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Multiple-Pathways Screening-Level Assessment of a Hazardous Waste Incineration Facility

> G. A. Holton C. C. Travis E. L. Etnier F. R. O'Donnell D. M. Hetrick E. Dixon

OPERATED BY MARTIN MARIETTA ENERGY SYSTEMS, INC. FOR THE UNITED STATES DEPARTMENT OF ENERGY



Printed in the United States of America. Available from National Technical Information Service U.S. Department of Commerce 5285 Port Royal Road, Springfield, Virginia 22161 NTIS price codes—Printed Copy: A04; Microfiche A01

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ORNL/TM-8652

Health and Safety Research Division

MULTIPLE-PATHWAYS SCREENING-LEVEL ASSESSMENT OF A HAZARDOUS WASTE INCINERATION FACILITY

G. A. Holton, C. C. Travis, E. L. Etnier, F. R. O'Donnell, D. M. Hetrick, and E. Dixon

Date of Issue -- September, 1984

Prepared for the Incineration Research Branch Industrial Environmental Research Laboratory U.S. ENVIRONMENTAL PROTECTION AGENCY Cincinnati, Ohio 45268 Under Interagency Agreement No. AD-89-F-1-768-0

> Prepared by the Oak Ridge National Laboratory Oak Ridge, Tennessee 37831 operated by Martin Marietta Energy Systems, Inc. for the U.S. DEPARTMENT OF ENERGY under Contract No. DE-AC05-840R21400

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ACKNOW LEDGMENTS

The authors acknowledge the support and encouragement given us by Ben Blaney of EPA's Incineration Research Branch. His many hours of technical assistance and review have substantially improved this document. The assistance of Lois Szluha in composition of the many drafts and final report is also gratefully acknowledged.

MULTIPLE-PATHWAYS SCREENING-LEVEL ASSESSMENT

OF A HAZARDOUS WASTE INCINERATION FACILITY

1. SUMMARY

The purpose of this assessment was to make a preliminary determination of the relative importance of air, food, and water pathways to human exposure from hazardous materials released from incineration facilities. These results are to be used to determine where more research on food and water pathways may be warrented. Identical 150 x 10^6 Btu/h rotary kiln incinerator facilities burning pesticide-related wastes were assumed to be sited in three different locations in the United States. This incinerator size represents an upper limit of heat capacity for U.S. incinerators (Travis et al., The locations studied for air and food chain exposures were a 1984). southern California site (S-1) at 33° 20' latitude and 115° 30' longitude; a northern Midwest site (S-2) at 44° 55' latitude and 89° 50' longitude, and a central Midwest site (S-3) at 38° 20' latitude and 94° 20′ longitude. These sites are in areas that lead the nation in production of leafy vegetables, milk, and beef, respectively, and were chosen to estimate possible worst-case population exposures from these In the water pathways assessments, screening-level foodstuffs. assessments were performed at sites S-1 and S-2.

The food chain and air pathway assessments considered average individual exposures and doses resulting from incineration of the ten most prevalent pesticide-related chemicals currently being incinerated

in the United States. Inhalation exposure estimates were made using ATM, an atmospheric transport model and CONEX, a model used to estimate population exposures. These codes make use of automated meteorological and population data bases. Estimates of maximum, minimum, and average individual inhalation intake were calculated for the ten pesticiderelated pollutants using annual-average ground-level air concentrations and site-specific population data obtained from the 1980 census.

Food chain ingestion intakes were estimated using TEREX, a terrestrial food chain exposure model. The code makes use of an automated agricultural data base consisting of parameters for the conterminous United States characterizing human food crops, livestock feeds, and livestock production. These data, together with deposition rates for each pollutant, and chemical-specific bioaccumulation factors, are used to calculate pollutant concentrations in various food items. Individual intakes (doses) were calculated for each site based on human dietary intakes of specific food items.

Estimates of human exposure via the drinking water pathway were only calculated for one pesticide-related chemical: trichloroethylene. Drinking water ingestion intakes were calculated using a multi-media model, TOX-SCREEN. This model estimates surface water concentrations resulting from direct atmospheric deposition and runoff. Ingestion doses were estimated by employing average pollutant concentrations in surface water and daily water consumption data. Estimates were also made of annual pollutant transfer of trichloroethylene to groundwater aquifers.

Major conclusions to be drawn from this report are:

For certain organic chemicals the food chain pathway may be an 1. important contributor to total human exposure from incineration of hazardous wastes. Average individual inhalation and ingestion intake $(\mu g/y)$ from incineration of pesticide-related waste at site S-1 is given in Table 1.1. Table 1.2 presents the percent contribution of the food chain pathway to total average individual dose (inhalation and food chain) for the three sites studied. The contribution of the food chain to total dose is very chemicalspecific, depending on the octanol-water partitioning coefficient and the atmospheric degradation rate. The percent contribution of ingestion dose to total dose ranges from 0.7% for hexachlorobutadiene to 83% for carbon tetrachloride. Differences between sites result primarily from site-specific differences in productivity rates for the various food items. Although there is large uncertainty associated with ingestion exposure calculations, the fact that ingestion of compounds suggests that the injestion pathway is of comparable import to the direct inhalation pathway. A comparison of the results obtained in an earlier, related study (Travis et al., 1984) suggest that food chain exposure to emitted hydrocarbons will not be significant. This is because food chain and inhalation exposures are according to the present study, and inhalation comparable, exposures were shown by Travis et al. to be small in terms of cancer risk and average daily intake. (This assumes, of course.

Pollutant	Inhalation (µg/y)	Ingestion (µg/y)
1,1,1,2-Tetrachloroe thane	7.74E-2	2.85E-2
Chloroform	7.15E-2	3.83E-3
Ethylene dichloride	2.23E-1	4.25E-3
Hexachlorobutadiene	1.08E-1	8.04E-4
1,1,2,2-Tetrachloroethane	2.82E-2	4.49E-3
Hexachloroethane	2.69E-2	1.38E-2
Carbon tetrachloride	1.05E-2	4.30E-2
Hexachlorobenzene	1.99E-2	8.07E-3
Trichloropropane	1.38E-1	4.00E-3
Trichloroethylene	3.16E-2	1.41E-3

Table 1.1 Comparison of average individual inhalation and ingestion intake $(\mu g/y)$ from incineration of pesticide-related waste at site S-1

5-1 S-2	S-3	
/ 60	65	
5 57	73	
2 5	8	
0.7 2	3	
4 31	45	
4 60	71	
0 76	83	
9 60	70	
3 7	10	
4 11	13	
	7 60 5 57 2 5 0.7 2 4 31 4 60 0 76 9 60 3 7 4 11	$\begin{array}{cccccccccccccccccccccccccccccccccccc$

Table 1.2 Percent contribution of food chain pathway to total average individual dose (inhalation and food chain)

that hydrocarbon compound potency values for food injestion are not significantly higher than for direct inhalation.) On the other hand, metal emissions from incinerators were found by Travis et al. to have potentially significant health risks. Metal emissions were not considered in the present study, but should be the focus of a future study.

2. For trichloroethylene, the drinking water pathway appears to be a small contributor to total human dose (Table 1.3). This pathway contributes 2 and 4% of total intake at sites S-1 and S-3, respectively. On the basis of this narrow preliminary assessment, it does not appear that the drinking water pathway is an important route of human exposure for hazardous materials released from incineration facilities.

from incineration of trichloroethylene								
Exposure Pathway								
Site	Inhalation	Ingestion	Drinking Water					
S-1	3.2E-2	1.4E-3	9.4E-4					
S-3	1.8E-2	2.8E-3	9.8E-4					

Table 1.3 Human intake $(\mu g/y)$ resulting from incineration of trichloroethylene

3. The present assessment did not determine human exposure from chemicals leached into groundwater after release from a hazardous waste incinerator. However, we did estimate annual transfer $(\mu g/y)$ of trichloroethylene into groundwater aquifers 15 and 50 m below the surface at sites S-1 and S-3, respectively. For site S-1, no groundwater contamination occurred within the 10-year period investigated, but at site S-3, the groundwater aquifer was contaminated within 10 years. Transfer to groundwater at this latter site in the 10th year was estimated to be 3.6 x 10^4 µg/y, which represents 4.5 x 10^{-6} times the assumed annual stack release of trichloroethylene. On the basis of this preliminary assessment, it does not appear that hazardous waste incineration poses a significant threat to groundwater quality.

2. INTRODUCTION

Previous studies of population exposures resulting from releases of air pollutants from hazardous waste incinerators (Staley et al., 1982; Holton et al., 1982; and Travis et al., 1984) have focused on the inhalation pathway to man. Little attention has been given to other exposure pathways even though studies of synthetic fuel production (Walsh, 1983) and coal-fired power plants (McBride et al., 1978) have shown that the food chain can be an important contributor to total population exposure. The present assessment is performed to determine the relative importance of air, food, and water pathways for human exposure to hazardous materials released from an incineration facility in the form of air pollutants. The inhalation and terrestrial food chain pathways are examined for transport of ten pesticide-related wastes. Due to resource limitations, the drinking water and groundwater pathways are examined for only one organic chemical: trichloroethylene.

This study did not consider the impact of fugitive emissions on the relative importance of the air, food, and water pathways. Preliminary investigation indicates that fugitive emissions would not change the relative importance of the three pathways. This is because air concentrations resulting from fugitive emissions drop off rapidly inside of 5 km as one moves away from the area source and then remain approximately constant out to 100 km. Thus, in the area between 5-100 km, the spatial distribution of populations and food crops has little effect on total inhalation and ingestion intakes. Even though air concentrations from fugitive emissions may be appreciably larger within 5 km of the source, the contribution to average individual ingestion intake is small since this area represents only 0.25% of the total area available for crop production.

It should be emphasized that the exposure assessment methodologies presented in this report are very generalized, and caution should be exercised in interpreting the results. It is not currently possible, nor is it necessarily desirable, to develop predictive methodologies which address all processes affecting movement of contaminants through the environment. Many environmental transport processes are extremely complex and not well understood. In addition, even when a sufficient conceptual basis exists for developing complex, process-oriented models, accurate physical and environmental data are generally not available to parameterize them. It is, therefore, often most appropriate to use simplifying assumptions when attempting to predict the environmental fate of pollutants.

The methodologies presented here represent a reasonable compromise between model complexity and the ability to obtain realistic data characterizing model parameters. We have attempted to make reasonably conservative assumptions regarding environmental transport of materials released by incineration facilities; if anything, the absolute value of exposures present worse case situations. The principal pathways considered are atmospheric and aquatic transport and transformation, ingestion of toxic materials that have passed through the and terrestrial food chain. However, the inhalation and food chain pathways are only investigated for ten chemicals at three sites, and results obtained may not be representative of other waste streams and Furthermore, a detailed analysis of the drinking water and locations. groundwater pathways has not been performed. Site-specific application of our results would require careful evaluation of the extent to which the models and parameter values used in this report are representative of conditions prevailing at the specific site.

2.1 INHALATION EXPOSURE

Inhalation exposure estimates were made using an atmospheric transport model (ATM), a Gaussian plume model developed at ORNL (Raridon et al., in press) and the Concentration Exposure Model (CONEX) (O'Donnell et al., 1983). ATM is used to calculate average groundlevel air concentrations and deposition rates in each sector segment for each pollutant. The ATM model was selected since it specifically accounts for both wet and dry deposition rates, values necessary as

input into the terrestrial food chain model. Latitude and longitude coordinates for each incinerator site are used to access automated meteorological data (NOAA, 1974) and 1980 Census population data sets. These data are then employed by CONEX to estimate population exposure from inhalation by multiplying atmospheric concentration by local population estimates. Maximum, minimum, and average individual intakes (dose) were calculated.

2.2 FOOD CHAIN DOSE

Food chain ingestion doses resulting from releases of hazardous materials at waste incinerators are estimated using TEREX, a terrestrial food chain exposure model. This mode1 estimates concentrations of organic chemicals in various human and livestock food items. Four categories of vegetables are considered: leafy vegetables and fruit exposed to airborne material; vegetables; vegetables, fruits, and nuts protected from airborne materials; and grains. Livestock feeds considered are hay, pasture, and grains. Non-vegetable human food items represented are milk and beef. Once pollutant concentrations have been estimated, individual intakes of each chemical are calculated at each site based on dietary intake of specific foods.

2.3 WATER INGESTION DOSE

Drinking water ingestion dose for trichloroethylene is calculated using a multimedia, screening-level model, TOX-SCREEN (McDowell-Boyer

and Hetrick, 1982). This model begins with an atmospheric release of pollutant at the incineration facility and estimates air, water, and soil concentrations through computation of media interaction (air to ground and surface water deposition, surface runoff from ground to surface water, leaching from ground to groundwater, percolation to groundwater and groundwater runoff to surface water).

Drinking water ingestion intakes are estimated by employing average pollutant concentrations in surface water (a river) and average daily intake of water. Estimates of penetration of trichloroethylene into the groundwater table are also made.

3. INCINERATION FACILITY DESIGN

Design of the incineration facility used in this study was based on a review of existing incinerators and engineering judgment. For example, the hypothetical 150 x 10^6 Btu/h incinerator used in this study was assumed to possess one receiving tank for each of four categories of waste: clean or dirty high-Btu waste and clean or dirty low-Btu waste (dirty waste is any waste that requires pretreatment to enhance viscosity). Two additional tanks were included to provide extra storage capacity for irregular shipments. The storage area of the facility was designed with sufficient capacity to store waste for 14 days continuous operation. The feed area was assumed to have sufficient storage for three days of operation. Other design factors, such as piping or numbers of pumps, were also taken into consideration. A more detailed description of facility design appears in Travis et al.

(1984). The process flow diagram for the facility studied is shown in Figure 1.

4. WASTE CHARACTERIZATION

Operation of a commercial incinerator is characterized by receipt of wastes of widely varying composition. The EPA has conducted a survey of the composition of hazardous waste streams currently being incinerated (MITRE, 1983). A total of 237 different constituents have been identified as present in one or more of the 413 hazardous waste streams reviewed. Table 4.1 lists the ten most prevalent pesticiderelated chemicals found in hazardous waste streams currently being incinerated. The present assessment will focus on these ten chemicals. Note that it is highly unlikely that all ten of these pesticide-related chemicals would ever be found in a specific waste stream.

Constituent	Amount Incinerated ^a (MT/y)
1,1,1,2-tetrachloroethane	9.57E4
Chloroform	9.13E4
Ethylene dichloride	7.85E4
Hexachlorobutadiene	6.79E4
1,1,2,2-tetrachloroethane	2.10E4
Hexachloroethane	1.45E4
Carbon tetrachloride	1.35E4
Hexachlorobenzene	1.23E4
Trichloropropane	1.20E4
Trichloroethylene	1.15E4

Table 4.1Ten most prevalent pesticide-related chemicalsfound in incineration waste streams

^aFrom compilation of waste information (USEPA, 1980).

4.1 STACK EMISSION SOURCE TERMS

The rate of release (mass per unit time) of specific chemicals as stack emissions is controlled by three facility variables: waste throughput, chemical concentration in the waste stream, and destruction and removal efficiency (DRE). Waste throughput in an incineration facility is determined by the percent contribution of the waste to the total waste stream after supplementary addition of No. 2 fuel oil to insure combustibility. When it is necessary to add fuel oil to the waste stream to insure incinerability (as is the case with the pesticide-related waste streams), waste throughput (TP_W) and fuel oil throughput (TP_{fo}) can be calculated using equations 1 and 2 below.

$$TP_{w} = 7200 \left[\frac{CF}{10^{4}} (\Delta Hc)_{fo} - CF \right] / \rho_{Lw} \left[(\Delta Hc)_{fo} - (\Delta Hc)_{w} \right], \qquad (1)$$

$$TP_{F0} = 7200 \left[CFr10 \ tsup4(\Delta Hc)_{w} \right] \rho_{Lf0} \left[(\Delta Hc)_{f0} - (\Delta Hc)_{w} \right], \qquad (2)$$

where

7200 = operating time (h/y); CF = incinerator capacity (150 x 10⁶ Btu/h); (Δ Hc)_{fo} = heat of combustion of #2 fuel oil (19,000 Btu/lb); (Δ Hc)_w = heat of combustion of waste (3,000 Btu/lb); ρ_{Lw} = liquid density of waste (14 lb/gal); and ρ_{Lfo} = liquid density of #2 fuel oil (7.2 lb/gal).

Using these equations, waste and fuel oil throughput are estimated to be 2.76 x 10^{10} g/y and 4.23 x 10^{10} g/y, respectively.

A destruction and removal efficiency (DRE) of 99.99% (the proposed emission standard for hazardous waste incinerators -- USEPA, 1981a) was assumed for this assessment. To obtain stack emission rates, throughput was multiplied by the fractional representation of each pesticide in the waste stream and 10^{-4} to account for a 99.99% DRE. Predicted annual stack emission rates (g/y) are given in Table 4.2.

Constituent	Fraction of waste stream ^a (%)	Emission rate g/y
1,1,1,2 tetrachloroethane	6.6	1.95E4
Chloroform	6.1	1.80E4
Ethylene dichloride	19.0	5.61E4
Hexachlorobutadiene	9.2	2.72E4
1,1,2,2-tetrachloroethane	2.4	7.08E3
Hexachloroethane	2.3	6.79E3
Carbon tetrachloride	0.9	2.66E3
Hexachlorobenzene	1.7	5.02E3
Trichloropropane	11.7	3.45E4
Trichloroethylene	2.7	7.97E3

Table 4.2 Stack emission rates of the pesticide-related generic waste (99.99% DRE)

^aCalculated by averaging pesticide-related waste chemical concentrations (USEPA, 1980).

5. SITE SELECTION

Identical 150 x 10^6 Btu/h rotary kiln incinerator facilities burning pesticide-related wastes were assumed to be sited in three different locations in the United States. The three locations chosen for this assessment were a southern California site (S-1) at 33° 20' latitude and 115° 30' longitude; a northern Midwest site (S-2) at 44° 55' latitude and 89° 50' longitude, and a central Midwest site (S-3) at 38° 20' latitude and 94° 20' longitude. These sites are in areas that lead the nation in production of leafy vegetables, milk, and beef, respectively, and were chosen to estimate possible worst-case contaminations of these foodstuffs. The number of persons in each sector segment was obtained from 1980 Census data tapes that were reformatted into 0.1° -latitude by 0.1° -longitude rectangular grids. APORT2 was used to apportion this population data to the sector segments that were used by CONEX. The site-specific cumulative population distributions are given in Table 5.1. The central Midwest site was the most populous, with 1.46 million people, followed by the northern Midwest site with 0.45 million people, and the southern California site with 0.20 million people.

Area-specific meteorological, climatological, and geological data are employed to estimate pollutant concentrations in air, food, and water. A circular area of 100 km radius around each incinerator facility was assumed for the assessment. The assessment area was divided into 160 sector segments consisting of 11 concentric circles about the origin (site center) and sixteen radial direction vectors. The circles had radii of 0.1, 10, 20, 30, 40, 50, 60, 70, 80, 90, and 100 km. Radial vectors were 22.5° apart, proceeding clockwise, with the first vector being centered on due north (0°). Centers of sector segments were located midway between the circles on the radial vectors.

6. INHALATION DOSE

Human dose via the inhalation pathway from incineration of pesticide-related waste was estimated for stack emissions for the three sites (S-1, S-2, and S-3). Models, parameters, and results are discussed below.

Distance (m)	S-1	S-2	S-3
5,050	0	7,432	2,528
15,000	992	76,571	10,474
25,000	4,984	108,979	18,777
35,000	8,585	128,609	42,134
45,000	28,827	196,307	70,483
55,000	55,307	263,092	143,535
65,000	78,809	317,157	309,225
75,000	110,132	349,963	724,409
85,000	141,703	395,472	1,168,924
95,000	191,007	448,182	1,455,344

Table 5.1 Cumulative population at three incinerator sites

6.1 MODEL SELECTION

Annual-average ground-level air concentrations and ground deposition rates of a representative chlorinated hydrocarbon pollutant were estimated using ATM, which employs a Gaussian plume dispersion model. Gaussian plume models are generally applied for distances of 20-50 km around a site. However, this type of dispersion model has been validated out to 150 km (Buckner, 1981), predicting annual-average air concentrations within a factor of three of those measured. ATM calculates concentrations and deposition at specified receptor points. In this case, the points (called "grid" points) were located at the intersections of eleven concentric circles and sixteen equally spaced direction vectors.

CONEX (O'Donnell et al., 1983) was used to calculate human exposures to the representative pollutant in each sector segment and in various aggregates of the segments (i.e., by concentration level, sector, radial band, and all segments). Exposures in a sector segment are calculated by multiplying the average ground-level air concentration in the sector segment by the number of persons located in that segment, which, in this case, was obtained from 1980 Census data using APORT2, an adaptation of the APORT computer code (Fields and Little, 1978). Maximum, minimum, and average intakes (dose) of the pollutant were estimated by multiplying the individual maximum, minimum, and average sector-segment exposures by a breathing rate of 8,322 m³/y (ICRP, 1975) and a 0.65 absorption factor.

6.2 INPUT PARAMETERS

ATM input parameters include model-plant descriptors, pollutant behavior variables, and site-specific meteorological data. The stack was assumed to be located at the site origin. Stack parameters employed are summarized below (Table 6.1).

Table 6.1. Stack Parameters

Parameter

Height above ground, m	27.43
Gas temperature, ^o K	366.5
Release velocity, m/s	6.40
Stack radius, m	1.04

To minimize the number of ATM model runs, air concentrations and deposition rates for a unit release of only one chlorinated hydrocarbon gas were estimated using ATM. These results were then adjusted to reflect individual pollutant source strengths to obtain pollutantspecific air concentration and deposition values. This procedure employed a zero degradation rate and gravitational settling velocity. A dry deposition rate of 0.01 m/s was assumed and ATM automatically calculated wet deposition velocities based on rainfall rate and duration. These parameter values are representative of all pollutants in the generic waste and their uniform application to all these pollutants should not bias results. Area-specific meteorological data were obtained from Stability Array (STAR) data tapes (NOAA, 1974) and from a compendium of weather statistics (Ruffner, 1978). The STAR data were organized into six stability categories (A through F) and six wind speed classes having average wind speeds of 0.75, 2.5, 4.3, 6.8, 9.5, and 12.5 m/s. Location of meteorological stations from which STAR data were obtained are summarized below (Table 6.2).

Site		Station	File header	Years averaged
	Number	Name		
S-1	23158	Blythe/Riverside, CA	810	Sept. 1969-Aug. 1974
S-2	14991	Eau Claire, WI	715	Jan. 1969-Dec. 1973
S-3	3947	Kansas City, MO	1200	Jan. 1969-Dec. 1974

Table 6.2 Location of meteorological stations

Dispersion parameters used were those of Briggs-Smith formulated by Hosker (see Raridon et al., in press). The remaining meteorological parameters were obtained from Ruffner (1978), and are summarized below (Table 6.3).

6.3 RESULTS

Minimum, expected, and maximum individual inhalation intakes $(\mu g/y)$ for all three sites are given in Table 6.4. These estimates are based on an assumed breathing rate of 8,322 m³/y (ICRP, 1975) and 65% absorption through the lung. Although total population size and distribution vary between the three sites (see Table 5.1), expected

S-1	S-2	S-3
295.8 ⁸	280.2 ^b	286.3 ^c
3.16 ^a	28.72 ^b	35.54 [°]
15 ^d	120 ^e	107 ^f
0.0103	0.0822	0.0733
3.51	3.99	5.54
536	458	413
1210	1213	1349
	S-1 295.8 ^a 3.16 ^a 15 ^d 0.0103 3.51 536 1210	S-1 S-2 295.8 ^a 280.2 ^b 3.16 ^a 28.72 ^b 15 ^d 120 ^e 0.0103 0.0822 3.51 3.99 536 458 1210 1213

Table 6.3 Meteorological parameters input into ATM

^aAverage for three weather stations: Blythe/Riverside and Imperial, California (1931-1960) and Yuma, Arizona (1941-1970).

^bAverage for two weather stations: Eau Claire (1931-1960) and Green Bay, Wisconsin (1941-1970).

^cAverage of 1931-1960 and 1941-1970 data for Kansas City, Missouri.

^dAverage for station at Yuma, Arizona (1941-1970).

^eAverage for station at Green Bay, Wisconsin (1941-1970).

^fAverage for station at Kansas City, Missouri (1941-1970).

& Calculated as 0.25 x (number of days with <math display="inline">> = 0.01 in. of rainfall/365 d/y).

^hCalculated as annual average rainfall (in./y) / (8760 h/y x fraction of time that it rains).

		(S-1)			(S-2)	_		(S-3)	
Pollutant		Stack ^c			Stack ^c		Stack ^c		
	Minimumd	Expected ^e	Maximumf	Minimumd	Expected®	Maximumf	Minimumd	Expected®	Maximum ^f
1,1,1,2-Tetrachloroethane	2.18E-2	7.74E-2	3.37E-1	1.77E-2	1.16E-1	5.27E-1	1.95E-2	4.46E-2	6.37E-1
Chloroform	2.03E-2	7.15E-2	3.12E-1	1.63E-2	1.10E-1	4.87E-1	1.80E-2	4.13E-2	5.88E-1
Ethylene dichloride	6.30E-2	2.23E-1	9.71E-1	5,112-2	3.34E-1	1.52E+0	5.63E-2	1.29E-1	1.83E+0
Hexachlorobutadiene	3.04E-2	1.08E-1	4.69E-1	2.47E-2	1.61E-1	7.35E-1	2.73E-2	6.22E-2	8.87E-1
1,1,2,2-Tetrachloroethane	7.96E-3	2.82E-2	1.22E-1	6.45E-3	4.23E-2	1.92E-1	7.11E-3	1.62E-2	2.31E-1
Hexachloroethane	7.56E-3	2.69E-2	1.18E-1	6.17E-3	4.04E-2	1.84E-1	6.79E-3	1.55E-2	2.21E-1
Carbon tetrachloride	2.98E-3	1.05E-2	4.59E-2	2.42E-3	1.58E-2	7.19E-2	2.66E-3	6.08E-3	8.67E-2
Hexachlorobenzene	5.63E-3	1.99E-2	8.67E-2	4.56E-4	2.99E-2	1.35E-1	5.02E-3	1.15E-2	1.63E-1
Trichloropropane	3.89E-2	1.38E-1	6.00E-1	3.15E-2	2.06E-1	9.42E-1	3.47E-2	7.94E-2	1.13E+0
Trichloroethylene	8.95E-3	3.16E-2	1.38E-1	7.25E-3	4.75E-2	2.16E-1	8.00E-3	1.83E-2	2.60E-1

Table 6.4 Inhalation intake^{a,b} $(\mu g/y)$ from stack emissions

^aAbsorption for each pollutant assumed to be 0.65.

^bStandard man inhalation rate (8322 m^3/y) assumed (ICRP, 1975).

^cStack emissions calculated from expected throughput and pollutant concentrations in waste for the 150 \times 10⁶ Btu/h rotary kiln incinerator (99.99% DRE).

^dMinimum sector segment receptor uptake.

^eAverage uptake for the assessment region.

fMaximum sector segment receptor uptake.

(average) individual intakes of each chemical at all three sites are very similar. Inhalation dose $(\mu g/y)$ to the maximally exposed individual varies by a factor of 12 between the three sites. Differences in the predicted inhalation dose for each chemical at a specific site are due simply to differences in the source terms (see Table 4.2).

7. FOOD CHAIN DOSE

Human exposure via the food ingestion pathway from incineration of pesticide-related waste is estimated for stack emissions at each of the three sites (S-1, S-2, and S-3). Food items considered are beef, milk, grains, leafy vegetables, exposed produce, and protected produce.

7.1 MODEL SELECTION

Exposure and dose resulting from incinerator wastes released to the atmosphere and incorporated into the terrestrial food chain were estimated with the computer codes TEREX and FOODCHAIN. The computer code, TEREX, calculated food crop production for specific United States sites, and utilized crop pollutant uptake parameters to estimate pollutant concentrations in individual food items. Dose estimates via the human ingestion pathway were then calculated using FOODCHAIN, which incorporates a standard diet and Monte Carlo sampling procedure. Each program is briefly described below.

TEREX calculates concentrations of pollutants in various foodstuffs. This computer code requires as input the latitude and longitude coordinates of the site, the number and distances of circular rings that make up the grid, and the deposition rate of each pollutant in each sector segment as estimated by the computer codes ATM and CONEX. TEREX accesses an agricultural and environmental database to obtain 33 site parameters necessary to estimate production of foodstuffs in each sector segment. These agricultural and environmental parameters are then combined with chemical-specific parameters and the deposition rates to estimate the concentration (μ g/kg) of a pollutant in foodstuffs grown in each sector segment.

The methodology used in TEREX to predict the uptake of organic chemicals by food and forage crops is based on approaches previously used to describe uptake of radionuclides in foodstuffs (USNRC, 1977; Baes et al., 1983; Baes and Miller, 1984). The general equation describing uptake in food and forage is given by:

$$C_{p} = d(A_{d} + U_{s})$$

where

 C_p = concentration in plants (µg/kg), d = deposition rate (µg/m²-s), A_d = atmospheric deposition component (m²-s/kg), and U_s = uptake from soil component (m²-s/kg). The atmospheric deposition component is given by :

$$A_{d} = \frac{r[1 - exp(-\lambda_{a1} - t_{e})]}{Y \lambda_{a1}}$$

where

- r = interception fraction for the edible portion of the plant (unitless),
- λ_{a1} = atmospheric loss constant (s⁻¹),
- t = time of exposure of edible plant parts to atmospheric deposition (s), and
 - Y = yield or standing crop biomass of the edible portion of the plant (kg/m²).

The atmospheric loss constant is the sum of the losses due to weathering (λ_W) or degradation, including photodegradation, (λ_{ad}) . Thus,

$$\lambda_{a1} = \lambda_{w} + \lambda_{ad}$$

The uptake from soil component is given by :

$$U_{s} = \frac{B[1 - exp(-\lambda_{s} t_{b})]}{P \lambda_{s}}$$

where

B = soil-plant uptake factor (unitless), $\lambda_s = \text{ soil loss constant (s^{-1}),}$ $t_b = \text{ period of long-term buildup in soil (s), and}$ $P = \text{ density of soil in the root zone (kg/m^2).}$

The soil loss constant is the sum of all soil losses due to leaching (λ_{s1}) , or degradation, (λ_{sd}) , and thus :

$$\lambda_s = \lambda_{s1} + \lambda_{sd}$$

Transport to beef and milk from ingested forage and grains is modeled via:

$$C_{i} = F_{i}(Q_{F}C_{F} + Q_{G}C_{G})$$

where

- C_i = estimated concentration of the contaminant in milk or beef ($\mu g/kg$),
- F_i = fraction of contaminant consumed each day which is transported and retained in milk or beef (d/kg),
- $Q_{\rm F}$ = quantity of forage eaten by cattle each day (kg/d),
- Q_{G} = quantity of grain eaten by cattle each day (kg/d),
- C_F = estimated concentration of contaminant in forage (µg/kg), and
- C_G = estimated concentration of contaminant in grain ($\mu g/kg$).

The computer code FOODCHAIN uses output from TEREX (site-specific production and pollutant concentrations in six basic foodstuffs) to estimate human dietary intake of contaminants. It is assumed that each individual in the population consumes food grown locally, if available. Since even for locally grown food, all food items consumed by an individual would not likely be produced in the same sector segment, FOOD-CHAIN randomly selects the six dietary components from various sector segments; the probability of an individual sector segment being selected is based on production of each crop in the sector segment. Consumption of each dietary component is weighted by a factor (between 0.0 and 1.0) proportional to the total production of that dietary item in the assessment area. If local agricultural production cannot meet the dietary requirements of the population (a factor $\langle 1.0$ for each specific crop), unpolluted food is assumed to be imported to meet the demand.

The total intake of a pollutant via a sample diet is computed by summing the pollutant intake $(\mu g/y)$ for each of the dietary components. This sampling is performed in an iterative manner (1000 times) to develop a frequency distribution of intake for each pollutant. These distributions are then analyzed to determine minimum, maximum, and expected individual intake. Minimum and maximum individual intakes represent the minimum and maximum values obtained from the 1,000 iterative samples and do not necessarily represent actual possible extremes in the frequency distribution. For example, a true maximum dose to an individual would result from an individual who obtained his entire diet from crops grown in the sector segment of highest food concentrations (a "fencepost" individual). It is highly unlikely that the diet of a "fencepost" individual would appear in the 1,000-iteration sample.

7.2 INPUT PARAMETERS

Input parameters for the food chain assessment can be divided into two classes: site-specific and chemical-specific data. Site-specific parameters utilized in the TEREX code include population (see Table 5.1), local climatological (see Table 6.3), and agricultural data. Climatological parameters such as annual precipitation, mixing height, evapotranspiration, and number of frost-free days are considered.

7.2.1. Agricultural Parameters

Agricultural parameters were derived from the 1974 U.S. Department of Commerce agricultural census by county (Shor, Baes, and Sharp, 1982), and include inventory estimates for milk cows and beef cows, and productivity and yield data for seven vegetable and food crop categories. The selection of these latter categories was based on phenotypic and agricultural transport characteristics (Shor, Baes, and Sharp, 1982). These categories are leafy vegetables, exposed and protected produce, grains, pasture, hay, and silage. The first three are classed as human foods, and the last three as livestock feeds. Grains are classed as both.

Characteristics of vegetables and the two types of produce are as follows. Leafy vegetables present a broad flat leaf surface for direct interception of atmospherically deposited material. Furthermore, the edible portion of the plant is primarily concerned with vegetative growth (leaves and stems). Exposed produce items (snap beans, tomatoes, apples, etc.) intercept atmospherically deposited material on edible surfaces, but total surface area available for deposition is relatively small compared to leafy vegetables. Additionally, edible portions are typically concerned with reproductive functions (fruits and seeds). Protected produce items (potatoes, peanuts, citrus fruits, etc.) are not directly exposed to atmospherically deposited material because their growth is underground, or if aboveground, the edible portions are

protected by pods, shells, or non-edible skins or peels. Typically, edible portions are reproductive or storage organs.

Grains are similar to protected produce, but their use as both livestock feeds and food for man necessitates a separate category. The other three categories of livestock feeds are pasture grasses, hay, and silage (corn and sorghum). All of these feeds are composed primarily of vegetative growth. Silage is categorized separately from hay and pasture grass based on its interception characteristics. Hay and pasture grasses are separated because their residence times in the field are significantly different.

7.2.2. Chemical-Specific Parameters

Chemical-specific parameters describing food chain transport are necessary input into TEREX, but for the chemicals of interest in this assessment, measured values are not available. Thus it was necessary to calculate default values for these transfer coefficients from known physicochemical properties.

In recent years, the octanol/water partition coefficient (K_{ow}) has been correlated with water solubility, sediment adsorption coefficients, and bioconcentration (Kenaga and Goring, 1980; Briggs, 1981; Chlou et al., 1977; and others). These parameters and their relationship to K_{ow} are discussed below.

Octanol/Water Partition Coefficient, K_{ow}. The octanol/water partition coefficient is defined as the ratio of a chemical's concentration in the octanol phase to its concentration in the aqueous phase of

a two-phase octanol/water system (Lyman, Reehl, and Rosenblatt, 1982). Values of K_{ow} represent the tendency of a chemical to partition itself between an organic phase and an aqueous phase, and may be correlated to uptake of chemicals into biological systems. This parameter may be measured in the laboratory, although variability in measured values of K_{ow} for a given chemical may be affected by such factors as temperature, pH, time of mixing, purity of chemicals or solvents, etc. (Kenaga and Goring, 1980). Values reported in the literature for the organic chemicals considered in this study are listed and referenced in Table 7.1. If more than one value is reported, an average value was Leo's Fragment Constant Method (Hansch and Leo, 1979) was utilused. ized to derive $\log K$ values for the organic chemicals for which there are no reported observations. These are also listed in Table 7.1. This method uses empirically derived atomic or group fragment constants and structural factors (see Lyman, Reehl, and Rosenblatt, 1982) to estimate $\log K_{ow}$. Comparison between observed and calculated log K values results in an average error estimate of $\pm 0.12 \log K_{ow}$ units (Lyman, Reehl, and Rosenblatt, 1982).

<u>Distribution Coefficient</u>, K_d . The distribution coefficient, K_d , is a measure of the retention of a solute by the soil matrix, and is represented by the ratio of the elemental concentration in the soil to the concentration in the solute at equilibrium. This parameter is utilized to estimate soil concentrations which are then used to determine plant uptake from the soil. An extensive literature review of K_d values for organic compounds was performed, and an attempt was made to

Chemical	Log K	Reference			
1,1,1,2-Tetrachloroethane	3.05	Calculated, this report			
Chloroform	1.96 1.97	Valvani, Yalkowsky and Roseman, 1981 Hansch and Anderson, 1967			
Ethylene dichloride	1.48	Valvani, Yalkowsky and Roseman, 1981			
Hexachlorobutadiene	1.78	Calculated, this report			
1,1,2,2-Tetrachloroethane	2.66	Calculated, this report			
Hexachloroe thane	4.62	Calculated, this report			
Carbon tetrachloride	2.64 2.83 avg.=2.74	Neely, Branson and Blare, 1974 Valvani, Yalkowsky and Roseman, 1981			
Hexachlorobenzene	5.23 5.44 5.50 avg.=5.39	Kenaga and Goring, 1980 Briggs, 1981 Chlou and Schmedding, 1982			
Trichloropropane	2.01	Calculated, this report			
Trichloroe thy lene	2.29	Valvani, Yalkowsky and Roseman, 1981			

Table 7.1. Observed and calculated log K values for organic chemicals from incineration waste streams

correlate K_d to the reported K_{OW} for each of the compounds (Baes and Watson, personal communication). By plotting log K_d versus log K_{OW} , a straight line regression equation was derived:

$$\log K_{d} = -0.99 + 0.53 (\log K_{ow}).$$

Using this relationship, K_d values were estimated for the ten organic chemicals of interest and are listed in Table 7.2.

<u>Soil-to-Plant Uptake</u> <u>Parameters</u>, B_v and B_r . Root uptake of organic chemicals distributed in soil is described by the parameters B_v and B_r , representing soil-to-plant transfer coefficients for vegetative and non-vegetative portions of food crops, respectively. The parameters B_v and B_r are unitless as they represent the ratio of the pollutant concentration in plants to the concentration in soil at time of harvest.

Baes (1982) has related B_v to K_d , and derived the following regression equation using the relationship of log K_{OW} to log Kd reported by Briggs (1981):

$$\log B_{u} = 2.71 - 0.62 \ (\log K_{out})$$

Following an extensive review of the literature on inorganic compounds, Baes et al. (1982) conclude that the reproductive parts of plants take up only a small fraction of inorganic chemicals incorporated into the vegetative portion of the same plant. Baes et al (1982) have assumed that

$$B_{r} = 0.1 B_{v}$$
,

a relationship we also assume to hold for organic compounds. Values of

Chemical	K _d	B _v	F _f	F _m	λ ad
	(m1/g)		(d/kg)	(d/kg)	(S ⁻¹)
1,1,1,2-Tetrachloroethane	4.23	6.7	2.4E-4	2.5E-5	2.0E-8
Chloroform	1.12	30.0	6.9E-5	7.1E-6	6.5E-8
Ethylene dichloride	0.62	60.3	3.9E-5	4.1E-6	5.5E-6
Hexachlorobutadiene	0.90	40.4	5.5E-5	5.8E-6	1.1E-5
1,1,2,2-Tetrachloroethane	2.63	11.0	1.5E-4	1.6E-5	1.2E-7
Hexachloroe thane	28.8	0.67	1.4E-3	1.5E-4	1.0E-9
Carbon tetrachloride	2.90	10.0	1.7E-4	1.7E-5	1.0E-9
Hexachlorobenzene	70.1	0.24	3.3E-3	3.5E-4	1.0E-9
Trichloropropane	1.2	28.2	7.2E-5	7.5E-6	2.1E-6
Trichloroethylene	1.7	18.7	9.9E-5	1.0E-5	1.1E-6

Table 7.2. Estimated values of input parameters used in TEREX

B, and B, estimated using the above equations are listed in Table 7.2.

<u>Meat and Milk Uptake Parameters</u>, F_f and F_m . Kenaga (1980) has shown a positive correlation between the bioconcentration factor (BCF) in beef fat (the ratio of the quantity of chemical found in beef fat to the quantity in the diet) and K_{ow} . Based on the average fat content of various commonly ingested beef cuts and milk, and the average consumption of feed per head of cattle, the following regression equations were derived (Kenaga, 1980):

$$\log F_{f} = -5.15 + 0.50 \ (\log K_{ow})$$
$$\log F_{m} = -6.13 + 0.50 \ (\log K_{ow}).$$

Table 7.2 lists estimated values for F_f and F_m .

<u>Photochemical Transformation</u> λ_{ad} . Pollutants released by incineration facilities may undergo photochemical transformations which alter their chemical and physical nature. Photochemically-induced changes in toxicity were not considered in this report. No photochemical degradation was assumed in estimating inhalation exposures since the atmospheric residence times over the area of concern (100 km) were relatively short (a matter of hours). However, pollutants deposited on food items may be photodegraded over the entire growing season(s). Chemical-specific values for λ_{ad} were used in estimating concentrations of pollutants in food items, and are listed in Table 7.2.

<u>Dietary Intake.</u> EPA is currently estimating total dietary intake of major foodstuffs based on U.S.D.A. 1979 Household Survey data (Yang and Nelson, 1982 personal communication). The U.S.D.A. study (1980) provides estimates of daily intake of foodstuffs based on age and sex, and the EPA has combined this data with U.S. Bureau of Census data on population age and sex distributions to make their average daily intake estimates (Yang and Nelson, 1982, personal communication). Since the EPA study is not complete, the values they suggest have been adjusted somewhat to more closely approximate other estimates of dietary intake presented in the literature (USNRC, 1977). The values used for this report are listed in Table 7.3. Annual intake of drinking water and other liquids is based on a daily intake of 1.22 liters (NCRP, 1979).

Table 7.3. Estimated annual average dietary intake (kg/y)

Leafy Vegetables	16
Exposed Vegetables	35
Protected Vegetables	64
Grains	75
Total Dairy	112
Total Meat	89
Liquid Intake	445
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7.3 RESULTS

Table 7.4 lists minimum, maximum, and expected individual intake from the food chain pathway for each of the three sites assuming 95% absorption through the gastrointestinal tract. The minimum, maximum, and expected values listed in the table result from analyses of 1000 possible diets, each composed of random selections of the six dietary

		(5-1)			(8-2)			(S-3)	
Pollutant	Stack ^C			Stack ^c			Stack ^c		
	Minimum ^d	Expected ^e	Maximum ^f	Minimum ^d	Expected	Maximum ^f	Minimum ^d	Expected®	Maximumf
1,1,1,2-Tetrachloroethane	2.40E-3	2.85E-2	6.74E-1	2.55E-2	1.24E-1	2.52E+0	1.17E-2	8.37E-2	3.08E+0
Chloroform	2.82E-3	3.83E-3	8.35E-1	3.09E-2	1.46E-1	3.11E+0	1.37E-2	1.09E-1	3.94E+0
Ethylene dichloride	3.91E-4	4.25E-3	6.23E-2	3.46E-3	1.77E-2	2.74E-1	1.65E-3	1.18E-2	4.29E-1
Hexachlorobutadiene.	9.32E-5	8.04E-4	1.04E-2	6.50E-4	3.74E-3	4.95E-2	2.81E-4	1.95E-3	7.03E-2
1,1,2,2-Tetrachloroethane	4.17E-4	4.49E-3	6.65E-2	4.42E-3	1.88E-2	3.21E-1	1.73E-3	1.31E-2	4.11E-1
Hexachloroethane	1.33E-3	1.38E-2	2.79E-1	1.29E-2	6.04E-2	9.61E-1	4.86E-3	3.83E-2	1.14E+0
Carbon tetrachloride	2.72E-3	4.30E-2	1.62E+0	1.14E-2	5.08E-2	1.28E+0	4.10E-3	2.91E-2	1.23E+0
Hexachlorobenzene	9.70E-4	8.07E-3	1.12E-1	8.19E-3	4.48E-2	8.00E-1	4.71E-3	2.68E-2	5.15E-1
Trichloropropane	3,62E-4	4.00E-3	6.29E-2	3.49E-3	1.60E-2	2.22E-1	1.31E-3	9.21E-3	3.14E-1
Trichloroethylene	1.12E-4	1.41E-3	1.94E-2	1.04E-3	5.86E-3	7.48E-2	4.21E-4	2.82E-3	4.76E-2

Table 7.4 Ingestion intake^a, b (μ g/y) from stack emissions

^aAbsorption through gastrointestinal tract for each pollutant assumed to be 0.95.

^bStandard diet assumed.

^cStack emissions calculated from expected throughput and pollutant concentrations in waste for the 150 \times 10⁶ Btu/h rotary kiln incinerator (99,99% DRE).

d_{Minimum} sector segment receptor uptake.

^eAverage uptake for the assessment region.

^fMaximum sector segment receptor uptake.

components from various sector segments. Average individal ingestion intakes $(\mu g/y)$ at all three sites are very similar. However, for a "fencepost" individual, total dietary intakes can be somewhat higher. For example, the dietary intake of hexachlorobenzene by a fencepost individual residing at site S-2 is estimated to be 1.8 $\mu g/y$, as compared to a maximum predicted value of $8.0E-1 \mu g/y$ (Table 7.4). Table 7.5 lists the estimated dietary intake of hexachlorobenzene by a fencepost individual from each of the six food categories. Also listed is the percent contribution of each food item to total dietary intake. The beef pathway is the most important, contributing 49% to total intake; grain and leafy vegetables contribute 19% and 13%, respectively. Variability in individual dietary habits (for example, a vegetarian diet) could lead to significant changes in total intake.

Not all food produced at the three sites considered is consumed locally. The most productive site considered was the S-1 site, producing approximately 20 times more food (in kg/y) than can be consumed by the local population. Site S-2 produces about 16 times more than it can consume, while site S-3 only produces a fraction (0.84) of its local needs. The excess food production at sites S-1 and S-2 may be exported to other parts of the United States and thus could result in ingestion exposures to populations removed from these two sites. However, since most of the diet of an individual removed from the site would consist of uncontaminated food, these exposures can be expected to be much smaller then those of the maximum intakes (μ g/y) listed in Table 7.4.

Food item	Concentration (µg/kg)	Intake (µg/y)	Percent contribution
Leafy vegetables	1.4E-2	2.3E-1	13
Protected vegetables	1.0E-3	6.3E-2	4
Exposed vegetables	4.2E-3	1.5E-1	8
Grains	4.6E-3	3.4E-1	19
Beef	1.0E-2	8.8E-1	49
Milk	1.2E-3	1.4E-1	. 8
Total		1.8	100

Table 7.5 Hexachlorobenzene intake for a fencepost individual at site S-2

8. WATER INGESTION EXPOSURE

As a screening approach, human exposure via the drinking water pathway to trichloroethylene released from incineration facilities was estimated for stack emissions at two different sites, S-1 and S-3. These two sites were chosen to reflect differences in meteorological and hydrological parameters. For example, average annual rainfall varies from 2.85 in./y at S-1 to 38.87 in./y at site S-3. All drinking water is assumed to come from surface water (a river) located at the site. Annual input to the water table is also estimated. Models, parameters used, and results are discussed in the following sections.

8.1 MODEL SELECTION

A screening-level multimedia model TOX-SCREEN (McDowell-Boyer and Hetrick, 1982) provides a means of estimating pollutant concentrations in air, and soil, and rate of leaching into groundwater resulting from an atmospheric release. TOX-SCREEN uses simplifying assumptions to simulate dispersive processes. The multimedia nature of TOX-SCREEN requires that physical and chemical processes which drive transport of chemicals across air-water, air-soil, and soil-water interfaces be simulated. Such multimedia interactions are handled explicitly in the model by use of deposition velocities, transfer rate coefficients, and mass loading parameters.

8.1.1 Aquatic Dispersion

For dispersion in rivers, TOX-SCREEN requires that the user select the number and size of reaches to be simulated, with the restriction that each reach must be considered geometrically equivalent (i.e., indentical in length, width, and depth) and have the same flow rate. Breaking the river up into reaches allows estimation of pollutant concentration at various points downstream from an emission source. For the present application, the generic river was broken into three reaches.

In TOX-SCREEN, an equation similar to the EPA EXAMS model equation (Smith et al., 1977; Burns, Cline, and Lassiter, 1982) is used to estimate the monthly pollutant mass in each reach of the river. Since the equation assumes complete and instantaneous mixing in each reach upon introduction of a pollutant, monthly pollutant concentrations are calculated by dividing the introduced pollutant mass by the reach volume. To estimate adsorption onto sediment, TOX-SCREEN computes the concentration of the suspended sediment according to Laursen's formula (Laursen, 1958). Results in the present assessment show that the concentrations of pollutants considered adsorbed on suspended particulates in the water column are neglible. This is not unexpected since the adsorption coefficient (K_d) is small for tricbloroethyline.

In this assessment, the chemical was not introduced directly into the river but was introduced as a result of wet and dry deposition from the air compartment, and surface and groundwater runoff and sediment washload (due to storms) from the soil compartment.

8.1.2 Atmospheric Dispersion

A modification of the original Gaussian plume equation of Pasquill (1961) is used in TOX-SCREEN for estimating downwind concentrations of a chemical emitted from a point source. Modifications to the basic equation were made so that the TOX-SCREEN model considers plume depletion due to wet and dry deposition processes, gravitational settling, and chemical degradation. Sector-averaged and maximum ground-level atmospheric concentrations are calculated on a monthly average basis, assuming a constant Pasquill Stability Category D (i.e., neutral conditions). Also, the wind direction is constant throughout the model application time period.

8.1.3 Dispersion in Soil

The TOX-SCREEN model employs a hydrologic transport model, SESOIL (Bonazountas and Wagner, 1981), to estimate concentrations of a pollutant in soil media following introduction via direct application (not considered in this assessment) and/or interaction with other media (i.e., deposition from air). In this model, simulated hydrologic processes, volatilization, and erosion by wind all serve to transport the pollutant from its point of introduction (i.e., to the upper, middle, or lower region of a soil column) through the column to other media. The SESOIL model is statistical and seasonal, with respect to the hydrologic cycle, and provides estimates of pollutant distributions within the soil column on an annual or monthly basis (Bonazountas and Wagner, 1981). At present, the SESOIL model does not address pollutant movement in saturated groundwater.

Output of the SESOIL model includes pollutant concentrations in the soil water (μ g/ml), soil air (μ g/ml), and adsorbed phases (μ g/g) in both the upper, middle, and lower unsaturated soil zones. The amount of pollutant lost from the unsaturated soil zones per unit area (cm²) is provided in terms of μ g lost via surface runoff, percolation to groundwater, volatilization, biodegradation, chemical degradation, surface washload (erosion by water) and resuspension (erosion by wind).

8.1.4 Intermedia Transport

In order for the simulation of processes described above to result in a quantitative assessment of intermedia transport, the relative locations of the media as well as the size of the contaminated area must be designated. Such designations are detailed in McDowell-Boyer and Hetrick (1982). Briefly, in the application, the river and soil surfaces were contaminated from deposition of a plume (i.e., due to a point source), and the total contamination area was delineated in TOX-SCREEN by the shape of the plume which intercepted the ground and water surface. Also, in TOX-SCREEN, location of the contaminated water and land area relative to an atmospheric point source is always assumed to encompass the point of maximum downwind concentration. Contaminated soil areas are always assumed to be adjacent to water bodies to maximize subsequent water contamination, via surface and/or groundwater runoff.

8.2 INPUT PARAMETERS

Table 8.1 contains a list of parameter values required by TOX-SCREEN to implement the aquatic dispersion equations. Default or typical values were used for most of these parameters (McDowell-Boyer and Hetrick, 1982). The exceptions are the first-order rate constants (biodegradation, hydrolysis, oxidation, photolysis, and volatilization) and the sediment-water partition coefficient. The rate constants were set to 0.0 so that no chemical degradation in the water was allowed. Another conservative assumption made was that dilution in the river would be low. This was done by setting the width of the river reach (WWIDR) equal to 5.0 m, which represents the expected width during annual low river flow. The values shown in the table were used for both the S-1 site and the S-3 site.

Table 8.2 contains parameter values needed by TOX-SCREEN to implement the atmospheric dispersion equations. Whereas the table shows an average value for precipitation and wind speed, separate monthly values were input to the TOX-SCREEN model. These values were 30-year averages for each month (Ruffner, 1978). The mixing height values given are mean afternoon mixing heights and are also taken from Ruffner (1978). All other values are default or chemical specific values.

A list of the parameters required for the soil dispersion equations is given in Table 8.3. Again, the table shows average values for the parameters TA, NN, S, MTR, MN, and MT whereas separate monthly values were input to the TOX-SCREEN model. Values for L, TA, NN, S,

Table 8.1. User-specified parameters in river dispersion equations

Parameter	Definition	Value
DIASRD	Median sediment particle diameter (mm)	0.45
DENWR	Water Density (g/cm ³)	1.0
DENSDR	Sediment density (g/cm ³)	2.65
HPLUSR	Concentration of hydrogen ion (M)	1.0E-7
DISK	Acid dissociation constant (M)	0.0
SWKSWR	Soil-water partition coefficient (mol/kg/mol/l)	15.0
WKXR	First-order rate constants (s^{-1})	0.0
WLENR	Length of river reach (m)	500.0
WMINR	Source term to river (kg/s)	0.0
NR	Number of reaches	3
SLOPER	Slope of river	7.5E-5
WVELR	Flow velocity of river (m/s)	1.0
WWIDR	Width of river reach (m)	15.0
WDEPR	Water depth (m)	5.0

Parameter	Definition	Value
ENTPY	Enthalpy of stack gas (j/kg)	2.5E5
HMIX	Mixing height (m)	1210.0 Site-1 1349.0 Site-3
ĦS	Stack height (m)	27.4
AK	Chemical degradation constants (s^{-1})	0.0
МРМ	Precipitation (cm/month)	0.6 Site-1 8.23 Site-3
QS	Point source term (kg/s)	2.5E-7
SRAD	Cross-sectional radius of stack (m)	1.04
RHO	Stack gas density at temperature T (kg/m^3)	0.66
UW	Average wind speed (m/s)	2.93 Site-1 4.53 Site-3
UDG	Dry deposition velocity (m/s)	0.01
VG	Gravitational settling velocity (m/s)	0.00
VS	Stack gas exit velocity (m/s)	6.4
WRATG	Washout ratio	2.27

Table 8.2. User-specified parameters in atmospheric dispersion equations

Parameter	Definition	Va1 S-1	lue S-3
٤	Latitude of area (°N)	33.3	38.3
TA	Temperature of area (°C)	22.6	13.5
NN	Fraction of sky covered by clouds	0.47	0.58
S	Relative humidity of the area as a fraction	0.69	0.68
A	Shortwave albedo of the surface (dimensionless)	0.05	0.10
MTR	Mean time of each rain event (d)	0.1	0.17
MN	Mean number of storm events per month	1.5	8.75
MT	Mean length of rain season (d)	1.5	30.4
RS	Soil density (g/cm ³)	1.3	1.3
K1	Soil intrinsic permeability (cm ²)	1.2E-9	7.0E-9
С	Soil disconnectedness index (dimensionless)	5.0	6.0
N	Effective soil porosity (dimensionless)	0.35	0.35
0C	Organic content of the soil (% oc)	2.9	2.9
SL	Compound solubility in water (μ g/ml)	1100.0	1100.0
KOC	Adsorption coefficient of the compound on organic carbon $(\mu/g \text{ oc})/(\mu g/m1)$	100.0	100.0
DA	Diffusion coefficient in air (cm^2/s)	0.083	0.083
H	Henry's law constant (m ³ atm/mol)	9.4E-3	9.4E-3
Z	Depth to the ground water table (m)	15.0	50.0
DU	Depth of the upper unsaturated soil zone (cm)	15.0	15.0
DM	Depth of the middle unsaturated soil zone (cm)	10.0	10.0
FRN	Freundlich equation exponent (dimensionless)	1.0	1.0
PH	pH of the upper soil zone (dimensionless)	8.0	8.0
ISRM	Monthly index for pollutant appearance in pollutant runoff (dimensionless)	1.0	1.0

Table 8.3. User-specified parameters in soil dispersion equations

NOTE: The parameters A2PH, APH, A2OC, AOC, A2KDE, AKDE, A2CC, ACC, A2CEC, and ACEC (Bonazountas and Wagner, 1981; Hetrick and McDowell-Boyer, 1984 were all set to 1.0. These are ratios of different properties (e.g., pH) of the compound in the middle and lower soil zones to the upper soil zone. All other input parameters required by the SESOIL portion of TOX-SCREEN that were not listed here were set to 0.0.

MTR, and MN were compiled from Ruffner (1978). The S-1 site values for RS, K1, C, and N were those given in Bonazountas and Wagner (1981) for an arid climate soil system (Santa Paula, California). These values were judged to be reasonable for site S-1 since the only available data found for this area was for K1, which ranged from 4.32×10^{-10} cm² (Zimmerman, 1981). The depth to the groundwater table for site S-1 was input as 15 m, which is the median of values reported by Loeltz et al. (1975). The S-3 site values for RS, K1, C, N, and Z were those given in Bonazountas, Wagner, and Goodwin (1982) for an industrial land treatment site in Topeka, Kansas. All other values given in Table 8.3 are default values from Bonazountas and Wagner (1981).

8.3 RESULTS

Surface water concentrations and annual pollutant transfer to a groundwater aquifer following incineration of trichloroethylene at the S-1 and S-3 sites are listed in Table 8.4.

Drinking water estimates are based on an assumed intake of 2.0L/d for an individual living 1.5 km below the site, and obtaining all of his drinking water from the river (ignoring water treatment). These assumptions lead to intake estimates of $9.4E-4 \mu g/y$ for the S-1 site, and $9.8E-4 \mu g/y$ for the S-3 site.

TOX-SCREEN estimates pollutant transfer to the groundwater aquifer. For the S-1 site, there is no groundwater contamination after 10 years. However, due to different geological and climatological parameters at the S-3 site, the groundwater aquifer becomes

S-1	S-3
1.28E-3	1.33E-3
0	0
1.28E-3	1.33E-3
0	0.0
1.28E-3	1.33E-3
0	3.55E-4
	S-1 1.28E-3 0 1.28E-3 0 1.28E-3 0

Table 8.4 Surface water concentrations and transfer to groundwater following incineration of trichloroethylene

contaminated within 10 years. Input into groundwater at this site in the tenth year is estimated to be $3.6E+4 \mu g/y$. This input represents 4.5E-6 times the annual release from the stack.

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