VOLUME II: CHAPTER 5

PREFERRED AND ALTERNATIVE METHODS FOR ESTIMATING AIR EMISSIONS FROM WASTEWATER COLLECTION AND TREATMENT

Final Report

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DISCLAIMER

As the Environmental Protection Agency has indicated in Emission Inventory Improvement Program (EIIP) documents, the choice of methods to be used to estimate emissions depends on how the estimates will be used and the degree of accuracy required. Methods using site-specific data are preferred over other methods. These documents are non-binding guidance and not rules. EPA, the States, and others retain the discretion to employ or to require other approaches that meet the requirements of the applicable statutory or regulatory requirements in individual circumstances.

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1

INTRODUCTION

The purposes of the preferred methods guidelines are to describe emissions estimation techniques for stationary point sources in a clear and unambiguous manner and to provide concise example calculations to aid in the preparation of emission inventories. This chapter describes the procedures and recommended approaches of estimating volatile organic compound (VOC) emissions from wastewater collection and treatment (WWCT).

Section 2 of this chapter contains a general description of the WWCT source category, a listing of common emission sources associated with WWCT, and an overview of the available air pollution control technologies for WWCT. Section 3 of this chapter provides an overview of available emission estimation methods. It should be noted that the use of site-specific emissions data is always preferred over the use of industry-averaged data such as default data, available in several of the current WWCT air emissions models. However, depending upon available resources, obtaining site-specific data may not be cost effective. Section 4 presents the preferred emission estimation methods for WWCT, while Section 5 presents alternative emission estimation techniques. Quality assurance and quality control procedures are described in Section 6, and Section 7 lists references. Appendix A contains an example data collection form for WWCT sources, and Appendix B contains the *AP-42* WWCT equations and example calculations (Environmental Protection Agency [EPA], 1995). Appendix C contains a list of references that may be consulted for more detailed, technical evaluations and comparisons of the emission estimation techniques and emissions software models discussed in this chapter.

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GENERAL SOURCE CATEGORY DESCRIPTION

2.1 SOURCE CATEGORY DESCRIPTION

This section provides a brief overview discussion of the WWCT category. In addition to wastewater generated at the municipal level, many industries generate large quantities of contaminated water as a byproduct of production processes. These wastewaters typically pass through a series of on-site collection and treatment units before discharge to a receiving water body or publicly owned treatment works (POTW). Many of these collection and treatment units are open to the atmosphere and allow for volatilization of VOCs from the wastewater.

The information presented in this document is applicable to any source, municipality, or industry treating wastewater on-site.

The following sections describe the various types of wastewater collection and treatment devices. The type of unit (collection or treatment) is provided, as is a brief description of each. Table A-1, Appendix A lists approximate physical dimensions of several units.

2.2 WWCT DEVICES

2.2.1 DRAINS (COLLECTION UNIT)

Wastewater streams from various sources throughout a given process are normally introduced into the collection system through process drains. Drains may be of a trapped or untrapped design. 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 (EPA, 1990).

2.2.2 MANHOLES (COLLECTION UNIT)

Manholes are service entrances into sewer lines that 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 4 feet to allow adequate space for workers. The upper portion tapers to the diameter of the opening at ground level. The opening is normally about 2 feet in diameter and covered with a heavy cast-iron plate with two to four holes for ventilation and for cover removal.

2.2.3 REACHES (COLLECTION UNIT)

A reach is a segment of sewer channel that conveys wastewater between two manholes or other sewer components such as lift stations or junction boxes. Sanitary sewers are naturally ventilated through holes in manhole covers, gooseneck vents (which are sometimes included to enhance ventilation), and vent risers on buildings that are connected to sewers. (Sanitary sewers are sometimes mechanically ventilated; i.e., fans or blowers are used to remove hydrogen sulfide.) Combined sanitary/storm sewers are generally well-ventilated, and include openings associated with street-level storm drains.

2.2.4 JUNCTION BOXES (COLLECTION UNIT)

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 that flows downstream from the junction box. Liquid level in the junction box depends on the flow rate of the wastewater. Junction boxes are either square or rectangular and are sized based on the flow rate of the entering streams. They may also be water-sealed or covered and vented.

2.2.5 LIFT STATIONS (COLLECTION UNIT)

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 the head pressure and is generally designed to operate or cut off based on preset high and low liquid levels.

2.2.6 TRENCHES (COLLECTION UNIT)

Trenches are 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 to accommodate 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.

2.2.7 SUMPS (COLLECTION UNIT)

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

2.2.8 WEIRS (COLLECTION UNIT)

Weirs act as dams in open channels in order to maintain constant water level upstream. 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 that influence the supply of water to the channel.

2.2.9 OIL/WATER SEPARATORS (TREATMENT UNIT)

Oil/water separators are often the first step in the wastewater treatment plant but may also be found in the process area. The purpose of these units is to separate liquid phases of different specific gravities; they also serve to remove free oil and suspended solids contained in the wastewater. Most of the separation occurs as the wastewater stream passes through a quiescent zone in the unit. Oils and scum with specific gravities less than water float to the top of the aqueous phase. Heavier solids sink to the bottom. Most of the organics contained in the wastewater tend to partition to the oil phase. For this reason, most of these organic compounds are removed with the skimmed oil leaving the separator. The wastewater stream leaving the separator, therefore, is reduced in organic loading.

2.2.10 EQUALIZATION BASINS (TREATMENT UNIT)

Equalization basins are used to reduce fluctuations in the wastewater flow rate and organic content to the downstream treatment processes and may be covered, stirred, or aerated. Equalization of wastewater flow rate results in more uniform effluent quality from downstream settling units such as clarifiers. Biological treatment performance can also benefit significantly from the damping of concentration and flow fluctuations. This damping protects biological processes from upset or failure due to shock loadings of toxic or treatment-inhibiting compounds.

2.2.11 CLARIFIERS (TREATMENT UNIT)

The primary purpose of a clarifier is to separate any oils, grease, scum, and solids contained in the wastewater. Most clarifiers are equipped with surface skimmers to clear the water of floating oil deposits and scum. Clarifiers also have sludge raking arms that prevent accumulation of organic solids collected at the bottom of the tank.

2.2.12 BIOLOGICAL TREATMENT BASINS (TREATMENT UNIT)

Biological waste treatment is normally accomplished through the use of aeration basins. Microorganisms that metabolize aerobically require oxygen to carry out the biodegradation of organic compounds that results in energy and biomass production. The aerobic environment in the basin is normally achieved by the use of diffused or mechanical aeration. This aeration also serves to maintain the biomass in a well-mixed regime. The goal is to maintain the biomass concentration at a level where the treatment is efficiently optimized and proper growth kinetics are induced.

2.2.13 SLUDGE DIGESTERS (TREATMENT UNIT)

Sludge digesters are used to treat organic sludges produced from various treatment operations. Two types of digesters are used: anaerobic digesters and aerobic digesters.

In the anaerobic digestion process, the organic material in mixtures of primary settled and biological sludges is converted biologically, under anaerobic conditions, to a variety of byproducts including methane (CH_4), carbon dioxide (CO_2), and hydrogen sulfide (H_2S). The process is carried out in an airtight reactor. Sludge, introduced continuously or intermittently, is retained in the reactor for varying periods of time. The stabilized sludge, withdrawn continuously or intermittently from the reactor, is reduced in organic and pathogen content and is nonputrescible.

In aerobic digestion, the sludge is aerated for an extended period of time in an open, unheated tank using conventional air diffusers or surface aeration equipment. The process may be operated in a continuous or batch mode. Smaller plants use the batch system in which sludge is aerated and completely mixed for an extended period of time, followed by quiescent settling and decantation. In continuous systems, a separate tank is used for decantation and concentration. High-purity oxygen aerobic digestion is a modification of the aerobic digestion process in which high-purity oxygen is used in lieu of air. The resultant sludge is similar to conventional aerobically digested sludge (Burton and Tchobanoglous, 1991).

2.2.14 TREATMENT TANKS (TREATMENT UNIT)

Flocculation tanks and pH adjustment tanks may be used for treatment of wastewater after and before biological treatment, respectively. In flocculation tanks, flocculating agents are added to the wastewater to promote formation of large-particle masses from the fine solids formed during biological treatment. These large particles will then precipitate out of the wastewater in the clarifier that typically follows. Tanks designed for pH adjustment typically precede the biological treatment step. In these tanks, the wastewater pH is adjusted, using acidic or alkaline additives, to prevent shocking of the biological system downstream.

2.2.15 SURFACE IMPOUNDMENTS (TREATMENT UNIT)

Surface impoundments are typically used for evaporation, polishing, equalization, storage prior to further treatment or disposal, leachate collection, and as emergency surge basins. They may be either quiescent or mechanically agitated.

2.2.16 AIR AND STEAM STRIPPING (TREATMENT UNIT)

Air stripping and steam stripping may be used to remove organic constituents in industrial wastewater streams prior to secondary and tertiary treatment devices.

Air stripping involves the contact of wastewater and air to strip out volatile organic constituents. As the volume of air contacting the contaminated water increases, an increase in the transfer rate of the organic compounds into the vapor phase is achieved. Removal efficiencies vary with volatility and solubility of organic impurities. For highly volatile compounds, average removal ranges from 90 to 99 percent, for medium- to low-volatility compounds, removal ranges from less than 50 to 90 percent, though a higher air flow rate may be needed (EPA, 1995).

Steam stripping is the distillation of wastewater to remove volatile organic constituents, with the basic operating principle being the direct contact of steam with wastewater. The steam provides the heat of vaporization for the more volatile organic constituents. Removal efficiencies vary with the amount of steam applied for a given wastewater flow rate and the volatility and solubility of the organic impurities. For highly volatile compounds (Henry's Law constant [HLC] greater than 10^{-3} atm-m^3/gmol), VOC removal ranges from 95 to 99 percent and can easily be achieved with a sufficient amount of steam. For medium-volatility compounds (HLC between 10^{-5} and 10^{-3} atm-m^3/gmol), average VOC removal ranges from 90 to 95 percent and would require more steam than needed for more volatile compounds. For low-volatility compounds (HLC less than 10^{-5} atm-m^3/gmol), average removal ranges from less than 50 to 90 percent (EPA, 1995).

2.3 EMISSION SOURCES

Wastewater streams are collected and treated in a variety of ways. Many of these collection and treatment system units are open to the atmosphere and allow organic-containing wastewaters to contact ambient air. Whenever this happens, there is a potential for VOC emissions. The organic pollutants volatilize in an attempt to exert their equilibrium partial pressure above the wastewater. In doing so, the organics are emitted to the ambient air surrounding the collection and treatment units. The magnitude of VOC emissions depends greatly on many factors such as the physical properties of the pollutants, pollutant concentration, flow rate, the temperature of the wastewater, and the design of the individual collection and treatment units. All of these factors, as well as the general scheme used to collect and treat facility wastewater, have a major effect on VOC emissions.

Collection and treatment schemes are facility specific. The flow rate and organic composition of wastewater streams at a particular facility are functions of the processes used. The wastewater flow rate and composition, in turn, influence the sizes and types of collection and treatment units that must be employed at a given facility.

Figure 5.2-1 illustrates a typical scheme for collecting and treating process wastewater generated at a facility and the opportunity for volatilization of organics.

Drains are often open to the atmosphere and provide an opportunity for volatilization of organics in the wastewater. The drain is normally connected to the process sewer line that carries the wastewater to the downstream collection and treatment units. Figure 5.2-1 illustrates the wastewater being carried past a manhole and on to a junction box where two process wastewater streams are joined. The manhole provides an escape route for organics volatilized in the sewer line. In addition, the junction box may also be open to the atmosphere, allowing organics to volatilize. Wastewater is discharged from

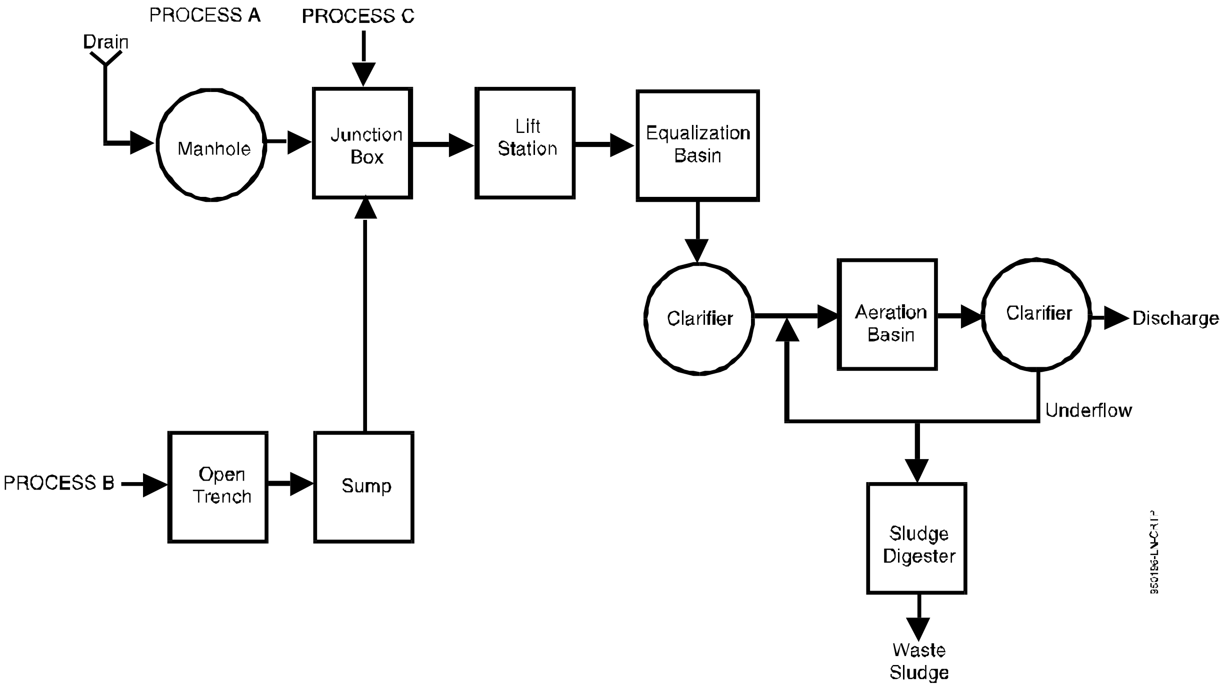

FIGURE 5.2-1. TYPICAL WASTEWATER COLLECTION AND TREATMENT SYSTEM

the junction box to a lift station where it is pumped to the treatment system. The lift station is also likely to be open to the atmosphere, allowing volatilization of organics.

The equalization basin, the first treatment unit shown in Figure 5.2-1, regulates the wastewater flow and pollutant compositions to the remaining treatment units. The equalization basin also typically provides a large area for wastewater contact with ambient air. For this reason, emissions may be relatively high from this unit. Suspended solids are removed in the clarifier, and the wastewater then flows to the aeration basin where microorganisms act on the organic constituents. Both the clarifier and the aeration basin may be open to the atmosphere. In addition, the aeration basin is normally aerated either mechanically or with diffused air. Wastewater leaving the aeration basin normally flows through a secondary clarifier for solids removal before it is discharged from the facility. The secondary clarifier is also likely to be open to the atmosphere. The solids that settle in the clarifier are discharged partly to a sludge digester and partly recycled to the aeration basin. Finally, waste sludge from the sludge digester is generally hauled off for land treatment or to a landfill.

In addition to VOC emissions from volatilization, sulfur oxides (SO_x) emissions from the thermal destruction of hydrogen sulfide can occur if methane gas from digesters is used in on-site combustion equipment. Chlorine and chlorinated compounds may be released if the wastewater stream is disinfected using chlorine prior to discharge.

2.4 FACTORS AND DESIGN CONSIDERATIONS INFLUENCING EMISSIONS

2.4.1 PROCESS OPERATING FACTORS

During wastewater treatment, the fate mechanisms of volatilization/stripping, sorption, and biotransformation primarily determine the fate of VOCs (Mihelcic et al., 1993). Of these, it is volatilization and stripping that result in air emissions. Biodegradation and sorption onto sludge serve to suppress air emissions.

Stripping may be defined as pollutant loss from the wastewater due to water movement caused by mechanical agitation, head loss, or air bubbles, while volatilization may be defined as quiescent or wind-driven loss (Mihelcic et al., 1993). The magnitude of emissions from volatilization/stripping depends on factors such as the physical properties of the pollutants (vapor pressure, Henry’s Law constants, solubility in water, etc.), the temperature of the wastewater, and the design of the individual collection and treatment units. WWCT unit design is important in determining the surface area of the air-water interface and the degree of mixing occurring in the wastewater.

Biodegradation by microorganisms occurs in biological treatment devices such as aeration basins. Due to the high level of biomass present in aeration basins, organic compounds may also be removed via sorption mechanisms. Parameters important in determining the rate of biodegradation and sorption occurring in aeration basins include the degree of biodegradability of the compound, the affinity of the compound for the organic or aqueous phase, and the biomass concentration in the basin (EPA, 1990). EPA has developed several methods for determining site-specific biodegradation rates for regulatory purposes. These include batch tests (aerated reactor and sealed reactor), as well as EPA Test Methods 304A and 304B. However, if site-specific rate constants are not available, default biodegradation rates are available for many pollutants in several of the emissions models used to estimate emissions. The use of site-specific biodegradation rates will result in a more accurate emission estimate.

Detailed information on the rates of organic removal through biodegradation, sorption, and volatilization are required for accurate emission estimates.

2.4.2 CONTROL TECHNIQUES

The types of control technologies generally used in reducing VOC emissions from wastewater include: steam stripping or air stripping (when followed by a collection device such as a carbon adsorber or a control device such as a flare), carbon adsorption (vapor or liquid phase), chemical oxidation, biotreatment (aerobic or anaerobic), and process modifications. Several of the control techniques (steam/air stripping and carbon adsorption) do not destroy the VOCs, they capture them. VOCs captured by these methods should be recovered or destroyed to prevent air emission releases to the environment.

For efficient control, all control elements should be placed as close as possible to the point of wastewater generation, with all collection, treatment, and storage systems ahead of the control technology being covered to suppress emissions. Tightly covered, well-maintained collection systems can suppress emissions by 95 to 99 percent. However, if there is explosion potential, it can be reduced by a low-volume flow of inert gas into the collection component, followed by venting to a device such as an incinerator or carbon adsorber.

The following are brief descriptions of the control technologies listed above and of any secondary controls that may need to be considered for fugitive air emissions.

Air and Steam Stripping

Steam stripping and air stripping off gases most often are vented to a secondary control or collection device, such as a combustion device or gas-phase carbon adsorber, in order to prevent air emissions. Combustion devices may include incinerators, boilers, and flares. Vent gases of high fuel value can be used as an alternative fuel and may be combined with other fuels such as natural gas and fuel oil. If the fuel value of the vent gas stream is very low, vent gases may be preheated and combined with combustion air.

Liquid-phase Carbon Adsorption

Liquid-phase carbon adsorption takes advantage of compound affinities for activated carbon. Activated carbon is an excellent adsorbent because of its large surface area and because it is usually in granular or powdered form for easy handling. Two types of liquid-phase carbon adsorption are the fixed-bed and moving-bed systems. The fixed-bed system is used primarily for low-flow wastewater streams with contact times around 15 minutes, and it is a batch operation (i.e., once the carbon is spent, the system is taken off line). Moving-bed carbon adsorption systems operate continuously with wastewater typically being introduced from the bottom of the column and regenerated carbon from the top (countercurrent flow). Spent carbon is continuously removed from the bottom of the bed. Liquid-phase carbon adsorption is usually used to recover compounds present in low concentrations or for high concentrations of nondegradable compounds. Removal efficiencies depend on the compound's affinity for activated carbon. Average removal efficiency ranges from 90 to 99 percent, but is dependent on compound concentrations (EPA, 1995).

Chemical Oxidation

Chemical oxidation involves a chemical reaction between the organic compound and an oxidant such as ozone, hydrogen peroxide, permanganate, or chlorine dioxide. Ozone is usually added to the wastewater through an ultraviolet-ozone reactor. Permanganate and chlorine dioxide are added directly into the wastewater. It is important to note that adding chlorine dioxide can form chlorinated hydrocarbons in a side reaction. The applicability of this technique depends on the reactivity of the individual organic compound.

Biotreatment

Biotreatment is the aerobic or anaerobic chemical breakdown of organic chemicals by microorganisms. Removal of organics by biodegradation is highly dependent on the compound's biodegradability, volatility, and ability to be adsorbed onto solids. Removal efficiencies range from almost 0 to 100 percent. In an acclimated biotreatment system, the microorganisms easily convert available organics into biological cells or biomass, or CO_2. This often requires a mixed culture of organisms, where each organism utilizes the food source most suitable to its metabolism. The organisms will starve and the organics will not be biodegraded if a system is not acclimated (i.e., the organisms cannot metabolize the available food source).

Process Modifications

Emissions from wastewater collection or treatment units may also be reduced by process modifications such as the use of level control gates, closed piping, or covered process units. These techniques reduce emissions by minimizing weir drops, turbulence, and contact with air.

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3

OVERVIEW OF AVAILABLE METHODS

3.1 EMISSION ESTIMATION METHODOLOGIES

Several methodologies are available for calculating fugitive emissions from industrial and municipal wastewater treatment systems. The method used is dependent upon available data, available resources, and the degree of accuracy required in the estimate.

This section discusses the methods available for calculating emissions from WWCT and identifies the preferred method of calculation. The discussion focuses on estimating emissions that occur from stripping mechanisms and the volatilization of pollutants present in wastewater streams.

3.1.1 MANUAL CALCULATIONS

Several EPA documents are available that provide theoretical equations that may be used to calculate emissions from WWCT. These include *Industrial Wastewater Volatile Organic Compound Emissions - Background Information for BACT/LAER Determinations* (EPA-450/3-90-004), *AP-42*, and *Air Emissions Models for Waste and Wastewater* (EPA-453/R-94-080A). The equations are based on mass transfer and liquid-gas equilibrium theory and use individual gas-phase and liquid-phase mass transfer coefficients to estimate overall mass transfer coefficients. Calculating air emissions using these equations is a complex procedure, especially if several systems are present, because the physical properties of the numerous contaminants must be individually determined. Because of the great deal of complexity involved, computer programs are available that incorporate these equations to estimate emissions from WWCT.

3.1.2 EMISSION MODELS

Some emission models currently available are based on measured or empirical values. The computer model may be based on theoretical equations that have been calibrated using actual data. Or, the models may be purely empirical, in which case the equations are usually based on statistical correlations with independent variables. Emissions estimated using models are a function of the WWCT system configuration, the properties of the specific compounds present in the wastewater streams, and the emission estimation approaches used in the model algorithms.

3.1.3 GAS-PHASE MEASUREMENT

Measuring air emissions from large open surfaces common at industrial and municipal wastewater treatment facilities is extremely difficult and perhaps one of the most challenging air quantification problems. Several techniques have been developed for this purpose, including surface emission isolation flux chambers, and transect and fenceline methods. If the industrial process is enclosed and vented, it is possible to directly measure emissions using standard measurement techniques. (Refer to Chapter 1 of this volume for a discussion of available methods.) In particular, POTWs may be covered or enclosed to reduce odor and/or prevent freezing in which case gas-phase measurement may be appropriate.

3.1.4 EMISSION FACTORS

Emission factors have been or are being developed for WWCT for several source categories. These factors have been developed as part of regulatory development projects such as the National Emissions Standards for Hazardous Air Pollutants (NESHAP) for the pulp and paper industry and for petroleum refineries. In some cases, emission factors are based on emissions estimates obtained using models, but have been reduced to a more simplistic form (mass of pollutant per process rate).

In addition, emission factors were developed by a consortium of California POTW operators as part of the Pooled Emissions Estimation Program (PEEP). These factors are not publicly available but may be obtained through Jim Bewley of the South Bayside System Authority at (415) 594-8411.

The PEEP emission factors were developed from field samples at 20 POTWs and cover 18 compounds and 18 processes. Liquid- and gas-phase samples were collected to complete mass balances at plants with similar processes. The emission factors are medians of the measured offgas mass emissions divided by the influent mass. When no data were available, because of "nondetects" or other causes, emission factors were extrapolated by averaging the known emission factors of either chlorinated or nonchlorinated compounds. PEEP factors usually predict significantly lower emissions than BAAT or fate models.

3.1.5 MATERIAL BALANCE

The simplest estimation method, material balance, relies on wastewater flow rate and influent and effluent liquid-phase pollutant concentrations. Compound mass that cannot be accounted for in the effluent is assumed to be volatilized. However, it needs to be noted that this method does not account for biodegradation or sorption onto solids or other removal mechanisms.

3.2 COMPARISON OF AVAILABLE EMISSION ESTIMATION METHODOLOGIES

3.2.1 MANUAL CALCULATIONS

Estimating emissions from WWCT by hand (or by spreadsheets) using the equations presented in the various literature is a very labor-intensive process and increases the potential for manual calculation error. For this reason, the use of manual calculations is not a preferred method, and should only be used in cases where access to models is prohibitive. It should be noted that the equations presented in the EPA document *Air Emissions Model for Waste and Wastewater* (EPA, 1994) have been incorporated into EPA's WATER8 model (discussed in Section 4) to alleviate the burden of performing the calculations by hand.

3.2.2 EMISSIONS MODELS

The use of emissions software models to calculate emissions from WWCT provides a widely accepted method of calculation. Most models are based on the theoretical equations presented in various literature and provide an automated means of performing the calculations. It should be noted that models estimate average emissions over a period of time. Peak or maximum emission rates over a short term may be more accurately assessed using gas-phase measurement or material balance approaches. Also, an in-depth knowledge of the WWCT schemes including pollutant concentrations and flow rate information are needed in order to obtain an accurate emission estimate.

3.2.3 GAS-PHASE MEASUREMENT

Direct and indirect gas-phase measurements are alternative methods of calculating emissions from WWCT. Once pollutant concentrations are known at a specific point, atmospheric dispersion modeling equations may be used to estimate an emission rate. Two potential sources of uncertainty, pollutant measurement error and the representativeness of the statistical dispersion equations for this type of application, are present in this method. In addition, the monitoring equipment needed to perform this method may be cost-prohibitive unless already in place.

If the treatment plant is enclosed and vented through a limited number of vents, traditional stack testing may be used to estimate emissions and would be considered a preferred method.

3.2.4 EMISSION FACTORS

Emission factors may be used to calculate emissions where approximate figures are acceptable. However, due to the variability of emissions based on site-specific operational, physical, and chemical parameters, emission factors should be carefully chosen that are based on similar-type sources.

3.2.5 MATERIAL BALANCE

Material balance calculations are a simple method of estimating emissions where inlet and outlet pollutant concentrations are known.

Other variables also may affect an estimate. Effluent data can be used to account for compounds passing through the plant, but if chlorine is added during treatment, chlorinated compounds that form can result in higher emissions than predicted by a material balance approach. To compensate, intermediate samples must be taken to quantify chlorinated compound emissions.

As mentioned before, material balance does not account for fate mechanisms other than volatilization. For example, it can overestimate emissions if the compound is biodegradable or adsorbs onto sludge.

4

PREFERRED METHOD FOR ESTIMATING EMISSIONS

The preferred method for estimating emissions from WWCT is the use of computer-based emissions models. There are numerous emissions estimation models available to calculate emissions from WWCT. These include publicly available models as well as proprietary models. Differences in the models include applicability to the types of collection and treatment systems, the level of site-specific data accepted, the level of default data provided, and whether or not the models account for the full spectrum of pollutant pathways (volatilization, biodegradation, and sorption). Models may also contain different default data (e.g., Henry's Law constants, biodegradation rate constants).

Many of these models allow for user input of data. The use of site-specific data is always preferred over the use of default data. Typically, the types of data needed are the chemical and physical properties of the wastewater stream, as well as collection and treatment device parameters. At a minimum, wastewater stream characteristics are needed at the inlet to the treatment plant or collection device. However, if data are available for various points within the treatment plant, a more accurate emissions estimate may be obtained.

In order to obtain a reliable emissions estimate using a software model, the modeler needs to understand both the configuration and wastewater stream characteristics of the collection and/or treatment units, as well as the emissions estimation algorithm used by the model. Not all models can handle all collection/treatment devices and results are likely to vary between models. A more accurate emissions estimate will result if the user has confidence in the input data and understands the emission estimation approach used by the model.

NOTE: A brief summary of some currently available models is provided below. Work is ongoing to improve some of the current models and to develop new ones. The discussion presented in this document is not to be interpreted as an endorsement of one model over another, but is provided for informational purposes only. The reader should consult with their state regulatory agency for guidance on the selection and use of an appropriate model. Also, Appendix C contains a reference list of technical articles providing qualitative as well as quantitative comparisons between models and emission estimation techniques.

4.1 WATER8/CHEMDAT8 (TREATMENT AND COLLECTION)

WATER8 is a publicly available computer program model developed by EPA that models the

fate of organic compounds in various wastewater treatment units, including collection systems, aerated basins, and other units. WATER8 contains useful features such as the ability to link treatment units to form a treatment system, the ability for recycle among units, and the ability to generate and save site-specific compound properties. WATER8 has a database with compound-specific data for over 950 chemicals. The mathematical equations used to calculate emissions in this model are based on the approaches described in *Air Emissions Models for Waste and Wastewater* (EPA, 1994). The WATER8 model is publicly available on the Clearinghouse for Inventories and Emission Factors (CHIEF) system
. Many of the emissions models contained in WATER8 are also
presented in spreadsheet form in CHEMDAT8.

4.2 BASTE (TREATMENT ONLY)

This model was developed to estimate sewage treatment emissions from treatment plants in the Bay Area of California. BASTE is a computer-based model with menu-driven input and is structured to allow significant flexibility in simulating a wide range of treatment processes. It can simulate the fate of organic compounds in well-mixed to plug-flow reactors, diffused bubble and surface aeration, and emissions from weirs and drops. BASTE is available through the CH_2M Hill Company.

4.3 CORAL+ (COLLECTION ONLY)

CORAL+ is a model that predicts emissions from sewer reaches based on actual data from field experiments. CORAL+ allows for continuous or slug discharges to sewers, variations in depth of flow and temperature, sewer physical conditions, and retardation of mass transfer by gas accumulation in the sewer headspace. Emissions are based on inputs of ventilation rates and patterns. CORAL+ also estimates losses at sewer drop structures and is available through the Enviromega Ltd. Company.

4.4 PAVE (TREATMENT ONLY)

This model was developed for the Chemical Manufacturers Association. It simulates the fate of contaminants in both surface-aerated and diffused-air activated sludge systems. The PAVE model offers a selection of different biological kinetic models. It is based on traditional kinetic process modelling for biological reactors and performs the traditional calculations of dissolved oxygen concentration and waste-activated sludge flow. The PAVE model works with compounds that have low volatilities and, therefore, may be gas-phase mass transfer limited. Most other models use oxygen as a mass transfer surrogate so that only liquid-phase mass transfer resistance is considered. PAVE is available through the Chemical Manufacturers Association.

4.5 CINCI (EPA - CINCINNATI MODEL) - *INTEGRATED MODEL FOR PREDICTING THE FATE OF ORGANICS IN WASTEWATER TREATMENT PLANTS* (TREATMENT ONLY)

This model was developed with support from the EPA Risk Reduction Engineering Laboratory. The physical properties database of the model includes 196 chemicals and metals, Henry's Law constants, sorption coefficients, biodegradation rate constants, and diffusivities. Removal mechanisms included are stripping/volatilization, stripping, surface volatilization, sorption, and biodegradation. Unit operations included are primary treatment followed by secondary treatment with sludge recycle, secondary treatment with sludge recycle, and secondary treatment without sludge recycle. The model is written in FORTRAN and has three built-in default cases. CINCI is available at no charge through the U.S. EPA Risk Reduction Engineering Laboratory.

4.6 NOCEPM - *NCASI ORGANIC COMPOUND ELIMINATION PATHWAY MODEL* (TREATMENT ONLY)

This model was developed by the National Council of the Paper Industry for Air and Stream Improvement, Inc. (NCASI); components were chosen from published literature. This model is also in the public domain. The physical properties database includes 11 chemicals, Henry's Law constants, sorption coefficients, biodegradation rate constants, and diffusion coefficients for 9 chemicals. Conceptual removal mechanisms are stripping, surface aeration, subsurface aeration, surface volatilization, sorption, and biodegradation. NOCEPM simulates only the secondary treatment step, but can represent activated sludge or aerated stabilization. It is written in QuickBasic™ and has no built-in default cases. The model was validated with chloroform for activated sludge and aerated stabilization processes and is available through NCASI.

4.7 TORONTO - *A MODEL OF ORGANIC CHEMICAL FATE IN A BIOLOGICAL WASTEWATER TREATMENT PLANT* (TREATMENT ONLY)

This model was developed with the support of the Ontario Ministry of the Environment, from which copies are available. There are 18 chemicals, Henry's Law constants, sorption coefficients, and biodegradation rate constants in the physical properties database. Removal mechanisms include stripping, surface volatilization, sorption, and biodegradation. TORONTO simulates primary sedimentation and secondary (biological) treatment. According to the report, this is a relatively simple model that uses a "fugacity" approach that "takes advantage of the linear relationship of fugacity to concentration to derive a relatively simple set of linear material balance expressions." Fugacity capacities and rate parameters are calculated for the air, water, and biomass phases. TORONTO is available through the Ontario Ministry of the Environment.

4.8 TOXCHEM+ - *TOXIC CHEMICAL MODELING PROGRAM FOR WATER POLLUTION CONTROL PLANTS* (TREATMENT AND COLLECTION)

This model was developed by Enviromega Ltd. Company (Campbellville, Ontario), in cooperation with the Environment Canada Wastewater Technology Centre. The database includes 204 chemicals (including metals) and detailed information on physical properties. The model also includes Henry's Law constants, sorption coefficients, and biodegradation rate constants. The model simulates volatilization, stripping, sorption, and biodegradation removal mechanisms from weirs, surface volatilization, surface aeration, and subsurface aeration. A wide variety of wastewater unit operations can be represented including grit chambers, primary clarifiers, collection reaches, sludge digestion, aeration basins, and secondary clarifiers. Both steady-state and dynamic results can be obtained. TOXCHEM+ is available through the Enviromega Ltd. Company.

5

ALTERNATIVE METHODS FOR ESTIMATING EMISSIONS

5.1 EMISSION FACTORS

Emission factors for WWCT are presented in the literature in two forms: traditional emission factors that relate emissions of a particular pollutant to a process rate, and fraction emitted (Fe) emission factors that relate emissions of a particular pollutant to the total amount of that pollutant present in the wastewater stream.

Examples 5.5-1 and 5.5-2 show how process rate emission factors and Fe emission factors may be used to calculate emissions from WWCT.

Example 5.5-1

This example shows how toluene emissions can be calculated using Fe and the wastewater stream characteristics provided:

Wastewater flow into collection system = 4,575,000 gal/day

Toluene concentration = 4 µg/L

Fe = 0.35 (for the collection system)

Toluene mass flow rate = 4,575,000 gal/day * 3.785 L/gal * 4 µg/L * 10^{-6} g/µg * lb/453.6 g
= 0.153 lb/day

Toluene emissions = 0.35 * 0.153 lb/day
= 0.054 lb/day

Example 5.5-2

This example shows how VOC emissions can be calculated using process rate-based emission factors (EFs) and the process parameters provided:

EF_{VOC} = 0.17 kg VOC/Mg pulp

Process rate = 27 Mg pulp/hr

VOC emissions = 27 Mg pulp/hr * 0.17 kg VOC/Mg pulp * 1,000 g/1 kg * lb/453.6 g

= 10.1 lb VOC/hr

5.2 MATERIAL BALANCE

Using a material balance approach to calculate emissions from WWCT is straightforward if the data are available and if the emissions estimate does not require extreme accuracy. In most cases, a material balance calculation will provide an emission estimate that is biased toward overestimating emissions due to the fact that the other (nonair) pollutant removal mechanisms (sorption and biodegradation) are not considered. This approach may be a viable option for collection systems and nonbiologically activated treatment where inlet and outlet pollutant concentrations are known. Example 5.5-3 shows how a material balance approach may be used to calculate emissions from WWCT.

5.3 MANUAL CALCULATIONS

Appendix B provides example calculations using the mass transfer equations presented in *AP-42*. The equations, along with guidance on how to use them, are included. (Please note that while the *AP-42* section still refers to the SIMS model, this has been superseded by the WATER8 model, which is available on the CHIEF BBS. Therefore, as of the writing of this document, *AP-42* is not consistent with EPA's method of choice for estimating emissions from wastewater treatment.)

Example 5.5-3

This example shows how toluene emissions can be calculated using a material balance approach. The wastewater stream is the same as that considered in Example 5.5-1. However, in this example, it is known that the wastewater stream exiting the collection system has a toluene concentration of 2 µg/L:

Wastewater flow = 4,575,000 gal/day

Toluene concentration at inlet = 4 µg/L

Toluene concentration at outlet = 2 µg/L

Toluene lost through system = 4 µg/L - 2 µg/L = 2 µg/L

Toluene emissions = 4,575,000 gal/day * 3.785 L/gal * 2 µg/L * 10^{-6} g/µg * lb/453.6 g

= 0.0764 lb/day

5.4 GAS-PHASE MEASUREMENT

5.4.1 DIRECT MEASUREMENT

The surface isolation flux chamber is the only commonly accepted direct measurement technique available for open wastewater surfaces. When properly placed and operated, the flux chamber accurately measures surface emissions. Total surface emissions are calculated by multiplying the values from the individual flux chamber measurements by the surface area each measurement represents. This can be quite challenging for processes that are not completely mixed and may have unique emissions at every point on the surface. For these cases, modeling can be used to interpolate surface emission values between flux chamber measurement points. This method is not suitable for estimating emissions of compounds with low volatility.

Treatment processes that are enclosed or covered may lend themselves to traditional stack testing methods for emission estimation purposes. If a collection system or treatment plant is well covered and vented through a limited number of openings, direct measurement (such as the use of EPA Method 25) may be considered a preferred, rather than an alternative, method of emission estimation.

5.4.2 INDIRECT MEASUREMENT

Indirect measurement techniques, including transect and fenceline sensing, primarily are used for estimating fugitive emissions from area sources.

Transect and fenceline methods are both indirect measurement techniques that rely on dispersion modeling to predict the emission rate based on measurements of the ambient pollutant concentrations in the emission plume.

The transect method typically uses both vertically and horizontally dispersed measurement points positioned close to the source.

6

QUALITY ASSURANCE/QUALITY CONTROL

The consistent use of standardized methods and procedures is essential in the compilation of reliable emission inventories. Quality assurance (QA) and quality control (QC) of an inventory are accomplished through a set of procedures that ensure the quality and reliability of data collection and analysis. These procedures include the use of appropriate emission estimation techniques, applicable and reasonable assumptions, accuracy/logic checks of computer models, checks of calculations, and data reliability checks. Depending upon the technical approach used to estimate emissions, a checklist with all of the particular data needs should be prepared to verify that each piece of information is used accurately and appropriately.

This section discusses QA/QC procedures for specific emission estimation methods presented in Sections 4 and 5 of this chapter. Volume VI, *Quality Assurance Procedures*, of this series describes additional QA/QC methods and tools for performing these procedures. Also, Volume II, Chapter 1, *Introduction to Stationary Point Source Emission Inventory Development*, presents recommended standard procedures to follow to ensure that the reported inventory data are complete and accurate.

6.1 GENERAL FACTORS INVOLVED IN EMISSION ESTIMATION TECHNIQUES

All calculations, whether done manually or electronically, should be verified by repeating at least one complete set of calculations. If a computer model is being used, verification that the calculations are done correctly need only be done once (until the model is updated or modified). The model verification process should be documented carefully (see Volume VI, Chapter 3, Section 4). Although this level of checking for a program can require a significant amount of time, it is necessary. Furthermore, given that these programs are generally used many times over, the effort required to check the algorithms is relatively small.

Manual calculations should be checked even more carefully, although completely replicating the set of equations is overly burdensome. Because manual calculations introduce more possibility for errors, are difficult to quality assure, and are harder to revise or update later, use of a spreadsheet or other electronic tool is strongly advised.

Often, emissions inventories are developed and/or compiled in computerized emissions databases or models. Presumably, the methods, assumptions, and any data included with the software are documented in a user's or a technical manual. If not, the user should conduct extensive and careful QA of the model or find a better documented system.

Even if the validation of the system is well-documented, the user will need to provide information about the input data. Comment fields, if available and sufficiently large, can be used to record assumptions, data references, and any other pertinent information. Alternatively, this information can be recorded in a separate document, electronically or otherwise. If at all possible, the electronic database should record a cross-reference to the document. This cross-reference could be a file name (and directory or disk number), a notebook identification number, or other document.

6.1.1 EMISSIONS MODELS

Use of emission models and equations generally involves more effort than use of emission factors. The level of effort is related to the complexity of the equation, the types of data that must be collected, and the diversity of products manufactured at a facility. Typically, the use of emission models involves making one or more conservative assumptions if a complete set of site-specific data is unavailable. As a result, the use of models may result in an overestimation of emissions. However, the accuracy and reliability of models can be improved by ensuring that data collected for emission calculations (e.g., material speciation data) are of the highest possible quality.

The EIIP recommends that sensitivity analyses be used as part of the QA program for emissions models. A sensitivity analysis is a process for identifying the magnitude, direction, and form of the effect of an individual parameter on the model's result. It is usually done by repeatedly running the model and changing the value of one variable while holding the others constant. Sensitivity analyses may be used to select the most appropriate model for a given situation. For example, one model may be particularly sensitive to errors in a variable that is not reliably measured. An alternative model may be found that is better suited to the available data. Sensitivity analyses also aid QC by identifying the key variables to be checked.

6.1.2 GAS-PHASE MEASUREMENT

When applying this technique for estimating emissions, sampling and analytical procedures, use of data, preparation and use of a QA plan, and report preparation should be described and understood by the team conducting the test. A systems audit should be conducted on-site as a qualitative review of the various aspects of a total sampling and analytical system to assess its overall effectiveness. For detailed information pertaining to specific test methods, procedures described in the published reference methods should be reviewed, as well as, Chapter 1 of this volume.

6.1.3 EMISSION FACTORS

The use of emission factors is straightforward when the relationship between process data and emissions is direct and relatively uncomplicated. When using emission factors, the user should be aware of the quality indicator associated with the value. Emission factors published within EPA documents and electronic tools have a quality rating applied to them. The lower the quality indicator, the more likely that a given emission factor may not be representative of the source type. The reliability and uncertainty of using emission factors as an emission estimation technique are discussed in detail in the QA/QC section of Chapter 1 of this volume.

6.1.4 MATERIAL BALANCE

As stated in Section 5, the accuracy and reliability of emission values calculated using the material balance approach are biased toward overestimation. Uncertainty of emissions using the material balance approach is also related to the quality of material speciation data, which is typically extracted from Material Safety Data Sheets (MSDSs). To assess the level of uncertainty of such data, the user should verify if a standard analytical test method (e.g., one using a gas chromatograph) has been used to measure the concentrations of the constituents.

6.2 DATA ATTRIBUTE RATING SYSTEM (DARS) SCORES

One measure of emission inventory data quality is the DARS score. Four examples are given here to illustrate DARS scoring using the preferred and alternative methods presented in this document. The DARS provides a numerical ranking on a scale of 0.1 to 1.0 for individual attributes of the emission factor and the activity data. Each score is based on what is known about the factor and activity data, such as the specificity to the source category and the measurement technique employed. The composite attribute score for the emissions estimate can be viewed as a statement of the confidence that can be placed in the data. For a complete discussion of DARS and other rating systems, see the *Quality Assurance Procedures* (Volume VI, Chapter 4) and *Introduction to Stationary Point Sources Emission Inventory Development* (Volume II, Chapter 1).

Each of the examples below is hypothetical. A range is given where appropriate to cover different situations. Table 5.6-1 shows scores developed from the use of emission models. Table 5.6-2 demonstrates scores determined for gas-phase measurement. Table 5.6-3 gives a set of scores for an estimate made with an emission factor. Table 5.6-4 demonstrates scores developed from a material balance approach. The activity data are assumed to be measured directly or indirectly. These examples are given as an illustration of the relative quality of each method. If the same analysis were done for an actual site, the scores could be different but the relative ranking of methods should stay the same.

TABLE 5.6-1

DARS SCORES: EMISSION MODELS

Attribute	Scores		
	Factor[a]	**Activity[b]**	**Emissions**
Measurement	0.3 - 0.9	1.0	0.3 - 0.9
Specificity	0.5 - 0.9	0.9	0.45 - 0.81
Spatial	1.0	1.0	1.0
Temporal	1.0	0.5 - 0.9	0.5 - 0.9
Composite Scores	0.75 - 0.95	0.85 - 0.95	0.56 - 0.90

[a] Lower scores apply to purely theoretical models and/or use of defaults rather than site-specific input values.
[b] Scores assume activity is volume of wastewater processed and that it is measured.

TABLE 5.6-2

DARS SCORES: GAS-PHASE MEASUREMENT

Attribute	Scores		
	Factor[a]	**Activity[b]**	**Emissions**
Measurement	0.5 - 1.0	1.0	0.5 - 1.0
Specificity	0.7 - 1.0	0.9	0.63 - 0.9
Spatial	0.5 - 1.0	1.0	0.5 - 1.0
Temporal	0.5 - 1.0	0.7 - 1.0	0.35 - 1.0
Composite Scores	0.55 - 1.0	0.9 - 0.98	0.50 - 0.98

[a] Exact score will depend on sample size, method used, and whether scales are appropriate to inventory.
[b] Assumes activity is wastewater processed and measured.

TABLE 5.6-3

DARS SCORES: EMISSION FACTORS

Attribute	Scores		
	Factor	**Activity**[a]	**Emissions**
Measurement	0.3 - 0.5	1.0	0.3 - 0.5
Specificity	0.3 - 0.7	0.9	0.21 - 0.63
Spatial	1.0	1.0	1.0
Temporal	0.8	0.8	0.5 - 0.9
Composite Scores	0.45 - 0.85	0.78 - 0.98	0.40 - 0.76

[a] Scores assume activity is volume of wastewater processed and that it is measured.

TABLE 5.6-4

DARS SCORES: MATERIAL BALANCE

Attribute	Scores		
	Factor	**Activity**	**Emissions**
Measurement[a]	0.5 - 0.7	1.0	0.5 - 0.7
Specificity	1.0	1.0	1.0
Spatial	1.0	1.0	1.0
Temporal[b]	0.5 - 1.0	0.5 - 1.0	0.25 - 1.0
Composite Scores	0.75 - 0.93	0.88 - 1.0	0.69 - 0.93

[a] Score increases as sample sizes (influent and effluent) increase.

[b] If influent/effluent concentrations are scaled up or down, lower DARS scores.

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7

REFERENCES

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Mihelcic, James R., C. Robert Baillod, John C. Crittenden, and Tony N. Rodgers. January 1993. Estimation of VOC Emissions from Wastewater Facilities by Volatilization and Stripping. *Air & Waste, Journal of the Air & Waste Management Association*. 43: 97-105.

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APPENDIX A

EXAMPLE DATA COLLECTION FORMS-WASTEWATER TREATMENT UNITS

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EXAMPLE DATA COLLECTION FORMS INSTRUCTIONS

1. These forms may be used as work sheets to aid the plant engineer in collecting the information necessary to calculate emissions from wastewater treatment units. The information requested on the forms relates to the methods (described in Sections 3 through 5) for quantifying emissions. These forms may also be used by regulatory agency personnel to assist in area-wide inventory preparation.

2. The completed forms should be maintained in a reference file by the plant engineer with other supporting documentation.

3. If the information requested is unknown, write "unknown" in the blank. If the information requested does not apply to a particular unit, write "NA" in the blank.

4. If you want to modify the form to better serve your needs, an electronic copy of the form may be obtained through the EIIP on the Clearinghouse for Inventories and Emission Factors system (CHIEF).

5. Table A-1 can be used as a reference for typical dimensions associated with each unit design parameter.

6. Use the comments field on the form to record all useful information that will allow your work to be reviewed and reconstructed.

TABLE A-1

DIMENSIONS FOR WASTE STREAM COLLECTION AND TREATMENT UNITS[a]

Component	Design Parameter	Typical Dimensions
Drain	riser height (m)	0.6
	riser diameter (m)	0.2
	process drain pipe diameter (m)	0.1
	effective diameter of riser (m)	0.1
	riser cap thickness (cm)	0.6
	sewer diameter (m)	0.9
Manhole	diameter (m)	1.2
	height (m)	1.2
	cover diameter (m)	0.6
	diameter of holes in cover (cm)	2.5
	cover thickness (cm)	0.6
	sewer diameter (m^2)	0.9
Junction Box	effective diameter (m)	0.9
	grade height (m)	1.5
	water depth (m)	0.9
	surface area (m^2)	0.7
Lift Station	effective diameter (m)	1.5
	width (m)	1.8
	grade height (m)	2.1
	water depth (m)	1.5
	surface area (m^2)	1.8
Trench	length (m)	15.2
	water depth (m)	0.6
	depth (m)	0.8
	width (m)	0.6
Weir	height (m)	1.8
Oil/Water Separator	length (m)	13.7
	width (m)	7.6
	retention time (hr)	0.8

TABLE A-1

(CONTINUED)

Component	Design Parameter	Typical Dimensions
Clarifier	diameter (m) depth (m) retention time (hr)	18.3 3.5 4.0
Sump	effective diameter (m) water depth (m) surface area (m^2)	1.5 1.5 1.8
Equalization Basin	effective diameter (m) water depth (m) surface area (m^2) retention time (days)	109 2.9 9,290 5
Aeration Basin	effective diameter (m) water depth (m) surface area (m^2) retention time (days)	150 2.0 17,652 6.5
Treatment Tank	effective diameter (m) water depth (m) surface area (m^2) retention time (hr)	11 4.9 93 2

[a] EPA. 1990. *Industrial Wastewater Volatile Organic Compound Emissions-Background Information for BACT/LAER Determinations*. U.S. Environmental Protection Agency, EPA-450/3-90-004. Research Triangle Park, North Carolina.

EXAMPLE DATA COLLECTION FORM - WASTEWATER UNITS

GENERAL INFORMATION		
Facility/Plant Name:		
SIC Code:		
SCC:		
SCC Description:		
Location:		
County:	City:	State:
Plant Geographical Coordinates:		
Latitude:		
Longitude:		
UTM Zone:		
UTM Easting:		
UTM Northing:		
Contact Name:		
Title:		
Telephone Number:	Facsimile Number:	
Source ID Number:	Unit ID Number:	
Permit Number:		
Permitted Hours of Operation (per year):		
Actual Hours of Operation:		
Hours/Day:	Days/Weeks:	Weeks/Year:

EXAMPLE DATA COLLECTION FORM - WASTEWATER UNITS

UNIT DESCRIPTION[a]
UNIT NUMBER ___ of ___
Junction box:
Reach:
Drain:
Drain type:
Lift station:
Sump:
Weir:
Other:
CONFIGURATION
Flowthrough:
Disposal:
MECHANICAL AERATION
Diffused air:
Biodegradation:
Oil film layer:
DESIGN PARAMETERS
Volume flow rate (units):
Surface area (units):
Liquid depth (units):
Width (units):
Fetch length (units):
Retention time (turnover/yr):
Pollutant of interest:
Concentration before treatment:

[a] Refer to Table A-1 for typical dimensions associated with design parameters.

INPUT DATA FOR MODELING WASTEWATER TREATMENT SYSTEMS

COLLECTION SYSTEM

Please fill out the following information for each unit. Attach additional sheets as needed.

TRUNK/REACH	**UNIT NUMBER**	**UNIT NUMBER**	**UNIT NUMBER**
Wastewater flow:			
Open or closed channel:			
Reach (channel) diameter:			
Reach surface roughness: (e.g., smooth, concrete, tile, pipe)			
Reach slope:			
Reach length:			
Wastewater temperature:			
Water concentration of known organics:			
Manholes and drop structures:			
Manhole gas volume:			
Tailwater depth in manhole:			
Air concentration of VOCs (if available):			
Water drop height in drop structure (height of splashing flow):			
Wind speed or ventilation rate in sewer:			

INPUT DATA FOR MODELING WASTEWATER TREATMENT SYSTEMS (CONTINUED)

BASINS & TANKS	COMMENTS
Flow rates and composition:	
Influent flow rate to unit (gal/hr):	
Recycle flow rate from clarifier (gal/hr):	
Feed influent organics:	
Major components (mg/L):	
Total organics (mg/L):	
Microorganism level in recycle (mg/L MLVSS[a]):	
Microorganism level in basin (mg/L MLVSS):	
Microorganism level in feed (mg/L MLVSS):	
Microorganism level in clarifier effluent (mg/L MLVSS):	
Oxygen concentration in feed (ppm):	
Oxygen concentration in basin (ppm):	
Basin geometry and characteristics:	
Volume (gal):	
Depth (ft):	
Surface area (ft^2):	
Temperature of liquid in basin (°C):	
Number of turbines:	
Turbine speed (rpm):	
Delivered power of turbine (hp/turbine):	
Oxygen transfer rating of turbine (lb of O_2/hp-hr):	
Diameter of turbine blade (ft):	
For subsurface aeration:	
Air flow to basin (ft/min):	
Liquid injection rate (ft^3/hr):	
Biodegradation rates:	
Overall removal efficiency (%):	
Compound-specific biorates (if known):	

[a] MLVSS = mixed liquor volatile suspended solids.

EMISSION ESTIMATION RESULTS

Pollutant	Emission Estimation Method[a]	Annual Emissions	Emissions Units	Emission Factor[b]	Emission Factor Units	Comments
VOC						
Hazardous Air Pollutants (list individually)						

[a] Use the following codes to indicate which emission estimation method is used for each pollutant:

Emission Factor = EF; Other (indicate) = O; Model (indicate which model was used) = M.

[b] Where applicable, enter the emission factor and provide the full citation of the reference or source of information from where the emission factor came. Include edition, version, table, and page numbers if *AP-42* is used.

Please copy blank form and attach additional sheets as needed.

APPENDIX B

AP-42 EMISSION ESTIMATION ALGORITHM AND EXAMPLE CALCULATIONS

Source: EPA. January 1995. "Waste Water Collection, Treatment and Storage" (Section 4.3.2). In: *Compilation of Air Pollutant Emission Factors, Volume I: Stationary Point and Area Sources, Fifth Edition, AP-42*. U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards. Research Triangle Park, North Carolina.

Note: *AP-42* refers to the SIMS model although it has been superseded by the WATER8 model, which is available on the CHIEF BBS.

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EMISSIONS

Volatile organic compounds (VOCs) are emitted from wastewater collection, treatment, and storage systems through volatilization of organic compounds at the liquid surface. Emissions can occur by diffusive or convective mechanisms, or both. Diffusion occurs when organic concentrations at the water surface are much higher than ambient concentrations. The organics volatilize or diffuse into the air, in an attempt to reach equilibrium between aqueous and vapor phases. Convection occurs when air flows over the water surface, sweeping organic vapors from the water surface into the air. The rate of volatilization relates directly to the speed of the air flow over the water surface.

Other factors that can affect the rate of volatilization include wastewater surface area, temperature, and turbulence; wastewater retention time in the system(s); the depth of the wastewater in the system(s); the concentration of organic compounds in the wastewater and their physical properties, such as volatility and diffusivity in water; the presence of a mechanism that inhibits volatilization, such as an oil film; or a competing mechanism, such as biodegradation.

The rate of volatilization can be determined by using mass transfer theory. Individual gas phase and liquid phase mass transfer coefficients (k_g and k_ℓ, respectively) are used to estimate overall mass transfer coefficients (K, K_{oil}, and K_D) for each VOC.[1-2] Figure 5.B-1 presents a flow diagram to assist in determining the appropriate emissions model for estimating VOC emissions from various types of wastewater treatment, storage, and collection systems. Tables 5.B-1 and 5.B-2, respectively, present the emission model equations and definitions.

VOCs vary in their degree of volatility. The emission models presented in this section can be used for high-, medium-, and low-volatility organic compounds. The Henry’s Law constant (HLC) is often used as a measure of a compound’s volatility, or the diffusion of organics into the air relative to diffusion through liquids. High-volatility VOCs are HLC > 10^{-3} atm-m^3/gmol; medium-volatility VOCs are 10^{-3} < HLC < 10^{-5} atm-m^3/gmol; and low-volatility VOCs are HLC < 10^{-5} atm-m^3/gmol.[1]

The design and arrangement of collection, treatment, and storage systems are facility-specific; therefore the most accurate wastewater emissions estimate will come from actual tests of a facility (i.e., tracer studies or direct measurement of emissions from openings). If actual data are unavailable, the emission models provided in this section can be used.

Emission models should be given site-specific information whenever it is available. The most extensive characterization of an actual system will produce the most accurate

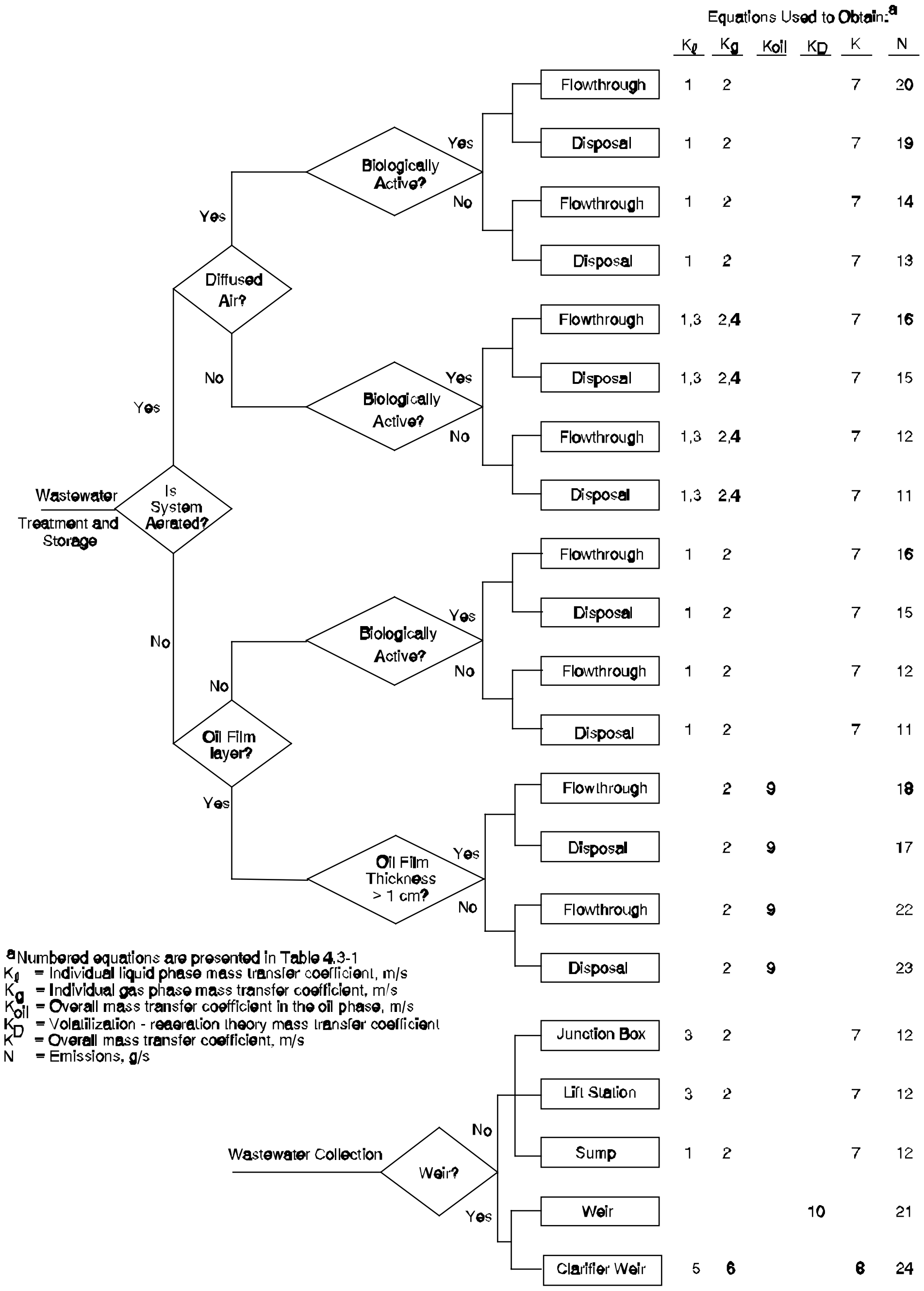

Figure 5.B-1. Flow diagram for estimating VOC emissions from wastewater collection, treatment, and storage systems.

[a] Citation refers to table assignment number in *AP-42*.

TABLE 5.B-1

MASS TRANSFER CORRELATIONS AND EMISSIONS EQUATIONS[a]

Equation No.	Equation
Individual liquid (k_ℓ) and gas (k_g) phase mass transfer coefficients	
1	k_ℓ (m/s) = $(2.78 \times 10^{-6})(D_w/D_{ether})^{2/3}$ For: $0 < U_{10} < 3.25$ m/s and all F/D ratios k_ℓ (m/s) = $[(2.605 \times 10^{-9})(F/D) + (1.277 \times 10^{-7})](U_{10})^2(D_w/D_{ether})^{2/3}$ For: $U_{10} > 3.25$ m/s and $14 < F/D < 51.2$ k_ℓ (m/s) = $(2.61 \times 10^{-7})(U_{10})^2(D_w/D_{ether})^{2/3}$ For: $U_{10} > 3.25$ m/s and $F/D > 51.2$ k_ℓ (m/s) = $1.0 \times 10^{-6} + 144 \times 10^{-4} (U^*)^{2.2} (Sc_L)^{-0.5}$; $U^* < 0.3$ k_ℓ (m/s) = $1.0 \times 10^{-6} + 34.1 \times 10^{-4} U^* (Sc_L)^{-0.5}$; $U^* > 0.3$ For: $U_{10} > 3.25$ m/s and $F/D < 14$ where: U^* (m/s) = $(0.01)(U_{10})(6.1 + 0.63(U_{10}))^{0.5}$ $Sc_L = \mu_L/(\rho_L D_w)$ $F/D = 2\ (A/\pi)^{0.5}$
2	k_g (m/s) = $(4.82 \times 10^{-3})(U_{10})^{0.78}\ (Sc_G)^{-0.67}\ (d_e)^{-0.11}$ where: $Sc_G = \mu_a/(\rho_a D_a)$ d_e(m) = $2(A/\pi)^{0.5}$
3	k_ℓ (m/s) = $[(8.22 \times 10^{-9})(J)(POWR)(1.024)^{(T-20)}(O_t)(10^6)\ *$ $(MW_L)/(Va_v \rho_L)](D_w/D_{O2,w})^{0.5}$ where: POWR (hp) = (total power to aerators)(V) Va_v(ft^2) = (fraction of area agitated)(A)
4	k_g (m/s) = $(1.35 \times 10^{-7})(Re)^{1.42}\ (P)^{0.4}\ (Sc_G)^{0.5}\ (Fr)^{-0.21}(D_a\ MW_a/d)$ where: $Re = d^2\ w\ \rho_a/\mu_a$ $P = [(0.85)(POWR)(550\ \text{ft-lb}_f/\text{s-hp})/N_I]\ g_c/(\rho_L (d^*)^5 w^3)$ $Sc_G = \mu_a/(\rho_a D_a)$ $Fr = (d^*)w^2/g_c$

TABLE 5.B-1

(CONTINUED)

Equation No.	Equation
5	k_ℓ (m/s) = $(f_{air,\ell})(Q)/[3600\ s/min\ (h_c)(\pi d_c)]$ where: $f_{air,\ell} = 1 - 1/r$ $r = \exp\ [0.77(h_c)^{0.623}(Q/\pi d_c)^{0.66}(D_w/D_{O2,w})^{0.66}]$
6	k_g (m/s) = $0.001 + (0.0462(U^{**})(Sc_G)^{-0.67})$ where: U^{**} (m/s) = $[6.1 + (0.63)(U_{10})]^{0.5}(U_{10}/100)$ $Sc_G = \mu_a/(\rho_a D_a)$
Overall mass transfer coefficients for water (K) and oil (K_{oil}) phases and for weirs (K_D)	
7	$K = (k_\ell\ Keq\ k_g)/(Keq\ k_g + k_\ell)$ where: $Keq = H/(RT)$
8	K (m/s) = $[[MW_L/(k_{\ell\rho L}{*}(100\ cm/m)] + [MW_a/(k_g\rho_a H{*}$ $55{,}555(100\ cm/m))]]^{-1}\ MW_L/[(100\ cm/m)\rho_L]$
9	$K_{oil} = k_g Keq_{oil}$ where: $Keq_{oil} = P^{*}\rho_a MW_{oil}/(\rho_{oil}\ MW_a\ P_o)$
10	$K_D = 0.16h\ (D_w/D_{O2,w})^{0.75}$
Air emissions (N)	
11	N(g/s) = (1 - Ct/Co) V Co/t where: Ct/Co = exp[-K A t/V]

TABLE 5.B-1

(CONTINUED)

Equation No.	Equation
12	$N(g/s) = K\ C_L\ A$ where: $C_L(g/m^3) = Q\ Co/(KA + Q)$
13	$N(g/s) = (1 - Ct/Co)\ V\ Co/t$ where: $Ct/Co = \exp[-(KA + KeqQ_a)t/V]$
14	$N(g/s) = (KA + Q_aKeq)C_L$ where: $C_L(g/m^3) = QCo/(KA + Q + Q_aKeq)$
15	$N(g/s) = (1 - Ct/Co)\ KA/(KA + Kmax\ b_i\ V/K_s)\ V\ Co/t$ where: $Ct/Co = \exp[-Kmax\ b_i\ t/K_s - K\ A\ t/V]$
16	$N(g/s) = K\ C_L\ A$ where: $C_L(g/m^3) = [-b + (b^2 - 4ac)^{0.5}]/(2a)$ and: $a = KA/Q + 1$ $b = K_s(KA/Q + 1) + Kmax\ b_i\ V/Q - Co$ $c = -K_sCo$
17	$N(g/s) = (1 - Ct_{oil}/Co_{oil})V_{oil}Co_{oil}/t$ where: $Ct_{oil}/Co_{oil} = \exp[-K_{oil}\ t/D_{oil}]$ and: $Co_{oil} = Kow\ Co/[1 - FO + FO(Kow)]$ $V_{oil} = (FO)(V)$ $D_{oil} = (FO)(V)/A$

TABLE 5.B-1

(CONTINUED)

Equation No.	Equation
18	$N(g/s) = K_{oil}C_{L,oil}A$ where: $C_{L,oil}(g/m^3) = Q_{oil}Co_{oil}/(K_{oil}A + Q_{oil})$ and: $Co_{oil} = Kow\ Co/[1 - FO + FO(Kow)]$ $Q_{oil} = (FO)(Q)$
19	$N(g/s) = (1 - Ct/Co)(KA + Q_aKeq)/(KA + Q_aKeq + Kmax\ b_i\ V/K_s)\ V\ Co/t$ where: $Ct/Co = \exp[-(KA + KeqQ_a)t/V - Kmax\ b_i\ t/K_s]$
20	$N(g/s) = (KA + Q_aKeq)C_L$ where: $C_L(g/m^3) = [-b +(b^2 - 4ac)^{0.5}]/(2a)$ and: $a = (KA + Q_aKeq)/Q + 1$ $b = K_s[(KA + Q_aKeq)/Q + 1] + Kmax\ b_i\ V/Q - Co$ $c = -K_sCo$
21	$N\ (g/s) = (1 - \exp[-K_D])Q\ Co$
22	$N(g/s) = K_{oil}C_{L,oil}A$ where: $C_{L,oil}(g/m^3) = Q_{oil}(Co_{oil}^*)/(K_{oil}A + Q_{oil})$ and: $Co_{oil}^* = Co/FO$ $Q_{oil} = (FO)(Q)$

TABLE 5.B-1

(CONTINUED)

Equation No.	Equation
23	$N(g/s) = (1 - Ct_{oil}/Co_{oil}^*)(V_{oil})(Co_{oil}^*)/t$ where: $Ct_{oil}/Co_{oil}^* = \exp[-K_{oil}\ t/D_{oil}]$ and: $Co_{oil}^* = Co/FO$ $V_{oil} = (FO)(V)$ $D_{oil} = (FO)(V)/A$
24	$N\ (g/s) = (1 - \exp[-K\ \pi\ d_c\ h_c/Q])Q\ Co$

[a] All parameters in numbered equations are defined in Table 5.B-2.

TABLE 5.B-2

PARAMETER DEFINITIONS FOR MASS TRANSFER CORRELATIONS AND EMISSIONS EQUATIONS

Parameter	Definition	Units	Code[a]
A	Wastewater surface area	m^2 or ft^2	A
b_i	Biomass concentration (total biological solids)	g/m^3	B
C_L	Concentration of constituent in the liquid phase	g/m^3	D
$C_{L,oil}$	Concentration of constituent in the oil phase	g/m^3	D
Co	Initial concentration of constituent in the liquid phase	g/m^3	A
Co_{oil}	Initial concentration of constituent in the oil phase considering mass transfer resistance between water and oil phases	g/m^3	D
Co_{oil}^*	Initial concentration of constituent in the oil phase considering no mass transfer resistance between water and oil phases	g/m^3	D
Ct	Concentration of constituent in the liquid phase at time = t	g/m^3	D
Ct_{oil}	Concentration of constituent in the oil phase at time = t	g/m^3	D
d	Impeller diameter	cm	B
D	Wastewater depth	m or ft	A,B
d^*	Impeller diameter	ft	B
D_a	Diffusivity of constituent in air	cm^2/s	C
d_c	Clarifier diameter	m	B
d_e	Effective diameter	m	D
D_{ether}	Diffusivity of ether in water	cm^2/s	$(8.5x10^{-6})$[b]
$D_{O2,w}$	Diffusivity of oxygen in water	cm^2/s	$(2.4x10^{-5})$[b]
D_{oil}	Oil film thickness	m	B

TABLE 5.B-2

(CONTINUED)

Parameter	Definition	Units	Code[a]
D_w	Diffusivity of constituent in water	cm^2/s	C
$f_{air,\ell}$	Fraction of constituent emitted to the air, considering zero gas resistance	dimensionless	D
F/D	Fetch to depth ratio, d_e/D	dimensionless	D
FO	Fraction of volume which is oil	dimensionless	B
Fr	Froude number	dimensionless	D
g_c	Gravitation constant (a conversion factor)	lb_m-ft/s^2-lb_f	32.17
h	Weir height (distance from the wastewater overflow to the receiving body of water)	ft	B
h_c	Clarifier weir height	m	B
H	Henry's Law constant of constituent	atm-m^3/gmol	C
J	Oxygen transfer rating of surface aerator	lb O_2/(hr-hp)	B
K	Overall mass transfer coefficient for transfer of constituent from liquid phase to gas phase	m/s	D
K_D	Volatilization-reaeration theory mass transfer coefficient	dimensionless	D
Keq	Equilibrium constant or partition coefficient (concentration in gas phase/concentration in liquid phase)	dimensionless	D
Keq_{oil}	Equilibrium constant or partition coefficient (concentration in gas phase/concentration in oil phase)	dimensionless	D
k_g	Gas phase mass transfer coefficient	m/s	D
k_ℓ	Liquid phase mass transfer coefficient	m/s	D
Kmax	Maximum biorate constant	g/s-g biomass	A,C
K_{oil}	Overall mass transfer coefficient for transfer of constituent from oil phase to gas phase	m/s	D

TABLE 5.B-2

(CONTINUED)

Parameter	**Definition**	**Units**	**Code**[a]
Kow	Octanol-water partition coefficient	dimensionless	C
K_s	Half saturation biorate constant	g/m^3	A,C
MW_a	Molecular weight of air	g/gmol	29
MW_{oil}	Molecular weight of oil	g/gmol	B
MW_L	Molecular weight of water	g/gmol	18
N	Emissions	g/s	D
N_I	Number of aerators	dimensionless	A,B
O_t	Oxygen transfer correction factor	dimensionless	B
P	Power number	dimensionless	D
P^*	Vapor pressure of the constituent	atm	C
P_o	Total pressure	atm	A
POWR	Total power to aerators	hp	B
Q	Volumetric flow rate	m^3/s	A
Q_a	Diffused air flow rate	m^3/s	B
Q_{oil}	Volumetric flow rate of oil	m^3/s	B
r	Deficit ratio (ratio of the difference between the constituent concentration at solubility and actual constituent concentration in the upstream and the downstream)	dimensionless	D
R	Universal gas constant	atm-m^3/gmol-K	8.21×10^{-5}
Re	Reynolds number	dimensionless	D
Sc_G	Schmidt number on gas side	dimensionless	D
Sc_L	Schmidt number on liquid side	dimensionless	D

TABLE 5.B-2

(CONTINUED)

Parameter	Definition	Units	Code[a]
T	Temperature of water	°C or Kelvin (K)	A
t	Residence time of disposal	s	A
U^*	Friction velocity	m/s	D
U^{**}	Friction velocity	m/s	D
U_{10}	Wind speed at 10 m above the liquid surface	m/s	B
V	Wastewater volume	m^3 or ft^3	A
Va_v	Turbulent surface area	ft^2	B
V_{oil}	Volume of oil	m^3	B
w	Rotational speed of impeller	rad/s	B
ρ_a	Density of air	g/cm^3	$(1.2x10^{-3})^b$
ρ_L	Density of water	g/cm^3 or lb/ft^3	1^b or 62.4^b
ρ_{oil}	Density of oil	g/m^3	B
μ_a	Viscosity of air	g/cm-s	$(1.81x10^{-4})^b$
μ_L	Viscosity of water	g/cm-s	$(8.93x10^{-3})^b$

[a] Code:
A = Site-specific parameter.
B = Site-specific parameter. For default values, see Table 5.B-3.
C = Parameter can be obtained from literature. See Table 5.B-4 for a list of ~150 compound chemical properties at T = 25°C (298°K).
D = Calculated value.

[b] Reported values at 25°C (298°K).

estimates from an emissions model. In addition, when addressing systems involving biodegradation, the accuracy of the predicted rate of biodegradation is improved when site-specific compound biorates are input. Reference 3 contains information on a test method for measuring site-specific biorates, and Table 5.B-4 presents estimated biorates for approximately 150 compounds.

To estimate an emissions rate (N), the first step is to calculate individual gas phase and liquid phase mass transfer coefficients k_g and k_ℓ. These individual coefficients are then used to calculate the overall mass transfer coefficient, K. Exceptions to this procedure are the calculation of overall mass transfer coefficients in the oil phase, K_{oil}, and the overall mass transfer coefficient for a weir, K_D. K_{oil} requires only k_g, and K_D does not require any individual mass transfer coefficients. The overall mass transfer coefficient is then used to calculate the emissions rates. The following discussion describes how to use Figure 5.B-1 to determine an emission rate. An example calculation is presented in Part B-1 below.

Figure 5.B-1 is divided into two sections: wastewater treatment and storage systems, and wastewater collection systems. Wastewater treatment and storage systems are further segmented into aerated/nonaerated systems, biologically active systems, oil film layer systems, and surface impoundment flowthrough or disposal. In flowthrough systems, wastewater is treated and discharged to a publicly owned treatment works (POTW) or a receiving body of water, such as a river or stream. All wastewater collection systems are by definition flowthrough. Disposal systems, on the other hand, do not discharge any wastewater.

Figure 5.B-1 includes information needed to estimate air emissions from junction boxes, lift stations, sumps, weirs, and clarifier weirs. Sumps are considered quiescent, but junction boxes, lift stations, and weirs are turbulent in nature. Junction boxes and lift stations are turbulent because incoming flow is normally above the water level in the component, which creates some splashing. Wastewater falls or overflows from weirs and creates splashing in the receiving body of water (both weir and clarifier weir models). Wastewater from weirs can be aerated by directing it to fall over steps, usually only the weir model.

Assessing VOC emissions from drains, manholes, and trenches is also important in determining the total wastewater facility emissions. As these sources can be open to the atmosphere and closest to the point of wastewater generation (i.e., where water temperatures and pollutant concentrations are greatest), emissions can be significant. Currently, there are no well-established emission models for these collection system types. However, work is being performed to address this need.

Preliminary models of VOC emissions from waste collection system units have been developed.[4] The emission equations presented in Reference 4 are used with standard collection system parameters to estimate the fraction of the constituents released as the wastewater flows through each unit. The fractions released from several units are estimated for high-, medium-, and low-volatility compounds. The units used in the estimated fractions included open drains, manhole covers, open trench drains, and covered sumps.

The numbers in Figure 5.B-1 under the columns for k_ℓ, k_g, K_{oil}, K_D, K, and N refer to the appropriate equations in Table 5.B-1.[a] Definitions for all parameters in these equations are given in Table 5.B-2. Table 5.B-2 also supplies the units that must be used for each parameter, with codes to help locate input values. If the parameter is coded with the letter A, a site-specific value is required. Code B also requires a site-specific parameter, but defaults are available. These defaults are typical or average values and are presented by specific system in Table 5.B-3.

Code C means the parameter can be obtained from literature data. Table 5.B-4 contains a list of approximately 150 chemicals and their physical properties needed to calculate emissions from wastewater, using the correlations presented in Table 5.B-1. All properties are at 25°C (77°F). A more extensive chemical properties data base is contained in Appendix C of Reference 1.) Parameters coded D are calculated values.

Calculating air emissions from wastewater collection, treatment, and storage systems is a complex procedure, especially if several systems are present. Performing the calculations by hand may result in errors and will be time consuming. A personal computer program called the Surface Impoundment Modeling System (SIMS) is now available for estimating air emissions. The program is menu driven and can estimate air emissions from all surface impoundment models presented in Figure 5.B-1, individually or in series. The program requires for each collection, treatment, or storage system component, at a minimum, the wastewater flow rate and component surface area. All other inputs are provided as default values. Any available site-specific information should be entered in place of these defaults, as the most fully characterized system will provide the most accurate emissions estimate.

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[a] All emission model systems presented in Figure 5.B-1 imply a completely mixed or uniform waste water concentration system. Emission models for a plug flow system, or system in which there is no axial, or horizontal mixing, are too extensive to be covered in this document. (An example of plug flow might be a high waste water flow in a narrow channel.) For information on emission models of this type, see Reference 1.

TABLE 5.B-3

SITE-SPECIFIC DEFAULT PARAMETERS[a]

Default Parameter[b]	Definition	Default Value
General		
T	Temperature of water	298°K
U_{10}	Windspeed	4.47 m/s
Biotreatment Systems		
b_i	Biomass concentration (for biologically active systems)	
	Quiescent treatment systems	50 g/m^3
	Aerated treatment systems	300 g/m^3
	Activated sludge units	4000 g/m^3
POWR	Total power to aerators	
	(for aerated treatment systems)	0.75 hp/1000 ft^3 (V)
	(for activated sludge)	2 hp/1000 ft^3 (V)
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_v	Turbulent surface area	
	(for aerated treatment systems)	0.24 (A)
	(for activated sludge)	0.52 (A)
J	Oxygen transfer rating to surface aerator (for aerated treatment systems)	3 lb O_2/hp•hr
O_t	Oxygen transfer correction factor (for aerated treatment systems)	0.83
N_I	Number of aerators	POWR/75
Diffused Air Systems		
Q_a	Diffused air volumetric flow rate	0.0004(V) m^3/s

TABLE 5.B-3

(CONTINUED)

Default Parameter[b]	Definition	Default Value
Oil Film Layers		
MW_{oil}	Molecular weight of oil	282 g/gmol
D_{oil}	Depth of oil layer	0.001 (V/A) m
V_{oil}	Volume of oil	0.001 (V) m^3
Q_{oil}	Volumetric flow rate of oil	0.001 (Q) m^3/s
ρ_{oil}	Density of oil	0.92 g/cm^3
FO	Fraction of volume which is oil[c]	0.001
Junction Boxes		
D	Depth of Junction Box	0.9 m
N_I	Number of aerators	1
Lift Station		
D	Depth of Lift Station	1.5 m
N_I	Number of aerators	1
Sump		
D	Depth of sump	5.9 m
Weirs		
d_c	Clarifier weir diameter[d]	28.5 m
h	Weir height	1.8 m
h_c	Clarifier weir height[e]	0.1 m

[a] Reference 1.
[b] As defined in Table 5.B-2.
[c] Reference 4.
[d] Reference 2.
[e] Reference 5.

The SIMS program with user's manual and background technical document can be obtained through state air pollution control agencies and through the U.S. Environmental Protection Agency's Control Technology Center in Research Triangle Park, North Carolina, telephone (919) 541-0800. The user's manual and background technical document should be followed to produce meaningful results.

The SIMS program and user's manual also can be downloaded from EPA's Clearinghouse for Inventories and Emission Factors system (CHIEF). The CHIEF is
open to all persons involved in air emission inventories.

First-time users must register before access is
allowed.

Emissions estimates from SIMS are based on mass transfer models developed by Emissions Standards Division (ESD) during evaluations of treatment, storage, and disposal facilities (TSDFs) and VOC emissions from industrial wastewater. As a part of the TSDF project, a Lotus® spreadsheet program called CHEMDAT7 was developed for estimating VOC emissions from wastewater land treatment systems, open landfills, closed landfills, and waste storage piles, as well as from various types of surface impoundments. For more information about CHEMDAT7, contact the ESD's Chemicals And Petroleum Branch (MD-13), U.S. Environmental Protection Agency, Research Triangle Park, North Carolina 27711.

EXAMPLE CALCULATION

An example industrial facility operates a flowthrough, mechanically aerated biological treatment impoundment that receives wastewater contaminated with benzene at a concentration of 10.29 g/m^3.

The following format is used for calculating benzene emissions from the treatment process:

I. Determine which emission model to use
II. User-supplied information
III. Defaults
IV. Pollutant physical property data and water, air, and other properties
V. Calculate individual mass transfer coefficient
VI. Calculate the overall mass transfer coefficients
VII. Calculate VOC emissions

I. Determine Which Emission Model To Use — Following the flow diagram in Figure 5.B-1, the emission model for a treatment system that is aerated, but not by diffused air, is biologically active, and is a flowthrough system, contains the following equations:

Parameter	Definition	Equation Nos. from Table 5.B-1
K	Overall mass transfer coefficient, m/s	7
k_ℓ	Individual liquid phase mass transfer coefficient, m/s	1, 3
k_g	Individual gas phase mass transfer coefficient, m/s	2, 4
N	VOC emissions, g/s	16

II. User-supplied Information — Once the correct emission model is determined, some site-specific parameters are required. As a minimum for this model, site-specific flow rate, wastewater surface area and depth, and pollutant concentration should be provided. For this example, these parameters have the following values:

Q = Volumetric flow rate = 0.0623 m^3/s
D = Wastewater depth = 1.97 m
A = Wastewater surface area = 17,652 m^2
Co = Initial benzene concentration in the liquid phase = 10.29 g/m^3

III. Defaults — Defaults for some emission model parameters are presented in Table 5.B-3. Generally, site-specific values should be used when available. For this facility, all available general and biotreatment system defaults from Table 5.B-3 were used:

U_{10} = Wind speed at 10 m above the liquid surface = e = 4.47 m/s
T = Temperature of water = 25°C (298°K)
b_i = Biomass concentration for aerated treatment systems = 300 g/m^3
J = Oxygen transfer rating to surface aerator = 3 lb O_2/hp-hr
POWR = Total power to aerators = 0.75 hp/1,000 ft^3 (V)
O_t = Oxygen transfer correction factor = 0.83
Va_v = Turbulent surface area = 0.24 (A)
d = Impeller diameter = 61 cm
d^* = Impeller diameter = 2 ft
w = Rotational speed of impeller = 126 rad/s
N_I = Number of aerators = POWR/75 hp

IV. Pollutant Physical Property Data, And Water, Air and Other Properties — For each pollutant, the specific physical properties needed by this model are listed in Table 5.B-4. Water, air, and other property values are given in Table 5.B-2.

A. Benzene (from Table 5.B-4)

$D_{w,benzene}$ = Diffusivity of benzene in water = 9.8×10^{-6} cm^2/s
$D_{a,benzene}$ = Diffusivity of benzene in air = 0.088 cm^2/s
$H_{benzene}$ = Henry's Law constant for benzene = 0.0055 atm- m^3/gmol
$Kmax_{benzene}$ = Maximum biorate constant for benzene = 5.28×10^{-6} g/g-s
$K_{s,benzene}$ = Half saturation biorate constant for benzene = 13.6 g/m^3

B. Water, Air, and Other Properties (from Table 5.B-2)

ρ_a = Density of air = 1.2×10^3 g/cm^3
ρ_L = Density of water = 1 g/cm^3 (62.4 lb_m/ft^3)
μ_a = Viscosity of air = 1.81×10^{-4} g/cm-s
$D_{O2,w}$ = Diffusivity of oxygen in water = 2.4×10^{-5} cm^2/s
D_{ether} = Diffusivity of ether in water = 8.5×10^{-6} cm^2/s
MW_L = Molecular weight of water = 18 g/gmol
MW_a = Molecular weight of air = 29 g/gmol
g_c = Gravitation constant = 32.17 $lb_m\text{-ft}/lb_f\text{-}s^2$
R = Universal gas constant = 8.21×10^{-5} atm-m^3/gmol

V. Calculate Individual Mass Transfer Coefficients — Because part of the impoundment is turbulent and part is quiescent, individual mass transfer coefficients are determined for both turbulent and quiescent areas of the surface impoundment.

<u>Turbulent area of impoundment</u> — Equations 3 and 4 from Table 5.B-1.

A. Calculate the individual liquid mass transfer coefficient, k_ℓ:

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

The total power to the aerators, POWR, and the turbulent surface area, Va_v, are calculated separately [Note: some conversions are necessary.]:

1. Calculate total power to aerators, POWR (Default presented in III):

POWR (hp) = 0.75 hp/1,000 ft^3 (V)
V = wastewater volume, m^3
V (m^3) = (A)(D) = (17,652 m^2)(1.97 m)
V = 34,774 m^3
POWR = (0.75 hp/1,000 ft^3)(ft^3/0.028317 m^3)(34,774 m^3)
= 921 hp

2. Calculate turbulent surface area, Va_v (default presented in III):

$$\begin{aligned} Va_v\ (ft^2) &= 0.24\ (A) \\ &= 0.24(17{,}652\ m^2)(10.758\ ft^2/m^2) \\ &= 45{,}576\ ft^2 \end{aligned}$$

Now, calculate k_ℓ, using the above calculations and information from II, III, and IV:

$$\begin{aligned} k_\ell\ (m/s) &= [(8.22 \times 10^{-9})(3\ lb\ O_2/hp\text{-}hr)(921\ hp)\ * \\ &\quad (1.024)^{(25-20)}(0.83)(10^6)(18\ g/gmol)/ \\ &\quad ((45{,}576\ ft^2)(1\ g/cm^3))]\ * \\ &\quad [(9.8 \times 10^{-6}\ cm^2/s)/(2.4 \times 10^{-5}\ cm^2/s)]^{0.5} \\ &= (0.00838)(0.639) \\ k_\ell &= 5.35 \times 10^{-3}\ m/s \end{aligned}$$

B. Calculate the individual gas phase mass transfer coefficient, k_g:

$$k_g\ (m/s) = (1.35 \times 10^{-7})(Re)^{1.42}(P)^{0.4}(Sc_G)^{0.5}(Fr)^{-0.21}(D_a\ MW_a/d)$$

The Reynolds number, Re, power number, P, Schmidt number on the gas side, Sc_G, and Froude's number, Fr, are calculated separately:

1. Calculate Reynolds number, Re:

$$\begin{aligned} Re &= d^2\ w\ \rho_a/\mu_a \\ &= (61\ cm)^2(126\ rad/s)(1.2 \times 10^{-3}\ g/cm^3)/(1.81 \times 10^{-4}\ g/cm\text{-}s) \\ &= 3.1 \times 10^6 \end{aligned}$$

2. Calculate power number, P:

$$\begin{aligned} P &= [(0.85)(POWR)(550\ ft\text{-}lb_f/s\text{-}hp)/N_I]\ g_c/(\rho_L(d^*)^5\ w^3) \\ N_I &= POWR/75\ hp\ \text{(default presented in III)} \\ P &= (0.85)(75\ hp)(POWR/POWR)(550\ ft\text{-}lb_f/s\text{-}hp)\ * \\ &\quad (32.17\ lb_m\text{-}ft/lb_f\text{-}s^2)/[(62.4\ lb_m/ft^3)(2\ ft)^5(126\ rad/s)^3] \\ &= 2.8 \times 10^{-4} \end{aligned}$$

3. Calculate Schmidt number on the gas side, Sc_G:

$$\begin{aligned} Sc_G &= \mu_a/(\rho_a D_a) \\ &= (1.81 \times 10^{-4}\ g/cm\text{-}s)/[(1.2 \times 10^{-3}\ g/cm^3)(0.088\ cm^2/s)] \\ &= 1.71 \end{aligned}$$

4. Calculate Froude number, Fr:

$$\begin{aligned}\text{Fr} &= (d^*)w^2/g_c\\ &= (2\ \text{ft})(126\ \text{rad/s})^2/(32.17\ \text{lb}_m\text{-ft/lb}_f\text{-s}^2)\\ &= 990\end{aligned}$$

Now, calculate k_g using the above calculations and information from II, III, and IV:

$$\begin{aligned}k_g\ (\text{m/s}) &= (1.35 \times 10^{-7})(3.1 \times 10^6)^{1.42}(2.8 \times 10^{-4})^{0.4}(1.71)^{0.5} *\\ &\quad (990)^{-0.21}(0.088\ \text{cm}^2/\text{s})(29\ \text{g/gmol})/(61\ \text{cm})\\ &= 0.109\ \text{m/s}\end{aligned}$$

<u>Quiescent surface area of impoundment</u> — Equations 1 and 2 from Table 5.B-1.

A. Calculate the individual liquid phase mass transfer coefficient, k_ℓ:

$$\begin{aligned}F/D &= 2(A/\pi)^{0.5}/D\\ &= 2(17{,}652\ \text{m}^2/\pi)^{0.5}/(1.97\ \text{m})\\ &= 76.1\\ U_{10} &= 4.47\ \text{m/s}\end{aligned}$$

For $U_{10} > 3.25$ m/s and $F/D > 51.2$ use the following:

$$\begin{aligned}k_\ell\ (\text{m/s}) &= (2.61 \times 10^{-7})(U_{10})^2(D_w/D_{ether})^{2/3}\\ &= (2.61 \times 10^{-7})(4.47\ \text{m/s})^2[(9.8 \times 10^{-6}\ \text{cm}^2/\text{s})/\\ &\quad (8.5 \times 10^{-6}\ \text{cm}^2/\text{s})]^{2/3}\\ &= 5.74 \times 10^{-6}\ \text{m/s}\end{aligned}$$

B. Calculate the individual gas phase mass transfer coefficient, k_g:

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

The Schmidt number on the gas side, Sc_G, and the effective diameter, d_e, are calculated separately:

1. Calculate the Schmidt number on the gas side, Sc_G:

$$Sc_G = \mu_a/(\rho_a D_a) = 1.71 \text{ (same as for turbulent impoundments)}$$

2. Calculate the effective diameter, d_e:

$$\begin{aligned}
d_e\ (\mathrm{m}) &= 2(A/\pi)^{0.5} \\
&= 2(17{,}652\ \mathrm{m}^2/\pi)^{0.5} \\
&= 149.9\ \mathrm{m} \\
k_g(\mathrm{m/s}) &= (4.82 \text{ x } 10^{-3})(4.47\ \mathrm{m/s})^{0.78}\ (1.71)^{-0.67}\ (149.9\ \mathrm{m})^{-0.11} \\
&= 6.24 \text{ x } 10^{-3}\ \mathrm{m/s}
\end{aligned}$$

VI. Calculate The Overall Mass Transfer Coefficient — 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. (Equation 7 from Table 5.B-1).

Overall mass transfer coefficient for the turbulent surface area of impoundment, K_T

$$\begin{aligned}
K_T\ (\mathrm{m/s}) &= (k_\ell Keqk_g)/(Keqk_g + k_\ell) \\
Keq &= H/RT \\
&= (0.0055\ \text{atm-m}^3/\text{gmol})/[(8.21 \text{ x } 10^{-5}\ \text{atm-m}^3/\ \text{gmol-°K}) \\
&\quad (298°\mathrm{K})] \\
&= 0.225 \\
K_T\ (\mathrm{m/s}) &= (5.35 \text{ x } 10^{-3}\ \mathrm{m/s})(0.225)(0.109)/[(0.109\ \mathrm{m/s})(0.225) + \\
&\quad (5.35 \text{ x } 10^{-6}\ \mathrm{m/s})] \\
K_T &= 4.39 \text{ x } 10^{-3}\ \mathrm{m/s}
\end{aligned}$$

Overall mass transfer coefficient for the quiescent surface area of impoundment, K_Q

$$\begin{aligned}
K_Q\ (\mathrm{m/s}) &= (k_\ell Keqk_g)/(Keqk_g + k_\ell) \\
&= (5.74 \text{ x } 10^{-6}\ \mathrm{m/s})(0.225)(6.24 \text{ x } 10^{-3}\ \mathrm{m/s})/ \\
&\quad [(6.24 \text{ X } 10^{-3}\ \mathrm{m/s})(0.225) + (5.74 \text{ x } 10^{-6}\ \mathrm{m/s})] \\
&= 5.72 \text{ x } 10^{-6}\ \mathrm{m/s}
\end{aligned}$$

Overall mass transfer coefficient, K, weighted by turbulent and quiescent surface areas, A_T and A_Q

$$\begin{aligned}
K\ (\mathrm{m/s}) &= (K_T A_T + K_Q A_Q)/A \\
A_T &= 0.24(A)\ \text{(Default value presented in III: } A_T = Va_v) \\
A_Q &= (1 - 0.24)A \\
K\ (\mathrm{m/s}) &= [(4.39 \text{ x } 10^{-3}\ \mathrm{m/s})(0.24\ A) + (5.72 \text{ x } 10^{-6}\ \mathrm{m/s}) \\
&\quad (1 - 0.24)A]/A \\
&= 1.06 \text{ x } 10^{-3}\ \mathrm{m/s}
\end{aligned}$$

VII. Calculate VOC Emissions For An Aerated Biological Flowthrough Impoundment — Equation 16 from Table 5.B-1:

$$N\ (g/s) = K\ C_L\ A$$

where:

$$C_L\ (g/m^3) = [-b + (b^2 - 4ac)^{0.5}]/(2a)$$

and:

$$a = KA/Q + 1$$
$$b = K_s(KA/Q + 1) + Kmax\ b_i\ V/Q - Co$$
$$c = -K_sCo$$

Calculate a, b, c, and the concentration of benzene in the liquid phase, C_L, separately:

1. Calculate a:

$$\begin{aligned} a &= (KA/Q + 1) = [(1.06 \times 10^{-3}\ m/s)(17{,}652\ m^2)/(0.0623\ m^3/s)] + 1 \\ &= 301.3 \end{aligned}$$

2. Calculate b (V = 34,774 m^3 from IV):

$$\begin{aligned} b &= K_s\ (KA/Q + 1) + Kmax\ b_i\ V/Q - Co \\ &= (13.6\ g/m^3)[(1.06 \times 10^{-3}\ m/s)(17{,}652\ m^2)/(0.0623\ m^3/s)] + \\ &\quad [(5.28 \times 10^{-6}\ g/g\text{-}s)(300\ g/m^3)(34{,}774\ m^3)/(0.0623\ m^3/s)] - 10.29\ g/m^3 \\ &= 4{,}084.6 + 884.1 - 10.29 \\ &= 4{,}958.46\ g/m^3 \end{aligned}$$

3. Calculate c:

$$\begin{aligned} c &= -K_sCo \\ &= -(13.6\ g/m^3)(10.29\ g/m^3) \\ &= -139.94 \end{aligned}$$

4. Calculate the concentration of benzene in the liquid phase, C_L, from a, b, and c above:

$$
\begin{aligned}
C_L \text{ (g/m}^3\text{)} &= [-b + (b^2 - 4ac)^{0.5}]/(2a) \\
&= [(4{,}958.46 \text{ g/m}^3) + [(4{,}958.46 \text{ g/m}^3)^2 - \\
&\quad [4(301.3)(-139.94)]]^{0.5}]/(2(301.3)) \\
&= 0.0282 \text{ g/m}^3
\end{aligned}
$$

Now calculate N with the above calculations and information from II and V:

$$
\begin{aligned}
N \text{ (g/s)} &= K\ A\ C_L \\
&= (1.06 \text{ x } 10^{-3} \text{ m/s})(17{,}652 \text{ m}^2)(0.0282 \text{ g/m}^3) \\
&= 0.52 \text{ g/s}
\end{aligned}
$$

GLOSSARY OF TERMS

Basin -	an earthen or concrete-lined depression used to hold liquid.
Completely mixed -	having the same characteristics and quality throughout or at all times.
Disposal -	the act of permanent storage. Flow of liquid into, but not out of a device.
Drain -	a device used for the collection of liquid. It may be open to the atmosphere or be equipped with a seal to prevent emissions of vapors.
Flowthrough -	having a continuous flow into and out of a device.
Plug flow -	having characteristics and quality not uniform throughout. These will change in the direction the fluid flows, but not perpendicular to the direction of flow (i.e., no axial movement).
Storage -	any device to accept and retain a fluid for the purpose of future discharge. Discontinuity of flow of liquid into and out of a device.
Treatment -	the act of improving fluid properties by physical means. The removal of undesirable impurities from a fluid.
VOC -	volatile organic compounds, referring to all organic compounds except

the following, which have been shown not to be photochemically reactive: methane, ethane, trichlorotrifluoroethane, methylene chloride, 1,1,1,-trichloroethane, trichlorofluoromethane, dichlorodifluoromethane, chlorodifluoromethane, trifluoromethane, dichlorotetrafluoroethane, and chloropentafluoroethane.

TABLE 5.B-4
SIMS CHEMICAL PROPERTY DATA FILE (PART 1)

Chemical Name	CAS Number	Molecular Weight	Vapor Pressure At 25°C (mm Hg)	Henry's Law Constant At 25°C (atm·m^3/mol)	Diffusivity Of Chemical In Water At 25°C (cm^2/s)	Diffusivity Of Chemical In Air At 25°C (cm^2/s)
ACETALDEHYDE	75-07-0	44.00	760	0.000095	0.0000141	0.124
ACETIC ACID	64-19-7	60.05	15.4	0.0627	0.000012	0.113
ACETIC ANHYDRIDE	108-24-7	102.09	5.29	0.00000591	0.00000933	0.235
ACETONE	67-64-1	58.00	266	0.000025	0.0000114	0.124
ACETONITRILE	75-05-8	41.03	90	0.0000058	0.0000166	0.128
ACROLEIN	107-02-8	56.10	244.2	0.0000566	0.0000122	0.105
ACRYLAMIDE	79-06-1	71.09	0.012	0.00000000052	0.0000106	0.097
ACRYLIC ACID	79-10-7	72.10	5.2	0.0000001	0.0000106	0.098
ACRYLONITRILE	107-13-1	53.10	114	0.000088	0.0000134	0.122
ADIPIC ACID	124-04-9	146.14	0.0000225	0.00000000005	0.00000684	0.0659
ALLYL ALCOHOL	107-18-6	58.10	23.3	0.000018	0.0000114	0.114
AMINOPHENOL(-O)	95-55-6	109.12	0.511	0.00000367	0.00000864	0.0774
AMINOPHENOL(-P)	123-30-8	109.12	0.893	0.0000197	0.00000239	0.0774
AMMONIA	7664-41-7	17.03	7470	0.000328	0.0000693	0.259
AMYL ACETATE(-N)	628-37-8	130.18	5.42	0.000464	0.0000012	0.064
ANILINE	62-53-3	93.10	1	0.0000026	0.0000083	0.07
BENZENE	71-43-2	78.10	95.2	0.0055	0.0000098	0.088
BENZO(A)ANTHRACENE	56-55-3	228.30	0.00000015	0.00000000138	0.000009	0.051
BENZO(A)PYRENE	50-32-8	252.30	0.00568	0.00000000138	0.000009	0.043

TABLE 5.B-4 (PART 1)
(CONTINUED)

Chemical Name	CAS Number	Molecular Weight	Vapor Pressure At 25°C (mm Hg)	Henry's Law Constant At 25°C (atm·m^3/mol)	Diffusivity Of Chemical In Water At 25°C (cm^2/s)	Diffusivity Of Chemical In Air At 25°C (cm^2/s)
CRESYLIC ACID	1319-77-3	108.00	0.3	0.0000017	0.0000083	0.074
CROTONALDEHYDE	4170-30-0	70.09	30	0.00000154	0.0000102	0.0903
CUMENE (ISOPROPYLBENZENE)	98-82-8	120.20	4.6	0.0146	0.0000071	0.065
CYCLOHEXANE	110-82-7	84.20	100	0.0137	0.0000091	0.0839
CYCLOHEXANOL	108-93-0	100.20	1.22	0.00000447	0.00000831	0.214
CYCLOHEXANONE	108-94-1	98.20	4.8	0.00000413	0.00000862	0.0784
DI-N-OCTYL PHTHALATE	117-84-0	390.62	0	0.137	0.0000041	0.0409
DIBUTYLPHTHALATE	84-74-2	278.30	0.00001	0.00000028	0.0000079	0.0438
DICHLORO(-2)BUTENE(1,4)	764-41-0	125.00	2.87	0.000259	0.00000812	0.0725
DICHLOROBENZENE(1,2) (-O)	95-50-1	147.00	1.5	0.00194	0.0000079	0.069
DICHLOROBENZENE(1,3) (-M)	541-73-1	147.00	2.28	0.00361	0.0000079	0.069
DICHLOROBENZENE(1,4) (-P)	106-46-7	147.00	1.2	0.0016	0.0000079	0.069
DICHLORODIFLUOROMETHANE	75-71-8	120.92	5000	0.401	0.00001	0.0001
DICHLOROETHANE(1,1)	75-34-3	99.00	234	0.00554	0.0000105	0.0914
DICHLOROETHANE(1,2)	107-06-2	99.00	80	0.0012	0.0000099	0.104
DICHLOROETHYLENE(1,2)	156-54-2	96.94	200	0.0319	0.000011	0.0935
DICHLOROPHENOL(2,4)	120-83-2	163.01	0.1	0.0000048	0.0000076	0.0709
DICHLOROPHENOXYACETIC ACID(2,4)	94-75-7	221.00	290	0.0621	0.00000649	0.0588
DICHLOROPROPANE(1,2)	78-87-5	112.99	40	0.0023	0.0000087	0.0782

TABLE B-4 (PART 1)
(CONTINUED)

Chemical Name	CAS Number	Molecular Weight	Vapor Pressure At 25°C (mm Hg)	Henry's Law Constant At 25°C (atm·m^3/mol)	Diffusivity Of Chemical In Water At 25°C (cm^2/s)	Diffusivity Of Chemical In Air At 25°C (cm^2/s)
DIETHYL (N,N) ANILINE	91-66-7	149.23	0.00283	0.0000000574	0.00000587	0.0513
DIETHYL PHTHALATE	84-66-2	222.00	0.003589	0.0111	0.0000058	0.0542
DIMETHYL FORMAMIDE	68-12-2	73.09	4	0.0000192	0.0000103	0.0939
DIMETHYL HYDRAZINE(1,1)	57-14-7	60.10	157	0.000124	0.0000109	0.106
DIMETHYL PHTHALATE	131-11-3	194.20	0.000187	0.00000215	0.0000063	0.0568
DIMETHYLBENZ(A)ANTHRACENE	57-97-6	256.33	0	0.00000000027	0.00000498	0.0461
DIMETHYLPHENOL(2,4)	105-67-9	122.16	0.0573	0.000921	0.0000084	0.0712
DINITROBENZENE (-M)	99-65-0	168.10	0.05	0.000022	0.00000764	0.279
DINITROTOLUENE(2,4)	121-14-2	182.10	0.0051	0.00000407	0.00000706	0.203
DIOXANE(1,4)	123-91-1	88.20	37	0.0000231	0.0000102	0.229
DIOXIN	NOCAS2	322.00	0	0.0000812	0.0000056	0.104
DIPHENYLAMINE	122-39-4	169.20	0.00375	0.00000278	0.00000631	0.058
EPICHLOROHYDRIN	106-89-8	92.50	17	0.0000323	0.0000098	0.086
ETHANOL	64-17-5	46.10	50	0.0000303	0.000013	0.123
ETHANOLAMINE(MONO-)	141-43-5	61.09	0.4	0.000000322	0.0000114	0.107
ETHYL ACRYLATE	140-88-5	100.00	40	0.00035	0.0000086	0.077
ETHYL CHLORIDE	75-00-3	64.52	1200	0.014	0.0000115	0.271
ETHYL-(2)PROPYL-(3) ACROLEIN	645-62-5	92.50	17	0.0000323	0.0000098	0.086
ETHYLACETATE	141-78-6	88.10	100	0.000128	0.00000966	0.0732

TABLE 5.B-4 (PART 1)
(CONTINUED)

Chemical Name	CAS Number	Molecular Weight	Vapor Pressure At 25°C (mm Hg)	Henry's Law Constant At 25°C (atm·m^3/mol)	Diffusivity Of Chemical In Water At 25°C (cm^2/s)	Diffusivity Of Chemical In Air At 25°C (cm^2/s)
ETHYLBENZENE	100-41-4	106.20	10	0.00644	0.0000078	0.075
ETHYLENEOXIDE	75-21-8	44.00	1250	0.000142	0.0000145	0.104
ETHYLETHER	60-29-7	74.10	520	0.00068	0.0000093	0.074
FORMALDEHYDE	50-00-0	30.00	3500	0.0000576	0.0000198	0.178
FORMIC ACID	64-18-6	46.00	42	0.0000007	0.00000137	0.079
FREONS	NOCAS3	120.92	5000	0.401	0.00001	0.104
FURAN	110-00-9	68.08	596	0.00534	0.0000122	0.104
FURFURAL	96-01-1	96.09	2	0.0000811	0.0000104	0.0872
HEPTANE (ISO)	142-82-5	100.21	66	1.836	0.00000711	0.187
HEXACHLOROBENZENE	118-74-1	284.80	1	0.00068	0.00000591	0.0542
HEXACHLOROBUTADIENE	87-68-3	260.80	0.15	0.0256	0.0000062	0.0561
HEXACHLOROCYCLOPENTADIENE	77-47-4	272.80	0.081	0.016	0.00000616	0.0561
HEXACHLOROETHANE	67-72-1	237.00	0.65	0.00000249	0.0000068	0.00249
HEXANE(-N)	100-54-3	86.20	150	0.122	0.00000777	0.2
HEXANOL(-1)	111-27-3	102.18	0.812	0.0000182	0.00000753	0.059
HYDROCYANIC ACID	74-90-8	27.00	726	0.000000465	0.0000182	0.197
HYDROFLUORIC ACID	7664-39-3	20.00	900	0.000237	0.000033	0.388
HYDROGEN SULFIDE	7783-06-4	34.10	15200	0.023	0.0000161	0.176
ISOPHORONE	78-59-1	138.21	0.439	0.00000576	0.00000676	0.0623

TABLE 5.B-4 (PART 1)
(CONTINUED)

Chemical Name	CAS Number	Molecular Weight	Vapor Pressure At 25°C (mm Hg)	Henry's Law Constant At 25°C (atm·m^3/mol)	Diffusivity Of Chemical In Water At 25°C (cm^2/s)	Diffusivity Of Chemical In Air At 25°C (cm^2/s)
METHANOL	67-56-1	32.00	114	0.0000027	0.0000164	0.15
METHYL ACETATE	79-20-9	74.10	235	0.000102	0.00001	0.104
METHYL CHLORIDE	74-87-3	50.50	3830	0.00814	0.0000065	0.126
METHYL ETHYL KETONE	78-93-3	72.10	100	0.0000435	0.0000098	0.0808
METHYL ISOBUTYL KETONE	108-10-1	100.20	15.7	0.0000495	0.0000078	0.075
METHYL METHACRYLATE	80-62-6	100.10	39	0.000066	0.0000086	0.077
METHYL STYRENE (ALPHA)	98-83-9	118.00	0.076	0.00591	0.0000114	0.264
METHYLENE CHLORIDE	75-09-2	85.00	438	0.00319	0.0000117	0.101
MORPHOLINE	110-91-8	87.12	10	0.0000573	0.0000096	0.091
NAPHTHALENE	91-20-3	128.20	0.23	0.00118	0.0000075	0.059
NITROANILINE(-O)	88-74-4	138.14	0.003	0.0000005	0.000008	0.073
NITROBENZENE	98-95-3	123.10	0.3	0.0000131	0.0000086	0.076
PENTACHLOROBENZENE	608-93-5	250.34	0.0046	0.0073	0.0000063	0.057
PENTACHLOROETHANE	76-01-7	202.30	4.4	0.021	0.0000073	0.066
PENTACHLOROPHENOL	87-86-5	266.40	0.00099	0.0000028	0.0000061	0.056
PHENOL	108-95-2	94.10	0.34	0.000000454	0.0000091	0.082
PHOSGENE	75-44-5	98.92	1390	0.171	0.00000112	0.108
PHTHALIC ACID	100-21-0	166.14	121	0.0132	0.0000068	0.064
PHTHALIC ANHYDRIDE	85-44-9	148.10	0.0015	0.0000009	0.0000086	0.071

TABLE 5.B-4 (PART 1)
(CONTINUED)

Chemical Name	CAS Number	Molecular Weight	Vapor Pressure At 25°C (mm Hg)	Henry's Law Constant At 25°C (atm·m^3/mol)	Diffusivity Of Chemical In Water At 25°C (cm^2/s)	Diffusivity Of Chemical In Air At 25°C (cm^2/s)
PICOLINE(-2)	108-99-6	93.12	10.4	0.000127	0.0000096	0.075
POLYCHLORINATED BIPHENYLS	1336-36-3	290.00	0.00185	0.0004	0.00001	0.104
PROPANOL (ISO)	71-23-8	60.09	42.8	0.00015	0.0000104	0.098
PROPIONALDEHYDE	123-38-6	58.08	300	0.00115	0.0000114	0.102
PROPYLENE GLYCOL	57-55-6	76.11	0.3	0.0000015	0.0000102	0.093
PROPYLENE OXIDE	75-66-9	58.10	525	0.00134	0.00001	0.104
PYRIDINE	110-86-1	79.10	20	0.0000236	0.0000076	0.091
RESORCINOL	108-46-3	110.11	0.00026	0.0000000188	0.0000087	0.078
STYRENE	100-42-5	104.20	7.3	0.00261	0.000008	0.071
TETRACHLOROETHANE(1,1,1,2)	630-20-6	167.85	6.5	0.002	0.0000079	0.071
TETRACHLOROETHANE(1,1,2,2)	79-34-5	167.85	6.5	0.00038	0.0000079	0.071
TETRACHLOROETHYLENE	127-18-4	165.83	19	0.029	0.0000082	0.072
TETRAHYDROFURAN	109-99-9	72.12	72.1	0.000049	0.0000105	0.098
TOLUENE	109-88-3	92.40	30	0.00668	0.0000086	0.087
TOLUENE DIISOCYANATE(2,4)	584-84-9	174.16	0.08	0.0000083	0.0000062	0.061
TRICHLORO(1,1,2)TRIFLUOROETHANE	76-13-1	187.38	300	0.435	0.0000082	0.078
TRICHLOROBENZENE(1,2,4)	120-82-1	181.50	0.18	0.00142	0.0000077	0.0676
TRICHLOROBUTANE(1,2,3)	NOCAS5	161.46	4.39	4.66	0.0000072	0.066
TRICHLOROETHANE(1,1,1)	71-55-6	133.40	123	0.00492	0.0000088	0.078

TABLE 5.B-4 (PART 1)
(CONTINUED)

Chemical Name	CAS Number	Molecular Weight	Vapor Pressure At 25°C (mm Hg)	Henry's Law Constant At 25°C (atm·m^3/mol)	Diffusivity Of Chemical In Water At 25°C (cm^2/s)	Diffusivity Of Chemical In Air At 25°C (cm^2/s)
TRICHLOROETHANE(1,1,2)	79-00-5	133.40	25	0.000742	0.0000088	0.078
TRICHLOROETHYLENE	79-01-6	131.40	75	0.0091	0.0000091	0.079
TRICHLOROFLUOROMETHANE	75-69-4	137.40	796	0.0583	0.0000097	0.087
TRICHLOROPHENOL(2,4,6)	88-06-2	197.46	0.0073	0.0000177	0.0000075	0.0661
TRICHLOROPROPANE(1,1,1)	NOCAS6	147.43	3.1	0.029	0.0000079	0.071
TRICHLOROPROPANE(1,2,3)	96-18-4	147.43	3	0.028	0.0000079	0.071
UREA	57-13-6	60.06	6.69	0.000264	0.0000137	0.122
VINYL ACETATE	108-05-4	86.09	115	0.00062	0.0000092	0.085
VINYL CHLORIDE	75-01-4	62.50	2660	0.086	0.0000123	0.106
VINYLIDENE CHLORIDE	75-35-4	97.00	591	0.015	0.0000104	0.09
XYLENE(-M)	1330-20-7	106.17	8	0.0052	0.0000078	0.07
XYLENE(-O)	95-47-6	106.17	7	0.00527	0.00001	0.087

TABLE 5.B-4
SIMS CHEMICAL PROPERTY DATA FILE (PART 2)

Chemical Name	Antoine's Equation Vapor Pressure Coefficient A	Antoine's Equation Vapor Pressure Coefficient B	Antoine's Equation Vapor Pressure Coefficient C	Maximum Biodegradation Rate Constant (g/g Biomass-s)	Half Saturation Constant (g/m^3)	Octanol-Water Partition Coefficient At 25°C
ACETALDEHYDE	8.005	1600.017	291.809	0.0000228944	419.0542	2.69153
ACETIC ACID	7.387	1533.313	222.309	0.0000038889	14.2857	0.48978
ACETIC ANHYDRIDE	7.149	1444.718	199.817	0.0000026944	1.9323	1
ACETONE	7.117	1210.595	229.664	0.0000003611	1.1304	0.57544
ACETONITRILE	7.119	1314.4	230	0.00000425	152.6014	0.45709
ACROLEIN	2.39	0	0	0.0000021667	22.9412	0.81283
ACRYLAMIDE	11.2932	3939.877	273.16	0.00000425	56.2388	6.32182
ACRYLIC ACID	5.652	648.629	154.683	0.0000026944	54.7819	2.04174
ACRYLONITRILE	7.038	1232.53	222.47	0.000005	24	0.12023
ADIPIC ACID	0	0	0	0.0000026944	66.9943	1.20226
ALLYL ALCOHOL	0	0	0	0.0000048872	3.9241	1.47911
AMINOPHENOL(-O)	0	0	0	0.00000425	68.1356	3.81533
AMINOPHENOL(-P)	-3.357	699.157	-331.343	0.00000425	68.1356	3.81533
AMMONIA	7.5547	1002.711	247.885	0.00000425	15.3	1
AMYL ACETATE(-N)	0	0	0	0.0000026944	16.1142	51.10801
ANILINE	7.32	1731.515	206.049	0.0000019722	0.3381	7.94328
BENZENE	6.905	1211.033	220.79	0.0000052778	13.5714	141.25375
BENZO(A)ANTHRACENE	6.9824	2426.6	156.6	0.0000086389	1.7006	407380.2778

TABLE 5.B-4 (PART 2)
(CONTINUED)

Chemical Name	Antoine's Equation Vapor Pressure Coefficient A	Antoine's Equation Vapor Pressure Coefficient B	Antoine's Equation Vapor Pressure Coefficient C	Maximum Biodegradation Rate Constant (g/g Biomass-s)	Half Saturation Constant (g/m^3)	Octanol-Water Partition Coefficient At 25°C
BENZO(A)PYRENE	9.2455	3724.363	273.16	0.0000086389	1.2303	954992.58602
BENZYL CHLORIDE	0	0	0	0.0000049306	17.5674	199.52623
BIS(2-CHLOROETHYL)ETHER	0	0	0	0.0000029889	20.0021	38.01894
BIS(2-CHLOROISOPROPYL)ETHER	0	0	0	0.0000029889	8.3382	380.1894
BIS(2-ETHYLHEXYL)PHTHALATE	0	0	0	0.0000002139	2.2	199526.2315
BROMOFORM	0	0	0	0.0000029889	10.653	199.52623
BROMOMETHANE	0	0	0	0.0000029889	30.4422	12.58925
BUTADIENE-(1,3)	6.849	930.546	238.854	0.0000042534	15.3	74.32347
BUTANOL (ISO)	7.4743	1314.19	186.55	0.0000021667	70.9091	5.62341
BUTANOL-(1)	7.4768	1362.39	178.77	0.0000021667	70.9091	5.62341
BUTYL BENZYL PHTHALATE	0	0	0	0.0000086389	14.1364	60255.95861
CARBON DISULFIDE	6.942	1169.11	241.59	0.0000042534	5.8175	1
CARBON TETRACHLORIDE	6.934	1242.43	230	0.0000004167	1	524.80746
CHLORO(-P)CRESOL(-M)	0	0	0	0.0000029889	5.2902	1258.92541
CHLOROACETALDEHYDE	0	0	0	0.0000029889	49.838	3.4405
CHLOROBENZENE	6.978	1431.05	217.55	0.0000001083	.039	316.22777
CHLOROFORM	6.493	929.44	196.03	0.0000008167	3.7215	91.20108
CHLORONAPHTHALENE-(2)	0	0	0	0.0000029889	2.167	13182.56739

TABLE 5.B-4 (PART 2)
(CONTINUED)

Chemical Name	Antoine's Equation Vapor Pressure Coefficient A	Antoine's Equation Vapor Pressure Coefficient B	Antoine's Equation Vapor Pressure Coefficient C	Maximum Biodegradation Rate Constant (g/g Biomass-s)	Half Saturation Constant (g/m^3)	Octanol-Water Partition Coefficient At 25°C
CHLOROPRENE	6.161	783.45	179.7	0.0000029968	6.3412	1
CRESOL(-M)	7.508	1856.36	199.07	0.0000064472	1.3653	93.32543
CRESOL(-O)	6.911	1435.5	165.16	0.0000063278	1.34	95.49926
CRESOL(-P)	7.035	1511.08	161.85	0.0000064472	1.3653	87.09636
CRESYLIC ACID	0	0	0	0.0000041667	15	1
CROTONALDEHYDE	0	0	0	0.0000026944	27.6285	12.36833
CUMENE (ISOPROPYLBENZENE)	6.963	1460.793	207.78	0.0000086458	16.5426	1
CYCLOHEXANE	6.841	1201.53	222.65	0.0000042534	15.3	338.0687
CYCLOHEXANOL	6.255	912.87	109.13	0.0000026944	18.0816	37.74314
CYCLOHEXANONE	7.8492	2137.192	273.16	0.0000031917	41.8921	6.45654
DI-N-OCTYL PHTHALATE	0	0	0	0.000000083	0.02	141253.7
DIBUTYLPHTHALATE	6.639	1744.2	113.59	0.0000001111	0.4	158489.31925
DICHLORO(-2)BUTENE(1,4)	0	0	0	0.0000029889	9.8973	242.1542
DICHLOROBENZENE(1,2) (-O)	0.176	0	0	0.0000006944	4.3103	2398.83292
DICHLOROBENZENE(1,3) (-M)	0	0	0	0.0000017778	2.7826	2398.83292
DICHLOROBENZENE(1,4) (-P)	0.079	0	0	0.0000017778	2.7826	2454.70892
DICHLORODIFLUOROMETHANE	0	0	0	0.0000029889	12.0413	144.54398
DICHLOROETHANE(1,1)	0	0	0	0.0000029889	4.6783	61.6595
DICHLOROETHANE(1,2)	7.025	1272.3	222.9	0.0000005833	2.1429	61.6595

TABLE 5.B-4 (PART 2)
(CONTINUED)

Chemical Name	Antoine's Equation Vapor Pressure Coefficient A	Antoine's Equation Vapor Pressure Coefficient B	Antoine's Equation Vapor Pressure Coefficient C	Maximum Biodegradation Rate Constant (g/g Biomass-s)	Half Saturation Constant (g/m^3)	Octanol-Water Partition Coefficient At 25°C
DICHLOROETHYLENE(1,2)	6.965	1141.9	231.9	0.0000029889	6.3294	1
DICHLOROPHENOL(2,4)	0	0	0	0.0000069444	7.5758	562.34133
DICHLOROPHENOXYACETIC ACID(2,4)	0	0	0	0.0000029889	14.8934	82.61445
DICHLOROPROPANE(1,2)	6.98	1380.1	22.8	0.0000047222	12.1429	1
DIETHYL (N,N) ANILINE	7.466	1993.57	218.5	0.00000425	27.0047	43.57596
DIETHYL PHTHALATE	0	0	0	0.000000753	1.28	1412.537
DIMETHYL FORMAMIDE	6.928	1400.87	196.43	0.00000425	15.3	1
DIMETHYL HYDRAZINE(1,1)	7.408	1305.91	225.53	0.00000425	15.3	1
DIMETHYL PHTHALATE	4.522	700.31	51.42	0.0000006111	0.7097	74.13102
DIMETHYLBENZ(A)ANTHRACENE	0	0	0	0.0000086389	0.3377	28680056.33087
DIMETHYLPHENOL(2,4)	0	0	0	0.0000029722	2.2766	263.0268
DINITROBENZENE (-M)	4.337	229.2	-137	0.00000425	29.9146	33.28818
DINITROTOLUENE(2,4)	5.798	1118	61.8	0.00000425	19.5233	102.3293
DIOXANE(1,4)	7.431	1554.68	240.34	0.0000026944	24.7001	16.60956
DIOXIN	12.88	6465.5	273	0.0000029968	6.3412	1
DIPHENYLAMINE	0	0	0	0.0000052778	8.4103	1659.58691
EPICHLOROHYDRIN	8.2294	2086.816	273.16	0.0000029968	6.3412	1.07152
ETHANOL	8.321	1718.21	237.52	0.0000024444	9.7778	0.47863
ETHANOLAMINE(MONO-)	7.456	1577.67	173.37	0.00000425	223.0321	0.16865

TABLE 5.B-4 (PART 2)
(CONTINUED)

Chemical Name	Antoine's Equation Vapor Pressure Coefficient A	Antoine's Equation Vapor Pressure Coefficient B	Antoine's Equation Vapor Pressure Coefficient C	Maximum Biodegradation Rate Constant (g/g Biomass-s)	Half Saturation Constant (g/m^3)	Octanol-Water Partition Coefficient At 25°C
ETHYL ACRYLATE	7.9645	1897.011	273.16	0.0000026944	39.4119	4.85667
ETHYL CHLORIDE	6.986	1030.01	238.61	0.0000029889	22.8074	26.91535
ETHYL-(2)PROPYL-(3) ACROLEIN	0	0	0	0.000004425	15.3	1
ETHYLACETATE	7.101	1244.95	217.88	0.0000048833	17.58	1
ETHYLBENZENE	6.975	1424.255	213.21	0.0000018889	3.2381	1412.53754
ETHYLENEOXIDE	7.128	1054.54	237.76	0.0000011667	4.6154	0.50003
ETHYLETHER	6.92	1064.07	228.8	0.0000026944	17.1206	43.57596
FORMALDEHYDE	7.195	970.6	244.1	0.0000013889	20	87.09636
FORMIC ACID	7.581	1699.2	260.7	0.0000026944	6.3412	0.1191
FREONS	0	0	0	0.0000029968	6.3412	1
FURAN	6.975	1060.87	227.74	0.0000026944	14.1936	71.37186
FURFURAL	6.575	1198.7	162.8	0.0000026944	18.0602	37.86047
HEPTANE (ISO)	6.8994	1331.53	212.41	0.0000042534	15.3	1453.372
HEXACHLOROBENZENE	0	0	0	0.0000029889	0.6651	295120.92267
HEXACHLOROBUTADIENE	- 0.824	0	0	0.000003	6.3412	5495.408
HEXACHLOROCYCLOPENTADIENE	0	0	0	0.0000029968	0.3412	9772.372
HEXACHLOROETHANE	0	0	0	0.0000029889	3.3876	4068.32838
HEXANE(-N)	6.876	1171.17	224.41	0.0000042534	15.3	534.0845
HEXANOL(-1)	7.86	1761.26	196.66	0.0000026944	15.2068	59.52851

TABLE 5.B-4 (PART 2)
(CONTINUED)

Chemical Name	Antoine's Equation Vapor Pressure Coefficient A	Antoine's Equation Vapor Pressure Coefficient B	Antoine's Equation Vapor Pressure Coefficient C	Maximum Biodegradation Rate Constant (g/g Biomass-s)	Half Saturation Constant (g/m^3)	Octanol-Water Partition Coefficient At 25°C
HYDROCYANIC ACID	7.528	1329.5	260.4	0.0000026944	1.9323	1
HYDROFLUORIC ACID	7.217	1268.37	273.87	0.0000026944	1.9323	1
HYDROGEN SULFIDE	7.614	885.319	250.25	0.0000029889	6.3294	1
ISOPHORONE	0	0	0	0.00000425	25.6087	50.11872
METHANOL	7.897	1474.08	229.13	0.000005	90	0.19953
METHYL ACETATE	7.065	1157.63	219.73	0.0000055194	159.2466	0.81285
METHYL CHLORIDE	7.093	948.58	249.34	0.0000029889	14.855	83.17638
METHYL ETHYL KETONE	6.9742	1209.6	216	0.0000005556	10	1.90546
METHYL ISOBUTYL KETONE	6.672	1168.4	191.9	0.0000002056	1.6383	23.98833
METHYL METHACRYLATE	8.409	2050.5	274.4	0.0000026944	109.2342	0.33221
METHYL STYRENE (ALPHA)	6.923	1486.88	202.4	0.0000008639	11.12438	2907.589
METHYLENE CHLORIDE	7.409	1325.9	252.6	0.0000061111	54.5762	17.78279
MORPHOLINE	7.7181	1745.8	235	0.00000425	291.9847	0.08318
NAPHTHALENE	7.01	1733.71	201.86	0.0000117972	42.47	1
NITROANILINE(-O)	8.868	336.5	273.16	0.00000425	22.8535	67.6083
NITROBENZENE	7.115	1746.6	201.8	0.0000030556	4.7826	69.1831
PENTACHLOROBENZENE	0	0	0	0.0000029889	0.4307	925887.02902
PENTACHLOROETHANE	6.74	1378	197	0.0000029889	0.4307	925887.02902
PENTACHLOROPHENOL	0	0	0	0.0000361111	38.2353	102329.29923

TABLE 5.B-4 (PART 2)
(CONTINUED)

Chemical Name	Antoine's Equation Vapor Pressure Coefficient A	Antoine's Equation Vapor Pressure Coefficient B	Antoine's Equation Vapor Pressure Coefficient C	Maximum Biodegradation Rate Constant (g/g Biomass-s)	Half Saturation Constant (g/m^3)	Octanol-Water Partition Coefficient At 25°C
PHENOL	7.133	1516.79	174.95	0.0000269444	7.4615	28.84032
PHOSGENE	6.842	941.25	230	0.00000425	70.8664	3.4405
PHTHALIC ACID	0	0	0	0.0000026944	34.983	6.64623
PHTHALIC ANHYDRIDE	8.022	2868.5	273.16	0.0000048872	3.9241	0.23988
PICOLINE(-2)	7.032	1415.73	211.63	0.00000425	44.8286	11.48154
POLYCYLORINATED BIPHENYLS	0	0	0	0.000005278	20	1
PROPANOL (ISO)	8.117	1580.92	219.61	0.0000041667	200	0.69183
PROPIONALDEHYDE	16.2315	2659.02	-44.15	0.0000026944	39.2284	4.91668
PROPYLENE GLYCOL	8.2082	2085.9	203.5396	0.0000026944	109.3574	0.33141
PROPYLENE OXIDE	8.2768	1656.884	273.16	0.0000048872	3.9241	1
PYRIDINE	7.041	1374.8	214.98	0.0000097306	146.9139	4.4684
RESORCINOL	6.9243	1884.547	186.0596	0.0000026944	35.6809	6.30957
STYRENE	7.14	1574.51	224.09	0.0000086389	282.7273	1445.43977
TETRACHLOROETHANE(1,1,2)	6.898	1365.88	209.74	0.0000029889	6.3294	1
TETRACHLOROETHANE(1,1,2,2)	6.631	1228.1	179.9	0.0000017222	9.1176	363.07805
TETRACHLOROETHYLENE	6.98	1386.92	217.53	0.0000017222	9.1176	398.10717
TETRAHYDROFURAN	6.995	1202.29	226.25	0.0000026944	20.3702	27.58221
TOLUENE	6.954	1344.8	219.48	0.0000204111	30.6167	489.77882
TOLUENE DIISOCYANATE(2,4)	0	0	0	0.0000425	15.3	1

TABLE 5.B-4 (PART 2)
(CONTINUED)

Chemical Name	Antoine's Equation Vapor Pressure Coefficient A	Antoine's Equation Vapor Pressure Coefficient B	Antoine's Equation Vapor Pressure Coefficient C	Maximum Biodegradation Rate Constant (g/g Biomass-s)	Half Saturation Constant (g/m^3)	Octanol-Water Partition Coefficient At 25°C
TRICHLORO(1,1,2)TRIFLUOROETHANE	6.88	1099.9	227.5	0.0000029889	3.3876	4068.32838
TRICHLOROBENZENE(1,2,4)	0	0	0	0.0000029889	2.4495	9549.92586
TRICHLOROBUTANE(1,2,3)	0	0	0	0.0000029968	6.3412	1450901.06626
TRICHLOROETHANE(1,1,1)	8.643	2136.6	302.8	0.0000009722	4.7297	309.02954
TRICHLOROETHANE(1,1,2)	6.951	1314.41	209.2	0.0000009722	4.7297	1
TRICHLOROETHYLENE	6.518	1018.6	192.7	0.0000010833	4.4318	194.98446
TRICHLOROFLUOROMETHANE	6.884	1043.004	236.88	0.000003	6.3412	338.8441
TRICHLOROPHENOL(2,4,6)	0	0	0	0.0000425	58.8462	4897.78819
TRICHLOROPROPANE(1,1,1)	0	0	0	0.0000029889	10.7719	193.7827
TRICHLOROPROPANE(1,2,3)	6.903	788.2	243.23	0.0000029889	10.7719	193.7827
UREA	0	0	0	0.00000425	4.8169	4068.32838
VINYL ACETATE	7.21	1296.13	226.66	0.0000026944	31.8363	8.51722
VINYL CHLORIDE	3.425	0	0	0.000003	6.3412	1.14815
VINYLIDENE CHLORIDE	6.972	1099.4	237.2	0.0000029968	6.3412	1
XYLENE(-M)	7.009	1426.266	215.11	0.0000086389	14.0094	1584.89319
XYLENE(-O)	6.998	1474.679	213.69	0.0000113306	22.8569	891.25094

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APPENDIX C

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