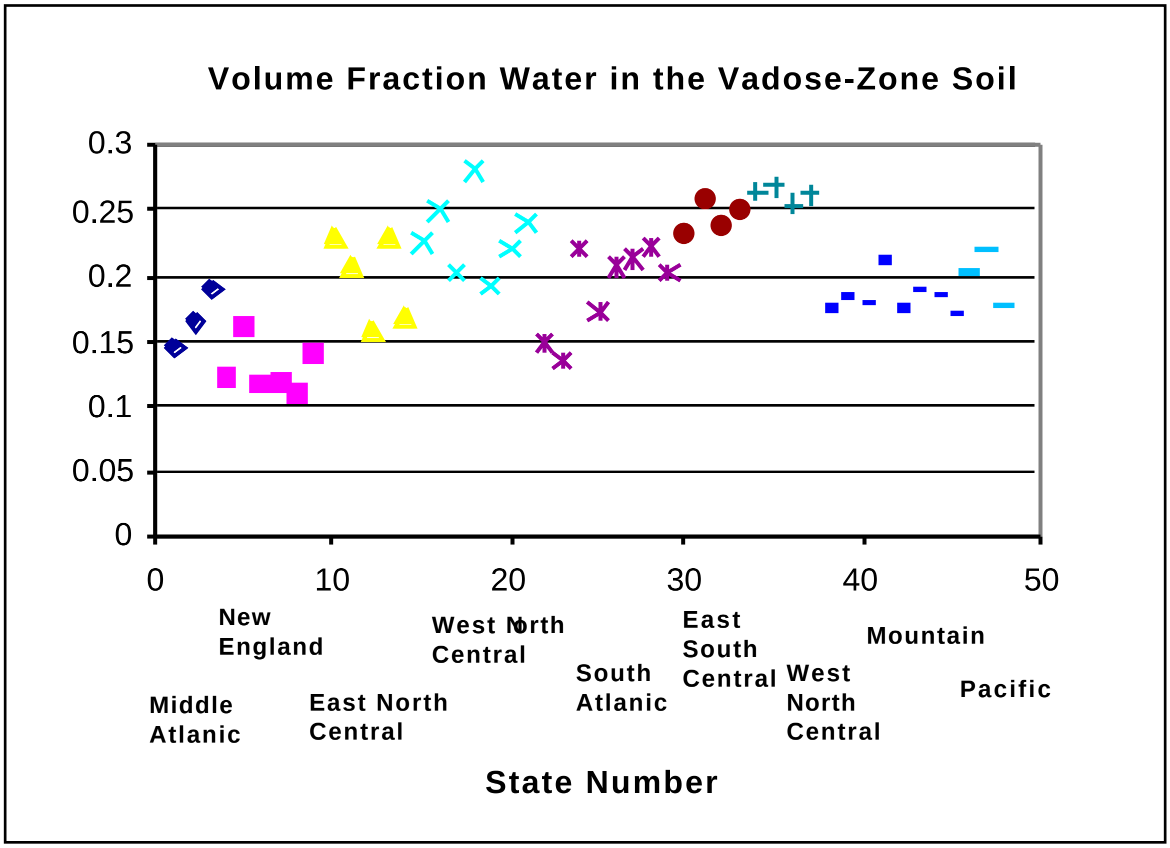

Figure 13. Variation among the 48 contiguous United States in the area-weighted average vadose-zone soil volumetric water content as derived from PATRIOT.

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.

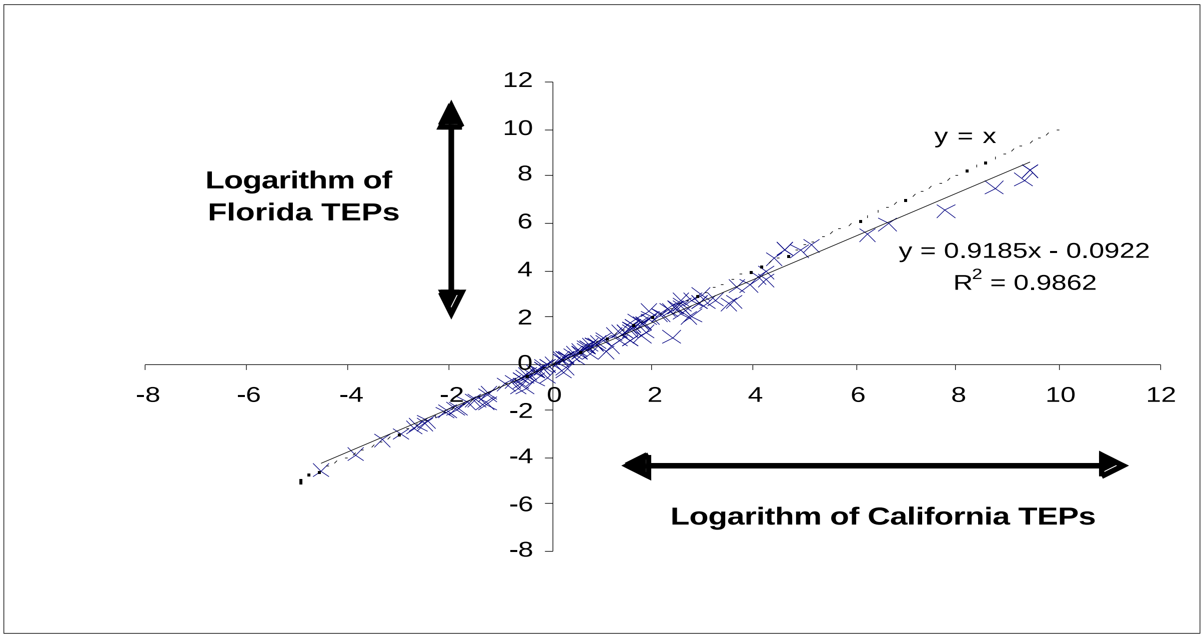

Figure 14(a) Logarithm of Florida carcinogen TEP's (in benzene equivalents) vs. logarithm of California carcinogen TEP's for 1 mol/d **air** emissions.

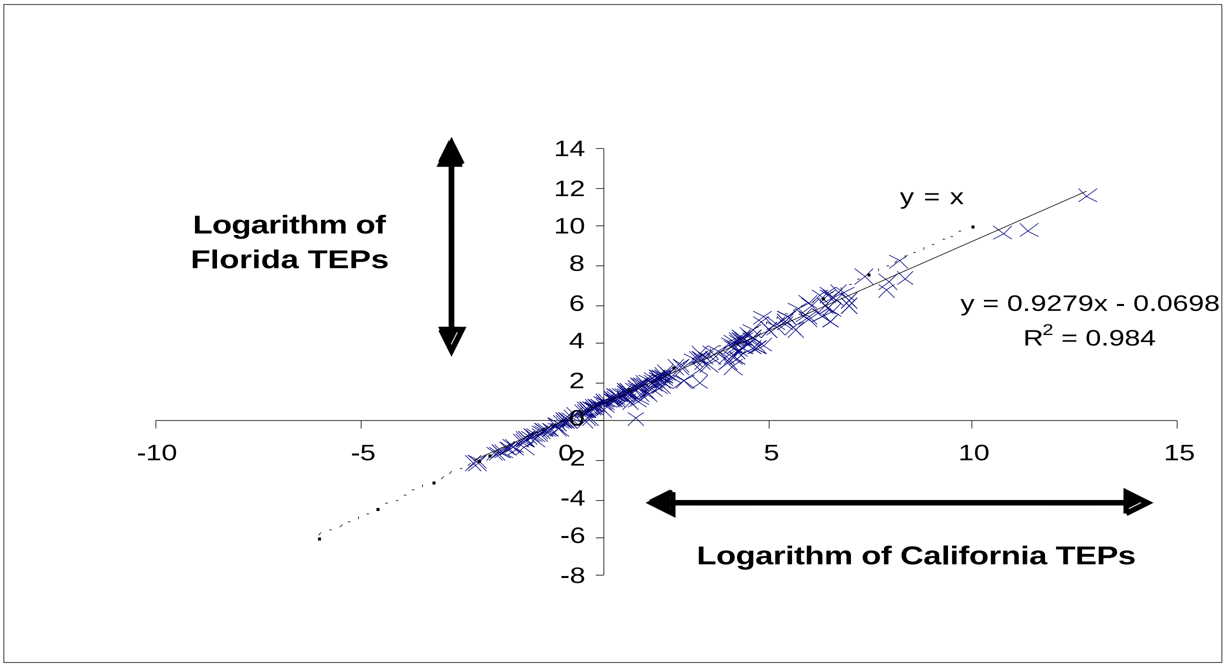

Figure 14(b) Logarithm of Florida non-carcinogen TEP's (in toluene equivalents) vs. logarithm of California non-carcinogen TEP's for 1 mol/d **air** emissions.

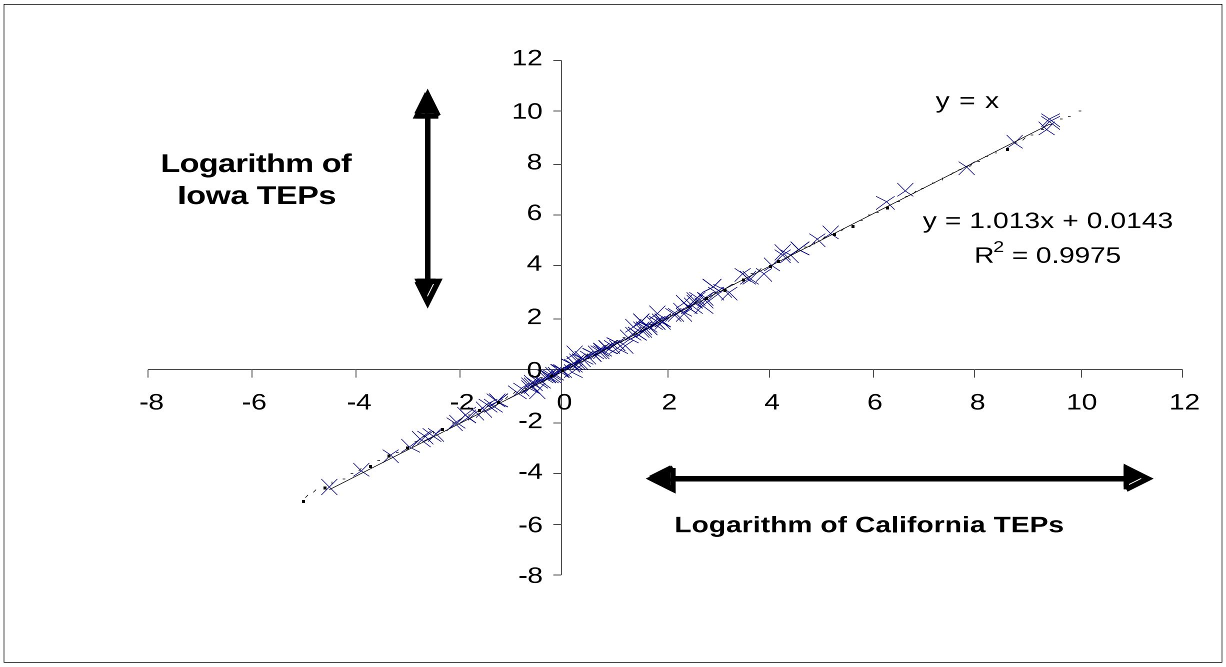

Figure 15(a) Logarithm of Iowa carcinogen TEP's (in benzene equivalents) vs. logarithm of California carcinogen TEP's for 1 mol/d **air** emissions.

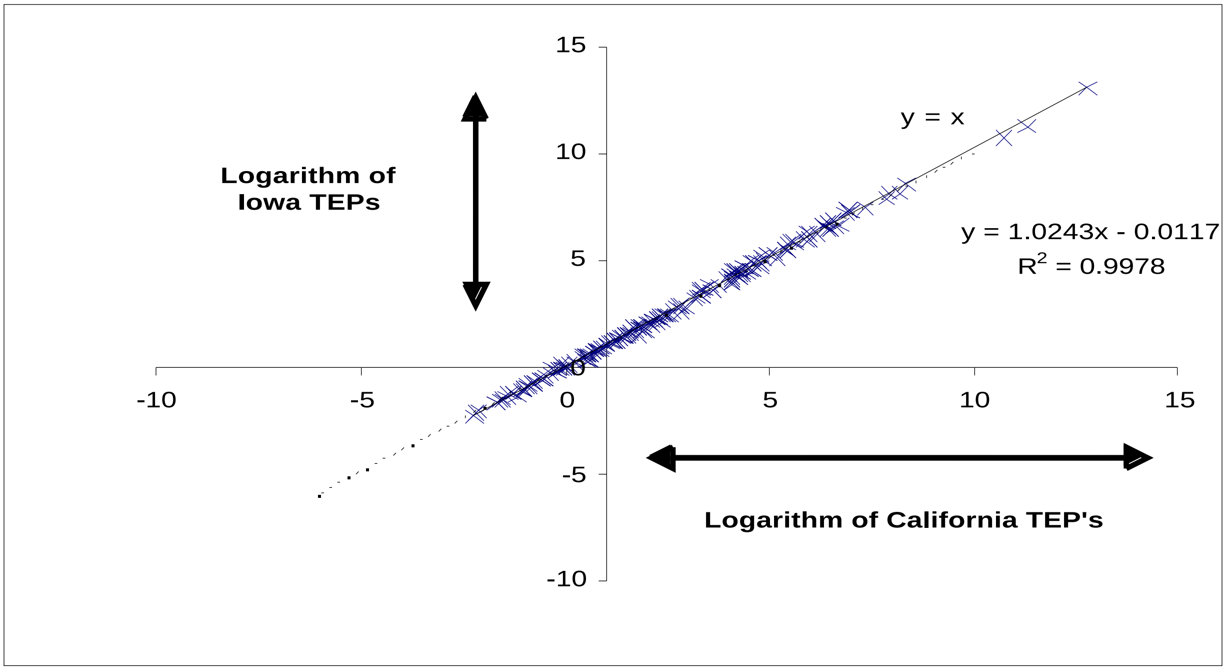

Figure 15(b) Logarithm of Iowa non-carcinogen TEP's (in toluene equivalents) vs. logarithm of California non-carcinogen TEP's for 1 mol/d **air** emissions.

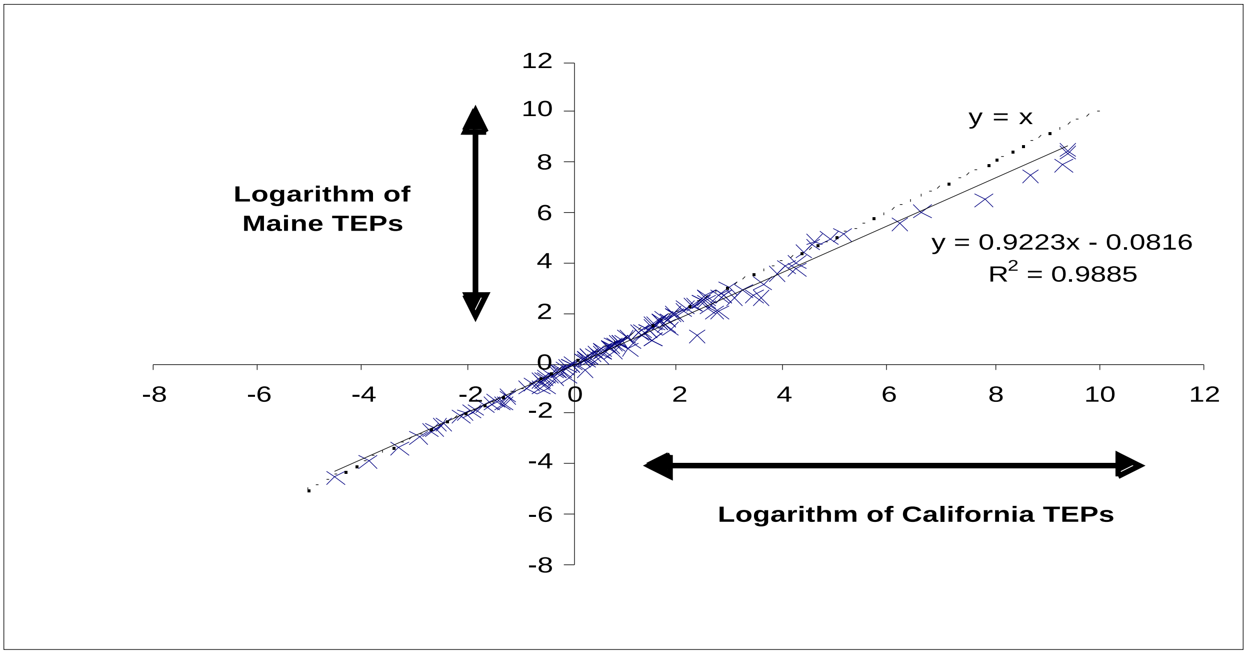

Figure 16(a) Logarithm of Maine carcinogen TEP's (in benzene equivalents) vs. logarithm of California carcinogen TEP's for 1 mol/d **air** emissions.

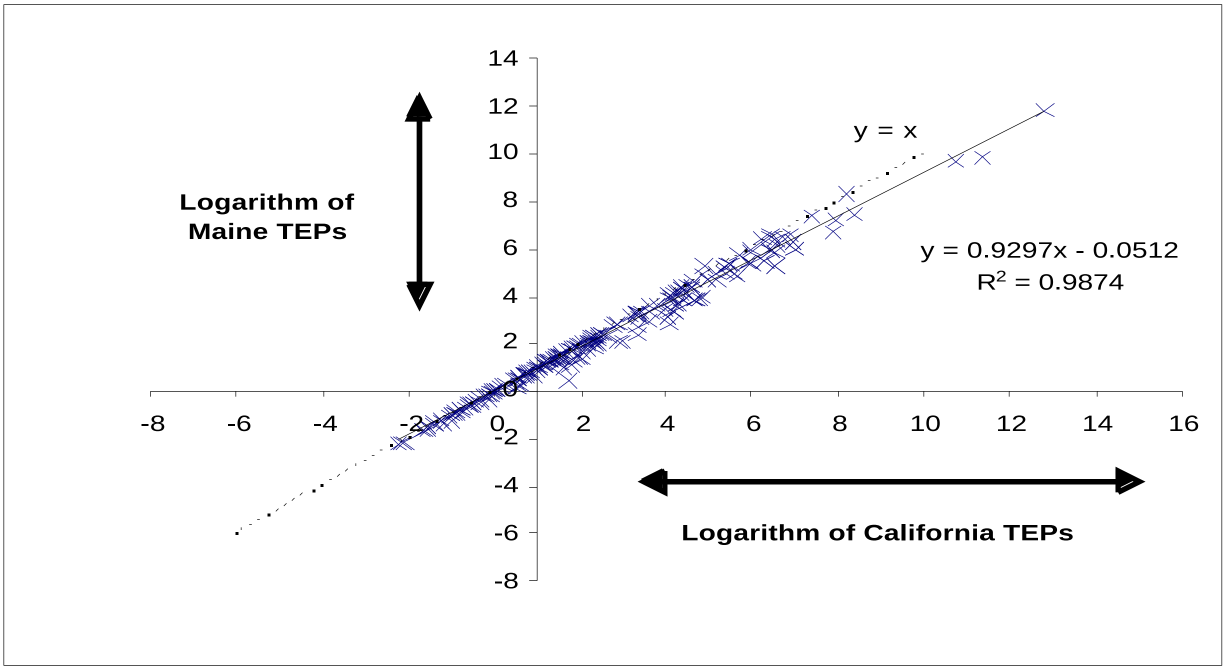

Figure 16(b) Logarithm of Maine non-carcinogen TEP's (in toluene equivalents) vs. logarithm of California non-carcinogen TEP's for 1 mol/d **air** emissions.

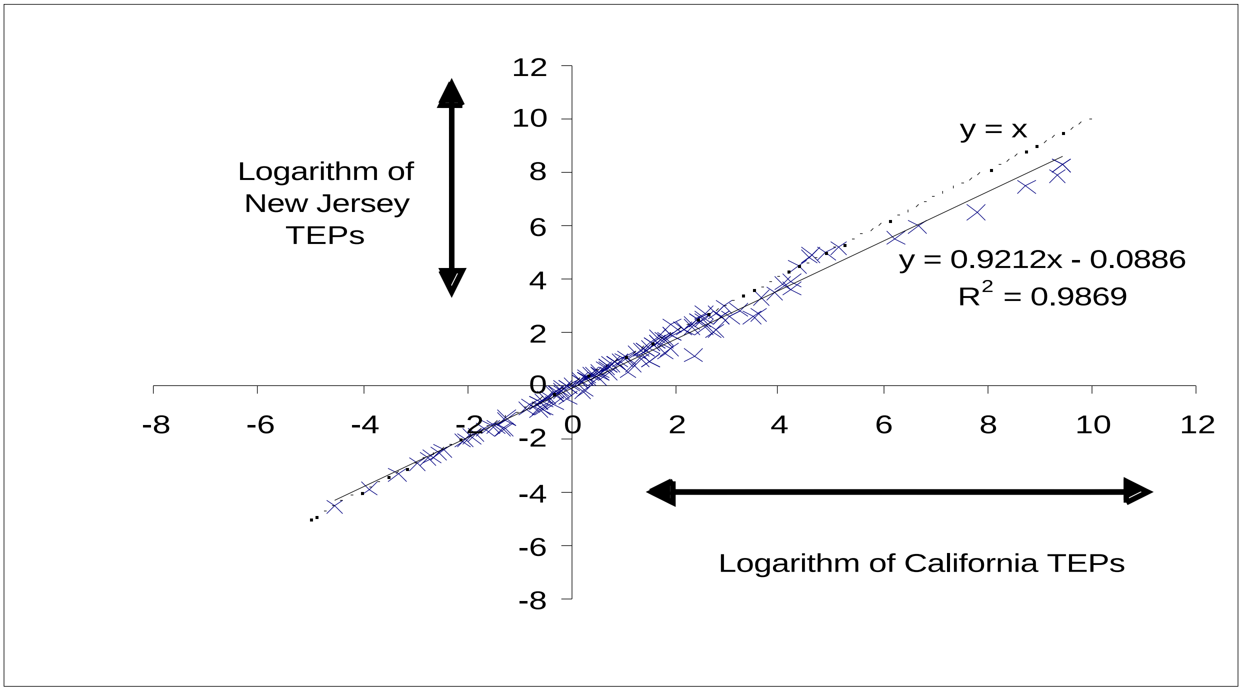

Figure 17(a) Logarithm of New Jersey carcinogen TEP's (in benzene equivalents) vs. logarithm of California carcinogen TEP's for 1 mol/d **air** emissions.

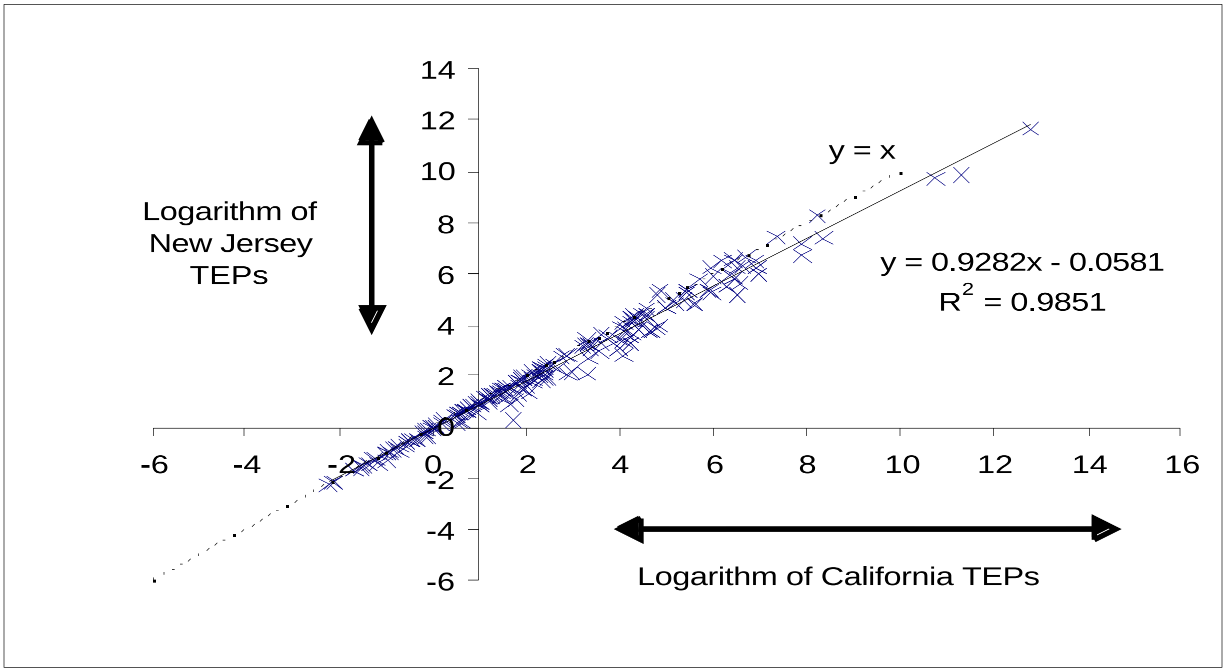

Figure 17(b) Logarithm of New Jersey non-carcinogen TEP's (in toluene equivalents) vs. logarithm of California non-carcinogen TEP's for 1 çmol/d **air** emissions.

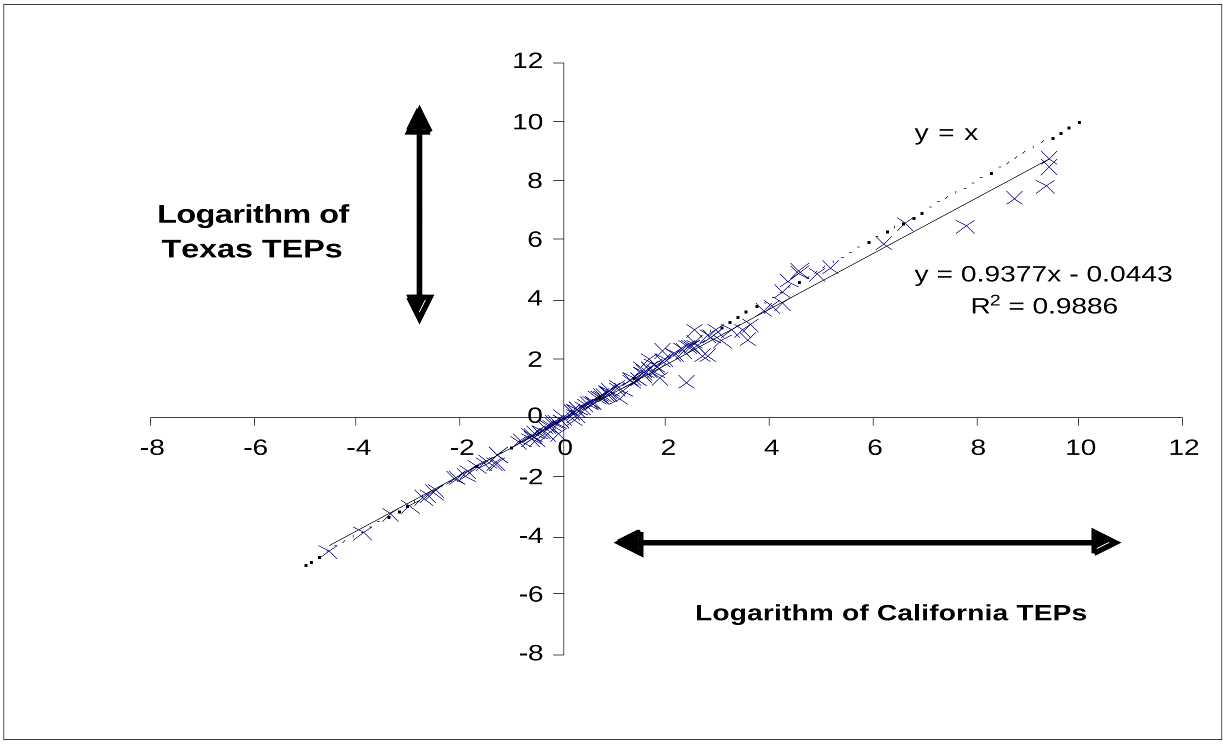

Figure 18(a) Logarithm of Texas carcinogen TEP's (in benzene equivalents) vs. logarithm of California carcinogen TEP's for 1 mol/d **air** emissions.

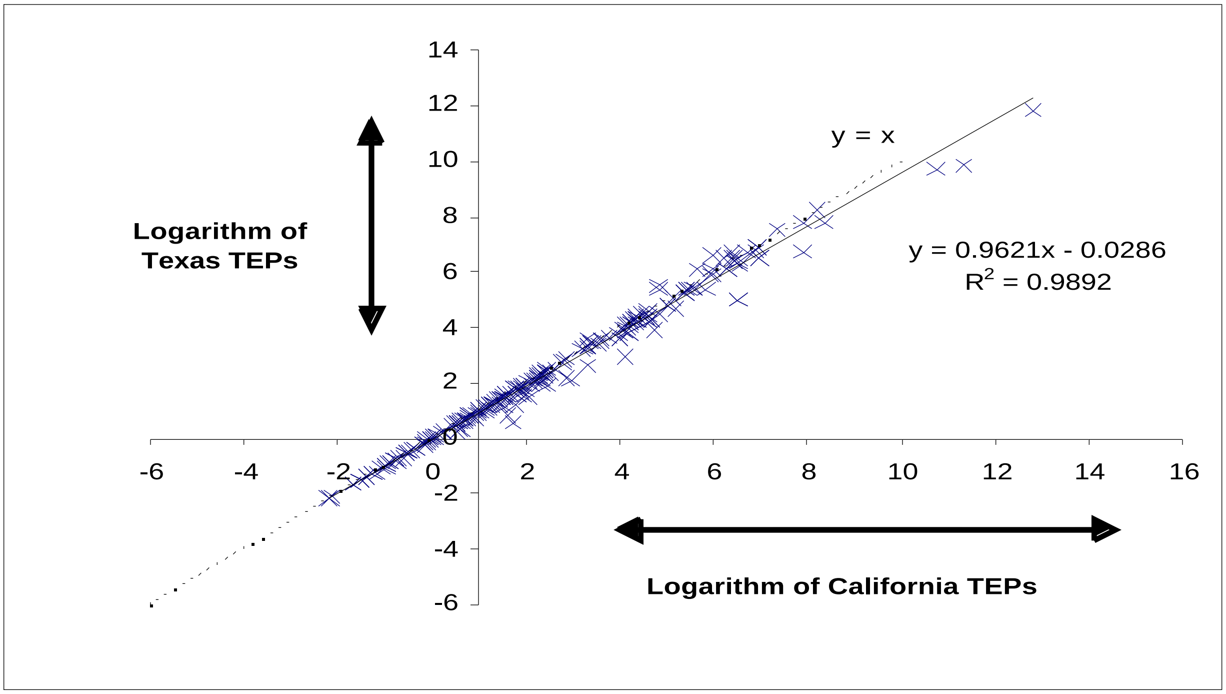

Figure 18(b) Logarithm of Texas non-carcinogen TEP's (in toluene equivalents) vs. logarithm of California non-carcinogen TEP's for 1 mol/d **air** emissions.

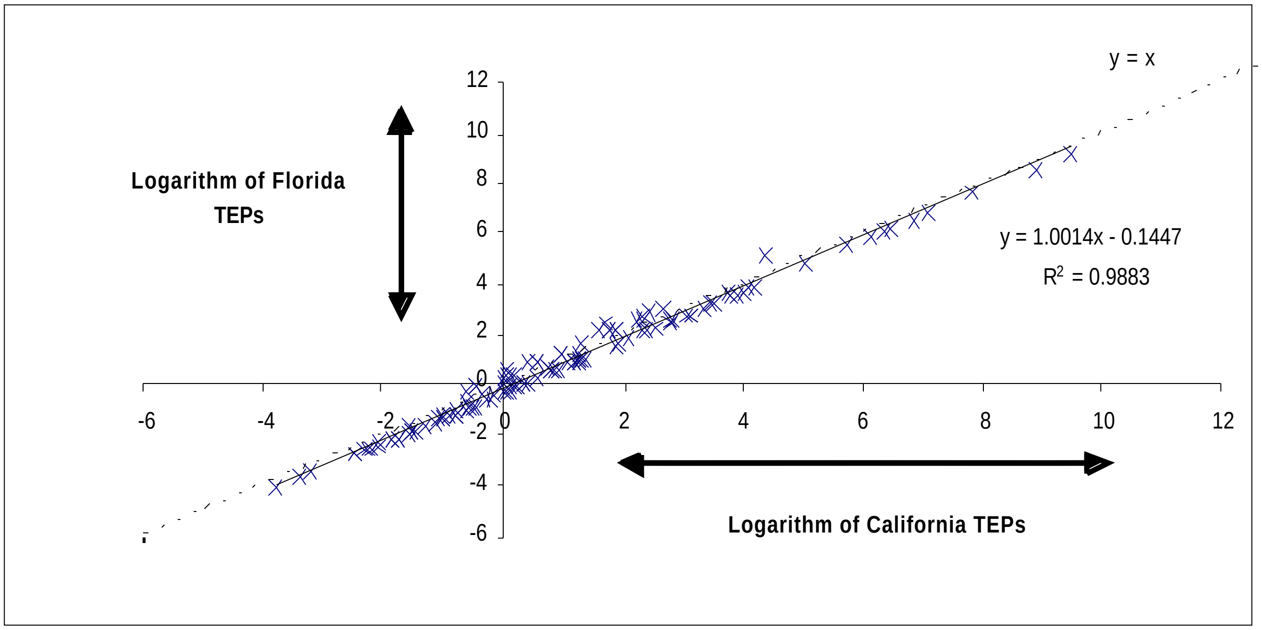

Figure 19(a) Logarithm of Florida carcinogen TEP's (in benzene equivalents) vs. logarithm of California carcinogen TEP's for 1 mol/d **surface-water** emissions.

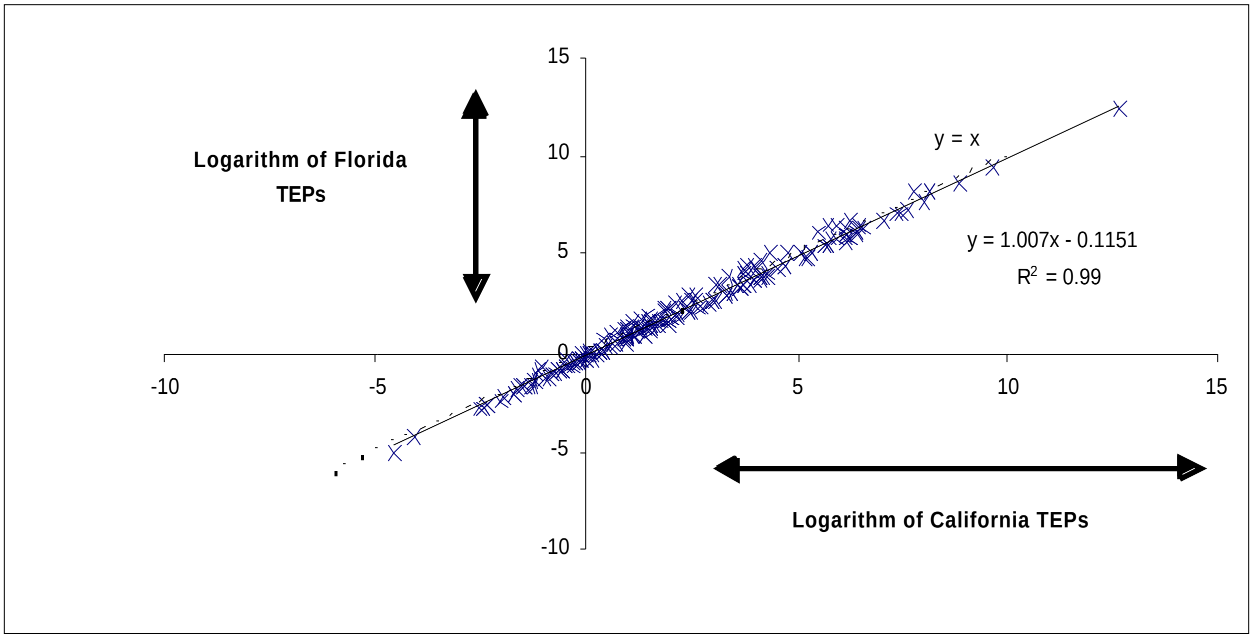

Figure 19(b) Logarithm of Florida non-carcinogen TEP's (in toluene equivalents) vs. logarithm of California non-carcinogen TEP's for 1 mol/d **surface-water** emissions.

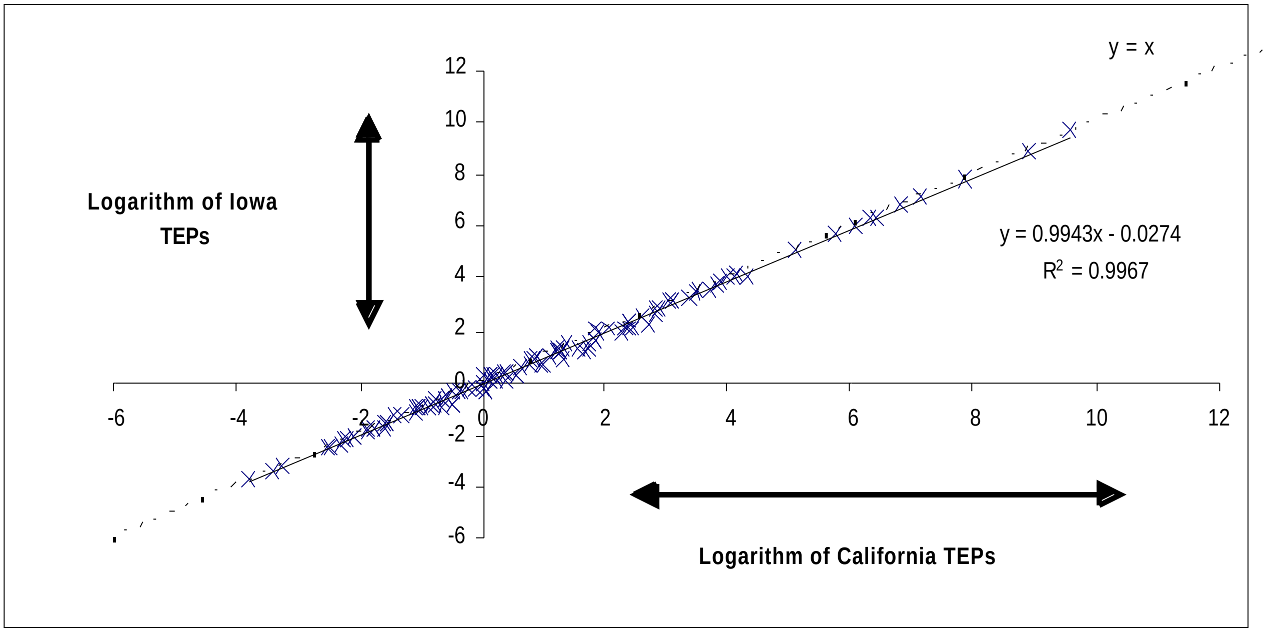

Figure 20(a) Logarithm of Iowa carcinogen TEP's (in benzene equivalents) vs. logarithm of California carcinogen TEP's for 1 mol/d **surface-water** emissions.

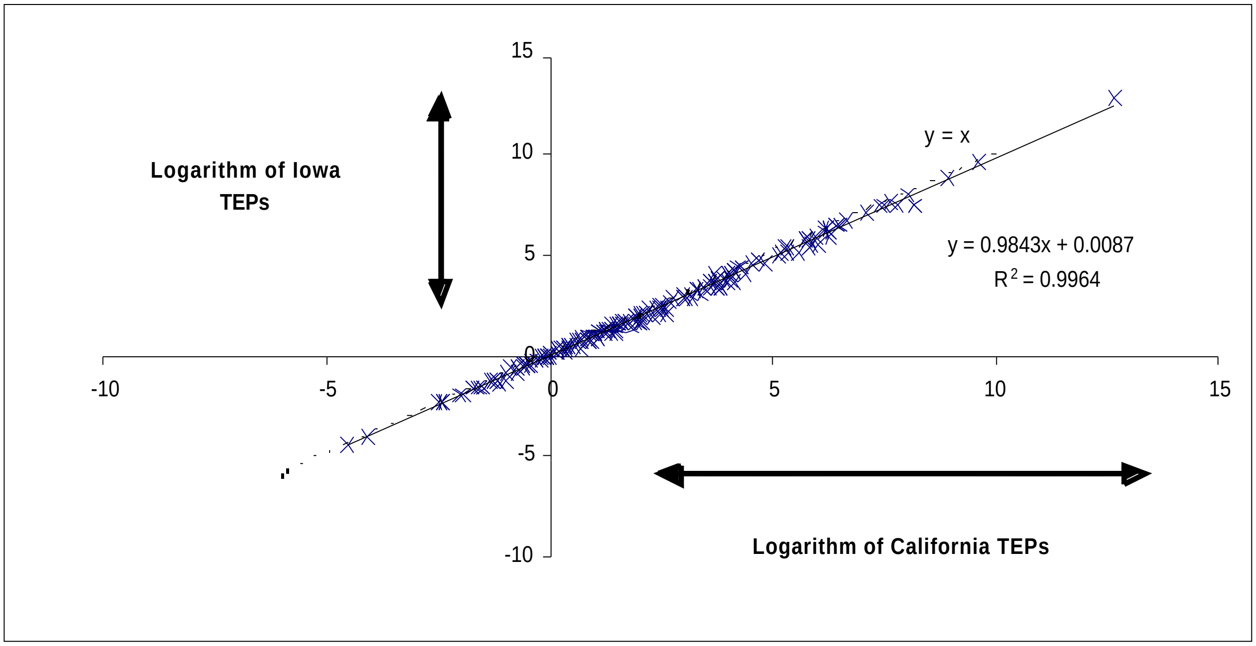

Figure 20(b) Logarithm of Iowa non-carcinogen TEP's (in toluene equivalents) vs. logarithm of California non-carcinogen TEP's for 1 mol/d **surface-water** emissions.

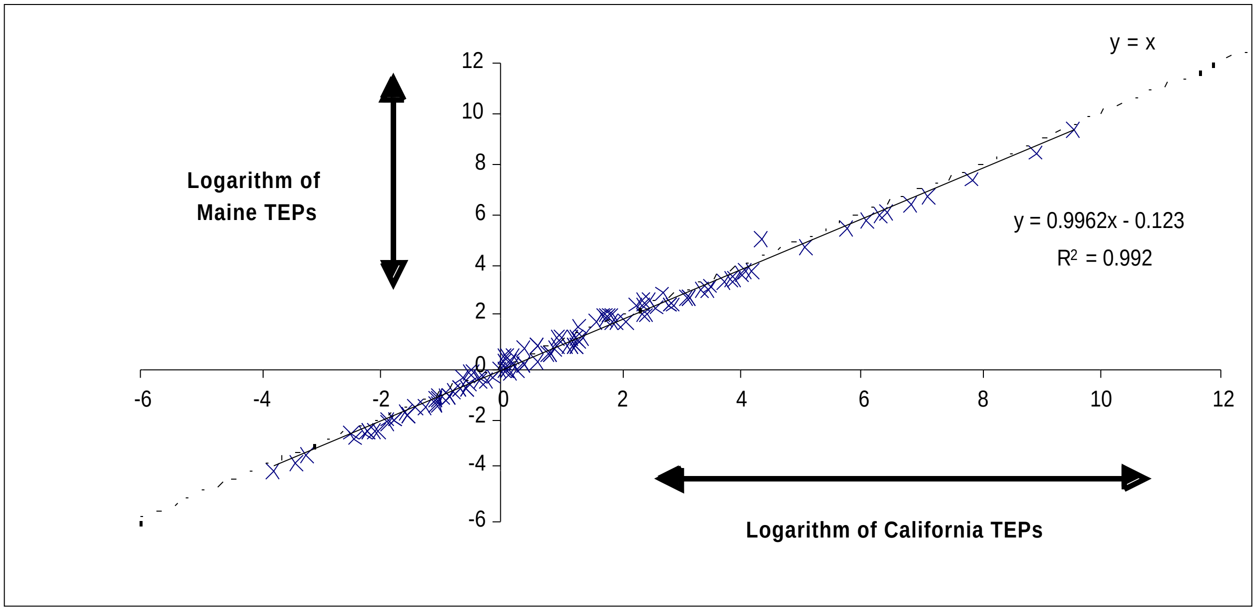

Figure 21(a) Logarithm of Maine carcinogen TEP's (in benzene equivalents) vs. logarithm of California carcinogen TEP's for 1 mol/d **surface-water** emissions.

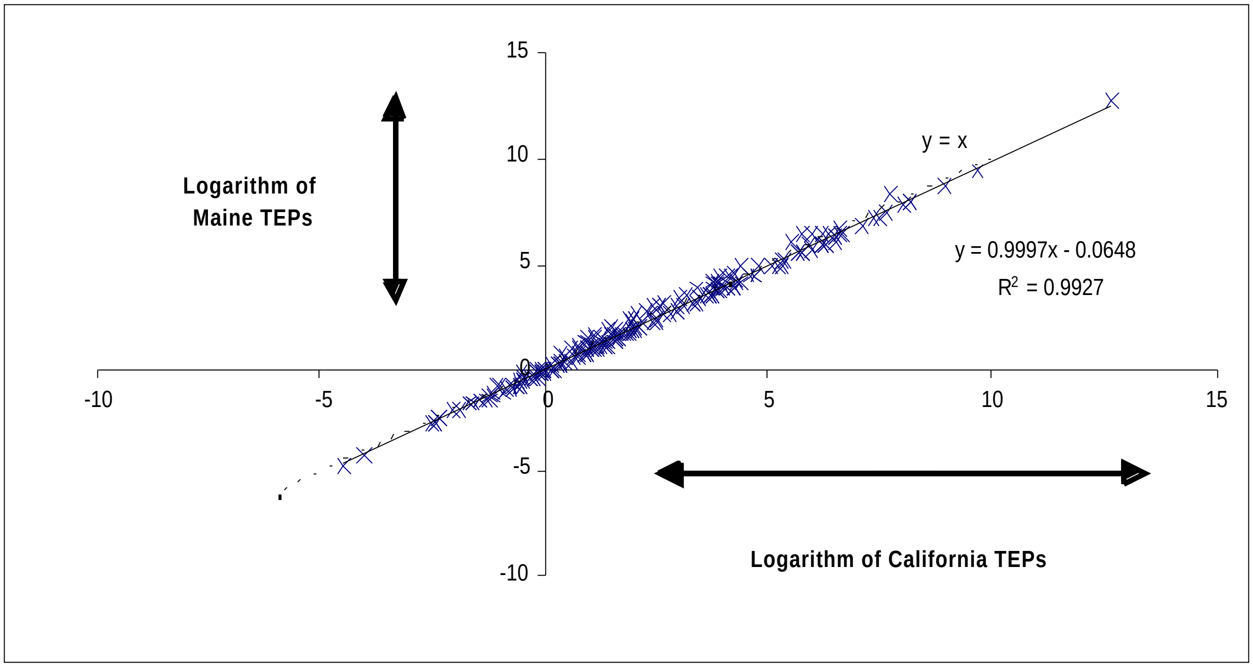

Figure 21(b) Logarithm of Maine non-carcinogen TEP's (in toluene equivalents) vs. logarithm of California non-carcinogen TEP's for 1 mol/d **surface-water** emissions.

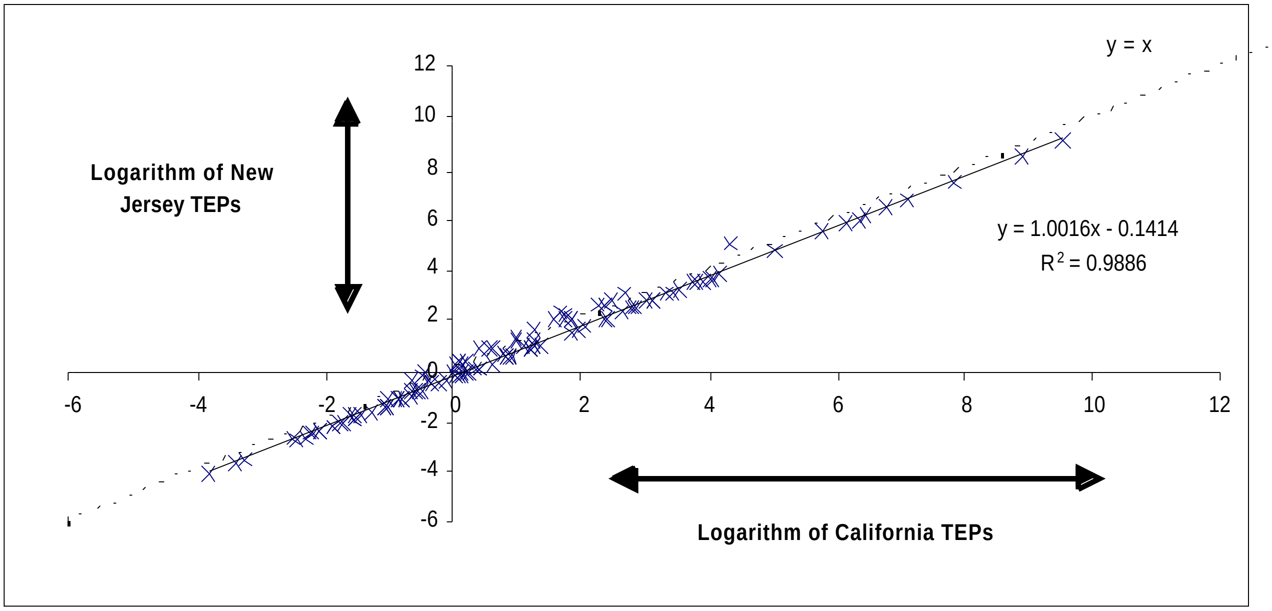

Figure 22(a) Logarithm of New Jersey carcinogen TEP's (in benzene equivalents) vs. logarithm of California carcinogen TEP's for 1 mol/d **surface-water** emissions.

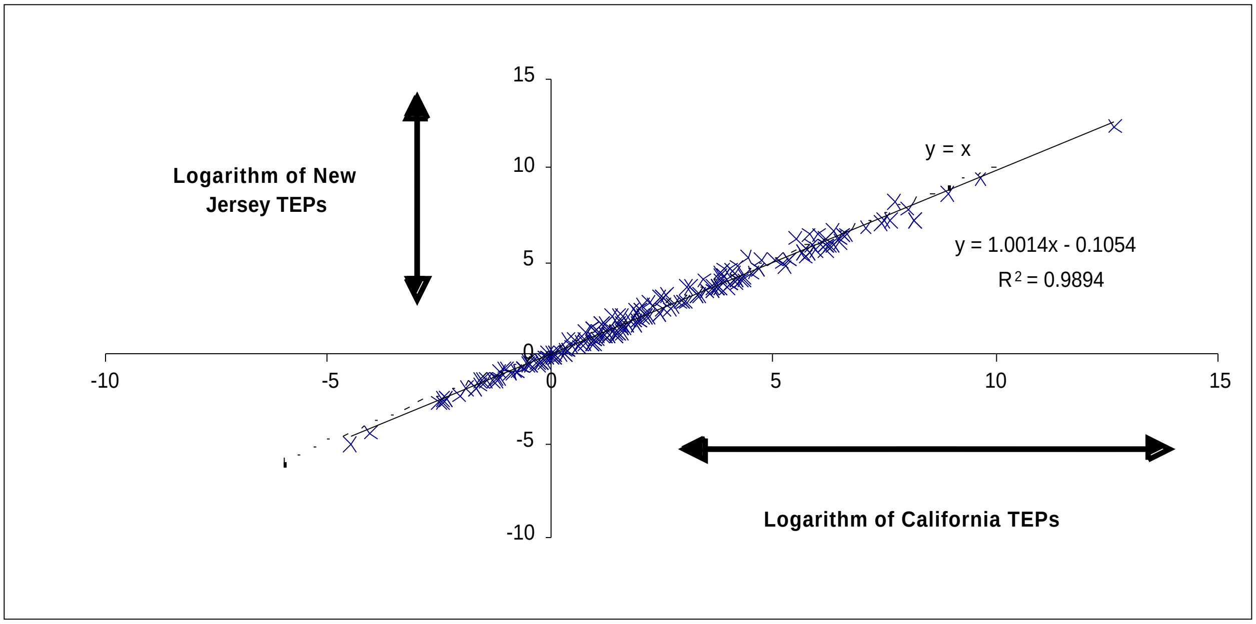

Figure 22(b) Logarithm of New Jersey non-carcinogen TEP's (in toluene equivalents) vs. logarithm of California non-carcinogen TEP's for 1 mol/d **surface-water** emissions.

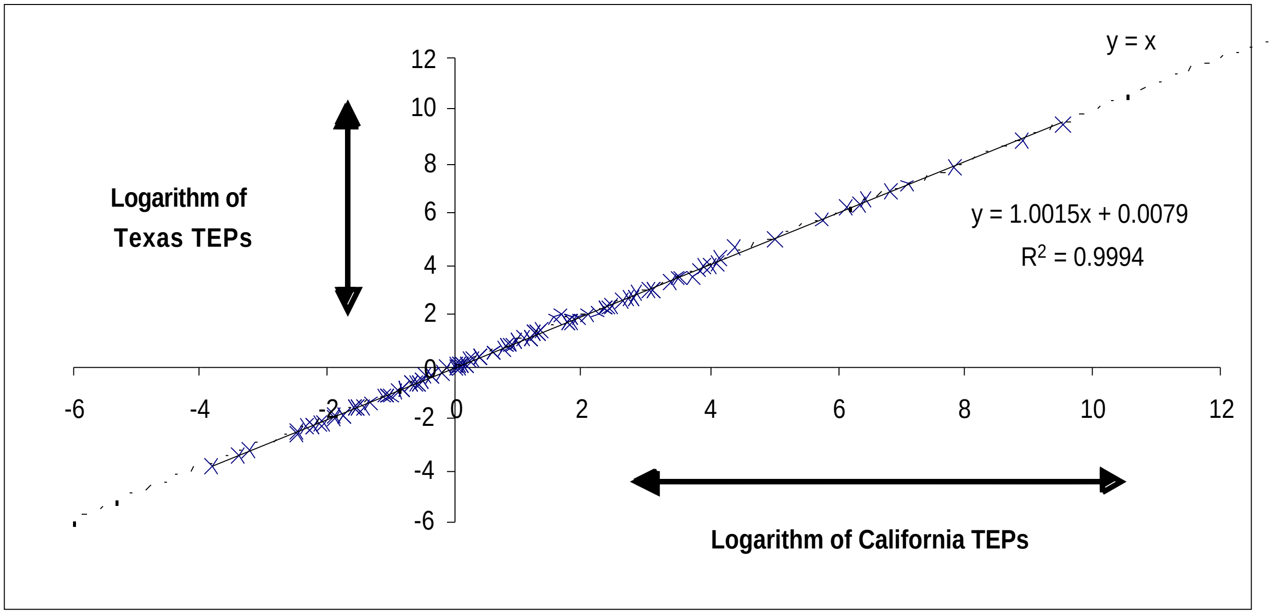

Figure 23(a) Logarithm of Texas carcinogen TEP's (in benzene equivalents) vs. logarithm of California carcinogen TEP's for 1 mol/d **surface-water** emissions.

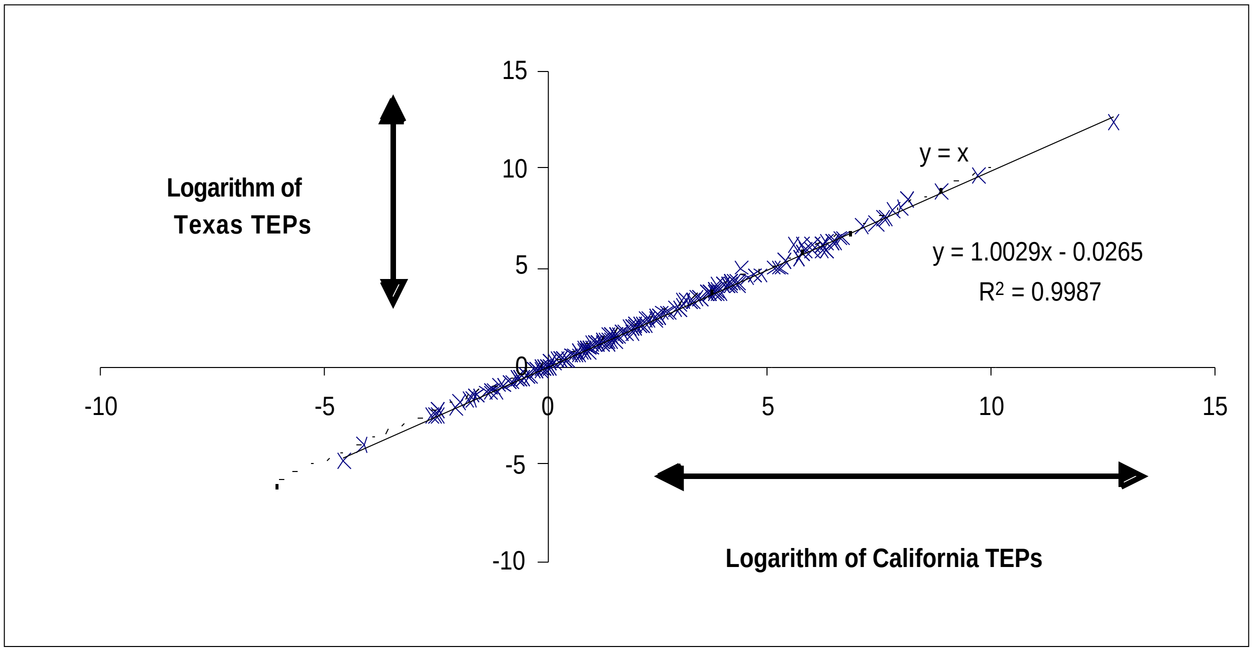

Figure 23(b) Logarithm of Texas non-carcinogen TEP's (in toluene equivalents) vs. logarithm of California non-carcinogen TEP's for 1 mol/d **surface-water** emissions.

6.0 References

Bare, J., G. Norris, T.E. McKone, and E. Hertwich (1998) "Development of TRACI: Tool for the Reduction and Assessment of Chemical Impacts," A presentation prepared for the Topical Conference on Pollution Prevention and Environmental Risk Reduction at the AIChE 1998 Annual Meeting.

Davis, G. A., M. Swanson, et al. (1994) *Comparative Evaluation of Chemical Ranking and Scoring Methodologies*. a report prepared for the US EPA Sustainable Technologies Division by the University of Tennessee, Knoxville, Tennessee.

Department of Toxic Substances Control (DTSC) (1992a) Guidance for Site Characterization and Multimedia Risk Assessment for Hazardous Substances Release Sites, Volume 2, Chapter 2 Documentation of Assumptions Used in the Decision to Include and Exclude Exposure Pathways, a report prepared for the State of California, Department of Toxic Substances Control, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-CR-103462.

Department of Toxic Substances Control (DTSC) (1992b) Guidance for Site Characterization and Multimedia Risk Assessment for Hazardous Substances Release Sites, Volume 2, Chapter 3, Guidelines for the Documentation of Methodologies, Justification, Input, Assumptions, Limitations, and Output for Exposure Models, a report prepared for the State of California, Department of Toxic Substances Control, by Lawrence Livermore National Laboratory, Livermore, CA, UCRL-CR-103460.

Environmental Defense Fund (EDF) (1998) *The Chemical Scorecard* available on the Internet at http://www.scorecard.org first issued in April 1998.

Eisenberg, J.N.S. and T.E. McKone, (1998 in press) "Decision Tree Method for the Classification of Chemical Pollutants: Incorporation of Across Chemical Variability and Within Chemical Uncertainty," accepted for publication in the Journal *Environmental Science and Technology*, August, 1998.

Guinée, J. and R. Heijungs (1993). "A Proposal for the Classification of Toxic Substances within the Framework of Life Cycle Assessment of Products." *Chemosphere* **26**(10): 1925-1944.

Hertwich, E.G., W. S. Pease, and T.E. McKone (1998) "Evaluating Toxic Impact Assessment Methods: What Works Best?" *Environ. Sci. & Technol.* **32**(5):A138-A144.

Imhoff, J.C., P.R. Hummel, J.L. Kittle jr., and R.F. Carsel (1994) "PATRIOT—A Methodology and Decision Support System for Evaluating the Leaching Potential of Pesticides," Environmental Research Brief, US Environmental Protection Agency (EPA) Environmental Research Laboratory Athens, GA, USA report EPA/600/S-93-10/, issued February, 1994. The PATRIOT model code and user help files can be obtained over the internet or by mail request from the US EPA Center for Exposure Assessment Modeling (CEAM), Athens GA, USA, 30605-2720.

D.W. Layton, T.E. McKone, C.H. Hall, M.A. Nelson, and Y.E. Ricker, *Demilitarization of Conventional Ordnance: Priorities for Data-Base Assessments of Environmental Contaminants*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-15902 (1986).

Maddalena, R.L., T.E. McKone, D.W. Layton, D.P.H. Hsieh (1995) "Comparison of Multi-Media Transport and Transformation Models: Regional Fugacity Model vs. CalTOX," *Chemosphere*, **30**, 869-889.

McKone, T.E. (1993a) *CalTOX, A Multimedia Total-Exposure Model for Hazardous-Wastes Sites Part I: Executive Summary*, prepared for the State of California, Department Toxic Substances Control, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-CR-111456PtI. (Currently available on the Internet at http://www.cwo.com/~herd1/.)

McKone, T.E. (1993b) *CalTOX, A Multimedia Total-Exposure Model for Hazardous-Wastes Sites Part II: The Dynamic Multimedia Transport and Transformation Model,* prepared for the State of California, Department Toxic Substances Control, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-CR-111456PtII. (Currently available on the Internet at http://www.cwo.com/~herd1/.)

McKone, T.E. (1993c) *CalTOX, A Multimedia Total-Exposure Model for Hazardous-Wastes Sites Part III: The Multiple-Pathway Exposure Model,* prepared for the California Department Toxic Substances Control, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-CR-111456PtIII. (Currently available on the Internet at http://www.cwo.com/~herd1/.)

NOAA (1998) National Climate Data Center (NCDC)—National Oceanic and Atmospheric Administration (NOAA) climate data online available at: http://www.ncdc.noaa.gov/ol/climate/online/ccd/

Pankow, J.F., et al, (1997) "The Urban Atmosphere as a Non-Point Source for the Transport of MTBE and Other Volatile Organic Compounds (VOCs) to Shallow Groundwater," *Environ, Sci, & Technol*. **31**(10):2821-2828)

Pease, W.S., E.G. Hertwich S. Mateles, and T.E. McKone (1998) "Human Health Impact Indicators for Life Cycle Analysis," in press.

Saxton, K.E. et al. (1986) “Estimating Generalized Soil-Water Characteristics From Texture.” *Soil Sci. Soc. Amer. J.* **50**(4):1031-1036.

Schwalen, E.T.; Kiefer, K.L.; Geng, S.; McKone, T.E.; and Hsieh, D.P.H., (1995) *The Distribution of California Landscape Variabiles for CalTOX*, a report prepared by the Risk Science Program, University of California, Davis for the State of California Department of Toxic Substances Control.

US Bureau of the Census (1997) *Statistical Abstract of the U.S.*, (U.S. Government Printing Office) p 227, Table No 367, “Land and Water Area of States and Other Entities.”

USDA (1998) US Department of Agriculture, Agriculture Research Service (ARS) Soil Texture Triangle Hydraulic Properties Calculator, at internet address: http://www.bsyse.wsu.edu/~saxton/saxton/grphtext.htm

USEPA (1989). *Risk Assessment Guidance for Superfund Volume I Human Health Evaluation Manual (Part A)*. US Environmental Protection Agency, Office of Emergency and Remedial Response. Washington, DC. EPA/540/1-89/002.

USEPA (1992). “US Environmental Protection Agency, Guidelines for Exposure Assessment: Notice.” *Federal Register* **57**(104):22888-22938.

USEPA SAB (1997). *Human Exposure Assessment: A Guide to Risk Ranking, Risk Reduction and Research Planning*. US Environmental Protection Agency, Science Advisory Board. Washington, DC. EPA-SAB-IAQC-95-005.

USEPA (1997) *Exposure Factors Handbook*. Office of Research and Development, U.S. Environmental Protection Agency, 1997.

van der Leeden, F., F.L. Troise, and D.K. Todd (1991) *The Water Encyclopedia* (Lewis Publishers, Chelsea, MI).

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

BLANK PAGE