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Environmental Protection  
Agency

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Planning and Standards  
Research Triangle Park NC 27711

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Air

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# **Background Document for the Surface Impoundment Modeling System (SIMS) Version 2.0**

control technology center



# **BACKGROUND DOCUMENT FOR THE SURFACE IMPOUNDMENT MODELING SYSTEM (SIMS) VERSION 2.0**

**CONTROL TECHNOLOGY CENTER**

**SPONSORED BY:**

**Emission Standards Division  
Office of Air Quality Planning Standards  
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Research Triangle Park, NC 27711**

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Cincinnati, OH 45268**

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# **BACKGROUND DOCUMENT FOR THE SURFACE IMPOUNDMENT MODELING SYSTEM (SIMS) VERSION 2.0**

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## **NOTICE**

**This report was prepared by Radian Corporation, Research Triangle Park, NC. It has been reviewed for technical accuracy by the Emission Standards Division and the Technical Support Division of the Office Of Air Quality Planning And Standards, and the Air And Energy Engineering Research Laboratory of the Office Of Research And Development, U. S. Environmental Protection Agency, and approved for publication. Mention of trade names or commercial products is not intended to constitute endorsement or recommendation for use.**

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## PREFACE

This document presents a brief description of the operation and design of specific surface impoundments and wastewater collection systems, and background information on the development of the Surface Impoundments Modeling System (SIMS). Development of the SIMS was funded jointly by the U.S. Environmental Protection Agency's (EPA) Monitoring and Reports Branch (MRB) and Control Technology Center (CTC).

MRB operates within the Technical Support Division of EPA's Office of Air Quality Planning and Standards (OAQPS) and is responsible for assisting State and local air pollution control agencies involved in the estimation of emissions from single sources and in the preparation of criteria pollutant emission inventories for various geographic areas. This assistance is provided through the development of emission factors and equations (in hard copy and/or computer software format), the issuance of emission inventory guidance documents, and telephone support for specific questions.

The CTC was established by EPA's Office of Research and Development (ORD) and OAQPS to provide technical assistance to State and local air pollution control agencies. Three levels of assistance can be accessed through the CTC. First, a CTC HOTLINE has been established to provide telephone assistance on matters relating to air pollution control technology. Second, more in-depth engineering assistance can be provided when appropriate. Third, the CTC can provide technical guidance through publication of technical guidance documents, development of personal computer software, and presentation of workshops on control technology matters.

The technical guidance projects, such as this one, focus on national or regional interests that are identified through contact with State and local agencies. In this case, the CTC and MRB became interested in automating and developing default parameters for calculations of volatile organic compound (VOC) emissions from surface impoundments and wastewater collection systems. The emission models were developed by the Emission Standards Division (ESD) during the evaluation of surface impoundments located in treatment, storage, and disposal facilities (TSDF) and during the evaluation of VOC emissions from industrial wastewater (IWW). SIMS allows the user to calculate emissions from an individual unit or from any combination of surface impoundments and/or

collection system components in series. As part of the TSDf project, a LOTUS 1-2-3® spreadsheet program called CHEMDAT7 was developed for estimating VOC emissions from wastewater and landfills. Wastewater emission models used in this program were incorporated into the SIMS. In addition, emission models for collection system components from the IWW CTC document were also incorporated into the SIMS.

The technical document discusses these emission models, surface impoundment and wastewater collection system design and operation, default parameter development, and the emission estimation procedures. In addition, a User's Manual and Programmer's Maintenance Manual were written to accompany the PC program. The User's Manual presents a complete reference for all features and commands in the SIMS, while the maintenance manual presents the documentation of the SIMS computer code.

This is the second version of the SIMS program and supporting documents. The following is a brief summary of the changes and/or additions to the program.

In October 1989, Version 1.0 of SIMS was completed and distributed to State/local agencies for estimating VOC and air toxics emissions from wastewater treatment facilities. Version 1.0 included models for quiescent and mechanically aerated surface impoundments. Since that time, numerous comments have been received concerning the usefulness of the system and modifications that would further improve/expand its use. This system addresses a number of those comments including:

- Expansion of the compound database from 40 to 150 compounds.
- Addition of emissions models for diffused air systems and systems with an oil film layer.
- Addition of the following emission models for collection system components: junction boxes, lift stations, sumps, and weirs.
- Capabilities for estimating emissions from associated treatment and collection system components in series.
- Improved reports.

These improvements are discussed in more detail herein and in the SIMS User's Manual.

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# LIST OF ABBREVIATIONS AND SYMBOLS

<u>Parameter</u>	<u>Definition</u>	<u>Units</u>
A	Surface area	m <sup>2</sup>
b <sub>i</sub>	Biomass concentration	g/m <sup>3</sup>
C <sub>L</sub>	Concentration of constituent in the liquid phase	g/m <sup>3</sup>
C <sub>L,oil</sub>	Concentration of constituent in the oil phase	g/m <sup>3</sup>
C <sub>o</sub>	Initial concentration of constituent in the liquid phase	g/m <sup>3</sup>
C <sub>o,oil</sub>	Initial concentration of constituent in the oil phase	g/m <sup>3</sup>
C <sub>t</sub>	Concentration of constituent in the liquid phase at time = t	g/m <sup>3</sup>
C <sub>t,oil</sub>	Concentration of constituent in the oil phase at time = t	g/m <sup>3</sup>
d	Impeller diameter	cm
D	Depth	m
d*	Impeller diameter	ft
D <sub>a</sub>	Diffusivity of constituent in air	cm <sup>2</sup> /s
d <sub>e</sub>	Effective diameter	m
D <sub>O<sub>2</sub>,w</sub>	Diffusivity of oxygen in water	cm <sup>2</sup> /s
D <sub>oil</sub>	Oil-film thickness	m
D <sub>w</sub>	Diffusivity of constituent in water	cm <sup>2</sup> /s
f <sub>air</sub>	Fraction of the compound emitted to the air	dimensionless
F <sub>O</sub>	Fraction of volume which is oil	dimensionless
Fr	Froude number	dimensionless
g <sub>c</sub>	Gravitation constant	32.17 lb <sub>m</sub> -ft/s <sup>2</sup> -lb <sub>f</sub>
h	Weir height (distance from the wastewater overflow to the receiving body of water)	ft

# LIST OF ABBREVIATIONS AND SYMBOLS (continued)

<u>Parameter</u>	<u>Definition</u>	<u>Units</u>
H	Henry's Law Constant of constituent	atm-m <sup>3</sup> /gmol
J	Oxygen transfer rating of surface aerator	lb O <sub>2</sub> /(hr-hp)
K	Overall mass transfer coefficient for transfer of constituent from liquid phase to gas phase	m/s
K <sub>D</sub>	Volatilization-re-aeration theory mass transfer coefficient	dimensionless
K <sub>eq</sub>	Equilibrium constant or partition coefficient (concentration in gas phase/concentration in liquid phase)	dimensionless
K <sub>eq<sub>oil</sub></sub>	Equilibrium constant or partition coefficient (concentration in gas phase/concentration in oil phase)	dimensionless
k <sub>g</sub>	Gas phase mass transfer coefficient	m/s
k <sub>l</sub>	Liquid phase mass transfer coefficient	m/s
K <sub>max</sub>	Maximum biorate constant	g/s-g biomass
K <sub>oil</sub>	Overall mass transfer coefficient for transfer of constituent from oil phase to gas phase	m/s
K <sub>ow</sub>	Octanol-water partition coefficient	dimensionless
K <sub>s</sub>	Half saturation biorate constant	g/m <sup>3</sup>
MW <sub>a</sub>	Molecular weight of air	g/gmol
MW <sub>oil</sub>	Molecular weight of oil	g/gmol
MW <sub>L</sub>	Molecular weight of water	g/gmol
N	Emissions	g/s
N <sub>A</sub>	Number of aerators	dimensionless
O <sub>c</sub>	Oxygen transfer correction factor	dimensionless
P	Power number	dimensionless
P*	Vapor pressure of the constituent	atm
P <sub>o</sub>	Total pressure	atm

# LIST OF ABBREVIATIONS AND SYMBOLS (continued)

<u>Parameter</u>	<u>Definition</u>	<u>Units</u>
POWER	Total power to aerators	hp
Q	Volumetric flow rate	m <sup>3</sup> /s
Q <sub>a</sub>	Diffused air flow rate	m <sup>3</sup> /s
Q <sub>oil</sub>	Volumetric flow rate of oil	m <sup>3</sup> /s
R	Universal gas constant	8.21 x 10 <sup>-5</sup> atm-m <sup>3</sup> /gmol-K
Re	Reynold's number	dimensionless
Sc <sub>g</sub>	Schmidt number on gas side	dimensionless
Sc <sub>L</sub>	Schmidt number on liquid side	dimensionless
T	Temperature of water	°C
t	Residence time of disposal	s
U*	Friction velocity	m/s
U <sub>10</sub>	Windspeed at 10 m above the liquid surface	m/s
V	Volume	m <sup>3</sup>
V <sub>a</sub>	Turbulent surface area	m <sup>2</sup>
V <sub>oil</sub>	Volume of oil	m <sup>3</sup>
w	Rotational speed of impeller	rad/s
ρ <sub>a</sub>	Density of air	g/cm <sup>3</sup>
ρ <sub>L</sub>	Density of liquid	g/cm <sup>3</sup>
ρ <sub>oil</sub>	density of oil	g/m <sup>3</sup>
μ <sub>a</sub>	Viscosity of air	g/cm-s
μ <sub>L</sub>	Viscosity of water	g/cm-s

## EXECUTIVE SUMMARY

The purpose of this document is to present background information on the data, equations, default development, and procedures used by the Surface Impoundment Modeling System (SIMS) Personal Computer (PC) Program. The PC Program estimates volatile organic compound (VOC) and toxic air pollutant emissions from surface impoundments (SI) and collection system components (CSC) individually or in series.

The SIMS program was written in response to the State and local need for a methodology to estimate emissions from SI and CSC located in treatment, storage, and disposal facilities (TSDF), publicly owned treatment works (POTW), and other similar processes. The emissions models contained in the program were developed by the Emission Standards Division (ESD) during the evaluation of TSDF. The program requires a minimum amount of information from the user which include the following:

- 1) Total flow rate to impoundment or collection system component;
- 2) Flow model (flowthrough or disposal);
- 3) Type of impoundment (mechanically aerated/diffused air/nonaerated/oil film layer and biodegradation/no biodegradation);
- 4) Impoundment or collection system component surface area;
- 5) Order of impoundments and/or collection system components in series; and
- 6) Industrial categories discharged to impoundment (a list is given).

Based on this minimum information and standard design practices for SI and CSC, the program assigns default values to all other input parameters required by the models. However, the program is designed to allow the user to replace most of the computer-assigned default values with actual values, when available.

The technical document provides a brief description of surface impoundment/collection system design and operation, summarizes the emission

models used by the program, discusses default program development, and discusses the emissions estimation procedure used by the program.

### Surface Impoundment/Collection System Design and Operation

SI are used for the treatment, storage, and disposal of liquid wastes. From available data, waste treatment is the primary application for SI in the municipal, industrial, and mining categories, while the majority of SI used for agricultural purposes are designated for storage. Only the oil and gas industry utilize the majority of SI for disposal. Current SI designs employ a combination of several application objectives such as treatment followed by temporary storage or by ultimate waste disposal.

Air emission rates are affected by the design and operation of the SI. The design and operating parameters considered most important in determining emissions are flow rate, surface area, liquid depth, retention time (for disposal SI), degree of mechanical aeration or diffused air rate (for mechanically aerated or diffused air SI), biomass concentration (where biodegradation is a competing mechanism), and any physical design characteristics that influence the effective wind speed across the liquid surface.

Collection system components are used to transport wastewater from the point of generation to treatment or storage systems. The number and types of collection system components are facility specific. Most collection system components are open to the atmosphere and thus create a potential for VOC emissions. The magnitude of VOC emissions depends greatly on many factors, such as the physical properties of the compounds in the wastewater, temperature of the wastewater, and the design of the component. Common collection system components include junction boxes, lift stations, sumps, weirs, drains, trenches, and manholes. The SIMS program estimates emissions from only the first four of these components; however, a brief discussion of the applications and design parameters are provided in Chapter 3 for all components mentioned.



## Surface Impoundment/Collection System Emission Models

VOC emissions from SI and CSC occur due to volatilization at the water or oil surface (for SI with an oil film layer). For all SI without an oil film layer and all CSC except weirs, the rate of volatilization is based on the two-film resistance theory. This theory assumes the rate limiting factor for volatilization is the overall resistance to mass transfer at the interface of the liquid surface and the ambient air. The overall resistance is due to individual resistances in the liquid and gas phase films at the interface. For SI with an oil film layer, the oil film is assumed thin and mass transfer is controlled by the gas phase resistance only. For weirs, volatilization-aeration theory is used. This theory assumes that emissions are based on diffusivities of oxygen and the constituent in the water.

Individual mass transfer coefficients account for resistances in the liquid and gas phase films. The individual mass transfer coefficients are used to estimate overall mass transfer coefficients for each pollutant. These overall coefficients are applied in mass balance equations to estimate air emissions from SI and CSC. The forms of the mass balance equations depend on type of flow (i.e., flowthrough or disposal), impoundment type (i.e., mechanically aerated, diffused air, nonaerated, oil film layer), and whether or not pollutants are biodegraded in the impoundment. For the emission models contained in SIMS, all SI and CSC are assumed to be well mixed (i.e., the pollutant concentration is the same throughout the SI).

The basic approach used by the models to estimate emissions is as follows:

- 1) estimate individual liquid and gas phase mass transfer coefficients for each pollutant,  $k_l$  (for collection system components and impoundments without an oil layer) and  $k_g$  (m/s);
- 2) estimate equilibrium constants for each pollutant from the following expressions:
  - A. Collection system components and surface impoundments without an oil layer.

$$K_{eq} = H/RT$$

where:

$K_{eq}$  = equilibrium constant, dimensionless

$H$  = Henry's Law constant, atm m<sup>3</sup>/gmol

$R$  = ideal gas law constant, atm m<sup>3</sup>/gmol - °K

$T$  = wastewater temperature, °K

B. Surface impoundments with an oil film layer.

$$K_{eq_{oil}} = P^* \rho_a MW_{oil} / (\rho_l MW_a P_o)$$

where:

$P^*$  = vapor pressure of the constituent, mmHg

$P_o$  = total pressure, mmHg

$\rho_a$  = density of air, g/cm<sup>3</sup>

$\rho_l$  = density of water, g/cm<sup>3</sup>

$MW_{oil}$  = molecular weight of oil, g/gmol

$MW_a$  = molecular weight of air, g/gmol

3) estimate overall mass transfer coefficient for each pollutant from the following expressions:

A. Collection system components and surface impoundments without an oil layer.

$$1/K = 1/k_l + 1/(k_g K_{eq})$$

where:

$K$  = overall mass transfer coefficient, m/s

B. Surface impoundments with an oil film layer.

$$K_{oil} = k_g K_{eq_{oil}}$$

where:

$K_{eq_{oil}}$  = oil phase equilibrium constant

$K_{oil}$  = oil phase overall mass transfer coefficient, m/s

4) apply a mass balance around the surface impoundment to estimate emissions

The emission rate,  $E$ , in g/s, is given in Table E-1 for all mass balance equation types included in SIMS.

TABLE E-1. EMISSION DATA EQUATIONS\*

Conditions	Emissions Rate, g/s
<u>Wastewater Treatment and Storage</u>	
Flowthrough, no biodegradation aerated or nonaerated	$(KAQ \text{ Co})/(Q + KA)$
Flowthrough, biodegradation aerated or nonaerated	$KA[-(K_s(KA/Q + 1) + VK_{maxb_i}/Q - Co) + \{(K_s(KA/Q + 1) + VK_{maxb_i}/Q - Co)^2 + 4(KA/Q + 1)(K_sCo)\}^{0.5}]/[2(KA/Q + 1)]$
Flowthrough, no biodegradation diffused air	$(KA + Q_A K_{eq})QCo/(KA + Q + Q_A K_{eq})$
Flowthrough, biodegradation diffused	$(KA + Q_A K_{eq})[-(K_s((KA + Q_A K_{eq})/Q + 1) + VK_{maxb_i}/Q - Co) + \{(K_s((KA + Q_A K_{eq})/Q + 1) + VK_{maxb_i}/Q - Co)^2 + 4((KA + Q_A K_{eq})/Q + 1)(K_sCo)\}^{0.5}]/[2((KA + Q_A K_{eq})/Q + 1)]$
Flowthrough, no biodegradation oil film layer	$K_{oil}AQ_{oil}Co_{oil}/(K_{oil}A + Q_{oil})$
Disposal, no biodegradation aerated or nonaerated	$[1 - \exp(-Kat/V)]VCo/t$
Disposal, biodegradation	$[1 - \exp(-K_{maxb_i}t/K_s - Kat/V)] [KA/(KA + K_{maxb_i}V/K_s)]VCo/t$
Disposal, no biodegradation diffused air	$[1 - \exp(-(KA + K_{eq}Q_A)t/V)] VCo/t$
Disposal, biodegradation diffused air	$[1 - \exp(-(KA + K_{eq}Q_A)t/V - K_{maxb_i}t/K_s)] (KA + Q_A K_{eq})/(KA + Q_A K_{eq} + K_{maxb_i}V/K_s)VCo/t$
Disposal, no biodegradation oil film layer	$[1 - \exp(-K_{oil}t/D_{oil})] V_{oil}Co_{oil}/t$

TABLE E-1. EMISSION DATA EQUATIONS (continued)<sup>a</sup>

Conditions	Emissions Rate, g/s
<u>Wastewater Collection</u>	
Junction boxes, lift stations and sumps	$(KAQCo)/(Q + KA)$
Weirs	$[1 - \exp(-K_o)]QCo$

<sup>a</sup>See Chapter 4 and the list of abbreviations and symbols (located at the front of the document) for use of the equations and for definitions of all parameters used, respectively.

## Default Parameter Development

Default values were developed using the evaluation of TSDF for many of the required inputs for the emissions models. However, default values were not developed for (1) the concentration profile in the wastewater feed to the SI, (2) the depth of the impoundment or CSC, and (3) certain physical property data.

Because concentration data may not be available to State and local agencies, methods were developed to assign default concentration values based on the minimum information expected to be available. Raw concentration profiles were developed for different industrial categories. These profiles are used to define the composition of the impoundment feed based on the industrial categories discharging to the SI. A listing of the 29 categories is presented in Table E-2. In cases where the impoundment is fed by process units in more than one type of industrial category, a flow weighting scheme is required. In addition, if the impoundment is located at a POTW, it is also necessary to know what percentage of the feed is from industrial (rather than municipal) sources. (SIMS does not estimate VOC emissions from municipal wastewater unless a concentration profile is provided).

A default depth of the impoundment was developed by plotting flow rate versus depth from data contained in recent literature. The correlation gives a linear relationship between flow rate and depth. Separate correlations were developed for flowthrough and disposal impoundments because of the great differences in data ranges. Given a specific flow rate, a default depth can be determined by the following equations.

### Flowthrough

$$\begin{array}{ll} Q = 4673.3 D - 3809.5 & Q \geq 1446 \text{ m}^3/\text{day} \\ Q = 863.8 D & 0 < Q < 1446 \text{ m}^3/\text{day} \end{array}$$

### Disposal

$$\begin{array}{ll} Q = 354.6 D - 700 & Q \geq 253 \text{ m}^3/\text{day} \\ Q = 101.2 D & 0 < Q < 253 \text{ m}^3/\text{day} \end{array}$$

Default depths for collection system components were obtained from average values reported in an EPA source (see Chapter 5).

TABLE E-2. INDUSTRIAL CATEGORIES

Industrial Category <sup>a</sup>	Industrial Category Code
Adhesives and Sealants	1
Battery Manufacturing	2
Coal, Oil, Petroleum Products, and Refining	3
Dye Manufacturing and Formulation	4
Electrical and Electronic Components	5
Electroplating and Metal Finishing	6
Equipment Manufacturing and Assembly	7
Explosives Manufacturing	8
Gum and Wood Chemicals, and Related Oils	9
Industrial and Commercial Laundries	10
Ink Manufacturing and Formulation	11
Inorganic Chemicals Manufacturing	12
Iron and Steel Manufacturing and Forming	13
Leather Tanning and Finishing	14
Nonferrous Metals Forming	15
Nonferrous Metals Manufacturing	16
Organic Chemicals Manufacturing	17
Paint Manufacture and Formulation	18
Pesticides Manufacturing	19
Pharmaceuticals Manufacturing	20
Photographic Chemicals and Film Manufacturing	21
Plastics Molding and Forming	22
Plastics, Resins, and Synthetic Fibers Manufacturing	23
Porcelain Enameling	24
Printing and Publishing	25
Pulp and Paper Mills	26
Rubber Manufacturing and Processing	27
Textile Mills	28
Timber Products Processing	29

<sup>a</sup>Pesticides Formulation has been omitted from the original list of 30 industry categories because of the lack of data available for this industrial category.

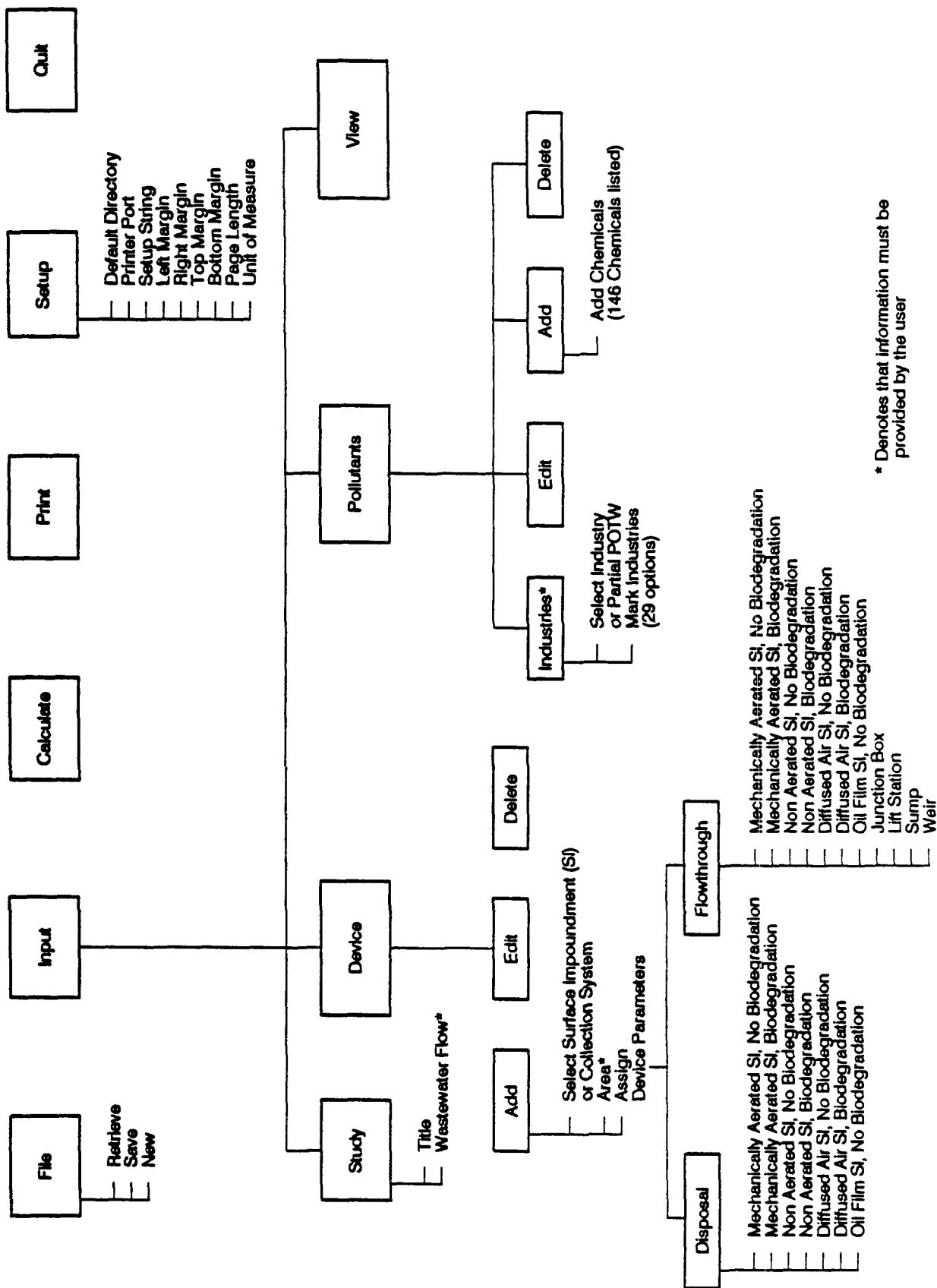
Physical property data for compounds in the SIMS were obtained from values reported in EPA sources where available. These properties include Henry's Law constants, diffusivities in air and water, biorates, vapor pressures, and octanol-water coefficients. (See Appendix B for listing).

#### Emission Estimation Procedure

There are eighteen potential emission estimation models for the SIMS:

- 1) Flowthrough, aerated, biological system,
- 2) Flowthrough, non-aerated, biological system,
- 3) Flowthrough, aerated, non-biological system,
- 4) Flowthrough, non-aerated, non-biological system,
- 5) Flowthrough, diffused air, biological system,
- 6) Flowthrough, diffused air, non-biological system,
- 7) Flowthrough, oil-film layer, non-biological system,
- 8) Flowthrough, junction box,
- 9) Flowthrough, lift station,
- 10) Flowthrough, sump,
- 11) Flowthrough, weir,
- 12) Disposal, aerated, biological system,
- 13) Disposal, non-aerated, biological system,
- 14) Disposal, aerated, non-biological system,
- 15) Disposal, non-aerated, non-biological system,
- 16) Disposal, diffused air, biological system,
- 17) Disposal, diffused air, non-biological system, and
- 18) Disposal, oil film layer, non-biological system.

Assuming the user has the minimum information discussed earlier, Figure E-1 presents a decision tree for estimating VOC emissions. It is important to realize that the accuracy of the emissions estimate decreases with the use of the defaults, especially concentration of organics and biorate constants. If a specific parameter is known or can be estimated with some accuracy, it is recommended that the estimated value be used in the SIMS program. Six detailed example calculations are presented in Chapter 6 of this document.



\* Denotes that information must be provided by the user

Figure E-1. SIMS Model Structure



## 1.0 INTRODUCTION

The assessment of volatile organic compound (VOC) emissions is essential in order to develop State implementation plans (SIP) for the control of atmospheric ozone. The assessment of toxic air pollutant emissions is essential in order to develop strategies for the control of toxic air emissions. Additionally, this information is basic to the review of Prevention of Significant Deterioration (PSD) applications and other Federal, State, and local agency programs involving assessment of air pollution.

The U.S. Environmental Protection Agency (EPA) has recently recognized the State and local need for a methodology to estimate emissions from surface impoundments and wastewater collection systems located in treatment, storage, and disposal facilities (TSDF), publicly owned treatment works (POTW), and other similar operations. A set of emission models for specific surface impoundments was developed by EPA's Emission Standards Division (ESD) within the Office of Air Quality Planning and Standards (OAQPS) during the evaluation of TSDF. These models can be used to estimate VOC emissions from surface impoundments based on input parameters such as impoundment type (aerated, nonaerated, diffused air, or oil film layer), impoundment dimensions, influent flow rate, and inlet pollutant concentrations. The CHEMDAT7 LOTUS 1-2-3® spreadsheet program, developed as part of the TSDF program, was designed to use these emission models. However, in some cases, State and local agency personnel may not have information on all the input parameters required by these models as presented in the CHEMDAT7 program.

For this reason, the air emission models were incorporated into a user friendly, personal computer-based program entitled Surface Impoundments Modeling System (SIMS). SIMS is a menu driven system that can be used by individuals with limited experience with personal computers (PC). In addition to estimating VOC emissions from specific surface impoundments, SIMS has incorporated emission models for estimating VOC emissions from specific collection system components. Emission models for these collection system components were developed by the ESD during the evaluation of VOC emissions from industrial wastewater (IWW). Most collection system emission models are based on the same mass transfer correlations developed under the TSDF program.

SIMS also uses an updated version of the oil film layer emission model used by CHEMDAT7. The CHEMDAT7 program does not make any correlation between the water and oil phases, assuming that the user can provide concentration information in the oil phase. SIMS has incorporated this correlation into the oil film emission model.

SIMS requires certain minimum information from the user. Based on this information, and standard design practices for surface impoundments and collection systems, the program assigns default values to all other input parameters required by the models. In addition, the program is designed to allow the user to replace most of the computer-assigned default values with actual data, when available.

SIMS allows the user to calculate emissions from an individual unit or from any combination of surface impoundments and/or collection system components in series. Results show input parameters and total VOC emissions, inlet and outlet concentrations, and the amount biodegraded (for impoundments with biodegradation only) in SI (Système Internationale d'Unités) or English units.

In some cases, there could be volatile inorganic compound emissions from surface impoundments. However, because the ESD emission models were developed for VOC emissions, they do not necessarily apply to volatile inorganic compound (VIC) emissions. For this reason, VIC emissions are not addressed in this document.

The purpose of this document is to present background information on the data, equations, and procedures used by the program to estimate emissions. A brief description of surface impoundment and wastewater collection system component design and operation is provided in Chapters 2 and 3, respectively. The air emissions models used by the program are summarized in Chapter 4. The development of the default parameters required by the emission models are discussed in Chapter 5. Chapter 6 presents the overall procedure employed by the SIMS to assign default values and estimate emissions.

SIMS data are primarily intended for regional studies. However, the program can be used as a screening tool for evaluating permits, keeping in mind that the models in SIMS do not represent EPA policy. These models are, however, based on the best information available to the EPA at this time.

## 2.0 SURFACE IMPOUNDMENT DESIGN AND OPERATION

Surface impoundments are used in a variety of applications by facilities in many different industrial categories. The design and operation of these impoundments are affected by the type of application in which they are used. A surface impoundment can be a basin, lagoon, treatment tank or any confinement where wastewater is held for a period of time. However, the Surface Impoundment Modeling System (SIMS) is limited to completely mixed surface impoundments. Therefore, the SIMS is not applicable to plug flow (no axial mixing) systems. (An example of a plug flow system is a narrow, fast moving canal). A brief discussion of the various applications and impoundment design and operating practices are provided in this chapter. Also discussed is how these design and operating practices are incorporated into the emission models developed by ESD and the computer program developed during this project.

### 2.1 APPLICATIONS

Surface impoundments are used for the treatment, storage, and disposal of liquid wastes. Table 2-1 shows the results of a national study surveying surface impoundment applications.<sup>1</sup> In this document, an impoundment with a retention time more than 30 days is considered a disposal impoundment. If the retention time is less than 30 days then it is considered a storage or treatment impoundment.

Table 2-1 shows that waste treatment is the primary application for the surface impoundments in the municipal, industrial, and mining categories. The majority of surface impoundments used for the agricultural purposes are designated for storage; only the oil and gas industry utilize the majority of their surface impoundments for disposal. Current surface impoundment design practices utilize a flexible applications approach, normally employing a combination of several application objectives (e.g., treatment followed by temporary storage or treatment followed by ultimate waste disposal).

As previously mentioned, impoundment applications vary depending on the type of industrial facility using the impoundment. Typical applications identified for different industries are detailed below:

TABLE 2-1. RESULTS OF A SURVEY ON SURFACE IMPOUNDMENT APPLICATIONS

	Storage	Disposal	Treatment
	(Percentage Use in Each Application, %)		
Agricultural	55	26	19
Municipal	5	31	64
Industrial	17	31	52
Mining	18	26	56
Oil & Gas	29	67	4

1. Mining and Milling Operations - production of various waste waters such as acid mine water, solvent wastes from solution mining, and wastes from dump leaching. Surface impoundments may be used for separation settling, washing, sorting of mineral products from tailings, and recovery of valuable minerals by precipitation.
2. Oil and Gas Industry - one of the largest users of surface impoundments. Surface impoundments may contain salt water associated with oil extraction and deep-well repressurizing operations, oil-water, and gas-fluids to be separated or stored during emergency conditions, and drill cuttings and drilling muds.
3. Textile and Leather Industry - Surface impoundments are primarily used for wastewater treatment and sludge disposal. Organic species impounded include dye carriers such as halogenated hydrocarbons and phenols; heavy metals impounded include chromium, zinc, and copper. Tanning and finishing wastes may contain sulfides and nitrogenous compounds.
4. Chemical and Allied Products Industry - Surface impoundments are used for wastewater treatment, sludge disposal, and residuals treatment and storage. Waste constituents are process-specific and include phosphates, fluoride, nitrogen, and assorted trace metals.
5. Other Industries - Surface impoundments are found at petroleum refining, primary metals production, wood treating, and metal finishing facilities. Surface impoundments are also used for the containment and/or treatment of air pollution scrubber sludge and dredging spoils sludge.

Surface impoundments can be flowthrough or disposal systems. Most waste treatment systems are flowthrough, while storage systems can be either flowthrough (i.e., as input to a treatment system) or disposal. Types of flowthrough or disposal surface impoundments include holding tanks or basins, equalization or pH adjustment basins, aerated basins (with or without biodegradation), activated sludge basins, clarifiers or any type of settling basin, diffused air systems (with or without biodegradation), oil film layer systems, and varying types of treatment tanks or basins where chemicals may be added.

## 2.2 DESIGN AND OPERATION

Air emission rates are affected by the design and operation of surface impoundments. The design and operating parameters considered most important in determining emissions are: influent flow rate; surface area; liquid depth; degree of aeration; retention time (or turnovers per year in the case of

disposal impoundments); physical design characteristics that influence the effective wind speed across the surface of the impoundment; and for impoundments where biodegradation is a factor, the biomass concentration.

### 2.2.1 Physical Design<sup>2</sup>

The most common and economical shape for a surface impoundment is rectangular with straight sides. The rectangular shape is normally preferred because it presents fewer problems during construction and lining. Circular shapes increase the costs of grading, liner installation, and construction. The three major positions of surface impoundments with respect to the natural grade are (1) below grade, (2) above-grade, and (3) a combination (below and above grades). A below-grade surface impoundment is excavated such that most of the capacity is below the natural grade of the surrounding land. An above-grade impoundment is built so that most of the capacity is at an elevation higher than the immediate surroundings. Combination types have characteristics of both the above and below-grade installations. The design chosen is determined by the economics of storage, containment, excavation difficulty, and material use. In general, most surface impoundments are constructed as the combination type because this design minimizes earthwork costs.

A knowledge of all the parameters which govern the depth of liquid in the impoundment are used to properly size the unit. These parameters include changes in liquid level due to storm surges as well as factors which influence the behavior of liquid while in the impoundment, such as wind speed and dike slope. Determination of these parameters will, in part, dictate the final design of the impoundment by establishing the maximum operating liquid level and minimum freeboard requirements.

Freeboard is typically defined as the distance between the actual liquid height in the impoundment and the top of the impoundment (height at which stored liquid would overflow). Freeboard has an affect on the air emission rate from an impoundment. As the freeboard height decreases, the liquid surface is more exposed to the ambient wind above the impoundment. For this reason, air emissions will increase as the freeboard height decreases. Determination of the design freeboard height requires that several specific parameters, including fetch, maximum liquid depth, and embankment slope, be accurately measured. Fetch is defined as the maximum unobstructed distance across a free liquid surface over which wind can act.

Figure 2-1 presents the relationship of freeboard to wind, surface area, depth, and fetch in a surface impoundment. Typically, the longest fetch will be the diagonal measurement across the surface of the impoundment. The calculation of fetch will be different depending on the shape of the impoundment (see Figure 2-1 for equations for circular or rectangular designs). The fetch to depth ratio for the impoundment is an important parameter in determining emissions.

It should be noted that the models described in Chapter 3 do not incorporate a variable for freeboard. If freeboard at a particular facility is significant, then the effective windspeed will be less than the measured windspeed. Currently no data are available to provide guidance on adjusting windspeed to account for freeboard.

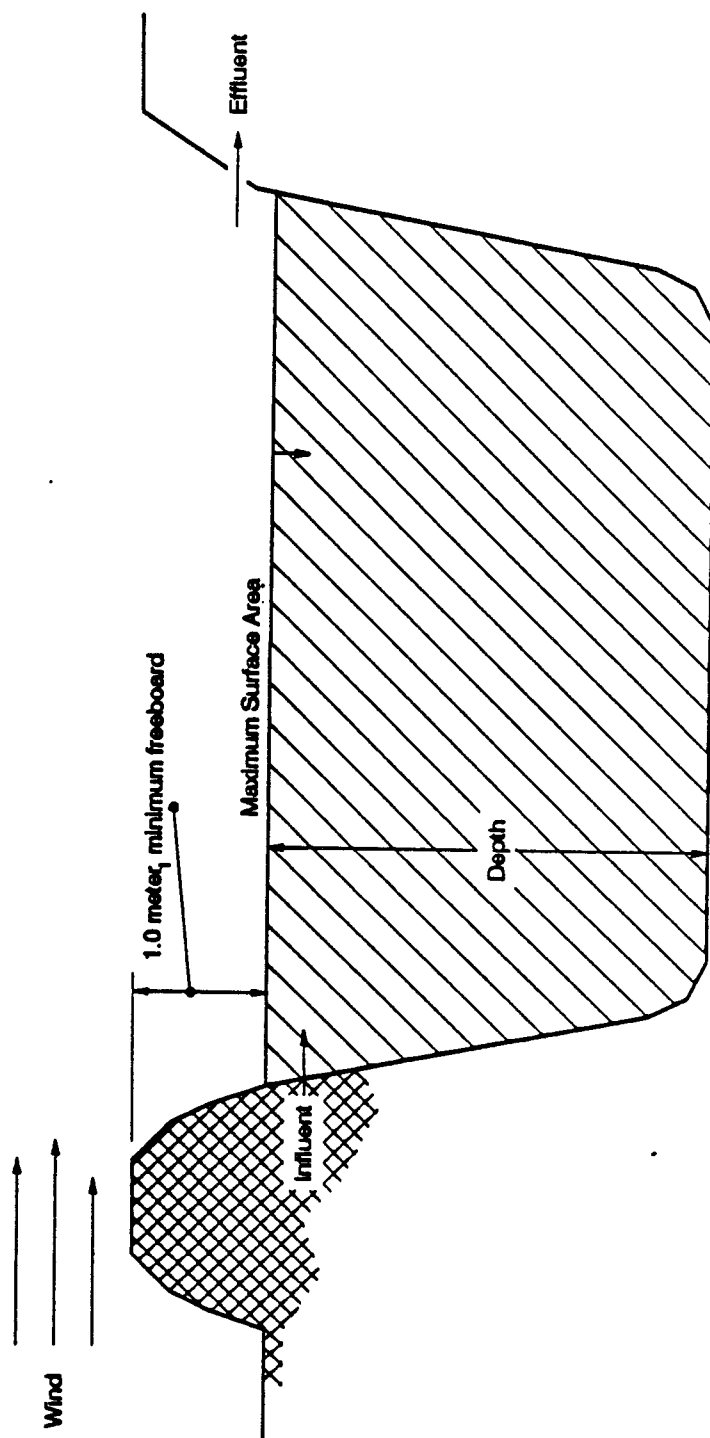
In addition to freeboard, the effective wind speed across the liquid surface of the impoundment is affected by other parameters. These include: the design of the dikes around the impoundment and whether the impoundment is constructed above or below grade. Design characteristics of the impoundment that significantly decreases the effective wind speed above the liquid surface will decrease air emissions.

The surface area and volume of the impoundment also have a significant effect on air emissions. A 1981 survey compiled by Westat<sup>3</sup> showed that the median surface area for storage impoundments was 1,500 m<sup>2</sup> and the median depth was 1.8 m. These median values for area and depth yield a total liquid volume of 2,700 m<sup>3</sup>.

#### 2.2.2 Flow and Level Control<sup>4</sup>

The flow of liquid into and out of an impoundment, and the need to control it, will be defined by the treatment process involved or the storage requirements of the surface impoundment. The major components which ultimately govern the flow into and out of an impoundment are the inflow and outflow structures. In some situations, such as flowthrough systems, inflow and outflow structures may have the same design. However, in most cases they will differ. Normally the inflow structure is a pipe equipped with a flow valve. Typical outflow structures are weirs, spillways, and drain pipes.

Some impoundments are equipped with active level control systems. Level sensing elements, such as floats, probes, and ultrasonic beams, detect changes in the liquid level. This level change causes a level control element such as



$$\text{Fetch} = 2 \sqrt{\frac{(\text{Surface Area})}{\pi}}$$

(circular impoundment)

$$\text{Fetch} = \sqrt{(\text{length})^2 + (\text{width})^2}$$

(rectangular impoundment)

Figure 2-1. Relationship of Freeboard to Wind, Surface Area, Depth, and Fetch in a Surface Impoundment



a pump or control valve to take action and influence the amount of liquid flowing into or out of the impoundment.

As discussed in the previous section, values for the median surface area and depth of impoundments were compiled during a survey by Westat. Information on retention times for impoundments were also gathered during the study. Based on the survey, retention times ranged from 1 to 550 days, with over half of the values at 46 days or less.<sup>5</sup> The flow range represented by this range in retention times can be determined from the median value for impoundment volume reported in the previous section (2,700 m<sup>3</sup>). A flow range of 5 to 2,700 cubic meters per day (m<sup>3</sup>/day) is obtained by dividing the median volume by the range in retention times. These ranges in flow and retention time have a significant impact on air emissions.

### 2.2.3 Biodegradation

Surface impoundments may be designed for biological activity. The major mechanisms of organic removal in biologically active impoundments include biodegradation, volatilization, removal with the effluent, and removal by adsorption on the waste sludge. A study of purgeable volatile organics in a pilot-scale wastewater treatment system showed that less than 0.4 percent (generally less than 0.1 percent) of the volatiles were found in the waste-activated sludge.<sup>6</sup> Another study of municipal wastewater treatment concluded that only a modest amount of purgeable toxics were transferred to the sludge.<sup>7</sup> A third study found that the concentrations of volatile organics in sludges from pilot-scale systems were generally comparable to or less than the corresponding concentrations in the process effluent.<sup>8</sup> This indicated that volatile organics do not have a high affinity for wastewater solids and do not concentrate in the sludges.

Biologically active impoundments are used to treat entire plant wastes as well as to polish the effluent from other treatment processes. Solids usually settle out in the impoundment or are removed in a separate vessel. Generally, the solids are not recycled; however, if the solids are returned, the process is the same as a modified activated sludge process.<sup>9</sup> For information purposes, typical design parameters for an activated sludge process are given in Table 2-2.<sup>10</sup> Typical parameters associated with biologically active impoundments are given in Table 2-3.<sup>11,12</sup> The loading parameter is expressed in terms of kg biological oxygen demand (BOD) per area or volume, and typical

TABLE 2-2. DESIGN PARAMETERS FOR ACTIVATED SLUDGE PROCESSES<sup>10</sup>

Process	F/M, <sup>a</sup> kg BOD/kg biomass day	Loading kg BOD/m <sup>3</sup> day	MLSS, <sup>b</sup> g/L	Retention time, h
Conventional <sup>c</sup>	0.2 - 0.4	0.3 - 0.6	1.5 - 3.0	4 - 8
CSTR <sup>d</sup>	0.2 - 0.6	0.8 - 2.0	3.0 - 6.0	3 - 5
Contact stabilization	0.2 - 0.6	1.0 - 1.2	1.0 - 3.0 <sup>e</sup> 4.0 - 10 <sup>f</sup>	0.5 - 1 <sup>e</sup> 3 - 6 <sup>f</sup>
Extended aeration	0.05 - 0.15	0.1 - 0.4	3.0 - 6.0	18 - 36
O <sub>2</sub> systems	0.25 - 1.0	1.6 - 3.3	6.0 - 8.0	1 - 3

<sup>a</sup>F/M = Food to microorganism ratio; BOD = Biological oxygen demand.

<sup>b</sup>MLSS = Mixed liquor suspended solids.

<sup>c</sup>Plug flow design.

<sup>d</sup>CSTR = Continuous stirred-tank reactor.

<sup>e</sup>Contact unit.

<sup>f</sup>Solids stabilization unit.

retention times in aerated impoundments range from 7 to 20 days. The level of suspended solids in these impoundments is over an order of magnitude less than the level in conventional activated sludge processes. Although the parameters in Table 2-3 are listed as "typical," large variations exist among facilities, and at a single facility the values may change with time. For example, a study conducted over 12 months at an aerobic impoundment used to treat municipal wastewater reported suspended solids levels of 0.02 to 0.1 g/L and volatile suspended solids of 0.01 to 0.06 g/L.<sup>13</sup> Another study of eight quiescent impoundments at four different sites with confirmed biological activity estimated active biomass concentrations from the rate of oxygen consumption that ranged from 0.014 to 0.22 g/L with an average of 0.057 g/L.<sup>14</sup>

The biomass concentration is an important parameter in estimating biodegradation rates. The best value to use for a specific site is a direct measurement such as volatile suspended solids for the system of interest. In the absence of site-specific data, a number may be chosen from the ranges for suspended solids given in Tables 2-2 and 2-3. Alternatively, typical or default values for biomass concentration given in Table 2-4 may be used.<sup>15</sup>

Numerous models have been proposed for the removal of organic compounds by biodegradation.<sup>16,17</sup> However, there is a general agreement that the biodegradation rate is zero-order with respect to concentration for high organic loadings relative to biomass, and becomes first-order with respect to concentration for low residual organic levels.

First-order or monod-type kinetics assumes that biodegradation of any one constituent is independent of the concentrations of other constituents. The significant features of this model are that at high concentrations, the biodegradation rate is independent of (or zero-order with respect to) the component concentration; and at low concentrations the rate becomes directly proportional (or first-order to) the component concentration. Biodegradation rates are also facility-specific since they are affected by the presence of other compounds in the wastewater. Therefore, site-specific biodegradation rates should be used if available. If site-specific rates are unavailable, default values provided by SIMS and presented in Appendix B can be used.

#### 2.2.4 Mechanical Aeration

Mechanical aerators are often used for the purpose of supplying oxygen required by the microorganisms to biodegrade pollutants in the impoundment.

TABLE 2-3. IMPOUNDMENTS DESIGNED FOR BIODEGRADATION<sup>11,12</sup>

Type	Application	Typical daily loading kg BOD <sub>5</sub> /m <sup>2</sup> day <sup>a</sup>	Retention Time, day	Typical depth, m	Suspended solids, g/L
Facultative	Raw municipal wastewater	0.0011 - 0.0034 <sup>a</sup>	25 - 180	1.2 - 2.5	0.11 - 0.40
	Effluent from primary treatment, trickling filters, aerated ponds, or anaerobic ponds				
Aerated	Industrial wastes	0.008 - 0.32	7 - 20	2 - 6	0.26 - 0.30
	Overloaded facultative ponds				
	Situations where limited land area is available				
Aerobic	Generally used to treat effluent from other processes, produces effluent low in soluble BOD <sub>5</sub> and high in algae solids	0.021 - 0.043 <sup>b</sup>	10 - 40	0.3 - 0.45	0.14 - 0.34
Anaerobic	Industrial wastes	0.16 - 0.80	20 - 50	2.5 - 5	0.08 - 0.16

<sup>a</sup>Five-day biological oxygen demand.

TABLE 2-4. TYPICAL OR DEFAULT VALUES FOR BIOMASS CONCENTRATION<sup>15</sup>

Units	Biomass concentration (g/L) <sup>a</sup>
Quiescent impoundments	0.05 <sup>b</sup>
Aerated impoundments	0.30 <sup>c</sup>
Activated sludge units	4.0 <sup>d</sup>

<sup>a</sup>These values are recommended for use in the emission equations when site-specific data are not available.

<sup>b</sup>Based on the range (0.0014 to 0.22) and average (0.057) from actual impoundments.

<sup>c</sup>From the data in Table 2-3 for aerated impoundments. Assumes biomass is approximated by the suspended solids level.

<sup>d</sup>Midrange value from Table 2-2 for CSTR based on mixed liquor suspended solids.

However, not all impoundments equipped with aeration devices contain biomass, which is necessary for biodegradation to occur. Some impoundments are aerated for purposes such as evaporative cooling.

The emission models used by the computer program require values for the parameters that describe the mechanical aeration system. Typical parameters for impeller speed and diameter are 126 rad/s (1,200 rpm) and 61 cm (2 ft), respectively. For impeller power, Metcalf and Eddy, Inc., suggest a range of 15 to 30 kw/1000 m<sup>3</sup> (0.6 to 1.15 hp/1,000 ft<sup>3</sup>) for mixing in impoundments.<sup>18</sup> However, more power may be needed to supply additional oxygen or to mix certain treatment solutions such as in activated sludge units. A review of information gathered during the evaluation of TSDF showed power usage as high as 92.2 kw/1000 m<sup>3</sup> (3.5 hp/1,000 ft<sup>3</sup>) at a specific TSDF impoundment.<sup>19</sup> Data included in the TSDF report show an average value of 52.67 kw/1000 m<sup>3</sup> (2.0 hp/1000 ft<sup>3</sup>) for activated sludge units.<sup>17</sup>

Data from Metcalf and Eddy indicated that an aerator with a 75-hp motor and a 61-cm diameter propeller turning at 126 rad/s (1200 rpm) would agitate a volume of 658 m<sup>3</sup> (23,240 ft<sup>3</sup>).<sup>20</sup> Assuming a uniform depth in the impoundment of 1.8 m, the agitated surface area was estimated as 366 m<sup>2</sup> (658/1.8). The agitated surface is assumed to be turbulent and comprises a 24 percent (366/1,500 x 100) of the total area. The balance of the surface area of the impoundment (76 percent) is assumed to be quiescent. As a comparison, Thibodeaux reported a turbulent area of 5.22 m<sup>2</sup>/hp and investigated a range of 0.11 to 20.2 m<sup>2</sup>/hp. The value of 5.22 m<sup>2</sup>/hp and a total of 75 hp yields an estimated turbulent area of 392 m<sup>2</sup> (26 percent), which compares favorably with the 24 percent turbulent area calculated by the alternative approach.<sup>21</sup> For activated sludge units, data presented in the TSDF report show an average agitated surface area of 52 percent.<sup>17</sup>

#### 2.2.5 Diffused Aeration

Diffused air or air sparging systems are generally used to promote biodegradation or air stripping. The diffused air emission model assumes that the concentration of the compound in the air bubbling through the liquid phase reaches equilibrium with the liquid-phase concentration.

The diffused air impoundment model uses the quiescent mass transfer correlation equations in the SIMS program (see Chapter 4 for quiescent impoundment mass transfer correlations). In addition to values required by these mass transfer correlations, the diffused air model requires a value for

the diffused air flow rate. Typically, diffused air flow rates range from 0.3 to 0.5 cubic meters per second per 1,000 cubic meters of total impoundment volume ( $0.3-0.5 \text{ m}^3/\text{s}-1,000 \text{ m}^3$ ).<sup>22</sup>

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### 3.0 COLLECTION SYSTEM DESIGN AND OPERATION

Collection system components are used to transport wastewater from the point of generation to treatment or storage systems. The number and types of collection system components are facility specific. Most collection system components are open to the atmosphere and thus create a potential for VOC emissions. The magnitude of VOC emissions depends greatly on many factors, such as the physical properties of the compounds in the wastewater, temperature of the wastewater, and the design of the component. Common collection system components include junction boxes, lift stations, sumps, weirs, drains, trenches, and manholes. The SIMS program estimates emissions from only the first four of these components; however, a brief discussion of the applications and design parameters are provided in this chapter for all components mentioned.

#### 3.1 JUNCTION BOXES<sup>1</sup>

A junction box normally serves several process sewer lines. Process lines meet at the junction box to combine the multiple wastewater streams into one stream which flows downstream from the junction box. Generally, the flow rate is controlled by the liquid level in the junction box. Junction boxes are normally either square or rectangular and are sized based on the flow rate of the entering streams. Typical junction box water depths range from 0.3 - 1.8 m, with an average of 0.9 m. Surface areas range from 0.007 - 2.5 m<sup>2</sup>, with an average of 0.7 m<sup>2</sup>.

Emissions occur from junction boxes predominantly by convective mass transfer. Organics in the wastewater volatilize into the ambient air just above the liquid surface in an attempt to reach equilibrium between the liquid and vapor phases.

Junction box design characteristics that affect emissions are: the fetch to depth ratio, the water turbulence in the junction box, and the liquid surface area. Depth is represented by the average liquid level in the junction box. As the liquid depth in the junction box increases, so does the resistance to liquid phase mass transfer. That is, organic compounds must overcome more resistance before they reach the water surface. Once these organics reach the surface, the fetch length, or linear distance across the

impoundment, provides the route for volatilization into the ambient air. Therefore, increases in the fetch to depth ratio for the junction box increase air emissions.

Water turbulence enhances liquid phase mass transfer.<sup>2</sup> In quiescent flow through the junction boxes, pollutants slowly diffuse to the water surface to replace the volatilizing pollutants. In turbulent flow through the junction box, the organic compounds are thoroughly mixed and pushed rapidly towards the surface. Therefore, more organic compounds are exposed to the surface air, and the emission rate is increased. If the sewer lines feed water to the junction box above the liquid surface, the exposure of organic compounds to the surface air is also increased. The water spills into the junction box causing splashing and additional turbulence at the liquid surface which increases emissions. This effect can be minimized by introducing water to the junction box below the liquid surface. The final design characteristic affecting emissions is surface area. An increase in surface area at constant depth increases the hydraulic (water) retention time in the junction box. Therefore, not only is the area for volatilization increased but so is the time available for volatilization.

The SIMS program uses the turbulent liquid phase mass transfer correlation and the quiescent gas phase mass transfer correlation for estimating VOC emissions from junction boxes (see Chapter 4).

### 3.2 LIFT STATIONS<sup>3</sup>

Lift stations are usually the last collection unit prior to the treatment system, accepting wastewater from one or several sewer lines. The main function of the lift station is to provide sufficient head pressure to transport the collected wastewater to the treatment system. A pump is used to provide this head pressure and is generally switched on and off by a preset high and low liquid level controller. Lift stations are usually rectangular in shape and greater in depth than length or width. Typical water depths for lift stations are 1.2 - 1.8 m, with an average of 1.5 m. Surface areas range from 1.1 - 1.7 m<sup>2</sup>, with an average of 1.8 m<sup>2</sup>.

Emissions occur from lift stations predominantly by convective mass transfer. Organics in the wastewater volatilize into the ambient air just above the liquid surface in an attempt to reach equilibrium between the liquid and vapor phases.

The characteristics affecting emissions from lift stations are the same as the characteristics affecting emissions from junction boxes. In addition to these design parameters, operation of the lift station affects air emissions. The liquid level in a lift station normally rises and falls based on the wastewater flow to the unit. As the level rises, the wastewater acts as a piston displacing organic vapors above the liquid surface into the ambient air. The linear distance between the low and high level limits in the lift station determine the amount of displacement during normal operation. As this distance increases, displacement increases and so does the emission rate. Also, at lower liquid levels, wastewater is normally spilling into the lift station above the liquid surface. This causes an increase in turbulence which increases liquid phase mass transfer. Therefore, volatilization occurs more rapidly above the surface of the rising liquid. At the higher liquid levels, the sewer lines feeding the lift station are often submerged which reduces splashing above the liquid surface.

The SIMS program also uses the turbulent liquid phase mass transfer correlation and the quiescent gas phase mass transfer correlation for estimating VOC emissions from lift stations (see Chapter 4).

### 3.3 SUMPS<sup>4</sup>

Sumps are typically used for collection and equalization of wastewater flow from trenches prior to treatment. (Trenches are discussed in Section 3.6). They are usually quiescent and open to the atmosphere. Typical diameters and depths are approximately 1.5 meters.

Emissions occur from sumps by both diffusive and convective mechanisms. As wastewater flows slowly through the sump, organics diffuse through the water to the liquid surface. These organics volatilize into the ambient air above the liquid, and can be swept into the air by wind blowing across the surface of the sump.

The design characteristics which affect air emission rates from sumps are: the fetch to depth ration, the liquid surface area, and the hydraulic retention time. Fetch to depth ratios vary widely for different sumps. As the fetch to depth ratio increases, so does the mass transfer rate of organics into the ambient air. The hydraulic retention time, which is a function of the wastewater flow rate and volume of the sump, also has an effect on emissions. An increase in retention time provides additional time for organic

compound volatilization to occur and, therefore, emissions increase. Likewise, an increase in the surface area of the sump increases the emissions rate.

The SIMS program uses the quiescent mass transfer correlations for estimating VOC emissions from sumps (see chapter 4).

### 3.4 WEIRS<sup>5</sup>

Weirs act as dams in open channels. The weir face is normally aligned perpendicular to the bed and walls of the channel. Water from the channel normally overflows the weir but may pass through a notch, or opening, in the weir face. Because of this configuration, weirs provide some control of the level and flow rate through the channel. This control, however, may be insignificant compared to upstream factors which influence the supply of water to the channel. Typical weir heights range from 0.9 - 2.7 m, with an average of 1.8 m. The weir height is the distance between the top of the liquid level and the point where the wastewater meets the receiving body of water.

Often the water overflowing the weir proceeds down stair steps, which serve to aerate the wastewater. The wastewater splashes off each step increasing the surface area of the water in contact with ambient air. This action increases diffusion of oxygen into the water which may be beneficial to the biodegradation process (often the next treatment step). However, this increased contact with air also accelerates emissions of volatile organics contained in the wastewater.<sup>6,7</sup> The organics volatilize from the surface of the falling water in an attempt to reach equilibrium between the liquid and vapor phases. The volatilizing organic compounds are swept into the ambient air surrounding the weir.

The concentration and physical properties of the organic compounds in the wastewater have a significant effect on VOC emissions. The diffusivity in water of the specific organic compounds present in the wastewater may be the most significant physical property. Organics must first diffuse through the liquid phase before volatilizing from the surface of the falling wastewater. Therefore, an increase in organic compound diffusivity in water tends to increase the air emissions rate.

The height of the weir is the most significant design characteristic affecting emissions.<sup>7</sup> The height of the weir determines the length of time that the wastewater stream is falling through the air. Because this is the

time period when the organics are being emitted to the air, an increase in weir height will increase the magnitude of air emissions.

The SIMS program uses mass transfer correlations developed from volatilization-re-aeration theory for estimating VOC emissions from weirs (see Chapter 4).

### 3.5 DRAINS<sup>8</sup>

Wastewater streams from various sources throughout a given process are normally introduced into the collection system through process drains. Individual drains are usually connected directly to the main process sewer line. However, they may also drain to trenches, sumps, or ditches. Some drains are dedicated to a single piece of equipment such as a scrubber, decanter, or stripper. Others serve several sources. These types of drains are located centrally between the pieces of equipment they serve and are referred to as area drains.

Emissions occur from drains by diffusive and convective mechanisms.<sup>9</sup> As wastewater flows through the drain, organics volatilize in an attempt to reach equilibrium between the aqueous and vapor phases. The organic vapor concentration in the headspace at the bottom of the drain riser is much higher than ambient concentrations. Due to this concentration gradient, organics diffuse from the drain into ambient air through the opening at the top of the drain riser. In addition, if the temperature of the wastewater flowing through the sewer is greater than the ambient air temperature, this temperature gradient will induce air flow from the vapor headspace in the sewer line. This air flow passes through the drain riser and into the ambient air. The convective forces created by this air flow establishes convective mass transfer of the organics. Air flows resulting from wind blowing over or into the drain, or from wind currents entering another sewer opening and flowing through the sewer, also aid the mass transfer.

Drain design characteristics such as diameter, and length of the drain riser affect emissions. The diameter of the drain riser must be large enough to prevent the wastewater from overflowing on to the ground. As the diameter increases, so does the surface area exposed to ambient air. This increase of the drain riser from the mouth of the drain to the process sewer is another design parameter which affects emissions. Pollutants are more readily emitted

to the atmosphere from a short drain riser due to the smaller resistance to diffusional and convective mass transfer.

### 3.6 TRENCHES<sup>10</sup>

Trenches are normally used to transport wastewater from the point of process equipment discharge to subsequent wastewater collection units such as junction boxes and lift stations. This mode of transport replaces the drain scenario as a method for introducing process wastewater into the downstream collection system. In older plants, trenches are often the primary mode of wastewater transportation in the collection system. Trenches are often interconnected throughout the process area and handle pad water runoff, water from equipment washes and spill cleanups, as well as process wastewater discharges. Normally, the length of the trench is determined by the general locations of the process equipment and the downstream collection system units. This length typically ranges from 50 to 500 feet. Trench depth and width are dictated by the wastewater flow rate discharged from process equipment. The depth and width of the trench must be sufficient to accommodate expected as well as emergency wastewater flows from the process equipment. Typical trench depths range from 0.4 to 1.2 m, with an average of 0.8 m.

Emissions from trenches, like junction boxes and lift stations, occur predominantly by convective mass transfer. As wastewater flows through the trench, organic compounds volatilize into the ambient air above the liquid surface in an attempt to reach equilibrium between the liquid and vapor phases.

The trench design characteristics which affect emission rate include the depth and width of the trench and the hydraulic retention time. Mass transfer rates increase as the depth of the trench becomes more shallow and the width of the trench becomes wider. The hydraulic retention time in the trench is a function of the wastewater flow rate and the volume of the trench. Longer trenches increase the hydraulic retention for mass transfer to take place and, therefore, will increase air emissions. The grade (slope) of the trench is also important. Grade will have an effect on the turbulence of the wastewater flowing through the trench. An increase in turbulence will reduce the liquid phase resistance to mass transfer and thus increase air emissions.

### 3.7 MANHOLES<sup>11</sup>

Manholes are service entrances into process sewer lines which permit inspection and cleaning of the sewer line. They are normally placed at periodic lengths along the sewer line. They may also be located where sewers intersect or where there is a significant change in direction, grade, or sewer line diameter. The lower portion of the manhole is usually cylindrical, with a typical inside diameter of four feet to allow adequate space for workmen. The upper portion tapers to the diameter of the opening at ground level. The opening is normally about two feet in diameter and covered with a heavy cast-iron plate. The cover usually contains two to four holes for ventilation so that the manhole cover can be grasped for removal.

Emissions occur from manholes by diffusive and convective mechanisms.<sup>9</sup> As wastewater moves through the sewer lines, organics volatilize in an attempt to reach equilibrium between the aqueous phase and the vapor headspace in the sewer line. The organic vapor concentration in the headspace above the wastewater is much higher than the concentration of organics in the ambient air above the manhole. Due to this concentration gradient, organics will diffuse from the sewer line into the ambient air through the manhole openings.

Manhole design characteristics that affect emission rates are: the manhole diameter, length from the manhole cover down to the sewer line, the thickness of the manhole cover, and the number and diameter of the vent holes in the manhole cover. The length from the manhole cover to the sewer line is the distance organics must diffuse from the wastewater before being emitted to the ambient air. Therefore, an increase in this length will decrease the emission rate. The thickness of the cover adds to this diffusional length. The diameter of holes in the cover along with the number of holes determine the ultimate surface area available for diffusion and convection of organics into the air.



### 3.8 REFERENCES

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## 4.0 SURFACE IMPOUNDMENT EMISSION MODELS

Mass transfer models were developed to estimate pollutant emissions from surface impoundments and collection system components during EPA's evaluation of hazardous waste TSD and VOC emissions from industrial wastewater, respectively.<sup>1,2</sup> Figure 4-1 presents a flow diagram for estimating VOC emissions from surface impoundments and collection system components. Table 4-1 presents a summary of all emission rate equations and Table 4-2 defines all mass transfer correlations given in Figure 4-1. The basic estimation approach, the form of the emission equations, and the input parameters required by the models are discussed in this chapter.

### 4.1 BASIC EMISSION ESTIMATION APPROACH

Emissions from surface impoundments and collection system components result from the volatilization of organic compounds at the water surface or at the oil film surface (for impoundments with an oil film layer). For surface impoundments without an oil film layer, and all collection system components presented in this document except weirs, models based on two-film resistance theory were developed to determine the rate of volatilization. This theory assumes the rate limiting factor for volatilization is the overall resistance to mass transfer at the liquid surface and the ambient air interface. The overall resistance is due to the individual resistances in both the liquid and gas phase films at the interface. For surface impoundments with an oil film layer, the oil film is assumed to be relatively thin, there is infinite resistance between the water and oil phases, and that mass transfer is controlled by the gas phase resistance only. For weirs, volatilization-re-aeration theory is assumed. This theory assumes that emissions are based on diffusivities of oxygen and the constituent in water.

Individual mass transfer coefficients account for the resistances in the liquid and gas phase films. These individual coefficients can be used to estimate overall mass transfer coefficients for each pollutant. Air emissions from the impoundment or collection system component are estimated by applying these overall coefficients in mass balance equations. The forms of the mass balance equations depend on a number of factors which are discussed in more detail in the next section (Section 4.2).

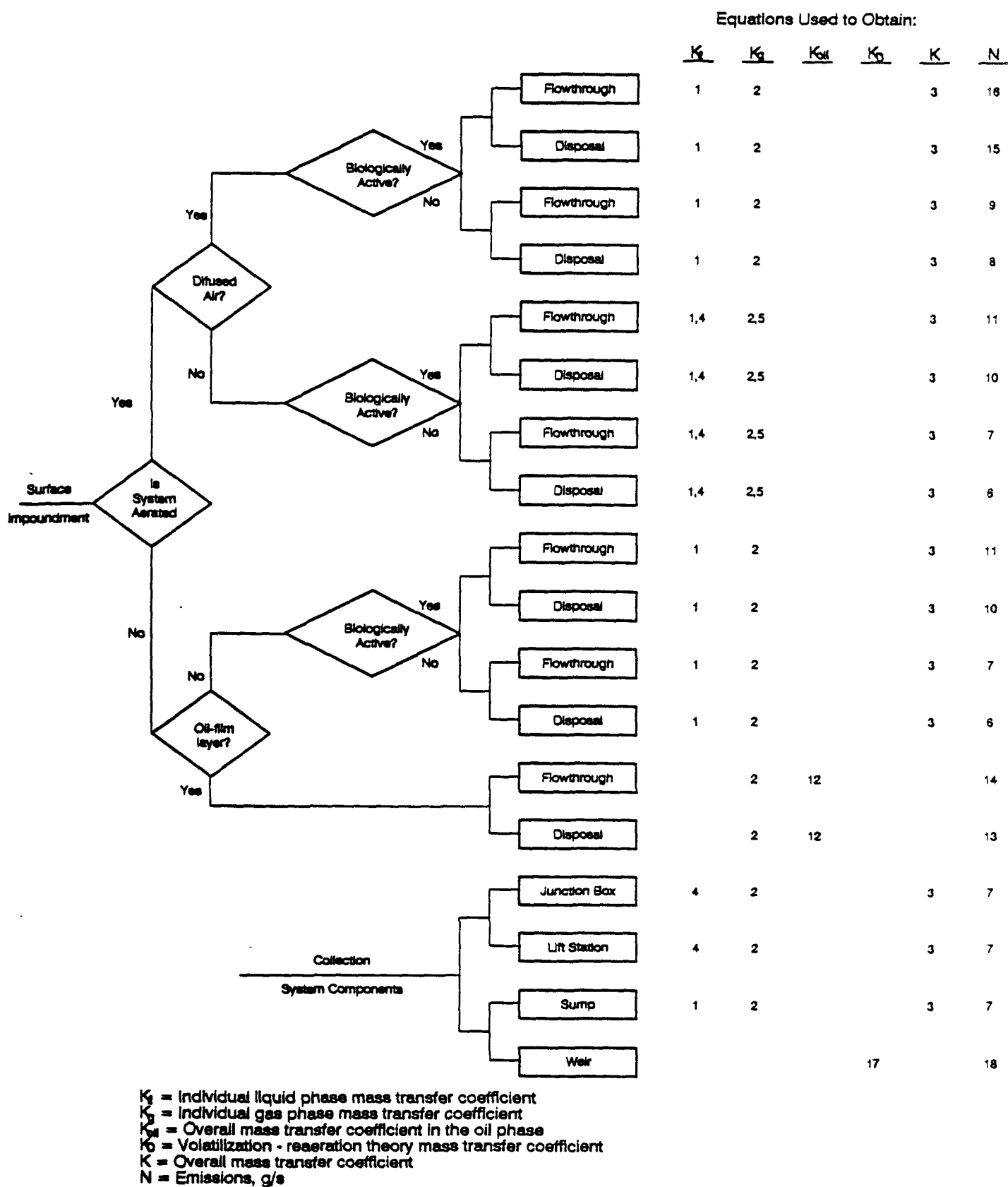


Figure 4-1. Flow Diagram for Estimating VOC Emissions from Surface Impoundments and Collection System Components

TABLE 4-1. EMISSION DATA EQUATIONS\*

Conditions	Emissions Rate, g/s
<u>Wastewater Treatment and Storage</u>	
Flowthrough, no biodegradation aerated or nonaerated	$(KAQ Co)/(Q + KA)$
Flowthrough, biodegradation aerated or nonaerated	$KA[-(K_s(KA/Q + 1) + VK_{maxb_1}/Q - Co) + \{(K_s(KA/Q + 1) + VK_{maxb_1}/Q - Co)^2 + 4(KA/Q + 1)(K_s Co)\}^{0.5}]/\{2(KA/Q + 1)\}$
Flowthrough, no biodegradation diffused air	$(KA + Q_A K_{eq})QCo/(KA + Q + Q_A K_{eq})$
Flowthrough, biodegradation diffused	$(KA + Q_A K_{eq})[-(K_s((KA + Q_A K_{eq})/Q + 1) + VK_{maxb_1}/Q - Co) + \{(K_s((KA + Q_A K_{eq})/Q + 1) + VK_{maxb_1}/Q - Co)^2 + 4((KA + Q_A K_{eq})/Q + 1)(K_s Co)\}^{0.5}]/\{2((KA + Q_A K_{eq})/Q + 1)\}$
Flowthrough, no biodegradation oil film layer	$K_{o11}AQ_{o11}Co_{o11}/(K_{o11}A + Q_{o11})$
Disposal, no biodegradation aerated or nonaerated	$[1 - \exp(-KAt/V)]VCo/t$
Disposal, biodegradation	$[1 - \exp(-K_{maxb_1}t/K_s - KAt/V)] [KA/(KA + K_{maxb_1}V/K_s)]VCo/t$
Disposal, no biodegradation diffused air	$[1 - \exp(-(KA + K_{eq}Q_A)t/V)] VCo/t$
Disposal, biodegradation diffused air	$[1 - \exp(-(KA + K_{eq}Q_A)t/V - K_{maxb_1}t/K_s)] (KA + Q_A K_{eq})/(KA + Q_A K_{eq} + K_{maxb_1}V/K_s)VCo/t$
Disposal, no biodegradation oil film layer	$[1 - \exp(-K_{o11}t/D_{o11})] V_{o11}Co_{o11}/t$

TABLE 4-1. EMISSION DATA EQUATIONS (continued)\*

Conditions	Emissions Rate, g/s
<u>Wastewater Collection</u>	
Junction boxes, lift stations and sumps	$(KAQCo)/(Q + KA)$
Weirs	$[1 - \exp(-K_D)]QCo$

\*See Figure 4-1, Table 4-2, and the list of abbreviations and symbols (located at the front of the document) for a flow diagram of specific mass transfer equations to use, the mass transfer correlations, and the definitions of all parameters used, respectively.

TABLE 4-2. MASS TRANSFER CORRELATIONS AND EMISSIONS EQUATIONS

Equation No.	Equations
1	$k_l \text{ (m/s)} = 2.78 \times 10^{-6} [D_w/D_{\text{ether}}]^{2/3}$ <p>For: <math>0 &lt; U_{10} &lt; 3.25 \text{ m/s}</math> and all <math>F/D</math> ratios</p> $k_l \text{ (m/s)} = [(2.605 \times 10^{-9})(F/D) + (1.277 \times 10^{-7})U_{10}^2][D_w/D_{\text{ether}}]^{2/3}$ <p>For: <math>U_{10} &gt; 3.25 \text{ m/s}</math> and <math>14 &lt; F/D &lt; 51.2</math></p> $k_l \text{ (m/s)} = 2.61 \times 10^{-7} U_{10}^2 [D_w/D_{\text{ether}}]^{2/3}$ <p>For: <math>U_{10} &gt; 3.25 \text{ m/s}</math> and <math>F/D &gt; 51.2</math></p> $k_l \text{ (m/s)} = 1.0 \times 10^{-6} + 144 \times 10^{-4} (U^*)^{2.2} (Sc_L)^{-0.5}; U^* < 0.3$ $k_l \text{ (m/s)} = 1.0 \times 10^{-6} + 34.1 \times 10^{-4} U^* (Sc_L)^{-0.5}; U^* > 0.3$ <p>For <math>U_{10} &gt; 3.25 \text{ m/s}</math> and <math>F/D &lt; 14</math></p> <p>where:</p> $U^* \text{ (m/s)} = 0.01 U_{10} (6.1 + 0.63 U_{10})^{0.5}$ $Sc_L = \mu_L / (\rho_L D_w)$
2	$k_g \text{ (m/s)} = 4.82 \times 10^{-3} (U_{10})^{0.78} (Sc_G)^{-0.67} (d_e)^{-0.11}$ <p>where:</p> $Sc_G = \mu_a / (\rho_a D_a)$ $d_e \text{ (m)} = 2(A/\pi)^{0.5}$
3	$K = \frac{k_l \text{ Keq } k_g}{\text{Keq } k_g + k_l}$ <p>where:</p> $\text{Keq} = H/(RT)$
4	$k_l \text{ (m/s)} = [8.22 \times 10^{-9} J (\text{POWR})(1.024)^{(T-20)} 0_t 10^6 MW_L (Va_v \rho_L)] (D_w/D_{o2,w})^{0.5}$ <p>where:</p> $\text{POWR (hp)} = (\text{Total Power to aerators})V$ $Va_v \text{ (ft}^2\text{)} = (\text{fraction of area agitated})A$
5	$k_g \text{ (m/s)} = 1.35 \times 10^{-7} (\text{Re})^{1.42} (P)^{0.4} (Sc_G)^{0.5} (\text{Fr})^{-0.21} (D_a \text{ MW}_a/d)$ <p>where:</p> $\text{Re} = d^2 w \rho_a / \mu_a$ $P = [0.85 (\text{POWR})(550 \text{ ft-lb}_f/\text{s-hp})/N_t] g_c / (\rho_L d^{*5} w^3)$

TABLE 4-2. MASS TRANSFER CORRELATIONS AND EMISSIONS EQUATIONS (continued)

Equation No.	Equations
	$Sc_G = \mu_a / (\rho_a D_a)$ $Fr = d^* w^2 / g_c$
6	$N(g/s) = (1 - Ct/Co) V Co/t$ <p>where:</p> $Ct/Co = \exp[-KAt/V]$
7	$N(g/s) = K C_L A$ <p>where:</p> $C_L(g/m^3) = Q Co/[KA + Q]$
8	$N(g/s) = (1 - Ct/Co) V Co/t$ <p>where:</p> $Ct/Co = \exp[-(KA + Keq Q_a)t/V]$
9	$N(g/s) = (KA + Q_a Keq) C_L$ <p>where:</p> $C_L(g/m^3) = QCo/(KA + Q + Q_a Keq)$
10	$N(g/s) = (1 - Ct/Co) KA/(KA + Kmaxb_i V/K_s) VCo/t$ <p>where:</p> $Ct/Co = \exp[-Kmaxb_i t/K_s - KAt/V]$
11	$N(g/s) = K C_L A$ <p>where:</p> $C_L(g/m^3) = [-b + (b^2 - 4ac)^{0.5}]/(2a)$ <p>and</p> $a = KA/Q + 1$ $b = K_s(KA/Q + 1) + Kmaxb_i V/Q - Co$ $c = -K_s Co$
12	$K_{oil} = k_g Keq_{oil}$ <p>where:</p> $Keq_{oil} = P^* \rho_a MW_{oil} / (\rho_{oil} MW_a P_o)$

TABLE 4-2. MASS TRANSFER CORRELATIONS AND EMISSIONS EQUATIONS (continued)

Equation No.	Equations
13	$N(g/s) = (1 - Ct_{oil}/Co_{oil})V_{oil}Co_{oil}/t$ <p>where:</p> $Ct_{oil}/Co_{oil} = \exp[-K_{oil}t/D_{oil}]$ <p>and:</p> $Co_{oil} = KowCo/((1 - FO) + FO(Kow))$ $V_{oil} = (FO)V$ $D_{oil} = (FO)V/A$
14	$N(g/s) = K_{oil}C_{L,oil}A$ <p>where:</p> $C_{L,oil}(g/m^3) = Q_{oil}Co_{oil}/(K_{oil}A + Q_{oil})$ <p>and:</p> $Co_{oil} = KowCo/((1 - FO) + FO(kow))$ $Q_{oil} = (FO)Q$
15	$N(g/s) = (1 - Ct/Co)(KA + Q_AKeq)/(KA + Q_AKeq + Kmaxb_iV/K_s)VCo/t$ <p>where:</p> $Ct/Co = \exp[-(KA + KeqQ_a)t/V - Kmaxb_it/K_s]$
16	$N(g/s) = (KA + Q_AKeq)C_L$ <p>where:</p> $C_L(g/m^3) = [-b + (b^2 - 4ac)^{0.5}]/(2a)$ <p>and</p> $a = (KA + Q_AKeq)/Q + 1$ $b = K_s[(KA + Q_AKeq)/Q + 1] + Kmaxb_iV/Q - Co$ $c = -K_sCo$
17	$K_p = 0.16h (D_w/D_{o2,w})^{0.75}$
18	$N(g/s) = [1 - \exp(-K_p)]QCo$



The basic approach used by the models to estimate emissions can be summarized as follows:

- (1) estimate individual liquid and gas phase mass transfer coefficients for each pollutant,  $k_l$  (for collection system components and impoundments without an oil layer) and  $k_g$  (m/s);
- (2) estimate equilibrium constants for each pollutant from the following expressions:

- A. Collection system components and surface impoundments without an oil layer.

$$K_{eq} = H/RT$$

where:

$K_{eq}$  = equilibrium constant, dimensionless

$H$  = Henry's Law constant, atm m<sup>3</sup>/gmol

$R$  = ideal gas law constant, atm m<sup>3</sup>/gmol - °K

$T$  = wastewater temperature, °K

- B. Surface impoundments with an oil film layer.

$$K_{eq_{oil}} = P^* \rho_a MW_{oil} / (\rho_l MW_a P_o)$$

where:

$P^*$  = vapor pressure of the constituent, mmHg

$P_o$  = total pressure, mmHg

$\rho_a$  = density of air, g/cm<sup>3</sup>

$\rho_l$  = density of water, g/cm<sup>3</sup>

$MW_{oil}$  = molecular weight of oil, g/gmol

$MW_a$  = molecular weight of air, g/gmol

- (3) estimate overall mass transfer coefficient for each pollutant from the following expressions:

- A. Collection system components and surface impoundments without an oil layer.

$$1/K = 1/k_l + 1/(k_g K_{eq})$$

where:

$K$  = overall mass transfer coefficient, m/s

B. Surface impoundments with an oil film layer.

$$K_{oil} = k_g K_{eq_{oil}}$$

where:

$K_{eq_{oil}}$  = oil phase equilibrium constant

$K_{oil}$  = oil phase overall mass transfer coefficient, m/s

- (4) apply a mass balance around the surface impoundment to estimate emissions

#### 4.2 EMISSION EQUATIONS

The emission models account for the following factors concerning the design and operation of a surface impoundment: (1) the flow regime through the impoundment (i.e., flowthrough or disposal), (2) the impoundment type (i.e., aerated, diffused air, nonaerated, or oil film layer), and (3) whether pollutants are biodegraded in the impoundment. These factors affect the correlations used to estimate the individual mass transfer coefficients as well as the forms of the mass balance emission equations.

Collection system components are flowthrough by nature and are aerated or nonaerated, depending on the characteristics of the incoming flow. Junction boxes and lift stations are characterized by turbulent flow, while sumps are typically quiescent. Weirs are characterized by volatilization-reaeration theory. Emission models for these collection system components are described briefly in Section 4.2.3.

##### 4.2.1 Flowthrough Impoundments

Flowthrough impoundments act as temporary storage for wastewater prior to subsequent treatment or discharge to a receiving body. Assuming a well-mixed system with no reactions and no separate organic phase, the mass balance for a flowthrough impoundment with a diffused air system (air sparging) yields the following equation:<sup>3</sup>

$$Q C_o = Q C_L + V K_{max} b_i C_L / (K_s + C_L) + K A C_L + Q_A K_{eq} C_L$$

where:

$Q$  = flow rate, m<sup>3</sup>/s

$C_o$  = inlet concentration, g/m<sup>3</sup>

$C_L$  = bulk liquid and effluent concentration, g/m<sup>3</sup>

$K_{max}$  = maximum rate constant, g/s-g biomass

$K_s$  = half saturation constant, g/m<sup>3</sup>

$b_i$  = biomass concentration, g/m<sup>3</sup>

$V$  = volume, m<sup>3</sup>

$K$  = overall mass transfer coefficient, m/s

$A$  = area, m<sup>2</sup>

$Q_A$  = air flow rate, m<sup>3</sup>/s

$K_{eq}$  = equilibrium constant, dimensionless

In the equation, the pollutant mass loading into the impoundment is represented by the term,  $QCo$ . The three predominant removal mechanisms accounted for in the equation are volatilization, biodegradation, and air sparging. The rates of removal by these three mechanisms are estimated from the terms,  $KA/V$  (for volatilization),  $VK_{max}b_iC_L/(K_s + C_L)$  (for biodegradation), and  $Q_AK_{eq}/V$  (for air sparging). Volatile organics not removed by these two mechanisms are assumed to leave with the effluent flowing from the impoundment. The rate of removal with the effluent is represented by the term,  $QC_L$ .

To determine the fraction of volatile organics emitted or biodegraded using the Monod model, the above equation is solved for the equilibrium or bulk concentration,  $C_L$ :

$$K'C_L^2 + [K_sK' + (V/Q)K_{max}b_i - Co]C_L - K_sCo = 0$$

where  $K' = (KA + Q_AK_{eq})/Q + 1$

Using the quadratic formula,

$$C_L = [-b + (b^2 - 4ac)^{0.5}]/2a$$

where:

$$a = K' = (KA + Q_AK_{eq})/Q + 1$$

$$b = K_s[(KA + Q_AK_{eq})/Q + 1] + (V/Q)K_{max}b_i - Co$$

$$c = -K_s Co$$

[NOTE: The plus sign in the quadratic equation is selected to ensure positive effluent concentrations.]

The fraction of the inlet organic emitted to the air is calculated by the following equation:

$$f_{air} = \frac{\text{Mass of pollutant } i \text{ emitted to the air}}{\text{Total mass of pollutant } i} = (KA + Q_A K_{eq}) C_L / (Q Co)$$

Therefore, for a well-mixed flowthrough impoundment with biodegradation and sparged air, the expression for estimating the air emission rate (N, g/s) of each pollutant is:

$$N = f_{air} Q Co = (KA + Q_A K_{eq}) \left[ - (K_s [(KA + Q_A K_{eq})/Q + 1] + VK_{max} b_i / Q - Co) + [(K_s [(KA + Q_A K_{eq})/Q + 1] + VK_{max} b_i / Q - Co)^2 + 4 ((KA + Q_A K_{eq})/Q + 1) (K_s Co)]^{0.5} \right] / [2 ((KA + Q_A K_{eq})/Q + 1)]$$

For impoundments which do not have diffused air systems, the air flow rate,  $Q_A$ , is zero. For this case, the air emission equation reduces to the following:

$$N = f_{air} Q Co = KA \left[ - (K_s (KA/Q + 1) + VK_{max} b_i / Q - Co) + ((K_s (KA/Q + 1) + VK_{max} b_i / Q - Co)^2 + 4 (KA/Q + 1) (K_s Co))^{0.5} \right] / [2 (KA/Q + 1)]$$

For flowthrough impoundments which contain no biomass, the biomass concentration ( $b_i$ ) equals zero and no biodegradation of pollutants occurs in the impoundment. For this case, the air emission equation reduces to the following:

$$N = f_{air} Q Co = [KA / (Q + KA)] Q Co$$

For flowthrough surface impoundments with an oil film layer, biodegradation is assumed to be negligible. As previously mentioned, to

simplify the emission model for an oil film layer the following was assumed: 1) infinite resistance between the water and oil phases; 2) thin oil film; and 3) mass transfer is controlled by the gas phase (i.e., the resistance in the liquid phase is infinite). Equilibrium exists initially between the water and oil phases (completely mixed system); however, the rate at which the compound diffuses into the oil phase approaches zero (the oil film layer model used in CHEMDAT7 assumes low resistance between the water and oil phases). The oil film layer mass balance and emission equation for flowthrough systems is presented in a memorandum to the file.<sup>4</sup> The emission model equation for flowthrough impoundments with an oil film is similar to that of a nonaerated, non-biological flowthrough system with all parameters referencing the oil phase:

$$N = fQ_{oil}Co_{oil} = [K_{oil}A/(K_{oil}A + Q_{oil})] (Q_{oil}Co_{oil})$$

where:

$K_{oil}$  = overall mass transfer coefficient in the oil phase, dimensionless

$Q_{oil}$  = flow rate of oil, m<sup>3</sup>/s

$Co_{oil}$  = initial concentration of constituent in oil phase, g/m<sup>3</sup>

and where  $Co_{oil}$  and  $Q_{oil}$  are approximated by:

$$Co_{oil} = CoKow/((1 - FO) + FO(Kow))$$

$$Q_{oil} = (FO)Kow$$

where:

$FO$  = fraction of impoundment volume as oil, dimensionless

$Kow$  = octanol water coefficient of constituent, dimensionless

As discussed in Section 4.1, individual liquid and gas phase mass transfer coefficients are used to estimate the overall mass transfer coefficient for each pollutant in the impoundment. Values for the individual mass transfer coefficients depend on whether or not the impoundment is aerated or nonaerated. Empirical correlations, available in the literature, can be used to estimate values for these individual coefficients. The correlations

used in the computer program for nonaerated impoundments and diffused air systems are presented in Table 4-3.<sup>5</sup> The oil film layer emission model also uses the quiescent individual gas phase mass transfer coefficient presented in Table 4-3 (MacKay and Matasugu).<sup>6</sup> The correlations presented in Table 4-3 relate the individual coefficients to the physical properties of the pollutants, the dimensions of the impoundment, and the ambient wind speed. The correlations used in the computer program for aerated impoundments are presented in Table 4-4.<sup>7</sup> These correlations relate the individual coefficients to the physical properties of the pollutants, the dimensions of the impoundment, and the characteristics of the aerators.

#### 4.2.2 Disposal Impoundments

Disposal impoundments are defined as units that receive wastewater for ultimate disposal rather than for storage or treatment. Generally, wastewater is not continuously fed to or discharged from these types of impoundments. Therefore, the assumption of an equilibrium bulk concentration, which is applicable for flowthrough impoundments, is no longer applicable for disposal impoundments; the concentration of volatile organics in a disposal impoundment decreases with time. The emission estimating procedure accounts for the decreasing liquid-phase concentration which is the driving force for air emissions. For a disposal impoundment that is filled with a batch of wastewater, the disappearance rate of a volatile pollutant due to air emissions, biodegradation, and air sparging can be expressed as:<sup>8</sup>

$$dC_t/C_t = (-K_{max}b_i/K_s - (K_A + Q_A K_{eq})/V) dt$$

where

$C_t$  = concentration in the impoundment at time =  $t$ ,  $g/m^3$

$t$  = time since disposal (residence time in the impoundment), sec

After integration from time = 0 to time =  $t$ , the above equation yields the following expression for the fraction of each pollutant emitted in the air:

$$f_{air} = \frac{\text{Mass of pollutant } i \text{ emitted to the air}}{\text{Total mass of pollutant } i}$$

$$(1 - C_t/C_o)(K_A + Q_A K_{eq}) / (K_A + Q_A K_{eq} + K_{max}b_i V / K_s)$$

where:

$$C_t/C_o = \exp [-(K_A + Q_A K_{eq})t/V - K_{max}b_i t/K_s]$$

TABLE 4-3. EQUATIONS FOR CALCULATING INDIVIDUAL MASS TRANSFER COEFFICIENTS FOR VOLATILIZATION OF ORGANIC SOLUTES FROM QUIESCENT SURFACE IMPOUNDMENTS

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Liquid phase

Springer et al. (for all cases except  $F/D < 14$  and  $U_{10} > 3.25$  m/s):

$$k_l = 2.78 \times 10^{-6} [D_w/D_{\text{ether}}]^{2/3} \quad (0 < U_{10} < 3.25) \text{ (m/s)}$$

(All F/D ratios)

$$k_l = [2.605 \times 10^{-9} (F/D) + 1.277 \times 10^{-7}] U_{10}^2 [D_w/D_{\text{ether}}]^{2/3} \quad (U_{10} > 3.25) \text{ (m/s)}$$

( $14 < F/D < 51.2$ )

$$k_l = 2.611 \times 10^{-7} U_{10}^2 [D_w/D_{\text{ether}}]^{2/3} \quad (U_{10} > 3.25) \text{ (m/s)}$$

( $F/D > 51.2$ )

where:

$U_{10}$  = windspeed at 10 m above the liquid surface, m/s

$D_w$  = diffusivity of constituent in water,  $\text{cm}^2/\text{s}$

$D_{\text{ether}}$  = diffusivity of ether in water,  $\text{cm}^2/\text{s}$

$F/D$  = Fetch-to-depth ratio (fetch is the linear distance across the impoundment or effective diameter,  $d_e$ ).

MacKay and Yeun (for  $F/D < 14$  and  $U_{10} > 3.25$  m/s):

$$k_l = 1.0 \times 10^{-6} + 34.1 \times 10^{-4} U^* Sc_L^{-0.5} \quad (U^* > 0.3) \text{ (m/s)}$$

$$k_l = 1.0 \times 10^{-6} + 144 \times 10^{-4} U^{*2.2} Sc_L^{-0.5} \quad (U^* < 0.3) \text{ (m/s)}$$

where:

$$U^* = \text{friction velocity (m/s)} = 0.01 U_{10} (6.1 + 0.63 U_{10})^{0.5}$$

$U_{10}$  = windspeed at 10 m above the liquid surface, m/s

$$Sc_L = \text{Schmidt number on liquid side} = \frac{\mu_L}{\rho_L D_w}$$

$\mu_L$  = viscosity of water, g/cm-s

$\rho_L$  = density of water,  $\text{g/cm}^3$

$D_w$  = diffusivity of constituent in water,  $\text{cm}^2/\text{s}$ .

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TABLE 4-3. EQUATIONS FOR CALCULATING INDIVIDUAL MASS TRANSFER COEFFICIENTS FOR VOLATILIZATION OF ORGANIC SOLUTES FROM QUIESCENT SURFACE IMPOUNDMENTS (continued)

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Gas phase

MacKay and Matasugu (in Hwang):

$$k_g = 4.82 \times 10^{-3} U_{10}^{0.78} Sc_g^{-0.67} d_e^{-0.11} (\text{m/s})$$

where:

$U_{10}$  = windspeed at 10m above the liquid surface, m/s

$Sc_g$  = Schmidt number on gas side =  $\frac{\mu_a}{\rho_a D_a}$

$\mu_a$  = viscosity of air, g/cm-s

$\rho_a$  = density of air, g/cm<sup>3</sup>

$D_a$  = diffusivity of constituent in air, cm<sup>2</sup>/s

$d_e$  = effective diameter of impoundment =  $(4A/\pi)^{0.5}$ , m

$A$  = area of impoundment, m<sup>2</sup>.

---



TABLE 4-4. EQUATIONS FOR CALCULATING INDIVIDUAL MASS TRANSFER COEFFICIENTS FOR VOLATILIZATION OF ORGANIC SOLUTES FROM TURBULENT SURFACE IMPOUNDMENTS

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Liquid phase

Thibodeaux:  

$$k_l = [8.22 \times 10^{-9} J (\text{POWR}) (1.024)^{T-20} O_t 10^6 MW_L / (Va_v \rho_L)] (D_w / D_{O_2,w})^{0.5} \text{ (m/s)}$$

where:

- J = oxygen transfer rating of surface aerator, lb O<sub>2</sub>/h-hp
- POWR = total power to aerators, hp
- T = water temperature, °C
- O<sub>t</sub> = oxygen transfer correction factor, dimensionless
- MW<sub>L</sub> = molecular weight of liquid, g/gmole
- Va<sub>v</sub> = turbulent surface area, m<sup>2</sup>
- ρ<sub>L</sub> = density of liquid, g/cm<sup>3</sup>
- D<sub>w</sub> = diffusivity of constituent in water, cm<sup>2</sup>/s
- D<sub>O<sub>2</sub>,w</sub> = diffusivity of oxygen in water = 2.4 x 10<sup>-5</sup> cm<sup>2</sup>/s.

Gas phase

Reinhardt:

$$k_g = 1.35 \times 10^{-7} Re^{1.42} p^{0.4} Sc_G^{0.5} Fr^{-0.21} D_g MW_g / d \text{ (m/s)}$$

where:

- Re = d<sup>2</sup>wρ<sub>g</sub>/μ<sub>g</sub> = Reynold's number
  - d = impeller diameter, cm
  - w = rotational speed of impeller, rad/s
-

TABLE 4-4. EQUATIONS FOR CALCULATING INDIVIDUAL MASS TRANSFER  
COEFFICIENTS FOR VOLATILIZATION OF ORGANIC SOLUTES FROM  
TURBULENT SURFACE IMPOUNDMENTS (Continued)

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$\rho_a$	= density of air, g/cm <sup>3</sup>
$\mu_a$	= viscosity of air, g/cm-s
	= $4.568 \times 10^{-7} T(^{\circ}\text{C}) + 1.7209 \times 10^{-4}$
$p$	= $P_i g_c / (\rho_L d^{*5} w^3)$ = power number
$P_i$	= power to impeller, ft-lb <sub>f</sub> /s
	= 0.85 (POWER) (550 ft-lb <sub>f</sub> /s-hp)/number of aerators ( $N_a$ ), where 0.85 = efficiency of aerator motor
$g_c$	= gravitation constant, 32.17 lb <sub>m</sub> -ft/s <sup>2</sup> /lb <sub>f</sub>
$\rho_L$	= density of liquid, lb/ft <sup>3</sup>
$d^*$	= impeller diameter, ft
$Sc_g$	= Schmidt number on gas side = $\mu_a / (\rho_a D_a)$
$Fr$	= $d^* w^2 / g_c$ = Froude number
$D_a$	= diffusivity of constituent in air, cm <sup>2</sup> /s
$MW_a$	= molecular weight of air.

---

Therefore, the average emission rate for each pollutant over the period of time = t is:

$$N = f_{air} VCo/t = (1 - \exp [-(Q_A K_{eq} + KA)t/V - K_{max} b_i t/K_s]) * (KA + Q_A K_{eq}) / (KA + Q_A K_{eq} + K_{max} b_i V/K_s) VCo/t$$

For disposal impoundments which do not have diffused air systems, the air flow rate is zero. For this case, the air emission equation reduces to:

$$N = f_{air} VCo/t = (1 - \exp [-KAt/V - K_{max} b_i t/K_s]) * KA / (KA + K_{max} b_i V/K_s) VCo/t$$

For disposal impoundments which contain no biomass, the biomass concentration ( $b_i$ ) equals zero and no biodegradation of pollutants occurs in the impoundment. For this case, the fraction emitted from the impoundment reduces to:

$$f_{air} = (1 - Ct/Co)$$

where:

$$Ct/Co = \frac{\text{Concentration of pollutant } i \text{ at time } t}{\text{Initial concentration of pollutant } i} = \exp [-KAt/V]$$

And, the average emission rate for each pollutant over the period of time = t is:

$$N = f_{air} VCo/t = \exp [-KAt/V] VCo/t$$

For disposal impoundments with an oil film layer, biodegradation is assumed to be negligible, the oil film is thin, and gas phase resistance is controlling. To calculate air emissions, the emission model equation for disposal impoundments is similar to that of a nonaerated, non-biological disposal impoundment with all parameters referencing the oil phase (The oil film layer mass balance and emission equation for disposal systems is presented in a memorandum to the file<sup>4</sup>:

$$N = f_{air} VCo_{oil}/t = (1 - \exp [-K_{oil} t/D_{oil}]) V_{oil} Co_{oil}/t$$

where:

$$K_{oil} = \text{overall mass transfer coefficient in the oil phase, dimensionless}$$

$Q_{oil}$  = flow rate of oil,  $m^3/s$   
 $Co_{oil}$  = initial concentration of constituent in oil phase,  $g/m^3$   
 $V_{oil}$  = volume of oil in impoundment,  $m^3$   
 and where  $K_{oil}$ ,  $Co_{oil}$ ,  $Q_{oil}$ , and  $V_{oil}$  are approximated by:

$$\begin{aligned}
 K_{oil} &= K_g K_{eq}^{oil} \\
 Co_{oil} &= CoKow / ((1 - FO) + FO(Kow)) \\
 Q_{oil} &= (FO)Kow \\
 V_{oil} &= (FO)V
 \end{aligned}$$

where:

$FO$  = fraction of impoundment volume as oil, dimensionless  
 $Kow$  = octanol water coefficient of constituent, dimensionless  
 $K_g$  = individual mass transfer coefficient in the gas phase,  $m/s$   
 $K_{eq}^{oil}$  = equilibrium mass transfer coefficient in the oil phase, dimensionless

Values for the overall mass transfer coefficients ( $K$  and  $K_{oil}$ ) in the above expressions are estimated by the same technique used to estimate overall coefficients for flowthrough impoundments. The individual liquid and gas phase mass transfer coefficients are based on the same correlations presented for flowthrough impoundments in Table 4-3 and Table 4-4. Therefore, values for the overall mass transfer coefficients in disposal impoundments depend only on whether the impoundment is aerated, air sparged, nonaerated, or whether the impoundment has an oil film layer.

#### 4.2.3 Collection System Components

Collection system component emission models for junction boxes, lift stations, and sumps, are the same as emission models for flowthrough surface impoundments. As mentioned in Chapter 3, emissions models for drains, manholes, and trenches are not presented in this document. See Reference 2 for more information on these types of collection system components. Weirs, however, are based on volatilization-reaeration theory.

Junction boxes and lift stations are modeled with turbulent liquid phase mass transfer correlations and quiescent gas phase mass transfer correlations (see Sections 3.1 and 3.2 for a description of these components). Table 4-3 presents mass transfer correlations for quiescent systems, and Table 4-4 presents mass transfer correlations for turbulent systems. The liquid phase mass transfer correlation assumes at least one surface aerator is present.

Although no aerator is present in reality, it can be assumed that the splashing made from incoming flow is similar to the splashing pattern made by a surface aerator.

Sumps are modeled using mass transfer correlations for quiescent impoundments (see Table 4-3). Section 3.3 presents a description of flow and emission patterns for sumps.

The emission model for weirs is based on volatilization-reaeration theory. This approach is based on reaeration studies.<sup>9</sup> The theory states that for estimating volatilization, a correlation is needed only for diffusivities for oxygen and the constituent in water.

The method has been demonstrated in particular for chemicals with high volatility, high molecular weight, and low solubility. Table 4-5 presents the mass transfer correlations used for weirs.

TABLE 4-5. EQUATIONS FOR CALCULATING INDIVIDUAL MASS TRANSFER COEFFICIENTS  
FOR VOLATILIZATION OF ORGANIC SOLUTES FROM WEIRS

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Volatilization - Reaeration Theory

$$K_D = K_D(O_2)[D_w/D_{O_2,w}]^{0.75}$$

where:

$$K_D(O_2) = 0.16h$$

$D_w$  = diffusivity of constituent in water,  $\text{cm}^2/\text{s}$

$D_{O_2,w}$  = diffusivity of oxygen in water,  $\text{cm}^2/\text{s}$

$h$  = height of the weir (distance from the wastewater overflow  
to the receiving body of water), ft

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### 4.3 REFERENCES

1. Office of Air Quality, Planning and Standards. U.S. Environmental Protection Agency. Hazardous Waste Treatment, Storage, and Disposal Facilities (TSDF) - Air Emission Models. EPA - 450/3-87-026. February 1989.
2. Industrial Wastewater Volatile Organic Compound Emissions -- Background Information for BACT/LAER Determinations. REVISED DRAFT. U.S. Environmental Protection Agency, Control Technology Center, Research Triangle Park, North Carolina, January 1990.
3. Reference 1. p. 4-26.
4. Memorandum to file. "Documentation of the Oil Film Layer Emission Model used in the SIMS Program." From Craig Berry, Radian Corporation, to David Misenheimer, U. S. Environmental Protection Agency. September 28, 1990.
5. Reference 1. p. 4-6 through 4-7.
6. Reference 1. p. 4-57 through 4-59.
7. Reference 1. p. 4-34 through 4-35.
8. Reference 1. p. 4-45 and 4-57 through 4-59.
9. Lyman, W. J., W. F. Reehl, and D. H. Rosenblatt. Handbook of Chemical Property Estimation Methods. McGraw-Hill Book Company, New York, New York, 1982.

## 5.0 DEFAULT PARAMETER DEVELOPMENT

In some cases, State and local air pollution control agencies may not have information available for some of the inputs required by the air emission models. However, State and local agencies should know at a minimum, the total flow to the impoundment, the industries which generate the influent, whether the impoundment is aerated, nonaerated, diffused air, or has an oil film layer, and the impoundment surface area.

Default values were developed during EPA's evaluation of TSDf for many of the required inputs. However, default values were not developed for: (1) the concentration profile in the wastewater feed to the impoundment, (2) the depth of the impoundment, and (3) certain physical property data. The purpose of this chapter is to discuss the methods and the data used to develop default values for these parameters. Default parameters developed during the evaluation of TSDf and industrial wastewater VOC emissions for the other inputs required by the emission models are also covered in the chapter.

It is important to realize that the accuracy of the emissions estimate decreases with the use of defaults and these values should only be used if no data are available.

### 5.1 CONCENTRATION PROFILES

As previously discussed, the emission models require inputs for the concentrations of each pollutant constituent in the feed to the surface impoundment. These concentration data may not be available to State and local agencies. For this reason, methods were developed to assign default concentration values based on the minimum information expected to be available in all cases. However, concentration defaults should not be used for estimating individual toxic emissions.

The first step was to develop raw concentration profiles for each industrial category. These profiles will be used to define the composition of the impoundment feed based on the industrial categories discharging to the impoundment. The development of the raw concentration profiles is discussed in Section 5.1.1.

In cases where wastewater from process units in more than one type of industrial category flow into the collection system component or impoundment,



a flow weighting scheme is required to use the raw concentration profiles developed for each industry. This flow weighting scheme is presented in Section 5.1.2. If the collection system component or impoundment is located at a publicly owned treatment works (POTW), it is also necessary to know what percentage of the feed to the impoundment is from industrial (rather than municipal) sources. The development of this factor is discussed in Section 5.1.3.

There are several terms which are important to the following discussion. These are defined as follows.

**Direct Discharge** - Industrial facilities which collect wastewater, treat it on-site, and discharge the treated water to a receiving stream are called direct dischargers. Their effluent flows are termed direct discharges.

**Indirect Discharge** - Some industrial facilities collect wastewater and send it to a POTW. The POTW then treats this wastewater along with any wastewater it receives and discharges the water to a receiving stream. In this case, the industrial facility is called an indirect discharger.

**Raw Concentration** - Raw concentration refers to the concentration of pollutants prior to any treatment. For a direct discharge, raw concentration is the concentration prior to the facilities on-site treatment facility.

**Current Concentration** - Current concentration refers to the concentration of pollutants after pretreatment. For an indirect discharge, current concentration is the concentration in the effluent sent to the POTW.

#### 5.1.1 Industrial Category Raw Concentrations

The raw concentration profiles for each of the industrial categories covered by this study were calculated directly from the Domestic Sewage Study (DSS)<sup>1</sup> data by dividing pollutant loadings (mass per unit time) by total indirect wastewater flows (volume per unit time). The DSS covers only indirect discharges.

It was assumed, however, that the raw concentrations for indirect discharges are approximately the same as direct discharges from these industrial categories. That is, the raw pollutant concentrations in process wastewater in each of these categories are not affected by whether wastewater treatment is conducted on-site or off-site. It is not expected that the types of processes used by facilities in the same industry are strongly affected by

whether the facility indirectly or directly discharges wastewater. For this reason, the average raw concentrations for indirect and direct dischargers should be reasonably similar.

Table 5-1 is a list of the 29 industrial categories and the industrial category code assigned to each category in the DSS. These industrial categories constitute the larger generators of hazardous wastes. Each of the industrial categories in Table 5-1 encompasses multiple Standard Industrial Classification (SIC) codes grouped together for the purposes of the DSS. A list of the SIC codes grouped in each of the industrial categories presented in Table 5-1 is shown in Appendix A.

The pollutant loadings used to develop default raw concentrations were obtained from Appendix G of the DSS.<sup>1</sup> Table 5-2 lists the 48 organic pollutants covered by the DSS. The pollutants are classified as priority pollutants (P), and/or volatile pollutants (V), and/or ignitable or reactive (I/R) pollutants. The indirect wastewater flow rates presented in the DSS for each industrial category are shown in Table 5-3. The primary data sources for the pollutant loadings and indirect wastewater flow rates presented in the DSS are OWRS, Industrial Technology Division (ITD) Development Documents, DSS Industry Profile Forms (updated data from the development documents), and the Industrial Studies Data Base (ISDB) developed by the Office of Solid Waste (OSW).

The ITD data bases were developed based on Section 308 surveys and sampling data gathered under the Clean Water Act (CWA). The ISDB was based on information gathered from Section 3007 surveys under authority of the Resource Conservation and Recovery Act (RCRA). In the DSS, data on loadings for four organic chemical industries were presented in both the ITD and the ISDB data bases. Loadings are available for more pollutants in the ISDB. Therefore, this data base was used in developing the default concentration profiles for these four industries. All other industrial categories contain data gathered only from the ITD development documents or an updated version in the DSS Industry Profile Forms.

#### 5.1.2 Flow Weighting of Concentration Profiles

At some facilities, wastewater generated by processes in more than one industrial category may feed an impoundment or collection system component. If the flows from each industrial category are known, then the average

TABLE 5-1. INDUSTRIAL CATEGORIES

Industrial Category <sup>a</sup>	Industrial Category Code
Adhesives and Sealants	1
Battery Manufacturing	2
Coal, Oil, Petroleum Products, and Refining	3
Dye Manufacturing and Formulation	4
Electrical and Electronic Components	5
Electroplating and Metal Finishing	6
Equipment Manufacturing and Assembly	7
Explosives Manufacturing	8
Gum and Wood Chemicals, and Related Oils	9
Industrial and Commercial Laundries	10
Ink Manufacturing and Formulation	11
Inorganic Chemicals Manufacturing	12
Iron and Steel Manufacturing and Forming	13
Leather Tanning and Finishing	14
Nonferrous Metals Forming	15
Nonferrous Metals Manufacturing	16
Organic Chemicals Manufacturing	17
Paint Manufacture and Formulation	18
Pesticides Manufacturing	19
Pharmaceuticals Manufacturing	20
Photographic Chemicals and Film Manufacturing	21
Plastics Molding and Forming	22
Plastics, Resins, and Synthetic Fibers Manufacturing	23
Porcelain Enameling	24
Printing and Publishing	25
Pulp and Paper Mills	26
Rubber Manufacturing and Processing	27
Textile Mills	28
Timber Products Processing	29

<sup>a</sup>Pesticides Formulation has been omitted from the original list of 30 industry categories because of the lack of data available for this industrial category.

TABLE 5-2. DSS SELECTED CONSENT DECREE POLLUTANTS

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Acrolein - P, I/R, V	Diethyl Phthalate - P
Benzene - P, I/R, V	2,4-Dimethyl Phenol - P
Bis-(2-Chloroethyl) Ether - P, I/R, V	Dimethyl Phthalate - P
Bis-(2-Ethyl Hexyl) Phthalate - P	Di-N-Octyl Phthalate - P
Bromomethane - P, V	Ethyl Benzene - P, I/R, V
Butyl Benzyl phthalate - P	Hexachloro-1,3-Butadiene - P
Carbon Tetrachloride - P, V	Hexachloroethane - P
Chlorobenzene - P, I/R	Methylene Chloride - P, V
p-Chloro-m-Cresol - P	Naphthalene - P
Chloroethane - P, I/R, V	Nitrobenzene - P
Chloroform - P, V	PCB (Polychlorinated biphenyls) - P
Chloromethane - P, I/R, V	Pentachlorophenol - P
2-Chloronaphthalene - P	Phenol - P
Di-N-Butyl Phthalate - P	1,1,2,2-Tetrachloroethane - P, V
1,2-Dichlorobenzene - P	Tetrachloroethylene - P, V
1,3-Dichlorobenzene - P	Toluene - P, I/R, V
1,4-Dichlorobenzene - P	Bromoform - P
1,1-Dichloroethane - P, I/R, V	1,2,4-Trichlorobenzene - P
1,2-Dichloroethane - P, I/R, V	1,1,1-Trichloroethane - P, V
1,1-Dichloroethylene - P, I/R, V	1,1,2-Trichloroethane - P, V

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TABLE 5-2. DSS SELECTED CONSENT DECREE POLLUTANTS (continued)

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Trans-1,2-Dichloroethylene - P, I/R, V	Trichloroethylene - P, V
2,4-Dichlorophenol - P	Trichlorofluoromethane - V
1,2-Dichloropropane - P, I/R, V	2,4,6-Trichlorophenol - P
Dichlorodifluoromethane - V	Vinyl Chloride - P, I/R, V

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P = CWA priority pollutant  
 I/R = Ignitable or reactive compound  
 V = Volatile compound

TABLE 5-3. TOTAL INDIRECT FLOW RATES BY INDUSTRIAL CATEGORY

Industrial Category	Total Indirect <sup>c</sup> Discharge Flow (MGD)
Adhesives and Sealants	2.7
Battery Manufacturing	7.9
Coal, Oil, Petroleum Products, and Refining	92.3
Dye Manufacturing and Formulation	11.3
Electrical and Electronic Components	33.5
Electroplating and Metal Finishing	575.7
Equipment Manufacturing and Assembly <sup>a</sup>	4,507.0
Explosives Manufacturing	1.0
Gum and Wood Chemicals, and Related Oils	3.5
Industrial and Commercial Laundries	526
Ink Manufacturing and Formulation	1.0
Inorganic Chemicals Manufacturing	18.5
Iron and Steel Manufacturing and Forming	430.7
Leather Tanning and Finishing	6.4
Nonferrous Metals Forming	36.0
Nonferrous Metals Manufacturing <sup>b</sup>	61.4
Organic Chemicals Manufacturing	65.9
Paint Manufacture and Formulation	0.8
Pesticides Manufacturing	4.3
Pharmaceuticals Manufacturing	48.0

TABLE 5-3. TOTAL INDIRECT FLOW RATES BY INDUSTRIAL CATEGORY (continued)

Industrial Category	Total Indirect <sup>c</sup> Discharge Flow (MGD)
Photographic Chemicals and Film Manufacturing	1.6
Plastics Molding and Forming	18.4
Plastics, Resins, and Synthetic Fibers Manufacturing	21.2
Porcelain Enameling	5.6
Printing and Publishing	46.4
Pulp and Paper Mills	1,029.3
Rubber Manufacturing and Processing	128.2
Textile Mills	339.2
Timber Products Processing	1.0

<sup>a</sup>Calculated from data found in Radian Memorandum, October 22, 1986; Subject: Estimate of Solvent Dischargers to POTW from the Electroplating and Metal Finishing and Equipment Manufacturing and Assembly Industrial Categories, p. 4 and 10.

<sup>b</sup>Calculated from Reference 2.

<sup>c</sup>Represents flow discharged from the industrial category to the POTW.

concentration can be calculated from the raw concentration profiles for each category and the flows for each category. If only the categories of the industrial dischargers are known then it is necessary to develop a default flow weighted concentration profile for the total flow stream.

To flow weight the raw concentration profiles developed for each industry, total flow rates (indirect plus direct) for each industry were used. Total industrial flow rates listed by SIC code are available in the 1982 Census of Manufacturers' (COM) subject series "Water Use in Manufacturing".<sup>2</sup> Flow rate data gathered from this source are summarized in Table 5-4 which lists the industrial categories, industrial category codes, total number of indirect plus direct industrial dischargers, and total industrial flow rates.

Total flow rates for Adhesives and Sealants, Battery Manufacturing, Explosives Manufacturing, Industrial and Commercial Laundries, Ink Manufacturing and Formulation, Leather Tanning and Finishing, and Printing and Publishing are not available in the COM. For these industries, total indirect flow rates from the DSS were divided by the total number of indirect dischargers to get an average flow rate per facility for these industrial categories. With this average flow rate per facility, a total industrial flow rate (by industrial category code) was obtained by multiplying this average flow per facility by the total number of facilities in that industry (direct plus indirect dischargers).

The following equation is used to determine the flow-weighted concentration of each pollutant in the feed:

$$C_{i,FV} = \frac{\text{sum of concentration of pollutant } i \text{ multiplied by the flow rate of industrial category code } j}{\text{sum of flow rate from industrial category code } j}$$

$$= (C_{i,1}F_1 + C_{i,2}F_2 + \dots + C_{i,n}F_n) / \sum_{i=1}^n F_i$$

where:

$C_{i,FV}$  = flow-weighted concentration of pollutant  $i$

$C_{i,1}$  = concentration of pollutant  $i$  in the first industrial category code

$C_{i,n}$  = Concentration of pollutant  $i$  in the  $n$ th industrial category code



TABLE 5-4. WATER DISCHARGE STATISTICS<sup>1</sup>

Industrial Category	Assigned Industrial Category Code	Total No. Dischargers (Direct and Indirect)	Total Flow <sup>a</sup> Discharged (MGD)
Adhesives and Sealants <sup>b</sup>	1	307	2.8
Battery Manufacturing <sup>b</sup>	2	170	9.0
Coal, Oil, Petroleum Products and Refining	3	236	692.4
Dye Manufacturing and Formulation	4	75	30.9
Electrical and Electronic Components	5	208	26.5
Electroplating and Metal Finishing	6	872	68.8
Equipment Manufacturing and Assembly	7	105,772	5,763.0
Explosives Manufacturing <sup>b</sup>	8	28	7.0
Gum and Wood Chemicals, and Related Oils	9	10	6.5
Industrial and Commercial Laundries <sup>b</sup>	10	68,800	528.0
Ink Manufacturing and Formulation <sup>b</sup>	11	460	2.1
Inorganic Chemicals Manufacturing	12	301	743.4
Iron and Steel Manufacturing and Forming	13	259	1,867.1
Leather Tanning and Finishing <sup>b</sup>	14	158	7.2
Nonferrous Metals Forming	15	201	76.1
Nonferrous Metals Manufacturing .	16	162	117.4
Organic Chemicals Manufacturing	17	211	343.5
Paint Manufacture and Formulation	18	41	2.1

TABLE 5-4. WATER DISCHARGE STATISTICS (continued)<sup>1</sup>

Industrial Category	Assigned Industrial Category Code	Total No. Dischargers (Direct and Indirect)	Total Flow <sup>a</sup> Discharged (MGD)
Pesticides Manufacturing	19	18	15.3
Pharmaceuticals Manufacturing	20	112	87.1
Photographic Chemicals and Film Manufacturing	21	25	15.7
Plastics Molding and Forming	22	219	33.6
Plastics, Resins, and Synthetic Fibers Manufacturing	23	184	331.3
Porcelain Enameling	24	91	10.8
Printing and Publishing <sup>b</sup>	25	38,763	46.5
Pulp and Paper Mills	26	600	1,760.2
Rubber Manufacturing and Processing	27	175	87.4
Textile Mills	28	620	103.7
Timber Products Processing	29	223	68.8

<sup>a</sup>Zero dischargers, or dischargers to the ground (well, spray, seepage) were not included.

<sup>b</sup>Calculation from Domestic Sewage Study (DSS).

- $F_1$  = relative flow rate of wastewater from the first industrial category code
- $F_n$  = relative flow rate of wastewater from the nth industrial category code

The relative flow rates ( $F_n$ ) used in the equation are the total wastewater flow rates obtained for each industry from the COM. The concentration variables used in the equation ( $C_{i,n}$ ) are obtained from the raw concentration profiles developed for each industrial category.

### 5.1.3 Surface Impoundments and Collection System Components at POTW

At POTW, the total flow to the collection system component or surface impoundment consists of both municipal and industrial wastewater. For this reason, the concentration of pollutants in the industrial wastewater will be diluted by the municipal flow. (SIMS assumes that municipal wastewater does not contain volatile organics. If this is not the case, a pollutant concentration profile for the municipal wastewater must be generated). Therefore, it was necessary to develop a default value for the percentage of industrial flow in wastewater to POTW. This value is used by the program to adjust the raw industrial concentrations to account for the municipal flow to the impoundment.

The contribution of municipal and industrial flow rates to the total feed for approximately 1,600 POTW are listed in the 1984 NEEDS data base.<sup>3</sup> Based on this source, industrial flow rates were found to compose 19.5 percent of the total flow rates to POTW on a national basis. This factor will be used to normalize the raw concentration profiles in cases where the impoundment or collection system component is located at a POTW. That is, if the total, but not the industrial flow to the impoundment or collection system component is known, the raw concentrations developed for each industrial category will be multiplied by 0.195 to account for the dilution by non-industrial wastewater sources.

## 5.2 DEPTH OF IMPOUNDMENT AND COLLECTION SYSTEM COMPONENT

Depth of the impoundment or collection system component is also needed as an input parameter for the emission models. A correlation for impoundments was developed for the default depth from data in Metcalf and Eddy's Wastewater Engineering.<sup>4</sup> Several approaches were evaluated. Plots of (1) retention time

versus depth, (2) depth versus the ratio of flow rate to surface area, and finally (3) flow rate versus depth were generated. Data were used for four types of treatment processes to generate the plots. Table 5-5 lists these processes and their applications. Table 5-6 lists the respective ranges for surface area, retention time, depth, and flow rate for each process. Each plot was generated by matching the minimum and maximum values in each range for each parameter and each process. That is, to generate the plot of flow rate versus depth, the minimum value of the depth parameter in each process was plotted versus the minimum value for flow rate in each process. The maximum value of the depth parameter in each process was plotted versus the maximum value for flow rate in each process.

The plot of flow rate versus depth was found to provide the best correlation, giving a linear relationship between flow rate and depth. The four processes were broken into two groups, flowthrough and non-flowthrough (or disposal) impoundments, because of the great differences in data ranges. Anaerobic processes have such long retention times that they can be considered as non-flowthrough, or disposal impoundments. The other three processes are flowthrough. Figure 5-1 shows the plot of flow rate,  $Q$ , versus depth,  $D$ , for flowthrough and disposal impoundments. Given a specific flow rate, a default depth can be determined by the following linear equations.

Flowthrough	$Q = 4673.30D - 3809.5$	$Q \geq 1446 \text{ m}^3/\text{day}$
	$Q = 863.8D$	$0 < Q < 1446 \text{ m}^3/\text{day}$
Disposal	$Q = 354.60D - 700$	$Q \geq 253 \text{ m}^3/\text{day}$
	$Q = 101.2D$	$0 < Q < 253 \text{ m}^3/\text{day}$

In order to insure that the calculated default depth produces a reasonable retention time for flowthrough impoundments, limits were placed on retention times. Table 5-7 presents the flowthrough impoundment retention times. These limits are used by the program to calculate minimum and maximum depths based on the input flow and surface area. The default depth is compared to the minimum and maximum depths. If the default depth does not fall between the minimum and maximum depth values, then the default depth is set equal to the minimum or maximum depth (whichever is closer). If the user

TABLE 5-5. SURFACE IMPOUNDMENTS

Type	Common	Application
Aerobic	Maturation or tertiary pond	Used for polishing effluents from conventional secondary treatment processes such as trickling filter or activated sludge.
Aerobic - Anaerobic (oxygen source: algae)	Facultative pond	Treatment of untreated, screened or primary settled wastewater and industrial wastes.
Aerobic - Anaerobic (oxygen source: surface aerators)	Facultative pond with mechanical aeration	Treatment of untreated screened or primary settled wastewater and industrial wastes.
Anaerobic	Anaerobic lagoon (pond), anaerobic pretreatment ponds	Treatment of domestic and industrial wastes.

TABLE 5-6. TYPICAL DESIGN PARAMETERS FOR SURFACE IMPOUNDMENTS

Type	Surface Area (A) (m <sup>2</sup> )	T (day)	Depth (m)	Flow Rate(Q) <sup>a</sup> (m <sup>3</sup> /day)
Aerobic	10120 - 40470	5 - 20	1 - 1.5	2024 - 3035
Aerobic/ Anaerobic (Oxygen Source: Algae)	10120 - 40470	7 - 30	1 - 2	1446 - 2698
Aerobic/ Anaerobic (Oxygen Source: Aerators)	10120 - 40470	3 - 10	2 - 6	6747 - 24282
Anaerobic	2020 - 10120	20 - 50	2.5 - 5	253 - 1012

<sup>a</sup>Flow rate calculated by using available ranges.  $Q = V/T = AD/T$

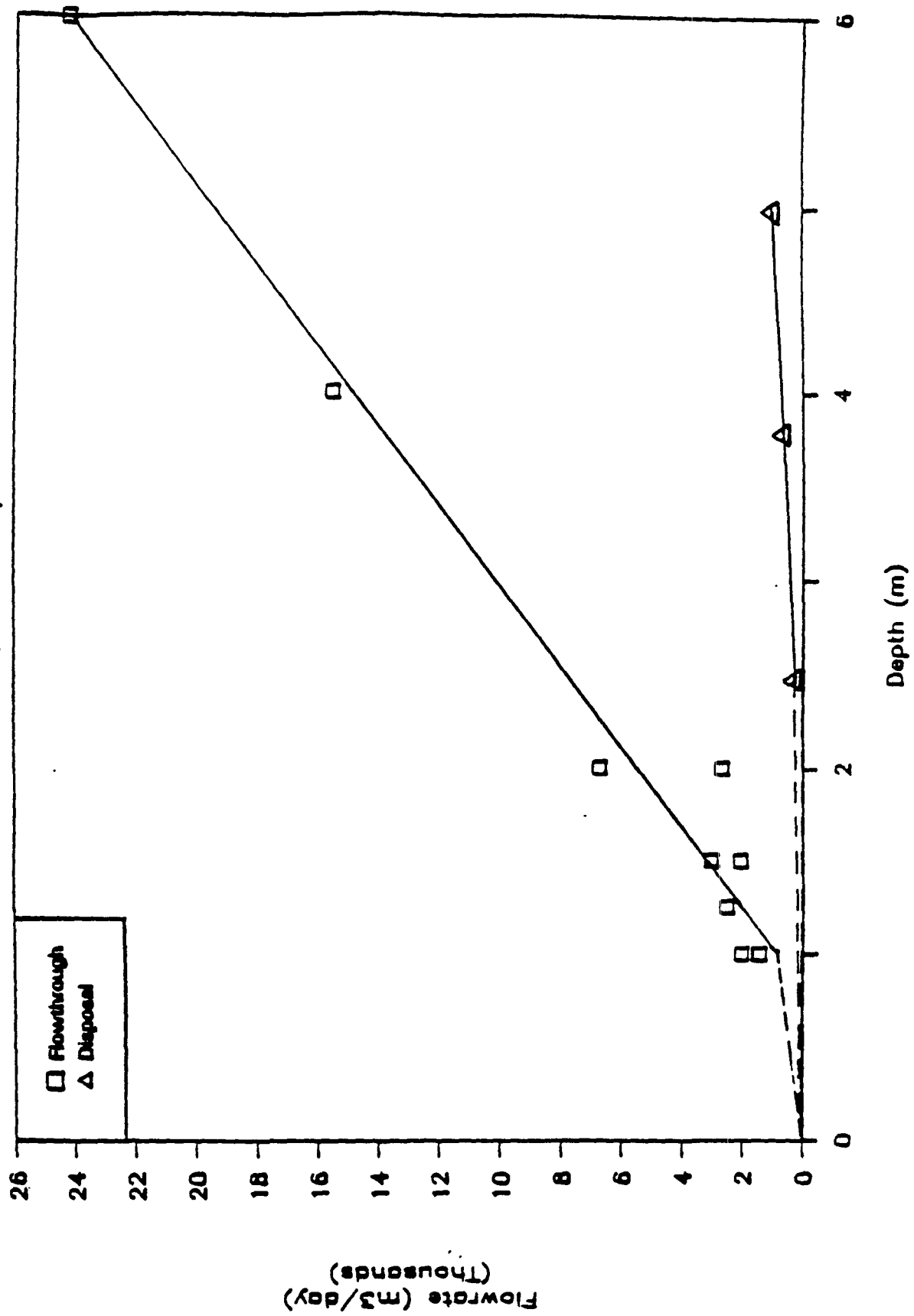


Figure 5-1. Flow Rate Versus Depth

TABLE 5-7. LIMITS ON FLOWTHROUGH IMPOUNDMENT RETENTION TIME

Impoundment Type	Retention Time Limits	
	Minimum	Maximum
Quiescent	10 days	30 days
Aerated	5 days	10 days
Activated Sludge	5 hours	10 hours
Diffused Air	1 hour	3 hours <sup>a</sup>
Oil Film Layer <sup>b</sup>	10 days	30 days <sup>a</sup>

<sup>a</sup>Reference 5.

<sup>b</sup>Retention times for oil film layer systems were assumed to be the same as for quiescent impoundments.



manually inputs a depth which falls outside the minimum and maximum values  $\pm 10$  percent, the program will use the manually input depth but will flag the input for the user.

The above correlations should only be used if no information is available to estimate the actual depth of the impoundment on-site. Most of the information used to develop these correlations was taken from data for impoundments such as lagoons, ponds or large biodegradation units where depth is variable and difficult to measure accurately. Therefore, if a facility can measure the depth or has a smaller impoundment or an impoundment which has a fairly constant depth, actual depth measurements should be used over the default.

Default depths used by SIMs for junction boxes, lift stations, and sumps are presented in Table 5-8.<sup>6</sup> In addition, the default weir height is also presented.<sup>6</sup> Table 5-8 also presents a range of depth and height for the above collection system components. Defaults should only be used if actual data is unavailable.

### 5.3 OTHER INPUT PARAMETERS REQUIRED BY THE EMISSION MODELS

Section 5.1 and 5.2 discussed the development of concentration and depth defaults required for use in the models. The purpose of this section is to provide information on the default values developed during the TSDF project for the other input parameters required by the model.

The types of other default parameters fall into two categories: 1) pollutant-specific parameters, and 2) site-specific parameters. The pollutant-specific default parameters are contained in Appendix C. These parameters include physical properties (i.e., diffusivities, vapor pressures) which are specific to a particular pollutant. Site-specific parameters and defaults for these parameters are provided in Table 5-9.

TABLE 5-8. COLLECTION SYSTEM DEFAULT DEPTH AND HEIGHT (WEIRS)<sup>6</sup>

Collection System Component	Defaults <sup>a</sup>		
	Depth (m)	Height (m)	Range (m)
Junction Box	0.9	---	0.6-1.2
Lift Station	1.5	---	1.2-1.8
Sump	1.5	---	NA
Weir	---	1.8	0.9-2.7

<sup>a</sup>Taken as the average of the dataset.

NA = Not Available

TABLE 5-9. SITE-SPECIFIC DEFAULT PARAMETERS<sup>6,7</sup>

Default Parameter	Definition	Default Value
<u>General</u>		
T	Temperature of water	25°C
U <sub>10</sub>	Windspeed	4.47 m/s
<u>Biotreatment Systems</u>		
b <sub>f</sub>	Biomass concentration (for biologically active systems)	
	Quiescent treatment systems	0.05 g/l
	Aerated treatment systems	0.30 g/l
	Activated sludge units	4.0 g/l
POWR	Total power to aerators (for aerated treatment systems) (for activated sludge)	0.75 hp/1000 ft <sup>3</sup> 2 hp/1000 ft <sup>3</sup>
W	Rotational speed of impeller (for aerated treatment systems)	126 rad/s (1200 rpm)
d(d*)	Impeller diameter (for aerated treatment systems)	61 cm (2 ft)
Va <sub>v</sub>	Turbulent surface area (for aerated treatment systems) (for activated sludge)	0.24 (A) m <sup>2</sup> 0.52 (A) m <sup>2</sup>
J	Oxygen transfer rating to surface aerator (for aerated treatment systems)	3 lb oxygen/hp-hr
O <sub>t</sub>	Oxygen transfer correction factor (for aerated treatment systems)	0.83
<u>Diffused Air Systems</u>		
Q <sub>A</sub>	Diffused air volumetric flow rate	0.0004 (V) m <sup>3</sup> /s

TABLE 5-9. SITE-SPECIFIC DEFAULT PARAMETERS (continued)<sup>6,7</sup>

Default Parameter	Definition	Default Value
<u>Oil Film Layers</u>		
MW <sub>oil</sub>	Molecular weight of oil	282 g/gmol
D <sub>oil</sub>	Depth of oil layer	0.001 (V/A) m
V <sub>oil</sub>	Volume of oil	0.001 (V) m <sup>3</sup>
Q <sub>oil</sub>	Volumetric flow rate of oil	0.001 (Q) m <sup>3</sup> /s
ρ <sub>oil</sub>	Density of oil	0.92 g/cm <sup>3</sup>
F <sub>O</sub>	Fraction of volume which is oil	0.001 <sup>a</sup>
<u>Junction Boxes</u>		
V <sub>aV</sub>	Turbulent surface area	1.0 (A) m <sup>2</sup>
<u>Lift Station</u>		
V <sub>aV</sub>	Turbulent surface area	1.0 (A) m <sup>2</sup>

<sup>a</sup>Reference 8.

## 5.4 REFERENCES

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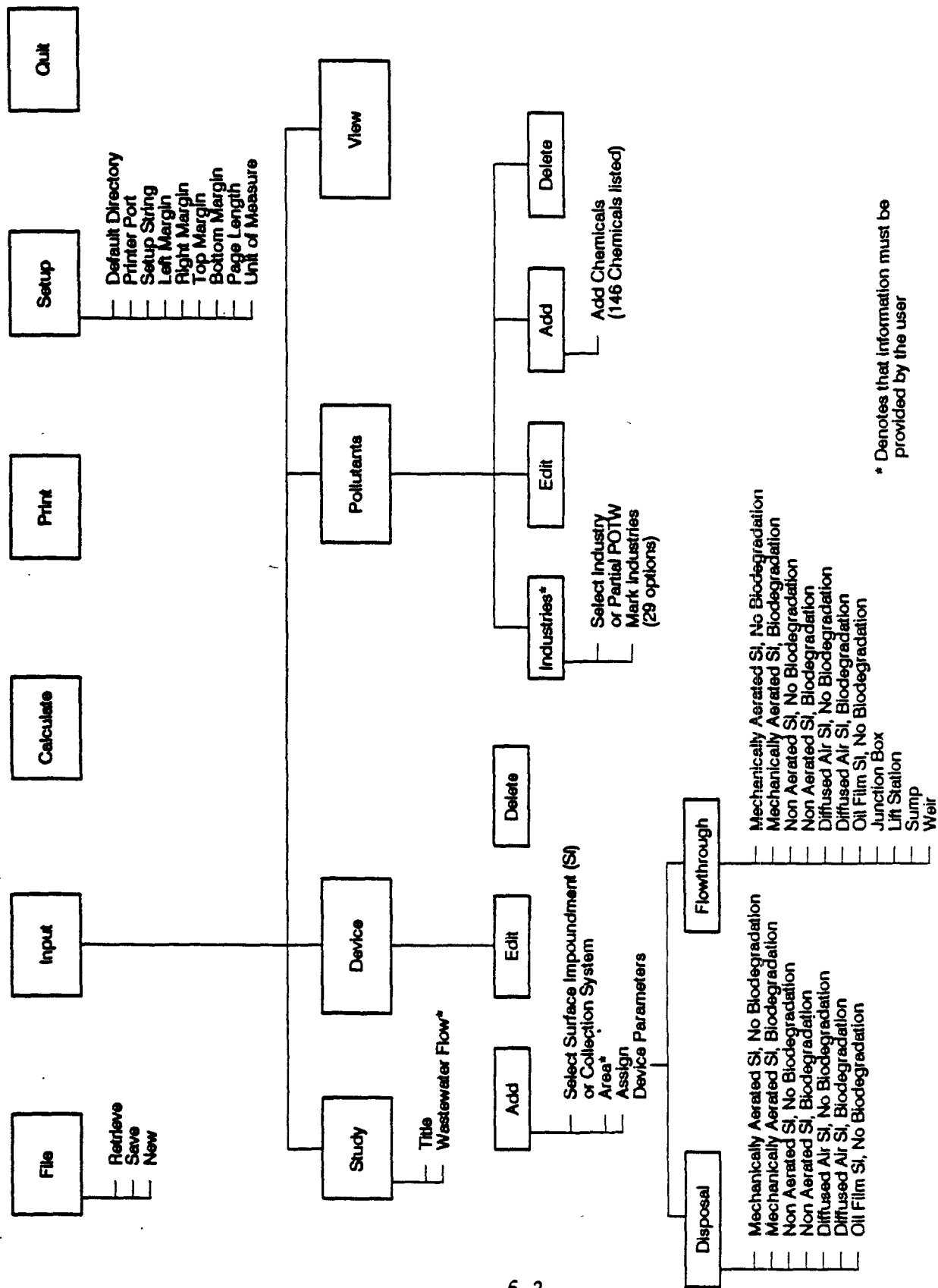
## 6.0 EMISSION ESTIMATION PROCEDURE

This section discusses the emissions estimation procedure used by the computer program. The equations used were previously discussed in Section 4.0, and the development of default parameters were discussed in Section 5.0. In this section the actual step by step calculation procedure is explained, and example calculations are presented.

SIMS is designed for collection and treatment systems in series. Although the default parameters for concentration assume the surface impoundment or collection system is the first portion of the treatment system, there may be cases where it is desired to estimate emissions from an impoundment or collection system component which is not the first unit. The model can still be used in these cases if all collection or treatment systems prior to the unit are modeled. The program then adjusts the concentration profile to account for the air emissions from the previous treatment or collection system cycle.

Figure 6-1 shows a flow diagram of the SIMS program structure used in defining the treatment and collection system components. After all parameters are defined for the user's system, VOC emissions can be estimated. There are 18 different potential estimation models:

- 1) Flowthrough, aerated, biological system,
- 2) Flowthrough, non-aerated, biological system,
- 3) Flowthrough, aerated, non-biological system,
- 4) Flowthrough, non-aerated, non-biological system,
- 5) Flowthrough, diffused air, biological system,
- 6) Flowthrough, diffused air, non-biological system,
- 7) Flowthrough, oil-film layer, non-biological system,
- 8) Flowthrough, junction box,
- 9) Flowthrough, lift station,
- 10) Flowthrough, sump,
- 11) Flowthrough, weir,
- 12) Disposal, aerated, biological system,
- 13) Disposal, non-aerated, biological system,
- 14) Disposal, aerated, non-biological system,



\* Denotes that information must be provided by the user

Figure 6-1. SIMS Model Structure



- 15) Disposal, non-aerated, non-biological system,
- 16) Disposal, diffused air, biological system,
- 17) Disposal, diffused air, non-biological system, and
- 18) Disposal, oil film layer, non-biological system.

For clarity of how the VOC emissions are estimated, six examples are presented in this chapter for the following scenarios:

- I. Disposal, non-aerated, non-biological impoundment,
- II. Flowthrough, aerated, biological impoundment,
- III. Flowthrough, diffused air, biological impoundment,
- IV. Disposal, oil film layer impoundment,
- V. Flowthrough, junction box, and
- VI. Flowthrough, weir.

The first step of the program is to INPUT information to define the system. STUDY is used to name the system and to input the wastewater flow rate. As noted in Figure 6-1, all bold type indicate minimum information required by SIMS. IMPOUNDMENTS is chosen next to define the impoundment or collection system component or series of impoundments and/or collection system components and their emission model parameters. ADD allows the user to select an impoundment or collection system type, define the surface area, and change any emission model default parameters. Once the impoundment is defined, POLLUTANTS is chosen to define the pollutant concentration profile. If the pollutant concentration profile is known, the user will simply ADD all pollutants and their respective concentrations to a pollutant list for the system. (There are 149 chemicals in the SIMS chemical database to choose from). If the user does not have information on the pollutant concentration profile, INDUSTRIES is chosen to define it. Under INDUSTRIES, the user is required to select the industry category(ies) which discharge to the system.

The user must first match SIC codes with the corresponding industrial category(ies), which are defined in Appendix A. The assigned code addresses data collected for that particular industrial category. For INDUSTRIES, the user must also specify if the impoundment or collection system component is at a publicly owned treatment work (POTW). If the impoundment is at a POTW and only the total flow is known, the percent industrial flow will be estimated

since the total flow is the sum of municipal and industrial wastewater. (SIMS assumes no volatile organics are present in municipal wastewater. If this is incorrect, the user must supply the concentration profile). These parameters will be given a default value if no information is supplied.

After the treatment and/or collection system is defined, CALCULATE runs the program to calculate the individual and overall mass transfer coefficients, and the total VOC emissions from the system.

The following six examples present the calculation steps involved to estimate VOC emissions using SIMS. All of the six example calculations will be performed using the information provided in Table 6-1. For clarity, the concentration profile for the six examples will be calculated first. (If the concentration profile has already been determined, INDUSTRIES need not be used. If only a partial list of pollutants and their concentrations is known, ADD allows the user to add pollutants or change the default concentration). Then, assuming each impoundment or collection system is independent, VOC emissions will be calculated for a selected compound. Calculation of impoundments and/or collection system components in series will not be shown in this chapter. However, all emission calculations for any one unit are identical if calculated in series. The effluent concentration from the first impoundment or collection system component is simply used as the inlet concentration to the next unit.

#### Calculation of Concentration Profile

From Table 6-1, there are three industrial flow rates discharging to the impoundment or collection system component. The industrial category codes for each discharge were obtained from Appendix A based on known SIC codes for each discharge. Based on inputted industry codes, SIMS will automatically assign a concentration profile.

If the impoundment is at a POTW, current concentrations will be assigned. A "current" concentration accounts for pretreatment of an industrial waste before it is discharged to a POTW. For this example, the surface impoundment is not at a POTW and the raw concentration is used. (See Section 5.1 for a description of "raw" and "current" concentrations). Table 6-2 presents the concentration profile for each industry category. To calculate the total concentration for each pollutant, the flow rate for each category is needed.

TABLE 6-1. EXAMPLE MODEL DATA

Scenario	Total Flow Rate (Q), m <sup>3</sup> /s	Total Surface Area (A), m <sup>2</sup>	Depth M
I. Disposal, non-aerated, non-biological impoundment	0.001 <sup>a</sup>	9,000 <sup>a</sup>	NA
II. Flowthrough, aerated, biological impoundment	0.0623 <sup>b</sup>	17,652 <sup>b</sup>	NA
III. Flowthrough, diffused air, biological impoundment	0.0075 <sup>c</sup>	100 <sup>c</sup>	4
IV. Disposal, oil film layer, impoundment	0.0623 <sup>b</sup>	900 <sup>c</sup>	2
V. Flowthrough, junction box	0.00252 <sup>d</sup>	0.656 <sup>d</sup>	0.9 <sup>d</sup>
VI. Flowthrough, weir	0.00252 <sup>e</sup>	height = 4 ft <sup>e</sup>	

-----  
Number of industrial flow rates discharged to impoundment<sup>c</sup> = 3

SIC codes and industrial category for each industrial flow rate into the impoundment<sup>c</sup>

<u>SIC Code</u>	<u>Description</u>	<u>Industrial Category Code<sup>f</sup></u>
2865	Dye Manufacture and Formulation	4
2879	Pesticides Manufacture	19
2869	Organic Chemicals Manufacturing	17

<sup>a</sup>Reference 2, disposal impoundments.

<sup>b</sup>Reference 1, aeration basin dimensions.

<sup>c</sup>Random choice.

<sup>d</sup>Reference 1, junction box dimensions.

<sup>e</sup>Reference 1, weir dimension.

<sup>f</sup>From Appendix A.

NA = Not Available by User.

TABLE 6-2. CONCENTRATION PROFILE

Industrial Category:	Dye Manufacture and Formulation	Organic Chemicals Manufacturing	Pesticides Manufacture	Total Concentration (g/m <sup>3</sup> )
Compound	Concentration (g/m <sup>3</sup> )	Concentration (g/m <sup>3</sup> )	Concentration (g/m <sup>3</sup> )	
Acrolein	--	$2.6 \times 10^{-4}$	--	$2.29 \times 10^{-4}$
Benzene	--	11.68	$9.13 \times 10^{-2}$	10.29
Bis(2-ethyl Hexyl)phthalate	--	8.02	--	7.07
Bromomethane	--	$4.25 \times 10^{-3}$	--	$3.74 \times 10^{-3}$
Butyl Benzyl phthalate	--	8.02	--	7.07
Carbon tetrachloride	--	1.06	0.143	0.940
Chlorobenzene	$7.86 \times 10^{-4}$	$2.0 \times 10^{-5}$	--	$7.97 \times 10^{-5}$
Chloroform	--	9.06	$1.3 \times 10^{-3}$	7.98
Chloromethane	--	0.15	0.02	0.133
Dibutylphthalate	--	$5 \times 10^{-6}$	--	$4.41 \times 10^{-6}$
1,2 dichlorobenzene	9.6	$1.45 \times 10^{-3}$	0.0878	0.763
1,4 dichlorobenzene	16.32	--	--	1.29
1,2 dichloroethane	--	--	$3.83 \times 10^{-4}$	$1.53 \times 10^{-5}$
2,4 dichlorophenol	--	--	0.724	$2.90 \times 10^{-2}$
Diethyl Phthalate	--	$3.50 \times 10^{-5}$	--	$3.08 \times 10^{-5}$
Ethyl Benzene	--	8.25	$5.44 \times 10^{-4}$	7.27
Methylene chloride	--	1.04	1.09	0.960
Napthalene	--	8.02	--	7.07
PCB's	0.0187	--	--	$1.48 \times 10^{-3}$
Phenol	0.179	27.30	0.108	24.07
1,1,2,2 tetrachloroethane	--	$9.98 \times 10^{-4}$	--	$8.79 \times 10^{-6}$
Tetrachloroethylene	1.67	1.04	4.35	1.22
Toluene	--	14.32	48.31	14.55
1,2,4 Trichlorobenzene	$8.44 \times 10^{-3}$	--	--	$6.67 \times 10^{-4}$
1,1,2 Trichloroethane	--	1.51	--	1.33
2,4,6 Trichlorophenol	--	--	$5.97 \times 10^{-3}$	$2.39 \times 10^{-4}$
Vinyl chloride	--	0.102	--	$8.99 \times 10^{-2}$

SIMS automatically assigns a default value for the industrial flow rates, depending on whether the impoundment is at a POTW or not. (Municipal flow must be accounted for if the impoundment is at a POTW). The user cannot override the percent of total flow from each industrial category, as this determines the default concentration profile. The default fraction of total industrial flow rates are the following:

<u>Industrial Category Code</u>	<u>Industrial Category</u>	<u>Fraction of Total Industrial Flow Rate</u>
4	Dye Manufacture and Formulation	0.079
17	Organic Chemicals	0.881
19	Pesticides Manufacturing	0.040

The total concentration for each pollutant as shown in Table 6-2 is weighted by flow rate as presented in Section 5.1.2.

The remainder of this chapter presents sample VOC emission calculations for six scenarios assuming the above concentration profile (Tables 6-3 through 6-8 provide scenarios for estimation models 15, 1, 5, 18, 8, and 11, respectively). For simplification, all emission calculations will be performed for benzene only. The following is the format for calculating emissions for each scenario:

- I. User Supplied Information
- II. Defaults
- III. Pollutant Physical Property Data and Water, Air, and Other Properties
- IV. Calculate Individual Mass Transfer Coefficients
- V. Calculate Equilibrium Mass Transfer Coefficient
- VI. Calculate the Overall Mass Transfer Coefficient
- VII. Calculate VOC Emissions

TABLE 6-3. VOC EMISSION CALCULATIONS FOR A NON-AERATED,  
NON-BIOLOGICAL, DISPOSAL IMPOUNDMENT

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I. User Supplied Information

$$Q = 0.001 \text{ m}^3/\text{s} \text{ (86.4 m}^3/\text{day)}$$

$$A = 9,000 \text{ m}^2$$

II. Defaults

A. Depth (from Section 5.2)

$$D = Q/101.2 \quad \text{for } 0 < Q < 253 \text{ m}^3/\text{day}$$

$$D = 86.4/101.2$$

$$D = 0.854 \text{ m}$$

B. Concentration (see Table 6-2)

$$C_0, \text{ Benzene} = 10.29 \text{ g/m}^3$$

C. Emission Model Parameters

$$U_{10} = 4.47 \text{ m/s}$$

$$T = 25^\circ\text{C} \text{ (298}^\circ\text{K)}$$

III. Pollutant Physical Property Data and Water, Air, and Other Properties

A. Benzene

$$D_{w,\text{benzene}} = 9.8 \times 10^{-6} \text{ cm}^2/\text{s}$$

$$D_{a,\text{benzene}} = 0.088 \text{ cm}^2/\text{s}$$

$$H_{\text{benzene}} = 0.0055 \text{ atm-m}^3/\text{gmol}$$

B. Water, Air, and Other Properties

$$\rho_a = 1.2 \times 10^{-3} \text{ g/cm}^3$$

$$\mu_a = 1.81 \times 10^{-4} \text{ g/cm-s}$$

$$D_{\text{ether}} = 8.5 \times 10^{-6} \text{ cm}^2/\text{s}$$

TABLE 6-3. VOC EMISSION CALCULATIONS FOR A NON-AERATED,  
NON-BIOLOGICAL, DISPOSAL IMPOUNDMENT (continued)

$$R = 8.21 \times 10^{-5} \text{ atm-m}^3/\text{gmol}$$

#### IV. Calculate Individual Mass Transfer Coefficients

##### A. Calculate $k_l$ (see Table 4-3)

For  $U_{10} > 3.25 \text{ m/s}$  and  $F/D > 51.2$

$$F/D = (4A/\pi)^{0.5}/D = (4(9,000)/\pi)^{0.5}/0.854 = 125.3$$

$$k_l (\text{m/s}) = 2.611 \times 10^{-7} (4.47 \text{ m/s})^2 [(9.8 \times 10^{-6} \text{ cm}^2/\text{s}) / 8.5 \times 10^{-6} \text{ cm}^2/\text{s}]^{2/3}$$

$$k_l = 5.74 \times 10^{-6} \text{ m/s}$$

##### B. Calculate $k_g$ (see Table 4-3)

$$k_g (\text{m/s}) = 4.82 \times 10^{-3} U_{10}^{0.78} Sc_G^{-0.67} d_e^{-0.11}$$

##### 1) Calculate Schmidt Number on the gas side, $Sc_G$ :

$$Sc_G = \mu_g / (\rho_g D_g)$$

$$Sc_G = (1.81 \times 10^{-4} \text{ g/cm-s}) / [(1.2 \times 10^{-3} \text{ g/cm}^3)(0.088 \text{ cm}^2/\text{s})]$$

$$Sc_G = 1.71$$

##### 2) Calculate the effective diameter, $d_e$ :

$$d_e (\text{m}) = (4A/\pi)^{0.5}$$

$$d_e (\text{m}) = (4(9,000)/\pi)^{0.5}$$

$$d_e = 107.0 \text{ m}$$

$$k_g (\text{m/s}) = 4.82 \times 10^{-3} (4.47 \text{ m/s})^{0.78} (1.71)^{-0.67} (107.0 \text{ m})^{-0.11}$$

$$k_g = 6.47 \times 10^{-3} \text{ m/s}$$

#### V. Calculate Equilibrium Mass Transfer Coefficient

$$K_{eq} = H/RT$$

TABLE 6-3. VOC EMISSION CALCULATIONS FOR A NON-AERATED,  
NON-BIOLOGICAL, DISPOSAL IMPOUNDMENT (continued)

$$K_{eq} = (0.0055 \text{ atm-m}^3/\text{gmol}) / [(8.21 \times 10^{-5} \text{ atm-m}^3/\text{gmol-}^\circ\text{K})(298^\circ\text{K})]$$

$$K_{eq} = 0.225$$

VI. Calculate the Overall Mass Transfer Coefficient

$$1/K \text{ (m/s)} = 1/k_l + 1/(k_g K_{eq})$$

$$1/K \text{ (m/s)} = 1/(5.74 \times 10^{-6} \text{ m/s}) + 1/[(6.47 \times 10^{-3} \text{ m/s})(0.225)]$$

$$K = 5.72 \times 10^{-6} \text{ m/s}$$

VII. Calculate VOC Emissions for a Non-Aerated, Non-Biological, Disposal  
Impoundment (see Table 4-1)

$$N \text{ (g/s)} = [1 - \exp(-KAt/V)]VC_0/t$$

1) Calculate volume, V:

$$V = A \cdot D = (9,000 \text{ m}^2)(0.854 \text{ m}) = 7,686 \text{ m}^3$$

2) Calculate retention time, t:

$$t = V/Q = (7,686 \text{ m}^3)/(0.001 \text{ m}^3/\text{s}) = 7,686,000 \text{ s}$$

$$N \text{ (g/s)} = [1 - \exp(-(5.72 \times 10^{-6} \text{ m/s})(9,000 \text{ m}^2)(7,686,000 \text{ s})/(7,686 \text{ m}^3))]$$

$$[(7,686 \text{ m}^3)(10.29 \text{ g/m}^3)/(7,686,000 \text{ s})]$$

$$N = 0.01029 \text{ g/s}$$



TABLE 6-4. VOC EMISSION CALCULATIONS FOR A FLOWTHROUGH,  
AERATED, BIOLOGICAL IMPOUNDMENT

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I. User Supplied Information

$$Q = 0.0623 \text{ m}^3/\text{s} \text{ (5382.7 m}^3/\text{day)}$$

$$A = 17,652 \text{ m}^2$$

II. Defaults

A. Depth (from Section 5.2)

$$D \text{ (m)} = (Q + 3809.5)/4673.3$$

$$D \text{ (m)} = (5382.7 + 3809.5)/4673.3$$

$$D = 1.97 \text{ m}$$

B. Concentration (see Table 6-2)

$$C_o, \text{ Benzene} = 10.29 \text{ g/m}^3$$

C. Emission Model Parameters

$$U_{10} = 4.47 \text{ m/s}$$

$$T = 25^\circ\text{C} \text{ (298}^\circ\text{K)}$$

$$b_1 = 0.3 \text{ g/l (300 g/m}^3\text{)}$$

$$J = 3 \text{ lb O}_2/\text{hp-hr}$$

$$\text{POWR} = 0.75 \text{ hp/1,000 ft}^3 \text{ (V)}$$

$$O_t = 0.83$$

$$V a_t = 0.24 \text{ (A)}$$

$$d = 61 \text{ cm, } d^* = 2 \text{ ft}$$

$$w = 126 \text{ rad/s}$$

$$N_s = \text{POWR}/75 \text{ hp}$$

TABLE 6-4. VOC EMISSION CALCULATIONS FOR A FLOWTHROUGH,  
AERATED, BIOLOGICAL IMPOUNDMENT (continued)

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III. Pollutant Physical Property Data and Water, Air, and Other Properties

A. Benzene

$$D_{u,\text{benzene}} = 9.8 \times 10^{-6} \text{ cm}^2/\text{s}$$

$$D_{a,\text{benzene}} = 0.088 \text{ cm}^2/\text{s}$$

$$H_{\text{benzene}} = 0.0055 \text{ atm-m}^3/\text{gmol}$$

$$K_{\text{max},\text{benzene}} = 5.28 \times 10^{-6} \text{ g/g-s}$$

$$K_{s,\text{benzene}} = 13.6 \text{ g/m}^3$$

B. Water, Air, and Other Properties

$$\rho_a = 1.2 \times 10^{-3} \text{ g/cm}^3$$

$$\rho_L = 1 \text{ g/cm}^3 (62.4 \text{ lb}_m/\text{ft}^3)$$

$$\mu_a = 1.81 \times 10^{-4} \text{ g/cm-s}$$

$$D_{O_2,u} = 2.4 \times 10^{-5} \text{ cm}^2/\text{s}$$

$$D_{\text{ether}} = 8.5 \times 10^{-6} \text{ cm}^2/\text{s}$$

$$MW_L = 18 \text{ g/gmol}$$

$$MW_a = 29 \text{ g/gmol}$$

$$g_c = 32.17 \text{ lb}_m\text{-ft/lb}_f\text{-s}^2$$

$$R = 8.21 \times 10^{-5} \text{ atm-m}^3/\text{gmol}$$

IV. Calculate Individual Mass Transfer Coefficients

Because part of the impoundment is turbulent and part is quiescent, the overall mass transfer coefficient is determined as an area weighted average of the turbulent and quiescent overall mass transfer coefficients.

TABLE 6-4. VOC EMISSION CALCULATIONS FOR A FLOWTHROUGH, AERATED, BIOLOGICAL IMPOUNDMENT (continued)

A. Calculate  $k_l$  (see Table 4-4)

$$k_l (\text{m/s}) = [(8.22 \times 10^{-9}) J(\text{POWR})(1.024)^{T-20} O_t (10^6) \\ MW_L / (V a_v \rho_L)] (D_w / D_{O2,w})^{0.5}$$

1) Calculate POWR:

$$\text{POWR (hp)} = 0.75 \text{ hp/1,000 ft}^3 \text{ (V)}$$

$$V (\text{m}^3) = A \cdot D = (17,652 \text{ m}^2)(1.97 \text{ m})$$

$$V = 34,774 \text{ m}^3$$

$$\text{POWR} = (0.75 \text{ hp/1,000 ft}^3)(\text{ft}^3/0.028317 \text{ m}^3)(34774 \text{ m}^3)$$

$$\text{POWR} = 921 \text{ hp}$$

2) Calculate  $V a_v$ :

$$V a_v (\text{ft}^2) = 0.24 A$$

$$V a_v = 0.24(17,652 \text{ m}^2)(10.758 \text{ ft}^2/\text{m}^2)$$

$$V a_v = 45,576 \text{ ft}^2$$

$$k_l (\text{m/s}) = [(8.22 \times 10^{-9})(3 \text{ lb}_{O2}/\text{hp-hr})(921 \text{ hp})(1.024)^{(25-20)}(0.83) \\ (10^6)(18 \text{ g/gmol}) / ((45,576 \text{ ft}^2)(1 \text{ g/cm}^3))] \\ [(9.8 \times 10^{-6} \text{ cm}^2/\text{s}) / (2.4 \times 10^{-5} \text{ cm}^2/\text{s})]^{0.5}$$

$$k_l (\text{m/s}) = (0.00838)(0.639)$$

$$k_l = 5.35 \times 10^{-3} \text{ m/s}$$

B. Calculate  $k_g$  (see Table 4-4)

$$k_g (\text{m/s}) = (1.35 \times 10^{-7}) \text{ Re}^{1.42} \rho^{0.4} S c_g^{0.5} \text{Fr}^{-0.21} D_s MW_g / d$$

1) Calculate Reynold's Number, Re:

$$\text{Re} = d^2 \omega \rho_s / \mu_s$$

$$\text{Re} = (61 \text{ cm})^2 (126 \text{ rad/s})(1.2 \times 10^{-3} \text{ g/cm}^3) / (1.81 \times 10^{-4} \text{ g/cm-s})$$

$$\text{Re} = 3.1 \times 10^6$$

TABLE 6-4. VOC EMISSION CALCULATIONS FOR A FLOWTHROUGH,  
AERATED, BIOLOGICAL IMPOUNDMENT (continued)

- 2) Calculate power number,  $p$ :

$$p = (0.85)(\text{POWR})(550 \text{ ft-lb}_f/\text{s-hp})/N_a g_c / (\rho_L d^{*5} w^3)$$

$$N_a = \text{POWR}/75 \text{ hp (default)}$$

$$p = [0.85 (75 \text{ hp})(550 \text{ ft-lb}_f/\text{s-hp})(32.17 \text{ lb}_m\text{-ft/lb}_f\text{-s}^2)] /$$

$$[(62.4 \text{ lb}_m/\text{ft}^3)(2 \text{ ft})^5(126 \text{ rad/s})^3]$$

$$p = 2.8 \times 10^{-4}$$

- 3) Calculate Schmidt Number on the gas side,  $Sc_g$ :

$$Sc_g = \mu_g / (\rho_g D_g)$$

$$Sc_g = (1.81 \times 10^{-4} \text{ g/cm-s}) / [(1.2 \times 10^{-3} \text{ g/cm}^3)(0.088 \text{ cm}^2/\text{s})]$$

$$Sc_g = 1.71$$

- 4) Calculate Froude Number,  $Fr$ :

$$Fr = d^* w^2 / g_c$$

$$Fr = (2 \text{ ft})(126 \text{ rad/s})^2 / (32.17 \text{ lb}_m\text{-ft/lb}_f\text{-s}^2)$$

$$Fr = 990$$

$$k_g (\text{m/s}) = (1.35 \times 10^{-7} (3.1 \times 10^6)^{1.42} (2.8 \times 10^{-4})^{0.4} (1.71)^{0.5} (990)^{-0.21}$$

$$(0.088 \text{ cm}^2/\text{s})(29 \text{ g/gmol}) / (61 \text{ cm})$$

$$k_g = 0.109 \text{ m/s}$$

#### Quiescent Surface Area of Impoundment

- A. Calculate  $k_l$  (see Table 4-3)

$$U_{10} > 3.25 \text{ m/s and } F/D > 51.2$$

$$F/D = (4A/\pi)^{0.5} / D$$

$$= (4(17,652 \text{ m}^2)/\pi)^{0.5} / 1.97 \text{ m}$$

$$= 76.1$$

TABLE 6-4. VOC EMISSION CALCULATIONS FOR A FLOWTHROUGH,  
AERATED, BIOLOGICAL IMPOUNDMENT (continued)

$$k_l \text{ (m/s)} = (2.611 \times 10^{-7}) U_{10}^2 [D_w/D_{\text{ether}}]^{2/3}$$

$$k_l \text{ (m/s)} = (2.611 \times 10^{-7}) (4.47 \text{ m/s})^2 [(9.8 \times 10^{-6} \text{ cm}^2/\text{s}) / (8.5 \times 10^{-6} \text{ cm}^2/\text{s})]^{2/3}$$

$$k_l = 5.74 \times 10^{-6} \text{ m/s}$$

B. Calculate  $k_g$  (see Table 4-3)

$$k_g = (4.82 \times 10^{-3}) U_{10}^{0.78} Sc_G^{-0.67} d_e^{-0.11}$$

1) Calculate the Schmidt Number on the gas side,  $Sc_G$ :

$$Sc_G = \mu_g / (\rho_g D_g) = 1.71 \text{ (same as for turbulent impoundments)}$$

2) Calculate the effective diameter,  $d_e$ :

$$d_e \text{ (m)} = (4A/\pi)^{0.5}$$

$$d_e \text{ (m)} = (4(17,652 \text{ m}^2)/\pi)^{0.5}$$

$$d_e = 149.9 \text{ m}$$

$$k_g \text{ (m/s)} = 4.82 \times 10^{-3} (4.47 \text{ m/s})^{0.78} (1.71)^{-0.67} (149.9 \text{ m})^{-0.11}$$

$$k_g = 6.24 \times 10^{-3} \text{ m/s}$$

V. Calculate Equilibrium Mass Transfer Coefficient

$$K_{eq} = H/RT$$

$$K_{eq} = (0.0055 \text{ atm-m}^3/\text{gmol}) / [(8.21 \times 10^{-5} \text{ atm-m}^3/\text{gmol-}^\circ\text{K})(298^\circ\text{K})]$$

$$K_{eq} = 0.225$$

TABLE 6-4. VOC EMISSION CALCULATIONS FOR A FLOWTHROUGH,  
AERATED, BIOLOGICAL IMPOUNDMENT (continued)

VI. Calculate the Overall Mass Transfer Coefficient

Turbulent Surface Area of Impoundment

$$1/K_T \text{ (m/s)} = 1/k_l + 1/(k_g K_{eq})$$

$$1/K_T \text{ (m/s)} = 1/(5.35 \times 10^{-3} \text{ m/s}) + 1/[(0.109)(0.225)]$$

$$K_T = 4.39 \times 10^{-3} \text{ m/s}$$

Quiescent Surface Area of Impoundment

$$1/K_Q \text{ (m/s)} = 1/k_l + 1/(k_g K_{eq})$$

$$1/K_Q \text{ (m/s)} = 1/(5.74 \times 10^{-6} \text{ m/s}) + 1/[(6.24 \times 10^{-3} \text{ m/s})(0.225)]$$

$$K_Q = 5.72 \times 10^{-6} \text{ m/s}$$

Overall Mass Transfer Coefficient Weighted by Area

$$K \text{ (m/s)} = (K_T A_T + K_Q A_Q)/A$$

$$A_T = 0.24A$$

$$A_Q = (1 - 0.24)A$$

$$K \text{ (m/s)} = [(4.39 \times 10^{-3} \text{ m/s})(0.24 A) + (5.72 \times 10^{-6} \text{ m/s})(1 - 0.24)A]/A$$

$$K = 1.06 \times 10^{-3} \text{ m/s}$$

VII. Calculate VOC Emissions for an Aerated, Biological, Flowthrough  
Impoundment (see Table 4-1)

$$N \text{ (g/s)} = KA[-(K_s(KA/Q + 1) + VK_{max}b_i/Q - C_o) +$$

$$((K_s(KA/Q + 1) + VK_{max}b_i/Q - C_o)^2 + 4(KA/Q + 1) \cdot$$

$$(K_s C_o))^{0.5}]/(2(KA/Q + 1))$$

TABLE 6-4. VOC EMISSION CALCULATIONS FOR A FLOWTHROUGH,  
AERATED, BIOLOGICAL IMPOUNDMENT (continued)

1) Calculate  $KA/Q + 1$ :

$$(KA/Q + 1) = (1.06 \times 10^{-3} \text{ m/s})(17,652 \text{ m}^2)/(0.0623 \text{ m}^3/\text{s}) + 1$$

$$(KA/Q + 1) = 301.3$$

2) Calculate  $VK_{\text{max}b_i}/Q$ :

$$VK_{\text{max}b_i}/Q = (34,774 \text{ m}^3)(5.28 \times 10^{-6} \text{ g/g-s})(300 \text{ g/m}^3)/$$

$$(0.0623 \text{ m}^3/\text{s})$$

$$VK_{\text{max}b_i}/Q = 884.1$$

$$N \text{ (g/s)} = (1.06 \times 10^{-3} \text{ m/s})(17,652 \text{ m}^2)[ -((13.6 \text{ g/m}^3)(301.3) + (884.1) -$$

$$10.29 \text{ g/m}^3) + (((13.6 \text{ g/m}^3)(301.3) + (884.1) - 10.29 \text{ g/m}^3)^2 +$$

$$4(301.3)((13.6 \text{ g/m}^3)(10.29 \text{ g/m}^3)))^{0.5}]/(2(301.3))$$

$$N \text{ (g/s)} = (18.71)[-4971.5 + 4988.4]/(602.6)$$

$$N = 0.52 \text{ g/s}$$

TABLE 6-5. VOC EMISSION CALCULATIONS FOR A DIFFUSED AIR,  
BIOLOGICAL, FLOWTHROUGH IMPOUNDMENT

---

I. User Supplied Information

$$Q = 0.0075 \text{ m}^3/\text{s}$$

$$A = 100 \text{ m}^2$$

$$D = 4\text{m}$$

$$b_i = 4,000 \text{ g/m}^3$$

II. Defaults

A. Depth - User has supplied the depth above.

B. Concentration (see Table 6-2)

$$C_{o,\text{benzene}} = 10.29 \text{ g/m}^3$$

C. Emission Model Parameters

$$U_{10} = 4.47 \text{ m/s}$$

$$T = 25^\circ\text{C} \quad (298^\circ\text{K})$$

$$b_i = 4.0 \text{ g/l} \quad (4,000 \text{ g/m}^3) - \text{User supplied}$$

$$Q_A = 0.0004(V) = (0.0004)(100\text{m}^2)(4\text{m}) = 0.16 \text{ m}^3/\text{s}$$

III. Pollutant Physical Property Data and Water, Air, and Other Properties

A. Benzene

$$D_{v,\text{benzene}} = 9.8 \times 10^{-6} \text{ cm}^2/\text{s}$$

$$D_{a,\text{benzene}} = 0.088 \text{ cm}^2/\text{s}$$

$$H_{\text{benzene}} = 0.0055 \text{ atm-m}^3/\text{gmol}$$

$$K_{\text{max},\text{benzene}} = 5.28 \times 10^{-6} \text{ g/g-s}$$

$$K_{s,\text{benzene}} = 13.6 \text{ g/m}^3$$



TABLE 6-5. VOC EMISSION CALCULATIONS FOR A DIFFUSED AIR,  
BIOLOGICAL, FLOWTHROUGH IMPOUNDMENT (continued)

B. Water, Air, and Other Properties

$$\rho_a = 1.2 \times 10^{-3} \text{ g/cm}^3$$

$$\rho_L = 1 \text{ g/cm}^3$$

$$\mu_a = 1.81 \times 10^{-4} \text{ g/cm-s}$$

$$\mu_L = 8.93 \times 10^{-3} \text{ g/cm-s}$$

$$D_{\text{ether}} = 8.5 \times 10^{-6} \text{ cm}^2/\text{s}$$

$$R = 8.21 \times 10^{-5} \text{ atm-m}^3/\text{gmol-}^\circ\text{K}$$

IV. Calculate Individual Mass Transfer Coefficients

A. Calculate  $k_l$  (see Table 4-3)

$$U_{10} > 3.25 \text{ m/s and } F/D < 14$$

$$F/D = (4A/\pi)^{0.5}/D$$

$$= (4(100 \text{ m}^2)/\pi)^{0.5}/4 \text{ m}$$

$$= 2.8$$

$$k_l \text{ (m/s)} = (1.0 \times 10^{-6}) + (144 \times 10^{-4})U^{*2.2}Sc_L^{-0.5}$$

$$\text{for } U^* < 0.3 \text{ m/s}$$

$$U^* \text{ (m/s)} = 0.01(U_{10})(6.1 + 0.63U_{10})^{0.5}$$

$$U^* \text{ (m/s)} = 0.01(4.47 \text{ m/s})(6.1 + 0.63(4.47 \text{ m/s}))^{0.5}$$

$$U^* = 0.133$$

1) Calculate Schmidt Number on the liquid side,  $Sc_L$ :

$$Sc_L = \mu_L/(\rho_L D_w)$$

$$Sc_L = (8.93 \times 10^{-3} \text{ g/cm-s})/[(1 \text{ g/cm}^3)(9.8 \times 10^{-6} \text{ cm}^2/\text{s})]$$

$$Sc_L = 911$$

$$k_l \text{ (m/s)} = (1.0 \times 10^{-6}) + (144 \times 10^{-4})(0.133)^{2.2}(911)^{-0.5}$$

TABLE 6-5. VOC EMISSION CALCULATIONS FOR A DIFFUSED AIR,  
BIOLOGICAL, FLOWTHROUGH IMPOUNDMENT (continued)

$$k_l = 6.64 \times 10^{-6} \text{ m/s}$$

B. Calculate  $k_g$  (see Table 4-3)

$$k_g \text{ (m/s)} = (4.82 \times 10^{-3}) U_{10}^{0.78} Sc_G^{-0.67} d_e^{-0.11}$$

1) Calculate Schmidt Number on the gas side,  $Sc_G$ :

$$Sc_G = \mu_g / (\rho_g D_a)$$

$$Sc_G = (1.81 \times 10^{-4} \text{ g/cm-s}) / [(1.2 \times 10^{-3} \text{ g/cm}^3)(0.088 \text{ cm}^2/\text{s})]$$

$$Sc_G = 1.71$$

2) Calculate the effective diameter,  $d_e$ :

$$d_e \text{ (m)} = (4A/\pi)^{0.5}$$

$$d_e \text{ (m)} = (4(100 \text{ m}^2)/\pi)^{0.5}$$

$$d_e = 11.3 \text{ m}$$

$$k_g \text{ (m/s)} = 4.82 \times 10^{-3} (4.47 \text{ m/s})^{0.78} (1.71)^{-0.67} (11.2 \text{ m})^{-0.11}$$

$$k_g = 8.29 \times 10^{-3} \text{ m/s}$$

V. Calculate Equilibrium Mass Transfer Coefficient

$$K_{eq} = H/RT$$

$$K_{eq} = (0.0055 \text{ atm-m}^3/\text{gmol}) / [(8.21 \times 10^{-5} \text{ atm-m}^3/\text{gmol-}^\circ\text{K})(298^\circ\text{K})]$$

$$K_{eq} = 0.225$$

VI. Calculate the Overall Mass Transfer Coefficient

$$1/K = 1/k_l + 1/(k_g K_{eq})$$

$$1/K = 1/(6.64 \times 10^{-6} \text{ m/s}) + 1/[(8.29 \times 10^{-3})(0.225)]$$

$$K = 6.62 \times 10^{-6} \text{ m/s}$$

TABLE 6-5. VOC EMISSION CALCULATIONS FOR A DIFFUSED AIR,  
BIOLOGICAL, FLOWTHROUGH IMPOUNDMENT (continued)

VII. Calculate VOC Emissions for a Diffused Air, Biological, Flowthrough Impoundment

$$N \text{ (g/s)} = (K_A + Q_A K_{eq}) [-(K_s((K_A + Q_A K_{eq})/Q + 1) + VK_{max} b_i/Q - C_o) + ((K_s((K_A + Q_A K_{eq})/Q + 1) + VK_{max} b_i/Q - C_o)^2 + 4((K_A + Q_A K_{eq})/Q + 1)(K_s C_o))^{0.5}] / (2((K_A + Q_A K_{eq})/Q + 1))$$

1) Calculate  $K_A + Q_A K_{eq}$ :

$$(K_A + Q_A K_{eq}) = (6.62 \times 10^{-6} \text{ m/s})(100 \text{ m}^2) + (0.16 \text{ m}^3/\text{s})(0.225)$$

$$(K_A + Q_A K_{eq}) = 0.03666 \text{ m}^3/\text{s}$$

2) Calculate  $(K_A + Q_A K_{eq})/Q$ :

$$(K_A + Q_A K_{eq})/Q = (0.03666 \text{ m}^3/\text{s}) / (0.0075 \text{ m}^3/\text{s})$$

$$(K_A + Q_A K_{eq})/Q = 4.888$$

3) Calculate  $VK_{max} b_i/Q$ :

$$VK_{max} b_i/Q = (400 \text{ m}^3)(5.28 \times 10^{-6} \text{ g/g-s})(4,000 \text{ g/m}^3) / (0.0075 \text{ m}^3/\text{s})$$

$$VK_{max} b_i/Q = 1126.4 \text{ g/m}^3$$

$$N \text{ (g/s)} = (0.03666 \text{ m}^3/\text{s}) [-(13.6 \text{ g/m}^3)(4.888 + 1) + 1126.4 \text{ g/m}^3 - 10.29 \text{ g/m}^3) + (((13.6 \text{ g/m}^3)(4.888 + 1) + 1126.4 \text{ g/m}^3 - 10.29 \text{ g/m}^3)^2 + 4(4.888 + 1)(13.6 \text{ g/m}^3)(10.29 \text{ g/m}^3))^{0.5}] / (2(4.888 + 1))$$

$$N \text{ (g/s)} = (0.03666) [-1196.2 + 1197.6] / 11.78$$

$$N = 4.28 \times 10^{-3} \text{ g/s}$$

TABLE 6-6. VOC EMISSION CALCULATIONS FOR A DISPOSAL IMPOUNDMENT  
WITH AN OIL FILM LAYER

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I. User Supplied Information

$$Q = 0.0623 \text{ m}^3/\text{s}$$

$$A = 900 \text{ m}^2$$

$$D = 2 \text{ M}$$

II. Defaults

A. Depth - User has supplied the depth above.

B. Concentration (see Table 6-2)

$$C_{\text{benzene}} = 10.29 \text{ g/m}^3$$

C. Emission Model Parameters

$$U_{10} = 4.47 \text{ m/s}$$

$$T = 25^\circ\text{C} \text{ (298}^\circ\text{K)}$$

$$FO = 0.001$$

III. Pollutant Physical Property Data and Water, Air, and Other Properties

A. Benzene

$$D_{\text{a,benzene}} = 0.088 \text{ cm}^2/\text{s}$$

$$D^*_{\text{benzene}} = 95.2 \text{ mmHg}$$

$$K_{\text{ow,benzene}} = 78.91$$

B. Water, Air, and Other Properties

$$\rho_{\text{a}} = 1.2 \times 10^{-3} \text{ g/cm}^3$$

$$\mu_{\text{a}} = 1.81 \times 10^{-4} \text{ g/cm-s}$$

$$\mu_{\text{oil}} = 0.92 \text{ g/cm}^3$$

$$MW_{\text{a}} = 29 \text{ g/gmol}$$

TABLE 6-6. VOC EMISSION CALCULATIONS FOR A DISPOSAL IMPOUNDMENT  
WITH AN OIL FILM LAYER (continued)

$$MW_{oil} = 282 \text{ g/gmol}$$

$$P_o = 760 \text{ mmHg}$$

IV. Calculate Individual Gas Phase Mass Transfer Coefficients

$$k_g = (4.82 \times 10^{-3}) U_{10}^{0.78} Sc_g^{-0.67} d_e^{-0.11}$$

- 1) Calculate Schmidt Number on the gas side,  $Sc_g$ :

$$Sc_g = \mu_g / (\rho_g D_g)$$

$$Sc_g = (1.81 \times 10^{-4} \text{ g/cm-s}) / [(1.2 \times 10^{-3} \text{ g/m}^3)(0.088 \text{ cm}^2/\text{s})]$$

$$Sc_g = 1.71$$

- 2) Calculate the effective diameter,  $d_e$ :

$$d_e \text{ (m)} = (4A/\pi)^{0.5}$$

$$d_e \text{ (m)} = (4(900 \text{ m}^2)/\pi)^{0.5}$$

$$d_e = 33.85 \text{ m}$$

$$k_g \text{ (m/s)} = (4.82 \times 10^{-3})(4.47 \text{ m/s})^{0.78}(1.71)^{-0.67}(33.85)^{-0.11}$$

$$k_g = 7.34 \times 10^{-3} \text{ m/s}$$

V. Calculate Equilibrium Mass Transfer Coefficient

$$K_{eq} = P^* \rho_o MW_{oil} / (\rho_{oil} MW_o P_o)$$

$$K_{eq} = (95.2 \text{ mmHg})(1.2 \times 10^{-3} \text{ g/cm}^3)(282 \text{ g/gmol}) /$$

$$[(0.92 \text{ g/cm}^3)(29 \text{ g/gmol})(760 \text{ mmHg})]$$

$$K_{eq} = 1.59 \times 10^{-3}$$

VI. Calculate the Overall Mass Transfer Coefficient

$$K_{oil} \text{ (m/s)} = k_g K_{eq}$$

TABLE 6-6. VOC EMISSION CALCULATIONS FOR A DISPOSAL IMPOUNDMENT  
WITH AN OIL FILM LAYER (continued)

$$K_{oil} \text{ (m/s)} = (7.34 \times 10^{-3} \text{ m/s})(1.59 \times 10^{-3})$$

$$K_{oil} = 1.17 \times 10^{-5} \text{ m/s}$$

VII. Calculate VOC Emissions for a Disposal Impoundment with an Oil Film Layer

$$N \text{ (g/s)} = [1 - \exp(-K_{oil}t/D_{oil})]V_{oil}Co_{oil}/t$$

- 1) Calculate the residence time, t:

$$t \text{ (s)} = V/Q$$

$$t \text{ (s)} = (1800 \text{ m}^3)/(0.0623 \text{ m}^3/\text{s})$$

$$t = 28892 \text{ s}$$

- 2) Calculate  $V_{oil}$ :

$$V_{oil} \text{ (m}^3\text{)} = FO(V)$$

$$V_{oil} \text{ (m}^3\text{)} = 0.001(1800 \text{ m}^3)$$

$$V_{oil} = 1.8 \text{ m}^3$$

- 3) Calculate  $Co_{oil}$ :

$$Co_{oil} \text{ (g/m}^3\text{)} = CoKow/[(1 - FO) + (FO)Kow]$$

$$Co_{oil} \text{ (g/m}^3\text{)} = (10.29 \text{ g/m}^3)(78.91)/[(1 - 0.001) + (0.001)(78.91)]$$

$$Co_{oil} = 753 \text{ g/m}^3$$

- 4) Calculate  $D_{oil}$ :

$$D_{oil} \text{ (m)} = 0.001(D)$$

$$D_{oil} \text{ (m)} = 0.001(2\text{m})$$

$$D_{oil} = 0.002 \text{ m}$$

$$N \text{ (g/s)} = [1 - \exp(-(1.17 \times 10^{-5} \text{ m/s})(28892 \text{ s})/(0.002 \text{ m}))]$$

$$(1.8 \text{ m}^3)(753 \text{ g/m}^3)/(28892 \text{ s})$$

$$N = 0.0469 \text{ g/s}$$

TABLE 6-7. VOC EMISSION CALCULATIONS FOR A  
FLOWTHROUGH JUNCTION BOX

---

I. User Supplied Information

$$Q = 0.00252 \text{ m}^3/\text{s}$$

$$A = 0.656 \text{ m}^2$$

$$D = 0.91 \text{ m}$$

II. Defaults

A. Depth - User has supplied the depth above.

B. Concentration (see Table 6-2)

$$C_{\text{benzene}} = 10.29 \text{ g/m}^3$$

C. Emission Model Parameters

$$U_{10} = 4.47 \text{ m/s}$$

$$T = 25^\circ\text{C} \quad (298^\circ\text{K})$$

$$J = 3 \text{ lb/hp-hr}$$

$$\text{POWR} = 0.75 \text{ hp/1,000 ft}^3(\text{v})$$

$$O_t = 0.83$$

$$V_{a_v} = 1.0 \text{ (A)}$$

$$d = 61 \text{ cm}, d^* = 2 \text{ ft}$$

$$w = 126 \text{ rad/s}$$

$$N_s = 1$$

$$MW_L = 18 \text{ g/gmol}$$

TABLE 6-7. VOC EMISSION CALCULATIONS FOR A  
FLOWTHROUGH JUNCTION BOX (continued)

III. Pollutant Physical Property Data and Water, Air, and Other Properties

A. Benzene

$$D_{w, \text{benzene}} = 9.8 \times 10^{-6} \text{ cm}^2/\text{s}$$

$$D_{a, \text{benzene}} = 0.088 \text{ cm}^2/\text{s}$$

$$H_{\text{benzene}} = 0.0055 \text{ atm m}^3/\text{gmol}$$

B. Water, Air, and Other Properties

$$\rho_a = 1.2 \times 10^{-3} \text{ g/cm}^3$$

$$\rho_L = 1 \text{ g/cm}^3 (62.4 \text{ lb}_m/\text{ft}^3)$$

$$\mu_a = 1.81 \times 10^{-4} \text{ g/cm-s}$$

$$D_{O_2, w} = 2.4 \times 10^{-5} \text{ cm}^2/\text{s}$$

$$R = 8.21 \times 10^{-5} \text{ atm-m}^3/\text{gmol}$$

IV. Calculate Individual Mass Transfer Coefficients

A. Calculate  $k_l$  (see Table 4-4)

$$k_l \text{ (m/s)} = [(8.22 \times 10^{-9})J(\text{POWR})(1.024)^{T-20}O_t(10^6) \\ MW_L/(V a_v \rho_L)](D_w/D_{O_2, w})^{0.5}$$

1) Calculate POWR:

$$\text{POWR (hp)} = 0.75 \text{ hp}/1,000 \text{ ft}^3 \text{ (V)}$$

$$V \text{ (ft}^3\text{)} = A \cdot D = (0.656 \text{ m}^2)(0.91 \text{ m}) (35.31 \text{ ft}^3/\text{m}^3)$$

$$V = 21.08 \text{ ft}^3$$

$$\text{POWR (hp)} = (0.75 \text{ hp}/1,000 \text{ ft}^3)(21.08 \text{ ft}^3)$$

$$\text{POWR} = 0.0158 \text{ hp}$$



TABLE 6-7. VOC EMISSION CALCULATIONS FOR A  
FLOWTHROUGH JUNCTION BOX (continued)

2) Calculate  $Va_v$ :

$$Va_v \text{ (ft}^2\text{)} = 1.0 A$$

$$Va_v \text{ (ft}^2\text{)} = 1.0(0.656 \text{ m}^2)(10.76 \text{ ft}^2/\text{m}^2)$$

$$Va_v = 7.06 \text{ ft}^2$$

$$k_l \text{ (m/s)} = [(8.22 \times 10^{-9})(3 \text{ lb}_{\text{O}_2}/\text{hp-hr})(0.0158 \text{ hp})(1.024)^{(25-20)}(0.83) \\ (10^6)(18 \text{ g/gmol})/(7.06 \text{ ft}^2)(1 \text{ g/cm}^3)]] \\ [(9.8 \times 10^{-6} \text{ cm}^2/\text{s})/(2.4 \times 10^{-5} \text{ cm}^2/\text{s})]^{0.5}$$

$$k_l \text{ (m/s)} = (0.000928)(0.639)$$

$$k_l = 5.93 \times 10^{-4} \text{ m/s}$$

B. Calculate  $k_g$  (see Table 4-3)

$$k_g \text{ (m/s)} = 4.82 \times 10^{-3} U_{10}^{0.78} Sc_g^{-0.67} d_e^{-0.11}$$

1) Calculate Schmidt Number on the gas side,  $Sc_g$ :

$$Sc_g = \mu_g/(\rho_g D_g)$$

$$Sc_g = (1.81 \times 10^{-4} \text{ g/cm-s})/[(1.2 \times 10^{-3} \text{ g/cm}^3)(0.088 \text{ cm}^2/\text{s})]$$

$$Sc_g = 1.71$$

2) Calculate the effective diameter,  $d_e$ :

$$d_e \text{ (m)} = (4A/\pi)^{0.5}$$

$$d_e \text{ (m)} = (4(0.656)/\pi)^{0.5}$$

$$d_e = 0.914 \text{ m}$$

$$k_g \text{ (m/s)} = 4.82 \times 10^{-3} (4.47 \text{ m/s})^{0.78} (1.71)^{-0.67} (0.914 \text{ m})^{-0.11}$$

$$k_g = 0.0109 \text{ m/s}$$

TABLE 6-7. VOC EMISSION CALCULATIONS FOR A  
FLOWTHROUGH JUNCTION BOX (continued)

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V. Calculate Equilibrium Mass Transfer Coefficient

$$K_{eq} = H/RT$$

$$K_{eq} = (0.0055 \text{ atm-m}^3/\text{gmol}) / [(8.21 \times 10^{-5} \text{ atm-m}^3/\text{gmol-}^\circ\text{K})(298^\circ\text{K})]$$

$$K_{eq} = 0.225$$

VI. Calculate the Overall Mass Transfer Coefficient

$$1/K \text{ (m/s)} = 1/k_l + 1/(k_g K_{eq})$$

$$1/K \text{ (m/s)} = 1/(5.93 \times 10^{-4} \text{ m/s}) + 1/[(0.0109 \text{ m/s})(0.225)]$$

$$K = 4.78 \times 10^{-4} \text{ m/s}$$

VII. Calculate VOC Emissions for a Flowthrough Junction Box

$$N \text{ (g/s)} = KAQCo / (Q + KA)$$

$$N \text{ (g/s)} = (4.78 \times 10^{-4} \text{ m/s})(0.656 \text{ m}^2)(0.00252 \text{ m}^3/\text{s})(10.29 \text{ g/m}^3) /$$

$$[0.00252 \text{ m}^3/\text{s} + (4.78 \times 10^{-4} \text{ m/s})(0.656 \text{ m}^2)]$$

$$N = 0.00287 \text{ g/s}$$

TABLE 6-8. VOC EMISSION CALCULATIONS FOR A  
FLOWTHROUGH WEIR

---

I. User Supplied Information

$$Q = 0.00252 \text{ m}^3/\text{s}$$

$$h = 4 \text{ ft}$$

II. Defaults

A. Depth - User has supplied the depth above.

B. Concentration (see Table 6-2)

$$C_{0,\text{benzene}} = 10.29 \text{ g/m}^3$$

C. Emission Model Parameters

$$T = 25^\circ\text{C} \quad (298^\circ\text{K})$$

III. Pollutant Physical Property Data and Water, Air, and Other Pollutants

A. Benzene

$$D_{w,\text{benzene}} = 9.8 \times 10^{-6} \text{ cm}^2/\text{s}$$

B. Water, Air, and Other Properties

$$D_{02,w} = 2.4 \times 10^{-5} \text{ cm}^2/\text{s}$$

VI. Calculate Overall Mass Transfer Coefficient

$$K_D = 0.16h[D_w/D_{02,w}]^{0.75}$$

$$K_D = 0.16(4 \text{ ft})[(9.8 \times 10^{-6} \text{ cm}^2/\text{s})/(2.4 \times 10^{-5} \text{ cm}^2/\text{s})]^{0.75}$$

$$K_D = 0.327$$

TABLE 6-8. VOC EMISSION CALCULATIONS FOR A  
FLOWTHROUGH WEIR (continued)

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VII. Calculate VOC Emissions for a Flowthrough Weir

$$N \text{ (g/s)} = [1 - \exp(-K_d)]QCo$$

$$N \text{ (g/s)} = [1 - \exp(-0.327)](0.0025 \text{ m}^3/\text{s})(10.29 \text{ g/m}^3)$$

$$N = 0.00718 \text{ g/s}$$

## 6.1 REFERENCES

1. Industrial Wastewater Volatile Organic Compound Emissions -- Background Information for BACT/LAER Determinations. REVISED DRAFT. U. S. Environmental Protection Agency, Control Technology Center, Research Triangle Park, North Carolina, January 1989.
2. Hazardous Waste TSDF - Background Information for Proposed RCRA Air Emission Standards Volume 2. U.S. Environmental Protection Agency Office of Air Quality Planning and Standards, March 1988.

APPENDIX A  
INDUSTRIAL CATEGORIES

Appendix A contains a listing of the industrial categories covered by the DSS. Each category is broken down into several subcategories which are labeled by SIC code. Because there may be more than one SIC code for each category, an industrial category code has been assigned to each industrial category to alleviate any confusion.

Industrial Category Code: 1

Category Name: Adhesives and Sealants - Manufacture of household and industrial adhesives and sealants.

<u>Subcategory</u>	<u>SIC Code</u>
Animal Glues and Other Protein Adhesives	2891
Starch Adhesives	2891
Synthetic Resin Adhesives - Rigid Thermosets	2891
Synthetic Resin Adhesives - Rubbery Thermosets	2891
Synthetic Resin Adhesives - Thermoplastics	2891
Copolymers and Mixtures	2891
Inorganic Adhesives	2891
Other Adhesives	2891



Industrial Category Code: 2

Category Name: Battery Manufacturing - Facilities engaged in the manufacture of primary and/or storage batteries.

<u>Subcategory</u>	<u>SIC Code</u>
Cadmium	3691 3692
Calcium	3691 3692
Lead	3691 3692
Lecclanche	3691 3692
Lithium	3691 3692
Magnesium	3691 3692
Zinc	3691 3692
Mercury	3691 3692
Other	3691 3692

Industrial Category Code: 3

Category Name: Coal, Oil, Petroleum Products, and Refining: - Petroleum refining, and production of paving, roofing, and lubricating materials.

<u>Subcategory</u>	<u>SIC Code</u>
Coal Coking and Oil and Tar Recovery	2951 2992 2999
Coal Tar Distillation	2951 2992 2999
Coal Gasification	2951 2992 2999
Coal Liquefaction	2951 2992 2999
Petroleum Distillation/ Fractionation-Fuel Gas Production	2911
Petroleum Distillation/ Fractionation-Light Distillates	2911
Petroleum Distillation/ Fractionation-Intermed. Prod. Distillates	2911
Petroleum Distillation/ Fractionation - Heavy Distillates	2911
Crude Feedstock Conversion to Petrochemical Production and Integrated Plants	2911

Industrial Category Code: 4

Category Name: Dye Manufacture and Formulation - Manufacture of chemicals which impart color to fabrics or other materials with which they come into contact.

<u>Subcategory</u>	<u>SIC Code</u>
Acid Dyes	2865
Azo Dyes	2865
Basic Dyes	2865
Direct Dyes	2865
Disperse Dyes	2865
Fiber-Reactive Dyes	2865
Fluorescent Dyes	2865
Mordant Dyes	2865
Solvent Dyes	2865
Vat Dyes	2865
Other Dyes	2865
Organic Pigments	2865

Industrial Category Code: 5

Category Name: Electrical and Electronic Components - Manufacture of components that enable devices to utilize electricity.

<u>Subcategory</u>	<u>SIC Code</u>
Semiconductors	3674
Electronic Crystals	3679 3339
Cathode Ray Tubes	3672 3673 3693
Receiving and Transmitting Tubes	3671 3673
Luminescent Materials	3641
Carbon and Graphite Products	3624
Transformers	3612 3677
Fuel Cells	3679
Electric Lamps	3641

Industrial Category Code: 6

Category Name: Electroplating/Metal Finishing - Industries engaged in electroplating, fabricating, and finishing of ferrous and nonferrous metal products.

<u>Subcategory</u>	<u>SIC Code</u>
Electroplating	3471
Electroless Plating	3679
Anodizing	3471
Coatings	3479
Chemical Etching and Milling	3479
Printed Circuit Board Manufacturing	3679
Cleaning/Degreasing	3471
Heat Treating	3398
Stamping	3465 3466 3469
Metal Fabrication/Metal Products Manufacture	3421 3422 3423 3425 3429 3433 3441 3442 3443 3444 3446 3448 3449 3451 3452 3493 3494 3495 3496 3498 3499 3910 3911 3914 3931 3961 3964

Industrial Category Code: 7

Category Name: Equipment Manufacture and Assembly - All activities relating to the manufacture and assembly of equipment, except those activities covered by other categories (e.g., electroplating/metal finishing operations).

<u>Subcategory</u>	<u>SIC Code</u>
Fabricated Metal products	all 3400 SIC codes, N.E.C. <sup>a</sup>
Machinery, Except Electrical	all 3500 SIC codes, N.E.C.
Electric and Electronic Equipment	all 3600 SIC codes, N.E.C.
Transportation Equipment	all 3700 SIC codes, N.E.C.
Instruments and Related Products	all 3800 SIC codes, N.E.C.
Miscellaneous Metal Products	2500 2520 2522 2540 3993

<sup>a</sup>N.E.C. = Not elsewhere classified.

Industrial Category Code: 8

Category Name: Explosives Manufacture - Manufacture, load, assemble, and pack (LAP) of explosives, initiating compounds and propellants.

<u>Subcategory</u>	<u>SIC Code</u>
Manufacture and Load, Assemble, and Pack (LAP) of Initiating Compounds	2892
Manufacture of Propellants	2892
Manufacture of Explosives	2892
Formulation and Packaging of Blasting Agents, Slurry Explosives and Pyrotechnics	2899
Load, Assemble, and Pack of Explosive Devices	2892
Load, Assemble, and Pack of Small Arms Ammunition	3482
Load, Assemble, and Pack of Other Ammunition	3483

Industrial Category Code: 9

Category Name: Gum and Wood Chemicals, Varnishes, Lacquers, and Related Oils - Industries which manufacture chemical products derived from wood, as well as oil and resin products applied to wood.

<u>Subcategory</u>	<u>SIC Code</u>
Char and Charcoal Products	2861
Gum Resin and Turpentine	2861
Wood Resin, Turpentine, and Pine Oil	2861
Tall Oil Resin, Fatty Acids, and Pitch	2861
Sulfate Turpentine (Turpentine from Spent Kraft Mill Liquors)	2861
Lignin, Cellulose, and Derivatives of Spent Pulping Liquors	2861
Other Gum and Wood Chemicals	2861
Linseed Oil and Other Drying Oils	2851
Oleoresinous Varnishes	2851
Spirit Varnishes, Shellac	2851
Enamels	2851
Lacquers	2851



Industrial Category Code: 10

Category Name: Industrial and Commercial Laundries - Laundering of garments, linens, household fabrics, and industrial fabrics.

<u>Subcategory</u>	<u>SIC Code</u>
Power Laundries, Family and Commercial	7211
Linen Supply	7213
Diaper Service	7214
Coin-Op Laundries and Dry Cleaning	7215
Dry Cleaning Plants, Except Rug Cleaning	7216
Carpet and Upholstery Cleaning	7217
Industrial laundries	7218
Laundry and Garment Services, not elsewhere classified	7219
Miscellaneous Laundries	7210

Industrial Category Code: 11

Category Name: Ink Manufacture and Formulation - Manufacture and formulation of chemicals applied to paper or other materials in printing operations.

<u>Subcategory</u>	<u>SIC Code</u>
Printing Inks	2893
Letterpress, Dry Offset, and Lithograph	2893
Radiation Cure Inks	2893
Flexographic and Rotogravure Inks	2893
Other Inks	2893

Industrial Category Code: 12

Category Name: Inorganic Chemicals Manufacturing - Industries which manufacture inorganic chemicals.

<u>Subcategory</u>	<u>SIC Code</u>
Acids	2819
Alkalies, Chlorine, Chlorine Chemicals	2812
Sodium, Potassium, Calcium and Magnesium Salts	2819
Inorganic Pigments	2816
Other Metal Salts	2819
Other Metal Oxides	2819
Nitrogen Inorganic	2819
Phosphorus and Phosphate Chemicals	2819
Silicon Chemicals	2819
Uranium and Radioactive Materials Manufacturing and Processing	2819
Boron Chemicals	2819
Miscellaneous Inorganic Chemicals	2810 2819
Industrial Gases	2813

Industrial Category Code: 13

Category Name: Iron and Steel Manufacturing and Forming - Industries engaged in the manufacture (including casting) and forming of ferrous metals.

<u>Subcategory</u>	<u>SIC Code</u>
Cokemaking	3312
Sintering	3312
Ironmaking	3312
Steelmaking	3312 3313
Vacuum Degassing	3312 3313
Continuous Casting	3312
Hot Forming	3312 3315 3317 3493
Salt Bath Descaling	3312
Acid Pickling	3312
Cold Forming	3315 3316 3317
Alkaline Cleaning	3312
Hot Coating	3312 3479
Electrometallurgical/Metallothermic Products	3313
Iron and Steel Forgings	3462 3312
Iron and Steel Casting	3321 3322 3324 3325
Miscellaneous Iron and Steel Operations	3300

Industrial Category Code: 14

Category Name: Leather Tanning and Finishing - Hair removal, tanning, retanning, finishing, and products processing of animal hides.

<u>Subcategory</u>	<u>SIC Code</u>
Hair Pulp, Chrome Tan, Retan, Wet Finish	3111
Hair Save, Chrome Tan, Retan, Wet Finish	3111
Hair Save, Nonchrome Tan, Retan, Wet Finish	3111
Retan, Wet Finish	3111
No Beamhouse	3111
Through-the-blue	3111
Shearling	3111
Pigskin	3111
Retan, Wet Finish-Splits	3111
Leather Products Processing	3100 3131 3140 3144 3149 3171 3172

Industrial Category Code: 15

Category Name: Nonferrous Metals Forming - Rolling, drawing, and extruding of metals (including copper and aluminum).

<u>Subcategory</u>	<u>SIC Code</u>
Copper/Aluminum Metal Powder Production and Powder Metallurgy	3399
Other Nonferrous Metals Forming	3350 3356 3497
Aluminum Forming	3353 3355 3354 3463
Copper Forming	3351 3357

Industrial Category Code: 16

Category Name: Nonferrous Metals Manufacturing - Facilities engaged in manufacture (including casting) of nonferrous metals.

<u>Subcategory</u>	<u>SIC Code</u>
Aluminum Casting	3361
Copper and Copper Alloy Casting	3362
Magnesium Casting	3369
Zinc Casting	3369
Primary Smelting and Refining of Copper	3331
Primary Smelting and Refining of Lead	3332
Primary Smelting and Refining of Zinc	3333
Primary Production of Aluminum	3334
Primary Smelting and Refining of Other Nonferrous Metals	3339
Secondary Smelting and Refining of Nonferrous Metals	3341
Other Nonferrous Metals Casting	3369

Industrial Category Code: 17

Category Name: Organic Chemicals Manufacturing - Manufacture of basic organic chemical feedstocks, (solvents and intermediates) and the manufacture of organometallics and other organic chemicals.

<u>Subcategory</u>	<u>SIC Code</u>
Solvents - Alcohol	2869
Solvents - Aliphatic Hydrocarbons	2869
Solvents - Alkyl Halides	2869
Solvents - Amines	2869
Solvents - Aromatic Hydrocarbons	2869
Solvents - Halogenated Aromatics	2869
Solvents - Esters	2869
Solvents - Glycol Ethers	2869
Solvents - Ketones	2869
Cyclic Intermediates	2869
Fermentation Products	2869
Organometallics	2869
Rubber and Plastics in Additives Manufacture	2869



Industrial Category Code: 18

Category Name: Paint Manufacture and Formulation - Industries engaged in formulating paints by mixing various constituent chemicals (solvents, drying oils, pigment extenders, etc.).

<u>Subcategory</u>	<u>SIC Code</u>
Paint Formulation - Water Based Paints	2851
Paint Formulation - Solvent-Based Paints	2851

Industrial Category Code: 19

Category Name: Pesticides Manufacture - Manufacture of compounds containing any technical grade ingredient used to control, prevent, destroy, repel, or mitigate pests.

<u>Subcategory</u>	<u>SIC Code</u>
Phosphates and Phosponates	2879
Ureas and Uracils	2879
Miscellaneous Pesticides	2879
Phosphorothioates	2879
Phosphorodithioates	2879
Other Organophosphates	2879
Carbamates, Thiocarbamates, and Dithiocarbamates	2879
Amides, Anilides, Imides, and Hydrazides	2879
Other Nitrogen Containing Compounds	2879
Triazines	2879
Amines, Nitro Compounds, and Quaternary Ammonium Compounds	2879
DDT and Related Compounds	2879
Chlorophenoxy Compounds	2879
Aldrin-Toxaphene Group	2879
Dihaloaromatic Compounds	2879
Highly Halogenated Compounds	2879

Industrial Category Code: 20

Category Name: Pharmaceutical Manufacturing - Production and processing of medicinal chemicals and pharmaceutical products.

<u>Subcategory</u>	<u>SIC Code</u>
Fermentation Products	2833
Extraction Products	2831 2833
Chemical Synthesis Products	2833
Mixing/Compounding and Formulation Processes	2834
Other	2830 2833

Industrial Category Code: 21

Category Name: Photographic Chemicals and Film Manufacturing - Solution mixing, emulsion or coating solution preparation, coating, packaging, and testing.

<u>Subcategory</u>	<u>SIC Code</u>
Silver Halide Sensitized Products	3861
Diazo Sensitized Products - Aqueous	3861
Diazo Sensitized Products - Solvent	3861
Thermally Sensitized Products	3861
Photographic Chemical Products	3861

Industrial Category Code: 22

Category Name: Plastics Molding and Forming - Molding primary plastics and manufacturing plastics products.

Subcategory

SIC Code

Miscellaneous Plastics Products

3000 3070 3079

Industrial Category Code: 23

Category Name: Plastics, Resins, and synthetic Fibers Manufacturing -  
Polymerization industries manufacturing resins, fibers, and films.

<u>Subcategory</u>	<u>SIC Code</u>
Thermosetting resins and Related Fibers and Films	2821
Thermoplastic Cellulosic Resins, and Related Fibers and Film	2823 2824
Thermoplastic Cellulosic - Cellulose Esters	2823 2824
Thermoplastic Resins - Synthetic	2821
Oil Soluble Resins	2821

Industrial Category Code: 24

Category Name: Porcelain Enameling - Manufacture of porcelain enameled products.

<u>Subcategory</u>	<u>SIC Code</u>
Steel Basis Materials	3431 3469 3631 3632 3633 3639
Cast Iron Basis Materials	3431 3631
Aluminum Basis Materials	3469 3631
Copper Basis Materials	3469 3631

Industrial Category Code: 25

Category Name: Printing and Publishing - All forms of publishing, commercial printing, and services for the printing trade.

<u>Subcategory</u>	<u>SIC Code</u>
Typesetting	2791
Photoengraving	2793
Electrotyping and Stereotyping	2794
Lithographic Platemaking and Related Services	2795
Commercial Printing, Letterpress	2771 2751
Commercial Printing, Lithographic	2752
Commercial Printing, Gravure	2754
Commercial Printing, Screen	2751
Newspapers	2710 2711
Periodicals	2721
Books	2730 2731
Miscellaneous	2700 2741 2750 2753 2760 2761 2771 2790
Blankbooks, Looseleaf Binders, and Devices	2782
Bookbinding	2789



Industrial Category Code: 26

Category Name: Pulp and Paper Mills - Manufacturing wood pulp and processing wood pulp into products.

<u>Subcategory</u>	<u>SIC Code</u>
Integrated Bleached Kraft Mills	2611 2621 2631
Integrated Unbleached Kraft Mills	2611 2621 2631
Integrated Semi-Chemical Mills	2611 2621 2631 2661
Integrated Sulfite	2611 2621
Groundwood Mills	2611 2621 2646
Nonintegrated Paper Mills	2621 2631
Secondary Fiber and De-Ink Mills	2621
Pulp Molding Mills	2646
Structure Board Manufacture	2661
Paper Products Processing	2600 2620 2640 2641 2642 2643 2645 2647 2648 2649 2650 2651 2653

Industrial Category Code: 27

Category Name: Rubber Manufacture and Processing - Production of elastomers and the molding and extruding processes which convert these elastomers into usable products.

<u>Subcategory</u>	<u>SIC Code</u>
Natural Rubber Manufacture - Latex Products	3011
Synthetic Rubber Manufacture - Butadiene/Styrene Rubber	2822 3011
Synthetic Rubber Manufacture - Butadiene/Acrylonitrile Rubber	2822 3069
Synthetic Rubber Manufacture - Chloroprene Rubber	2822 3069
Synthetic Rubber Manufacture - Butyl Rubber	2822 3011
Synthetic Rubber Manufacture - Thiokol Rubber	2822 3069
Synthetic Rubber Manufacture - Urethane Rubber	2822 3069
Synthetic Rubber Manufacture - Ethylene/Propylene Polymers, Terpolymers	2822 3041
Synthetic Rubber Manufacture - Synthetic Natural Rubber (Polyisoprene, Polybutadiene)	2822 3011
Synthetic Rubber Manufacture - Urethane Rubber	2822 3069
Synthetic Rubber Manufacture - Silicone Rubber	2822 9999
Rubber Processing and Fabricating (Compounding, Coating, Molding, Extruding)	3069
Manufacture of Other Rubbers	3069

Industrial Category Code: 28

Category Name: Textile Mills - Facilities which engage in the manufacture of natural or synthetic fiber and the processing of these fibers into usable products, particularly fabrics.

<u>Subcategory</u>	<u>SIC Code</u>
Processing of Natural Fibers	2211 2221 2231 2241
Synthetic Fibers, processing Cellulose Fibers	2221 2241
Synthetic Fibers, Processing Nylon Fibers	2221 2241
Synthetic Fibers, Processing Polyester Fibers	2221 2241
Synthetic Fibers, Processing Spandex Fibers	2221 2241
Synthetic Fibers, Processing Inorganic Fibers	2221 2241
Dyeing and Finishing of Processing Textiles	2261 2262 2269
Miscellaneous Textile Mill Operations	2200 2250 2252 2253 2254 2257 2258 2260 2270 2272

Industrial Category Code: 29

Category Name: Timber Products Processing - Production of lumber, wood, and basic board materials.

<u>Subcategory</u>	<u>SIC Code</u>
Veneer and Plywood Products	2435 2436
Structural Wood Members, not elsewhere classified	2439
Particleboard Manufacturing	2492
Wet Process Hardboard Manufacturing	2499
Insulation Board Manufacturing	2661
Miscellaneous Timber Products Processing	2400 2430 2434 2490

**APPENDIX B**  
**Pollutant Physical Properties Database**

## APPENDIX B

This Appendix presents a database of 146 compounds which can be modeled using SIMS. Compound physical property data used by the emission models to estimate VOC emissions include vapor pressure (PVAP), Henry's Law Constant (H\_CONST), diffusivity in water (DIFF\_WAT), diffusivity in air (DIFF\_AIR), maximum biorate constant (KMAX), biorate half saturation constant (KS), and octanol-water coefficients (KOW). In addition, the database lists molecular weight (MOLE\_WT) and Antoine coefficients for estimating vapor pressure at different temperatures where available.

All vapor pressure data was obtained from the CHEMDAT7 compound physical property database with the exception of polychlorinated biphenols, di-N-octyl phthalate, diethyl phthalate, and butyl benzyl phthalate.<sup>1,2</sup> All Henry's Law Constants were taken from the CHEMDAT7 database. Most compound diffusivities in water and in air were obtained from CHEMDAT7. If these values were unavailable, compound diffusivities in air were calculated using the FSG Method,<sup>3</sup> and diffusivities in water were estimated using the Hayduk and Laudie Method.<sup>4</sup>

All maximum biorate constants and half saturation biorate constants were also obtained from CHEMDAT7. It is important to note, however, that CHEMDAT7 has limited literature data, and defaults were provided by a physical properties database called CHEM7.<sup>2</sup> CHEM7 estimates unavailable physical properties based on compounds of similar structure and/or functional groups.

Almost all octanol-water coefficients (KOW) were also obtained from the CHEMDAT7. The exceptions were compounds not listed in CHEMDAT7 and include di-n-octyl phthalate and trichlorobutane (1,2,3). The KOW values for these compounds were obtained from the Domestic Sewage Study<sup>5</sup> and from the following correlation<sup>6</sup> (noted by KOW and SOL in the database), respectively:

$$KOW = \exp[7.494 - \ln C_s]$$

where:

$$C_s = \text{solubility in water, gmol/m}^3$$

and:

$$C_s = PVAP / (760 H\_LAW)$$

PVAP = compound vapor pressure, mmHg

H\_LAW = Henry's Law Constant, atm m<sup>3</sup>/gmol

Solubility data was obtained from CHEMDAT7 or CHRIS Hazardous Chemical Data.<sup>7</sup>

Antoine coefficients were obtained from CHEMDAT7 and are in the following form:

$$\text{Log}_{10}\text{PVAP}(\text{mmHg}) = A - B/(T + C)$$

where:

A, B, and C = Antoine coefficients

T = temperature, °C

CAS NO	CHEMNAME	MOLE WT	PVAP	H CONST	DIFF MAT	DIFF AIR	VP COEF A	VP COEF B	VP COEF C	KM1	KS	KOM	NOTE
Units		g/mol	satg	atm-g <sup>3</sup> /mol	cm <sup>2</sup> /s	cm <sup>2</sup> /s				g/g-s	g/s <sup>3</sup>		
75-07-9	ACETAL DEHYDE	44.06	746.00000000	0.0009500000	0.00001110	0.12400	8.0050	1400.0170	291.8090	0.000028944	419.0542	2.49133 CH7	
64-19-7	ACETIC ACID	60.05	15.40000000	0.0027000000	0.00001260	0.11300	7.3070	1533.3130	222.3090	0.000038089	14.2857	0.48978 CH7	
106-26-7	ACETIC ANHYDRIDE	102.09	5.29000000	0.0000591000	0.00000933	0.23500	7.1490	1446.7180	199.8170	0.000026944	1.9323	1.00000 CH7	
67-84-1	ACETONE	58.00	286.00000000	0.0000250000	0.00001140	0.12400	7.1190	1210.3950	229.4440	0.000003611	1.1304	0.57544 CH7	
75-05-8	ACETONITRILE	41.03	90.00000000	0.0000580000	0.00001440	0.12800	7.1190	1314.4000	230.0000	0.0000042500	152.6014	0.45709 CH7	
107-02-8	ACROLEIN	56.10	244.20000000	0.0000546000	0.00001220	0.10500	2.3900	0.0000	0.0000	0.0000021667	22.9412	0.81283 CH7	
79-04-1	ACRYLAMIDE	71.09	0.01200000	0.0000000052	0.00001040	0.09700	11.2932	3939.8778	273.1600	0.0000042500	56.2388	6.32182 CH7	
79-10-7	ACRYLIC ACID	72.10	5.20000000	0.0000010000	0.00001040	0.09800	5.6250	648.6290	154.4830	0.0000026944	54.7819	2.04174 CH7	
107-13-1	ACRYLONITRILE	53.10	114.00000000	0.0000080000	0.00001340	0.12200	7.0380	1232.3360	222.4700	0.0000050000	24.0000	0.12023 CH7	
124-04-9	ADIPIC ACID	146.14	0.0002250	0.0000000005	0.00000684	0.06590	0.0000	0.0000	0.0000	0.0000026944	66.9943	1.20226 CH7	
107-10-6	ALLYL ALCOHOL	58.10	23.30000000	0.0000180000	0.00001140	0.11400	0.0000	0.0000	0.0000	0.0000048872	3.9241	1.47911 CH7	
95-55-6	ANILINE	109.12	0.51100000	0.0000347000	0.00000844	0.07740	0.0000	0.0000	0.0000	0.0000042500	68.1356	3.81533 CH7	
123-30-8	ANISOPHENOL (P)	109.12	0.89300000	0.0000197000	0.00000239	0.07740	-3.3570	699.1570	-331.3430	0.0000042500	68.1356	3.81533 CH7	
7664-41-7	ANISOL	106.12	0.89300000	0.0000197000	0.00000239	0.07740	-3.3570	699.1570	-331.3430	0.0000042500	68.1356	3.81533 CH7	
628-37-8	AMYL ACETATE (M)	17.03	7470.00000000	0.0003280000	0.00006930	0.25900	7.5547	1002.7110	247.8850	0.0000042500	15.3000	1.00000 CH7	
62-53-3	ANILINE	109.12	0.89300000	0.0000197000	0.00000239	0.07740	-3.3570	699.1570	-331.3430	0.0000042500	68.1356	3.81533 CH7	
71-43-2	BENZENE	78.10	95.20000000	0.0000240000	0.00000830	0.07000	7.3200	1731.5150	204.0490	0.0000019272	0.3381	7.94328 CH7	
54-55-3	BENZOTRIANTRACENE	228.30	0.00000015	0.00000000138	0.00000900	0.05100	6.9824	2426.6000	154.6000	0.0000008439	1.7006	407380.27780 CH7	
50-32-8	BENZOTRIANTRACENE	252.30	0.00000000	0.00000000138	0.00000900	0.05100	6.9824	2426.6000	154.6000	0.0000008439	1.7006	407380.27780 CH7	
100-44-7	BENZYL CHLORIDE	126.60	1.21000000	0.0003300000	0.00000780	0.07500	9.2455	3724.3630	273.1600	0.0000008439	1.2303	954992.58602 CH7	
111-44-4	BIS(2-CHLOROETHYL) ETHER	143.00	1.40000000	0.0000130000	0.00000750	0.06920	0.0000	0.0000	0.0000	0.0000049306	17.5674	199.52623 CH7	
39638-32-9	BIS(2-CHLOROISOPROPYL) ETHER	171.10	0.85000000	0.0001100000	0.00000641	0.06020	0.0000	0.0000	0.0000	0.0000049306	20.0021	38.01894 CH7	
117-81-7	BROMODIFENYL ETHER	390.48	0.00000020	0.0000000000	0.00000370	0.03510	0.0000	0.0000	0.0000	0.00000002139	2.2000	199526.23150 CH7	
74-83-9	BROMODIFENYL ETHER	390.48	0.00000020	0.0000000000	0.00000370	0.03510	0.0000	0.0000	0.0000	0.00000002139	2.2000	199526.23150 CH7	
74-83-9	BROMODIFENYL ETHER	390.48	0.00000020	0.0000000000	0.00000370	0.03510	0.0000	0.0000	0.0000	0.00000002139	2.2000	199526.23150 CH7	
106-99-0	BUTADIENE (1,3)	54.09	2100.00000000	0.0000000000	0.00001080	0.24900	6.8490	920.5460	238.6540	0.0000042534	15.3600	74.32347 CH7	
78-83-1	BUTANOL (1S)	74.12	10.00000000	0.0000020000	0.00000930	0.08000	7.4768	1362.3900	178.7700	0.0000021667	70.9091	5.62341 CH7	
71-36-3	BUTANOL (1S)	74.12	10.00000000	0.0000020000	0.00000930	0.08000	7.4768	1362.3900	178.7700	0.0000021667	70.9091	5.62341 CH7	
85-48-7	BUTYL BENZYL PHthalate	312.39	0.00000080	0.010800000000	0.00000480	0.04580	0.0000	0.0000	0.0000	0.000000086389	14.1364	60255.95861 CH7	
75-15-0	CARBON DISULFIDE	76.10	366.00000000	0.016800000000	0.00001000	0.10400	6.9240	1169.1100	241.5900	0.0000042534	5.8175	1.00000 CH7	
54-23-5	CARBON TETRACHLORIDE	153.80	113.00000000	0.033000000000	0.00000880	0.07800	6.9240	1242.4300	230.0000	0.00000004167	1.0000	524.80746 CH7	
59-30-7	CHLORO (F) CRESOL (M)	142.60	0.00330000	0.000000164000	0.00000760	0.07090	0.0000	0.0000	0.0000	0.000000000000	5.2902	1258.92541 CH7	
107-20-0	CHLORACETAL DEHYDE	78.50	40.00000000	0.0000260000	0.00001150	0.09900	0.0000	0.0000	0.0000	0.000000000000	49.8380	3.44050 CH7	
108-90-7	CHLOROBENZENE	112.60	11.80000000	0.003930000000	0.00000870	0.07300	6.9780	1431.0500	217.5500	0.0000001083	0.0390	316.22777 CH7	
67-66-3	CHLOROPHENOL	119.40	208.00000000	0.003390000000	0.00001000	0.10400	6.9780	929.4400	186.0300	0.00000008167	3.7215	91.20108 CH7	
91-58-7	CHLOROPHTHALIC ACID	162.51	0.01700000	0.018000000000	0.00000740	0.06530	0.0000	0.0000	0.0000	0.000000000000	2.1670	13182.56739 CH7	
126-99-8	CHLOROPHTHALIC ACID	89.50	273.00000000	0.033100000000	0.00001600	0.10400	6.1810	783.4500	179.7000	0.00000029868	6.3412	1.00000 CH7	
108-39-4	CRESOL (M)	108.10	0.08000000	0.000000443000	0.00001000	0.07400	7.5080	1856.3600	199.0700	0.0000004472	1.3653	93.32543 CH7	
95-48-7	CRESOL (P)	108.10	0.24000000	0.000002600000	0.00000830	0.07400	6.9310	1435.5000	155.1600	0.0000003278	1.3400	95.49926 CH7	
106-44-5	CRESOL (P)	108.10	0.11000000	0.000000443000	0.00001000	0.07400	7.5080	1856.3600	199.0700	0.0000004472	1.3653	93.32543 CH7	
1319-77-3	CRESYLIC ACID	108.00	0.30000000	0.0000017000	0.00000830	0.07400	0.0000	0.0000	0.0000	0.000000041667	15.0000	1.00000 CH7	
4170-30-0	CROTONAL DEHYDE	70.09	30.00000000	0.000001540000	0.00001020	0.09030	0.0000	0.0000	0.0000	0.00000026944	27.6285	12.36833 CH7	
98-82-8	CUMENE (ISOPROPYL BENZENE)	120.20	4.60000000	0.014800000000	0.00000710	0.06530	6.9350	1460.7930	207.7800	0.0000008458	16.5426	1.00000 CH7	
110-82-7	CYCLOHEXANE	84.20	100.00000000	0.017300000000	0.00000910	0.08390	6.8410	1201.5300	222.4500	0.0000042534	15.3000	338.06870 CH7	
108-93-0	CYCLOHEXANOL	100.20	1.22000000	0.000004470000	0.00000831	0.21400	6.2550	912.8700	109.1300	0.0000026944	18.0816	37.74314 CH7	
117-84-1	D1-N-OCTYL PHthalate	390.20	4.80000000	0.000000413000	0.00000862	0.07840	7.8492	2137.1920	273.1600	0.0000031917	41.8921	6.45654 CH7	
84-74-2	DIBUTYL PHthalate	278.30	0.00001000	0.137000000000	0.00000470	0.04380	6.6390	1744.2000	113.5900	0.000000000000	0.0200	141253.70000 CH7	
744-41-0	DICHLORO (2-BUTENE) (1,4)	125.00	2.80000000	0.000259000000	0.00000812	0.07250	0.0000	0.0000	0.0000	0.000000000000	9.8975	242.15420 CH7	
93-50-1	DICHLOROPHTHALIC ACID	147.00	1.50000000	0.000000000000	0.00000790	0.06940	0.0000	0.0000	0.0000	0.000000000000	4.3103	2398.83292 CH7	
54-73-1	DICHLOROPHTHALIC ACID	147.00	2.28000000	0.000000000000	0.00000790	0.06940	0.0000	0.0000	0.0000	0.000000000000	2.7826	2398.83292 CH7	
106-46-7	DICHLOROPHTHALIC ACID	147.00	1.20000000	0.000000000000	0.00000790	0.06940	0.0000	0.0000	0.0000	0.000000000000	2.7826	2454.70892 CH7	
75-71-8	DICHLORODIFLUOROMETHANE	120.92	3000.00000000	0.401000000000	0.00000000	0.000000	0.0000	0.0000	0.0000	0.000000000000	12.0413	144.54398 CH7	



CAS_NO	CHEMNAME	MOLE WT g/mol	ρ <sub>25</sub> g/cc	H_DENSITY g/cm³ @ 25°C	DIFF. MAT cm²/s	DIFF. AIR VP cm²/s	VP_COEF_B	VP_COEF_C	KNAI g/g-s	KS g/s³	YOM	NOTE
75-34-3	BICHOROTHANE (1,1)	99.00	234.0000000	0.9654000000	0.00001050	0.0000	0.0000	0.0000	0.0000029889	4.6783	61.45950 CH7	
107-04-2	BICHOROTHANE (1,2)	99.00	80.00000000	0.0012000000	0.00000990	0.10400	1272.3000	222.9000	0.0000065833	2.1429	61.45950 CH7	
154-54-2	BICHOROTHANE (1,2)	96.94	200.0000000	0.0319000000	0.00001100	0.0000	1141.9000	231.9000	0.0000029889	6.3294	1.00000 CH7	
120-83-2	BICHOROTHANE (2,4)	163.01	0.10000000	0.00000000	0.00000740	0.07070	0.0000	0.0000	0.0000069444	7.5758	362.34133 CH7	
94-75-7	BICHOROTHANE (1,2)	221.00	280.0000000	0.0210000000	0.00000449	0.05800	0.0000	0.0000	0.0000029889	14.8934	82.41445 CH7	
78-87-5	BICHOROTHANE (1,2)	112.99	40.0000000	0.0023000000	0.00000870	0.07820	6.9800	22.8000	0.0000047222	12.1429	1.00000 CH7	
91-66-7	BICHOROTHANE (1,2)	112.99	40.0000000	0.0023000000	0.00000870	0.07820	6.9800	22.8000	0.0000047222	12.1429	1.00000 CH7	
84-66-2	BICHOROTHANE (1,2)	222.00	0.0023000	0.0111000000	0.00000587	0.05130	7.4600	1993.5700	0.0000042500	27.0047	43.57596 CH7	
68-12-2	BICHOROTHANE (1,2)	73.09	4.0000000	0.0001200000	0.00001030	0.09390	6.9280	1400.8700	0.0000042500	15.3000	1.00000 CH7	
57-14-7	BICHOROTHANE (1,1)	60.10	157.0000000	0.0001200000	0.00001090	0.10400	7.0680	1305.9100	0.0000042500	15.3000	1.00000 CH7	
131-11-3	BICHOROTHANE (1,1)	194.20	0.00018700	0.0000021500	0.00000630	0.06300	4.5220	700.3100	0.0000006111	0.7097	74.13102 CH7	
57-97-4	BICHOROTHANE (1,1)	254.33	0.00000000	0.00000000027	0.00000498	0.04100	0.0000	0.0000	0.00000086389	0.3377	2860056.33087 CH7	
105-47-9	BICHOROTHANE (2,4)	122.16	0.03730000	0.0002200000	0.00000840	0.07120	0.0000	0.0000	0.0000029722	2.2766	243.02480 CH7	
99-65-0	BICHOROTHANE (1,1)	168.10	0.03000000	0.0000220000	0.00000764	0.23900	4.3370	229.2000	0.0000042500	29.9146	33.28818 CH7	
121-14-2	BICHOROTHANE (2,4)	182.10	0.00310000	0.0000407000	0.00000704	0.20300	5.7980	1118.0000	0.0000042500	19.5233	102.32930 CH7	
123-91-1	BICHOROTHANE (1,4)	88.20	37.00000000	0.0002310000	0.00001020	0.22900	7.4310	1554.5800	0.0000026944	24.7001	16.40956 CH7	
MOCS2	BIDIN	372.00	0.00000000	0.0000012000	0.00000540	0.10400	12.8800	6465.5000	0.0000029968	6.3412	1.00000 CH7	
122-39-4	BIPHENYLAMINE	169.20	0.00375000	0.0000027800	0.00000631	0.05800	0.0000	0.0000	0.0000052778	8.4103	1659.58491 CH7	
106-89-8	EPICHLOROPHYLLIN	92.50	17.00000000	0.0000375000	0.00000980	0.08600	8.2294	2086.8160	0.0000029968	6.3412	1.07152 CH7	
64-17-5	ETHANOL	46.10	50.00000000	0.0000303000	0.00001300	0.12300	8.3210	1718.2100	0.0000024444	9.7778	0.47863 CH7	
141-43-5	ETHANOLAMINE (MONO-)	61.09	0.40000000	0.0000032200	0.00001140	0.10700	7.4560	1577.6700	0.0000042500	223.0321	0.16865 CH7	
140-88-5	ETHYL ACRYLATE	106.10	10.00000000	0.0003500000	0.00000860	0.07700	7.9645	1897.0110	0.0000026944	39.4119	4.85667 CH7	
645-42-5	ETHYL CHLORIDE	64.52	1200.0000000	0.0003250000	0.00001150	0.27100	4.9840	1030.0100	0.0000042500	22.8074	26.91335 CH7	
141-78-6	ETHYLENE	88.10	100.0000000	0.0002800000	0.00000960	0.08600	0.0000	0.0000	0.0000029889	15.3000	1.00000 CH7	
100-41-4	ETHYLENE	104.20	10.00000000	0.0004400000	0.00000780	0.07500	4.9750	1424.2550	0.0000048833	17.5800	1412.53754 CH7	
75-21-8	ETHYLENE	44.00	1250.0000000	0.0001450000	0.00001450	0.10400	7.1280	1054.5400	0.0000011667	4.6154	0.50003 CH7	
60-29-7	ETHYLENE	74.10	520.0000000	0.0000800000	0.00000930	0.07400	4.9200	1044.0700	0.0000026944	17.1206	43.57596 CH7	
50-00-0	FORMALDEHYDE	30.00	3500.0000000	0.0000000000	0.00001980	0.17800	7.1950	970.6000	0.0000033889	20.0000	87.09636 CH7	
44-18-6	FORMIC ACID	46.00	42.00000000	0.0000137000	0.00001000	0.10400	7.5810	1699.2000	0.0000026944	161.3977	0.11910 CH7	
MOCS3	FURAN	120.92	5000.0000000	0.0003400000	0.00001220	0.10400	4.9750	1046.8700	0.0000026944	6.3412	1.00000 CH7	
110-00-9	FURAN	68.08	596.0000000	0.0003400000	0.00001040	0.08720	4.5750	1198.7000	0.0000026944	18.0602	37.86047 CH7	
96-01-1	FURFURAL	96.09	2.00000000	0.0000811000	0.00000711	0.18700	6.8994	1331.5300	0.0000042534	15.3000	1453.37200 CH7	
142-87-5	HEPTANE (150)	100.21	66.00000000	1.8360000000	0.00000591	0.05420	-0.8240	0.0000	0.0000029889	0.6651	295120.92267 CH7	
118-74-1	HEXACHLOROBUTADIENE	284.80	0.15000000	0.0004800000	0.00000620	0.05610	0.0000	0.0000	0.0000030000	6.3412	5495.40800 CH7	
87-48-3	HEXACHLOROBUTADIENE	284.80	0.15000000	0.0004800000	0.00000620	0.05610	0.0000	0.0000	0.0000029968	0.3412	9772.37200 CH7	
77-47-4	HEXACHLOROCYCLOPENTADIENE	272.80	0.08100000	0.0160000000	0.00000616	0.05610	0.0000	0.0000	0.0000029889	3.3876	4068.32839 CH7	
67-72-1	HEXACHLORIDE	237.00	0.65000000	0.0000024700	0.00000680	0.00249	0.0000	0.0000	0.0000029889	15.3000	534.08450 CH7	
100-54-3	HEXANE (1)	86.20	150.00000000	0.0000000000	0.00000777	0.20600	6.8760	1171.1700	0.0000042534	15.3000	59.52851 CH7	
111-27-3	HEXANE (1)	102.18	0.81200000	0.0000182000	0.00000753	0.05900	7.8600	1761.2600	0.0000026944	15.2068	1.00000 CH7	
74-90-8	HYDROXYLIC ACID	27.00	726.0000000	0.0000045500	0.00000753	0.19700	7.5280	1379.5000	0.0000026944	1.9323	1.00000 CH7	
7644-39-3	HYDROXYLIC ACID	20.00	900.0000000	0.0000000000	0.000005300	0.38800	7.2170	1268.3700	0.0000026944	1.9323	1.00000 CH7	
7783-06-4	HYDROGEN SULFIDE	34.10	15200.0000000	0.0000000000	0.00001510	0.17600	7.6140	885.3190	0.0000029889	6.2294	1.00000 CH7	
78-59-1	ISOPHORONE	138.21	0.43500000	0.0000057600	0.00000676	0.06230	0.0000	0.0000	0.0000042500	25.6667	50.11872 CH7	
67-56-1	METHANOL	32.00	114.00000000	0.0000025000	0.00001640	0.15000	7.8970	1474.0800	0.0000050000	90.0000	0.19953 CH7	
79-20-9	METHYL ACETATE	74.10	275.0000000	0.0000000000	0.00001640	0.15000	7.8970	1474.0800	0.0000055194	159.2466	0.81783 CH7	
74-87-3	METHYL CHLORIDE	50.50	3830.0000000	0.0000000000	0.00000550	0.10400	7.0930	948.5800	0.0000029889	14.8550	83.17638 CH7	
108-10-1	METHYL ISOBUTYL FETONE	100.20	15.70000000	0.0004450000	0.00000730	0.07500	6.9742	129.9600	0.0000026944	1.6383	1.90346 CH7	
80-62-6	METHYL METHACRYLATE	100.10	36.00000000	0.0004450000	0.00000730	0.07500	6.9742	129.9600	0.0000026944	1.6383	23.98833 CH7	
98-83-9	METHYL STYRENE (ALPHA)	118.00	0.07500000	0.0004450000	0.00000730	0.07500	6.9742	129.9600	0.0000026944	1.6383	23.98833 CH7	
75-09-2	METHYLENE CHLORIDE	85.00	4.80000000	0.0004450000	0.00000730	0.07500	6.9742	129.9600	0.0000026944	1.6383	23.98833 CH7	
110-91-8	MORPHOLINE	87.12	16.00000000	0.0004450000	0.00000730	0.07500	6.9742	129.9600	0.0000026944	1.6383	23.98833 CH7	

CAS_NO Units	CHEMNAME	MOLE_WT g/mol	PWAP mwh	N_CONST atm-s <sup>3</sup> /g <sup>3</sup>	DIFF_INT cm <sup>2</sup> /s	DIFF_AIR cm <sup>2</sup> /s	VP_COEF_A	VP_COEF_B	VP_COEF_C	KMAI g/g-s	KS g/s <sup>3</sup>	KOM -	NOTE
91-20-3	NAPHTHALENE	128.20	0.23000000	0.0011800000	0.0000750	0.05900	7.0100	1733.7100	201.8400	0.0000117972	42.4700	1.00000	CH7
98-74-4	1-METHYLNAPHTHALENE (1-D)	138.14	0.00300000	0.0000005000	0.0000000	0.07100	8.8400	334.3000	273.1600	0.0000042500	22.8535	67.60030	CH7
98-95-3	2-METHYLNAPHTHALENE	128.14	0.00300000	0.0000005000	0.0000000	0.07100	7.1150	1746.4000	201.8000	0.0000030556	4.7826	69.18310	CH7
608-93-5	PENTACHLOROBENZENE	250.34	0.00400000	0.0030000000	0.0000030	0.05700	0.0000	0.0000	0.0000	0.0000029889	0.4307	925987.02902	CH7
76-01-7	PENTACHLOROTHRANE	202.30	4.40000000	0.0210000000	0.00000730	0.04600	6.7400	1378.0000	197.0000	0.0000029889	0.4307	925987.02902	CH7
97-86-5	PENTACHLOROPHENOL	246.40	0.00090000	0.0000028000	0.00000410	0.05600	0.0000	0.0000	0.0000	0.0000036111	38.2353	102329.29923	CH7
108-95-2	PHENOL	94.10	0.34000000	0.0000005400	0.00000910	0.08200	7.1330	1516.7900	174.9500	0.0000269444	7.4815	28.84032	CH7
75-44-3	PHOSGENE	98.92	1390.00000000	0.1710000000	0.0000112	0.10800	6.8420	941.2500	230.0000	0.0000042500	70.8664	3.44050	CH7
100-21-0	PHthalic ACID	146.14	121.00000000	0.0132000000	0.00000480	0.04400	0.0000	0.0000	0.0000	0.0000026944	34.9830	6.44623	CH7
85-44-9	PHthalic ANHYDRIDE	148.10	0.00150000	0.0000009000	0.00000860	0.07100	8.8220	2848.3000	273.1600	0.0000048872	3.9241	0.23988	CH7
108-99-6	PICOLINE (1-2)	93.12	10.40000000	0.0001270000	0.00000960	0.07500	7.0320	1415.7300	211.6300	0.0000042500	44.8286	11.48154	CH7
1334-34-3	POLYCHLORINATED BIPHENYLS	290.00	0.00185000	0.0040000000	0.0001000	0.10400	0.0000	0.0000	0.0000	0.0000052780	20.0000	1.00000	CH7
71-23-0	PROPANOL (1SD)	60.09	42.80000000	0.0001500000	0.00001040	0.09800	8.1170	1580.9200	219.6100	0.0000041667	200.0000	0.8183	CH7
123-38-6	PROPYLALDEHYDE	58.08	300.00000000	0.0011500000	0.00001140	0.10200	16.2315	2639.0200	-44.1500	0.0000026944	39.2284	4.91668	CH7
57-55-6	PROPYLENE GLYCOL	76.11	0.30000000	0.0000015000	0.00001020	0.09300	8.2082	2085.9000	203.5396	0.0000026944	109.3574	0.33141	CH7
75-66-9	PROPYLENE OXIDE	58.10	575.00000000	0.0013400000	0.0001000	0.07600	8.2748	1654.8840	273.1600	0.0000048872	3.9241	1.00000	CH7
110-86-1	PYRIDINE	79.10	20.00000000	0.0000236000	0.00000760	0.09100	7.0410	1373.8000	214.9800	0.000007306	146.9139	4.46884	CH7
108-44-3	RESORCINOL	110.11	0.00076000	0.0000001880	0.00000870	0.07800	6.9243	1884.5470	184.0596	0.0000026944	35.4809	4.30957	CH7
100-42-5	STYRENE	104.20	7.30000000	0.0026100000	0.00000800	0.07100	7.1400	1574.3100	229.7400	0.0000086389	282.7273	1445.43977	CH7
630-20-6	TETRACHLORIDE THANE (1,1,1,2)	167.85	6.50000000	0.0070000000	0.00000790	0.07100	6.8980	1365.8800	204.0900	0.0000029889	6.3294	1.00000	CH7
79-34-5	TETRACHLORIDE THANE (1,1,2,2)	167.85	6.50000000	0.0038000000	0.00000790	0.07100	6.4310	1228.1000	179.9000	0.0000017222	9.1176	363.07805	CH7
127-18-4	TETRACHLORIDE THYLENE	187.38	19.00000000	0.0290000000	0.00000820	0.07200	6.9800	1386.9200	217.5300	0.0000061722	9.1176	398.10717	CH7
109-99-9	TETRAHYDROFURAN	72.12	72.10000000	0.0000490000	0.0001050	0.09800	6.9950	1202.2900	226.2500	0.0000026944	20.3702	27.58221	CH7
109-98-3	TOLUENE	92.40	30.00000000	0.0000000000	0.00000860	0.08700	6.9240	1344.8000	219.4800	0.0000204111	30.6167	489.77882	CH7
584-84-9	TOLUENE DITSOXYMETHYLENE (2,4)	174.16	0.08000000	0.0000002000	0.00000620	0.06100	0.0000	0.0000	0.0000	0.0000042500	15.3000	1.00000	CH7
74-13-1	TRICHLORO (1,1,2) TRIFLUORIDE THANE	187.38	300.00000000	0.4750000000	0.00000820	0.07800	6.8800	1099.9000	227.5000	0.0000029889	3.3876	4068.37838	CH7
120-82-1	TRICHLOROBENZENE (1,2,4)	181.50	6.18000000	0.0014200000	0.00000770	0.06600	0.0000	0.0000	0.0000	0.0000029889	7.4495	9549.92586	CH7
MOCAS5	TRICHLOROBUTANE (1,2,3)	161.46	4.35000000	0.0040000000	0.00000720	0.06600	0.0000	0.0000	0.0000	0.0000029889	6.3412	1450901.04626	SOL
71-33-6	TRICHLORIDE THANE (1,1,1)	133.40	123.00000000	0.0049200000	0.00000880	0.07800	8.4430	2136.6000	302.8000	0.0000009722	4.7297	309.02954	CH7
74-80-5	TRICHLORIDE THANE (1,1,2)	133.40	25.00000000	0.0067420000	0.00000910	0.07800	6.9510	1314.4100	209.2000	0.0000009722	4.7297	1.00000	CH7
75-69-4	TRICHLORIDE THYLENE	131.40	75.00000000	0.0091000000	0.00000970	0.07900	6.5180	1018.6000	192.7000	0.0000010833	4.4318	194.98446	CH7
88-06-2	TRICHLOROPROPYLENE (2,4,6)	137.40	796.00000000	0.0523000000	0.00000970	0.08700	6.8840	1043.0040	236.8800	0.0000030000	6.3412	338.84410	CH7
MOCAS6	TRICHLOROPROPYLENE (1,1,1)	197.46	0.00730000	0.0000177000	0.00000750	0.06610	0.0000	0.0000	0.0000	0.0000042500	58.8462	4897.78819	CH7
76-18-4	TRICHLOROPROPANE (1,2,3)	147.43	3.10000000	0.0290000000	0.00000790	0.07100	0.0000	0.0000	0.0000	0.0000029889	10.7719	193.78270	CH7
57-13-6	UREA	60.06	3.00000000	0.0002840000	0.00000790	0.07100	6.9030	788.2000	243.2300	0.0000029889	10.7719	193.78270	CH7
108-03-4	VINYL ACETATE	86.09	115.00000000	0.0002840000	0.00001370	0.12200	0.0000	0.0000	0.0000	0.0000042500	4.8189	4068.37838	CH7
75-01-4	VINYL CHLORIDE	62.50	2680.00000000	0.0800000000	0.00000920	0.08500	7.2100	1296.1300	226.6400	0.0000026944	31.8363	9.51722	CH7
75-35-4	VINYLIDENE CHLORIDE	97.00	591.00000000	0.0050000000	0.00001230	0.10600	3.4250	0.0000	0.0000	0.0000030000	6.3412	1.14815	CH7
1330-20-7	VYLENE (H)	106.17	8.00000000	0.0052000000	0.00001040	0.09000	6.9700	1099.4000	237.2000	0.0000029968	6.3412	1.00000	CH7
95-47-6	VYLENE (D)	106.17	7.00000000	0.0052000000	0.00000780	0.07000	7.0090	1426.2660	213.1100	0.0000086389	14.0094	1584.89319	CH7
					0.00001000	0.08700	6.9980	1474.6790	213.6900	0.0000113306	22.8569	891.25094	CH7

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16. ABSTRACT  This document presents a brief description of the operation and design of surface impoundments and background information on the development of the Surface Impoundments Modeling System (SIMS). The SIMS was developed with funding from the U. S. Environmental Protection Agency's (EPA) Control Technology Center (CTC) and with project management provided by EPA's Technical Support Division of the Office of Air Quality Planning and Standards. SIMS is based on emission models developed by the Emission Standards Division (ESD) during the evaluation of surface impoundments located in treatment, storage, and disposal facilities (TSDF). The purpose of this latest update to SIMS is to add models for diffused air systems and several collection system devices, and to expand the compound database from 40 to 150. This technical document discusses these emission models, surface impoundment design and operation, default parameter development, and the emission estimation procedure. Another document entitled, <u>SIMS Version 2.0 User's Manual</u> , EPA-450/4-90-019a, presents a complete reference for all features and commands in the SIMS PC program.		
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