



National Pollutant Inventory

Emission Estimation Technique Manual

for

**Sewage and
Wastewater Treatment**

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**EMISSION ESTIMATION TECHNIQUES
FOR
SEWAGE AND WASTEWATER TREATMENT**

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1.0 INTRODUCTION

The purpose of all Emission Estimation Technique (EET) Manuals in this series is to assist Australian manufacturing, industrial, and service facilities to report emissions of listed substances to the National Pollutant Inventory (NPI). This Manual describes the procedures and recommended approaches for estimating emissions from facilities engaged in sewage and wastewater treatment.

The sewage and wastewater treatment operations covered in this Manual apply to facilities engaged in operating sewage or drainage systems, or sewage treatment plants.

EET MANUAL: Sewage and Wastewater Treatment

HANDBOOK: Sewerage and Drainage Services

ANZSIC CODES : 3702 and all codes within the 370 ANZSIC code group.

This Manual was drafted by the Queensland Environmental Protection Agency on behalf of the Commonwealth Government. It has been developed through a process of national consultation involving State and Territory environmental authorities and key industry stakeholders.

2.0 Processes Description

Sewage collection and treatment plays a critical role in the public health and environment of all Australian towns and cities. On average, each Australian produces 70 000 litres of sewage each year, with the majority of effluent from Australia's large coastal cities and towns discharged to coastal waters under environmental licence conditions.

Sewage and wastewater treatment plants are designed to utilise biological, chemical, and physical processes in order to remove pollutants. Treatment plants are designed to remove pollutants in the following order:

1. suspended solids,
2. dissolved biodegradable organic material, and
3. inorganic nutrients.

These three stages are referred to as primary, secondary, and advanced water, or tertiary, treatment respectively.

2.1 Physical or Primary Treatment

Physical treatment is an essential stage of most waste treatment processes, particularly those with large volumes of solid or organic material. This stage of the process involves physical separation by removing material that floats, or can settle out. It is generally termed 'primary' treatment, although some of the physical processes could be classified as 'secondary' or 'advanced water' treatment.

2.2 Secondary Treatment

In the context of sewage treatment, the process of biological degradation of organic wastes is typically used as secondary treatment. There are several processes in common use:

- activated sludge;
- trickling filter; and
- ponding.

2.3 Advanced Water or Tertiary Treatment

At this stage of treatment, additional combinations of unit operations and processes are used to remove other constituents, such as nitrogen and phosphorus, which are not reduced significantly by secondary treatment. These include, among others:

- Coagulation/air flotation or sedimentation;
- Filtration;

-
- Disinfection (UV, Chlorine, etc);
 - Very high level of nutrient removal (chemical or biological);
 - Activated carbon treatment; and
 - Reverse osmosis

2.4 Disinfection

In most instances, it is necessary to disinfect wastewater before it is discharged. The common methods of disinfection are:

- chlorination;
- UV disinfection;
- ozone treatment; and
- detention lagoons

Chlorination of wastewater will give rise to the emission of chlorine, an NPI-listed substance. Other disinfection methods do not typically give rise to emissions of NPI-listed substances.

2.5 Emissions to Water

Inland and marine waters are discussed separately because the chemical pathways differ considerably.

2.5.1 Inland Waters

Effluent discharge to inland waters in Australia is usually from smaller inland communities, with a few exceptions such as Canberra, and other regional cities and larger towns.

In Australia (with very few exceptions), discharge to inland waters occurs after a minimum of secondary treatment. Commonly, disinfection is a requirement. There is an increasing need for the removal of nitrogen and phosphorus, particularly for the large discharges, or where the effluent constitutes a significant proportion of total stream flow. Nutrient removal is desirable for discharges to the longer inland rivers, especially where there are other nutrient inputs from agriculture.

2.5.2 Ocean and Marine Waters

Effluent discharge to the ocean is common in Australia, particularly from the larger coastal cities. All of the state capital cities are located on the coast and discharge effluent directly, or indirectly, to the ocean. There are more than 50 ocean outfalls from these cities and other coastal centres. Discharge rates vary from about 500 megalitres per day from outfalls in Sydney and Melbourne, to less than 1 megalitre per day in smaller communities. The degree of purification before discharge varies from minimal, up to advanced water treatment with nutrient removal.

2.6 Emissions to Land

Discharge of sewage effluent to land is significantly influenced by land availability, climate, topography, and soil conditions. Many small, mainly inland communities discharge effluent to land. Land discharge in arid or inland regions is often associated with reuse of the effluent for other purposes, such as irrigation. When discharging sewage effluent to land, the goal is to return water and nutrients with the least adverse effect on the soil, on the pasture or crop, and on the ecosystems near the discharge site.

Emissions of NPI-listed substances to land from sewerage and wastewater treatment plants include the following three methods:

- lagoon treatment and effluent polishing through irrigation that rely on micro-organisms and sunlight to disinfect the effluent as it passes through the lagoons and irrigation ponds;
- land filtration that relies on evaporation and soil filtering; and
- pasture filtration disposal, or fate management, that relies on bacteria in the soil and pasture to treat the effluent.

Nutrients (nitrogen and phosphorus) do not require reporting when the emissions occur to land, as these pollutants only require reporting where the emissions are above threshold and the discharge is to a surface waterbody. However, other NPI-listed substances, contained in wastewater effluent and discharged to land need to be characterised and reported where thresholds for these substances have been tripped.

2.7 Emissions to Air

Volatile organic compounds (VOCs) are emitted from wastewater treatment, collection and storage systems, through the volatilisation of organic compounds at the liquid surface. Hydrogen sulfide can form under anaerobic conditions; low concentrations may be emitted and could be calculated using the WATER8 computer model (see Appendix II). Chlorine may also be emitted.

Emissions can occur through diffusive or convective mechanisms, or both. Diffusion occurs when organic concentrations at the water surface are much higher than ambient concentrations. The organics volatilise or diffuse into the air in an attempt to reach equilibrium between aqueous and vapour phases. Convection occurs when air flows over the water surface, thereby sweeping organic vapours from the surface into the air. The rate of volatilisation is directly related to the speed of the air flow over the water surface.

2.8 Leaks, Overflows and Spills

Most large sewerage systems comprise main sewers, pumping stations, and emergency relief structures. During times of rainfall, infiltration occurs into the sewerage system. Sewerage systems are designed to contain a certain volume of sewage flow under defined rainfall levels. When these levels are exceeded, sewage spills may occur because of insufficient capacity in the system.

Sewage spills are usually controlled by the location of emergency relief structures within the system. These are designed to control sewage flow, and to minimise the impact on the environment and public health. Measurement of spills, (or an estimation in the event that there are no emergency relief structures), will need to be undertaken where thresholds are triggered. Spills can occur to stormwater, surface waters, or to land.

Emissions of total nitrogen and total phosphorus to land via spills do not require reporting. However, where these nutrient pollutants are emitted to surface waters from spill events, characterisation and reporting is required when thresholds are exceeded.

3.0 Determining Thresholds

Estimates of emissions of NPI-listed substances to air, water and land should be reported for each substance that triggers a threshold. The reporting list and detailed information on thresholds are contained in *The NPI Guide* at the front of this Handbook.

Wastewater from domestic, commercial and industrial sources will contain a range of NPI-listed substances, including total nitrogen and total phosphorus, metals, inorganics and organics. Wastewater from commercial and industrial sources may contain higher levels of metals, inorganics and organics. Commercial and industrial waste is typically discharged into the sewerage system on the basis of trade-waste agreements between an individual business and the facility operator. Knowledge and characterisation of this waste is useful in determining whether NPI reporting thresholds have been tripped, and in calculating emissions.

The pricing of trade-waste agreements attempts to reflect the ‘true cost’ of the transfer and treatment of sewage, and encourages businesses to remove pollutants before they enter the sewerage system. It also requires the sewage facility operator to have a reasonable knowledge of the influent. An understanding of the different pollutants in the influent is important for determining thresholds and reporting obligations.

The first step for the operator of a sewage and wastewater treatment facility when preparing a report to the NPI, is to consider which methods of effluent discharge are used by the facility, and which listed substances may require reporting. This is important because some pollutants, such as nitrogen and phosphorus, only require reporting where the emissions are directly to water. Table 1 summarises the NPI-listed pollutants contained in sewage effluent in terms of both the threshold categories, and the likely emission media. Only those listed substances matched by ticks against emission media need to be factored into threshold determinations. The *NPI Guide* at the front of this Handbook, contains the complete NPI-list of substances, and explanatory notes on the reporting thresholds.

Table 1. Reporting Decision Matrix by Emission Media and NPI-Listed Substance Category

Sewerage Effluent Emission Media		NPI Pollutant and Threshold Categories				
		Total Phosphorus (3 t/yr) ^a	Total Nitrogen (15 t/yr) ^a	Metals (10 t/yr) ^b	Inorganic /Organics (10 t/yr) ^b	Total VOCs (25 t/yr) ^b
Water	coastal waters	✓	✓	✓	✓	✓
	inland waterways	✓	✓	✓	✓	✓
	aquifer recharge			✓	✓	✓
Land	irrigation reuse			✓	✓	✓
	lagoon filtration			✓	✓	✓
	pasture filtration			✓	✓	✓
Air	vaporisation				✓	✓
Spills	stormwater	✓	✓	✓	✓	✓
	surface waters	✓	✓	✓	✓	✓
	land			✓	✓	✓

Source: Queensland Environmental Protection Agency, 1999.

^a Threshold based on amount of substance emitted.

^b Threshold based on amount of substance accepted in receiving waters, or *used*.

3.1 Emission Based Thresholds – Total Nitrogen and Total Phosphorus

The next step in the reporting process is to determine total annual *emissions* to waterways of the major contributing NPI listed substances from sewage and wastewater treatment facilities, nitrogen and phosphorus. If these emissions exceed threshold levels they must be reported. Total Nitrogen and Total Phosphorus are the only substances in threshold Category 3, and as such are the only substances that require threshold evaluation on an emission basis.

Since threshold determination and emission estimation are analogous in this case, see Section 4.1 for Emission Estimation Techniques.

3.2 Usage Based Thresholds – Category 1 Substances

For those substances with a Category 1 threshold (metals, inorganics and organic substances), the threshold test is whether 10 tonnes or more of the substances are used annually. For the purpose of the NPI, ‘use’ includes:

- those substances present in the influent stream – a threshold will be tripped if more than 10 tonnes/yr of a substance is present in the influent;
- those substances added as part of the sewage treatment process, such as chlorine – a threshold will be tripped if more than 10 tonnes/yr is used;
- those substances that are produced as a by-product of the sewage treatment process, such as hydrogen sulfide – a threshold will be tripped if more than 10 tonnes/yr is produced.

Monitoring of the raw sewage influent stream for NPI listed substances is the most appropriate way to determine whether a Category 1 threshold has been tripped for substances in the influent. Equation (1) (located at the end of this section) allows such concentration data to be converted into annual influent loads, which can be compared against the Category 1 threshold quantities listed in the *NPI Guide*.

For most plants however, monitoring of the influent stream may not routinely cover all of the NPI listed substances. As a guide, Table 2 can be used to estimate a facility's likelihood of tripping a Category 1 threshold. This sets out typical composition data for raw sewage influent, and what this translates to as a daily usage figure at selected daily influent flows. This data is from a large industry-intensive city and therefore would be expected to show a 'worst case' for most 'typical' treatment plant situations. Knowledge of a facility's influent flow rate allows extrapolation to estimate which substances may trip the Category 1 threshold.

Since a particular facility's raw sewage composition may vary from 'typical' values, it is recommended that this method be used as a guide only. After determining those substances near or above threshold levels, sewage monitoring should then be carried out at the facility to determine the actual situation. Indeed, if a particular facility's influent is non-typical (such as those predominantly served by industrial inputs), then these indicative values may not be applicable, and direct monitoring may be required.

The usage of each of the substances listed as Category 1 and 1a under the NPI must be estimated to determine whether the 10 tonnes (or 25 tonnes for VOCs) reporting threshold is exceeded. If the threshold is exceeded, emissions of these Category 1 and 1a substances must be reported for all operations/processes relating to the facility, even if the actual emissions of the substances are very low or zero.

Table 2. Typical Concentrations and Annual Usage of Category 1 Substances in an Urban Sewage Treatment Plant at Selected Influent Flow Rates

Prefix	NPI-Listed Substance	Typical Raw Sewage Concentration (mg/L)	Predicted Annual Usage at Selected Influent Flow Rates (tonnes/year)		
			1 ML/day	10 ML/day	100ML/day
1,3-	Acetaldehyde	ND	ND	ND	ND
	Acetic acid (ethanoic acid)	ND	ND	ND	ND
	Acetone	0.025	0.009	0.09	0.9
	Acetonitrile	ND	ND	ND	ND
	Acrylamide	ND	ND	ND	ND
	Acrylic acid	ND	ND	ND	ND
	Acrylonitrile (2-propenenitrile)	0.0025	0.0009	0.009	0.09
	Ammonia (total)	26.1	9.53	95.3	953
	Aniline (benzenamine)	<0.005	<0.0018	<0.018	<0.18
	Antimony	0.0022	0.0008	0.008	0.08
	Arsenic	<0.005	<0.0018	<0.018	<0.18
	Benzene	0.0026	0.0009	0.009	0.09
	Benzene hexachloro- (HCB)	<0.010	<0.0036	<0.036	<0.36
	Beryllium	0.0006	0.0002	0.002	0.02
	Biphenyl (1,1-biphenyl)	ND	ND	ND	ND
	Boron	0.227	0.083	0.83	8.3
	Butadiene (vinyl ethylene)	ND	ND	ND	ND
	Cadmium	<0.0005	<0.0002	<0.002	<0.02
	Carbon disulfide	0.0574	0.021	0.21	2.1
	Carbon monoxide	ND	ND	ND	ND
	Chlorine	ND	ND	ND	ND
	Chlorine dioxide	ND	ND	ND	ND
	Chloroethane (ethyl chloride)	<0.005	<0.0018	<0.018	<0.18
	Chloroform	0.004	0.0016	0.016	0.16
	Chlorophenols (di, tri, tetra)	0.566	0.207	2.07	20.7
	Chromium (III) *	0.066	0.024	0.24	2.4
	Chromium (VI) *	0.066	0.024	0.24	2.4
	Cobalt	0.0039	0.0014	0.014	0.14
	Copper	0.123	0.045	0.45	4.5
	Cumene	ND	ND	ND	ND
	Cyanide (inorganic) compounds	ND	ND	ND	ND
	Cyclohexane	ND	ND	ND	ND
	1,2-Dibromoethane	<0.0005	<0.0002	<0.002	<0.02
	Dibutyl phthalate	0.044	0.016	0.16	1.6
	1,2-Dichloroethane	<0.0005	<0.0002	<0.002	<0.02
	Dichloromethane	0.006	0.002	0.02	0.22
	Ethanol	ND	ND	ND	ND
	2-Ethoxyethanol	ND	ND	ND	ND
	2-Ethoxyethanol acetate	ND	ND	ND	ND
	Ethyl acetate	ND	ND	ND	ND
	Ethyl butyl ketone	ND	ND	ND	ND
	Ethylbenzene	0.0019	0.0007	0.0068	0.068
	Ethylene glycol (1,2-ethanediol)	ND	ND	ND	ND
	Ethylene oxide	ND	ND	ND	ND

Table 2. Typical Concentrations and Annual Usage of Category 1 Substances in an Urban Sewage Treatment Plant at Selected Influent Flow Rates cont'

Prefix	NPI-Listed Substance	Typical Raw Sewage Concentration (mg/L)	Predicted Annual Usage at Selected Influent Flow Rates (tonnes/year)		
			1 ML/day	10 ML/day	100ML/day
n-	Di-(2-Ethylhexyl) phthalate (DEHP)	0.059	0.022	0.22	2.2
	Fluoride	ND	ND	ND	ND
	Formaldehyde	0.0002	0.00006	0.0006	0.006
	Glutaraldehyde	ND	ND	ND	ND
	Hexane	ND	ND	ND	ND
	Hydrochloric acid	ND	ND	ND	ND
	Hydrogen sulfide	2.86	1.04	10.4	104
	Lead & compounds	0.06	0.02	0.22	2.2
	Magnesium oxide fume	ND	ND	ND	ND
	Manganese	0.144	0.053	0.53	5.3
2-	Mercury	0.0006	0.0002	0.002	0.02
	Methanol	ND	ND	ND	ND
	Methoxyethanol	ND	ND	ND	ND
	Methoxyethanol acetate	ND	ND	ND	ND
4,4-	Methyl ethyl ketone	0.009	0.003	0.033	0.33
	Methyl isobutyl ketone	0.015	0.0055	0.055	0.55
	Methyl methacrylate	ND	ND	ND	ND
	Methylene bis 2,4 aniline (MOCA)	ND	ND	ND	ND
	Methylenebis (phenylisocyanate)	ND	ND	ND	ND
	Nickel	0.023	0.0083	0.083	0.83
	Nickel carbonyl	ND	ND	ND	ND
	Nickel subsulfide	ND	ND	ND	ND
	Nitric acid	ND	ND	ND	ND
	Organo-tin compounds	ND	ND	ND	ND
	Phenol	0.024	0.0088	0.088	0.88
	Phosphoric acid	ND	ND	ND	ND
	Selenium	0.0057	0.0021	0.021	0.21
	Styrene (ethenylbenzene)	0.0026	0.0009	0.009	0.09
	Sulfur dioxide	ND	ND	ND	ND
	Sulfuric acid	ND	ND	ND	ND

Table 2. Typical Concentrations and Annual Usage of Category 1 Substances in an Urban Sewage Treatment Plant at Selected Influent Flow Rates cont'

Prefix	NPI-Listed Substance	Typical Raw Sewage Concentration (mg/L)	Predicted Annual Usage at Selected Influent Flow Rates (tonnes/year)		
			1 ML/day	10 ML/day	100ML/day
1,1,1,2	Tetrachloroethane	<0.0005	<0.0002	<0.002	<0.02
	Tetrachloroethylene	0.03	0.011	0.11	1.1
	Toluene (methylbenzene)	0.007	0.0027	0.027	0.27
	Toluene-2,4-diisocyanate	ND	ND	ND	ND
1,1,2-	Trichloroethane	<0.0005	<0.0002	<0.002	<0.02
	Trichloroethylene	0.0075	0.0027	0.027	0.27
	Vinyl Chloride Monomer	<0.005	<0.002	<0.02	<0.2
	Xylenes	0.014	0.0052	0.052	0.52
	Zinc	0.213	0.078	0.78	7.8
	TOTAL VOC's **	1.49	0.546	5.46	54.6

Source: Melbourne Water, Western Treatment Plant, 1996

ND = Not Determined

Bolded numbers refer to potential threshold tripping substances

* Measured data refers to total chromium

** Total VOC's are an estimate only; calculated based on summing all VOC's covered by this analysis. The list of substances used could vary depending on the analytes chosen for the testing regime.

*** Concentrations are indicative only and are representative of the conditions at the time of sampling.

If monitoring data for raw sewage entering a particular facility is available, actual usage can be calculated using Equation (1) below. Similarly (using Equation (1)), concentration data from Table 2 can be multiplied by site specific influent flow rates to give indicative annual usage of substances at that facility.

$$I_{kpy,i} = C_i * V * OpHrs / 1\,000\,000 \quad (1)$$

where:

$$\begin{aligned}
 I_{kpy,i} &= \text{influent loading of pollutant i, kg/yr} \\
 C_i &= \text{concentration of pollutant i in influent wastewater, mg/L (from monitoring data or Table 2)} \\
 V &= \text{hourly volume of wastewater, L/hr} \\
 OpHrs &= \text{operating hours per year for which data apply, hr/yr} \\
 1\,000\,000 &= \text{conversion factor, mg/kg}
 \end{aligned}$$

Example 1. Influent Threshold Determination

The amount of zinc contained in influent wastewater can be determined from application of Equation (1) and the following data.

Total Influent Flow Rate, V	150 ML/day = 150 000 000/24 L/hr
Typical zinc concentration in sewage, C _{zn}	0.21 mg/L (from Table 2)
OpHrs (24hrs * 365 days)	8760 hr/yr
Conversion mg to kg	1 000 000

$$\begin{aligned} I_{zn} &= C_{zn} * V * \text{OpHrs} / 1\,000\,000 \\ &= 0.21 * (150\,000\,000/24) * 8\,760 / 1\,000\,000 \\ &= 11\,500 \text{ kg zinc/yr} \\ &= 11.5 \text{ tonnes zinc/yr} \end{aligned}$$

The influent threshold of 10 tonnes per year of zinc has been triggered, and reporting of zinc emissions in effluent streams is required.

3.3 Combustion Based Thresholds – Category 2 Substances

If your facility burns greater than a certain amount of fuel (or waste gases) or uses greater than a certain amount of electricity per year, you are required to report emissions from those substances listed as category 2a and/or 2b. For more information about these thresholds consult the NPI Guide.

4.0 Estimating Emissions

When a threshold has been triggered, emissions need to be calculated and reported to the NPI for each environmental medium to which emissions occur, (ie. to water, land, and atmosphere). The following sections describe emission estimation techniques for undertaking these calculations.

Effluent discharged into waterways or onto land from sewage and wastewater treatment plants is regularly monitored by the facility operator to ensure that it meets the standards of its environmental licence as required by the relevant State, Territory, and/or local government environment regulator. Emissions of volatile organic compounds (VOCs) can also occur to atmosphere because of vaporisation, although generally the triggering of VOC thresholds, and the reporting of these emissions will only be required from the largest sewage and wastewater treatment plants.

Most sewerage systems in Australia were originally designed to remove and treat domestic sewage. However, the introduction of tighter controls on the discharge of commercial and industrial waste into the environment means that the sewerage system, particularly in industrial and manufacturing districts, is required to treat industrial effluent as well.

In general, there are four types of emission estimation techniques (EETs) that may be used to estimate emissions from your facility.

The four types described in *The NPI Guide* are:

- sampling or direct measurement;
- mass balance;
- fuel analysis or other engineering calculations; and
- emission factors

Select the EET, (or mix of EETs), that is most appropriate for your purposes. For example, you might choose to use a mass balance to best estimate fugitive losses from pumps and vents, direct measurement for stack and pipe emissions, and emission factors when estimating losses from storage tanks and stockpiles.

If you estimate your emission by using any of these EETs, your data will be displayed on the NPI database as being of ‘acceptable reliability’. Similarly, if your relevant environmental authority has approved the use of EETs that are not outlined in this handbook, your data will also be displayed as being of ‘acceptable reliability’.

This Manual seeks to provide the most effective emission estimation techniques for the NPI substances relevant to this industry. However, the absence of an EET for a substance in this handbook does not necessarily imply that an emission should not be reported to the NPI. The obligation to report on all relevant emissions remains if reporting thresholds have been exceeded.

You are able to use emission estimation techniques that are not outlined in this document. You must, however, seek the consent of your relevant environmental authority. For example, if your company has developed site-specific emission factors, you may use these if approved by your relevant environmental authority.

You should note that the EETs presented in this manual relate principally to average process emissions. Emissions resulting from non-routine events are rarely discussed in the literature, and there is a general lack of EETs for such events. However, it is important to recognise that emissions resulting from significant operating excursions and/or accidental situations (eg. spills) will also need to be estimated. Emissions to land, air and water from spills must be estimated and added to process emissions when calculating total emissions for reporting purposes. The emission resulting from a spill is the net emission, ie. the quantity of the NPI reportable substance spilled, less the quantity recovered or consumed during clean up operations.

4.1 Estimating Emissions of Total Nitrogen and Total Phosphorus

4.1.1 Using Sampling Data

Because of the significant environmental hazards posed by the discharge of nutrients to waterbodies, sewage and wastewater treatment facilities emitting nitrogen and phosphorus to inland waterways and ocean outfalls are required by their relevant State or Territory environment agency to closely monitor and measure these emissions. A specific sampling program is usually developed for each treatment plant based on the nature and volume of the discharge. This existing monitoring data can be used to calculate annual emissions and therefore whether the threshold has been tripped.

Equation (2) illustrates a technique for using existing nutrient sampling data.

$$E_{kpy,i} = C_i * V * OpHrs / 1\,000\,000 \quad (2)$$

where:

$E_{kpy,i}$	= emissions of pollutant i, kg/yr
C_i	= concentration of pollutant i in wastewater, mg/L
V	= hourly volume of wastewater, L/hr
$OpHrs$	= operating hours per year for which data applies, hr/yr
1 000 000	= conversion factor, mg/kg

In applying Equation (2) for water emission calculations, monitoring data should be averaged and only representative concentrations used in emission calculations. For example, lagoons relying on biological processes and with long detention times are less likely to have sudden changes in effluent quality than plants with short detention times using mechanical and electrical equipment. The frequency of sampling is also dependent on plant size and the remoteness of the plant.

Normally, the larger the discharge, the more significant the potential impact on the environment, and consequently, there may be an increased need for more regular sampling. Other factors that can influence the sampling regime include the variability of the inflow, the composition and variability of the industrial waste component of the inflow, (and the level of competence of the operating staff).

Sampling for NPI reporting requirements should be done using the same methodology as outlined in the licence agreement. In instances where licence agreements do not stipulate sampling practices, grab samples should be used for small and medium sized plants, and taken within two hours of the normal time of the maximum daily flow. For larger facilities, composite samples are recommended. Details on the storage, transportation, and testing of samples can be found in Australian Standard AS2031.

For threshold determination purposes, if the Category thresholds are exceeded, you are required to report this emission for this substance.

4.1.2 Using Emission Factors

In instances where reliable sampling data is unavailable, emission factors can be used to estimate pollutant emissions. An emission factor can be defined as a pollutant emission rate relative to a level of source activity, (eg. daily wastewater volume). Emission factors are generally based on the results of source tests or sampling conducted at one or more sewage and wastewater treatment facilities.

The emission factors presented in Table 3 are an average of total nitrogen and total phosphorus concentrations in wastewater effluent from a range of Australian wastewater treatment facilities. These concentrations can be used in place of site-specific sampling data by the application of Equation (2).

Table 3. Typical Nutrient Emission Factors from Sewage and Wastewater Treatment Plants

Treatment Process	Nutrient Emission Factor	
	Total Nitrogen (mg/L)	Total Phosphorus (mg/L)
Wastewater		
A	35 - 60	6 - 16
B	30 - 55	6 - 14
C	20 - 50	6 - 12
D	10 - 20	< 2
E	NA	NA
F	< 10	< 1

Source: NWQMS, 1997.

NA = not applicable.

NOTES:

- A Removal of gross solids plus some of the readily settleable solids eg. microscreening.
- B Removal of gross solids plus readily settleable solids eg. primary sedimentation.
- C Removal of most solids and BOD eg. biological treatment, chemically assisted treatment, lagoons.
- D Nutrient removal after removal of solids eg. biological, chemical precipitation, etc.
- E Disinfection eg. lagooning, ultraviolet, chlorination.
- F Advanced wastewater treatment (tertiary, after nutrient removal, see D) eg. sand filtration, ion exchange, microfiltration.

For threshold determination purposes, if the Category thresholds are exceeded, you are required to report this emission for this substance.

4.2 Estimating Emissions of Category 1 Substances (Total VOCs, Speciated Organics, Metals and Inorganic Compounds)

4.2.1 Emissions to Water and Land

Sewage and wastewater treatment facilities using 10 tonnes or more per year of any listed Category 1 substance, and/or 25 tonnes of total VOCs are required to estimate and report emissions of these pollutants in the effluent stream, which includes water and land. This can be determined from monitoring data in the same manner as for Total Nitrogen and Total Phosphorus (see Section 4.1.1).

For organic chemicals in general, some degradation during wastewater treatment will occur so that not all the chemical received is transferred to water effluent and sludge. Wastewater facilities can estimate the amount of organic compounds in effluent by using measured data, or by subtracting the amount biodegraded from the total amount removed in treatment. The amount of removal can be determined from operating data, and the extent of biodegradation might be obtained from published studies (see Tables 10 & 11 *SIMS Chemical Property Data File*, Appendix III). If the biodegradability of the organic chemical cannot be measured, or is not known, reporting facilities should assume that all substances remain in the wastewater or are adsorbed into the sludge.

4.2.2 Emissions of Chlorine

Sewage and wastewater treatment plants may disinfect effluent before it is discharged into receiving waters to reduce and destroy the microbiological agents and pathogens that cause disease. This practice is not universal throughout Australia, but is common at sewage treatment plants in inland and arid regions. Facilities exceeding the 10 tonne threshold by using the disinfection process (or where the amount used for disinfecting and the amount received in influent equals or exceeds 10 tonnes annually) must report emissions of chlorine in effluent discharged to receiving waters.

For more information on measuring chlorine emissions, see Appendix I.

4.2.3 Emissions to Air

Volatile organic compounds (VOCs) are emitted from wastewater treatment, collection, and storage systems through the volatilisation of organic compounds at the liquid surface. Where the threshold for VOCs have been tripped (as determined with reference to Section 3.2), emissions to atmosphere will need to be estimated and reported.

Emissions can occur through diffusive or convective mechanisms, or both. Diffusion occurs when organic concentrations at the water surface are much higher than ambient concentrations. The organics volatilise (or diffuse) into the air in an attempt to reach equilibrium between aqueous and vapour phases. Convection occurs when air flows over the water surface, sweeping organic vapours from the surface into the air. The rate of volatilisation is directly related to the speed of the air flow over the water surface.

Factors that can affect the rate of volatilisation of VOCs from wastewater include:

- wastewater surface area;
- temperature;
- turbulence;
- wastewater retention time in the system(s);
- depth of the wastewater in the system(s);
- concentration of organic compounds in the wastewater;
- volatility and diffusivity in water of the substance;
- presence of a mechanism that inhibits volatilisation,(eg. an oil film) or a competing mechanism, (eg. biodegradation); and
- design of the wastewater treatment and collection units.

Emissions to air can be estimated using the EETs outlined in Appendices II and III.

Process gases, including methane and hydrogen sulfide, are commonly used in engines to pump the effluent and can be used in a turbine to produce electricity. Combustion by-products could include sulfur dioxide. (See EET Manual for Combustion Engines.)

5.0 References

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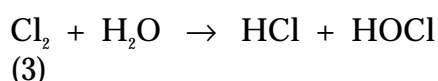
The following EET manuals referred in this manual can be obtained from your local Environment Protection Agency (see the front of the NPI Guide for details).

- Emission Estimation Technique Manual for Combustion Engines

APPENDIX I Measurement of Chlorine Emissions – Colourimetric Method

1.0 Introduction

Chlorine is a widely used disinfectant. Under normal conditions, chlorine is a green-yellow, corrosive gas with a density 2.5 times that of air. The gas is soluble in water, and is a potent disinfectant even at low concentrations. When dissolved in water, chlorine forms two acids by reaction with water. This reaction is shown in Equation (3).



Hypochlorous acid (HOCl) is a disinfecting agent, and its chlorine content is referred to as *free available chlorine*. Chlorine rapidly penetrates microbial cells and kills the micro-organism. However, its effectiveness is greatly influenced by the physical and chemical characteristics of the water, or wastewater. The presence of suspended solids, or the clustering of micro-organisms, may protect pathogens and so reduce the disinfecting ability.

Chlorine is a strong oxidising agent and when it reacts with a reducing agent, (eg. ammonia), the amount available to kill pathogens is depleted. In the case of ammonia, the reaction forms a series of end products, that will usually include nitrogen gas and nitrite ion. The reaction products present, and their relative amounts, depend on the molar ratio of chlorine to ammonia, the pH, and the contact time. The intermediates are a series of chlorinated ammonia compounds known as chloramines.

There are three possible chloramines - monochloramine, dichloroamine, and trichloramine. Although they form in a stepwise manner, not all three need be formed under given conditions. Chloramines are much less powerful disinfectants than free chlorine.

The term *free available chlorine* refers to chlorine gas (Cl_2), hypochlorite ion (OCl^-), and hypochlorous acid (HOCl). The term *combined available chlorine* refers to chloramines. The process of oxidation of ammonia by chlorine shows a unique dose-response curve. Initially, as the chlorine dose is increased, the residual chlorine rises to a maximum, at which point the molar concentrations of the chlorine and ammonia are roughly equal. This point represents the formation of chloramines. As further chlorine is added, the residual then decreases mainly because of conversion of monochloramine to nitrogen. Eventually, a stage is reached where all the ammonia has been converted to chloramines, and all the chloramines have been oxidised. At this stage (known as breakpoint), adding further chlorine will make the chlorine residual rise in proportion to the chlorine added. The solution composition at the breakpoint depends on the reaction conditions, including the molar ratio of the two reactants.

Other substances found in natural waters and wastes react with chlorine. These include organic carbon, ferrous ion, sulfide, and nitrite. This means the actual chlorine demand always exceeds that predicted from the ammonia concentration. For example, at sewage treatment plants that are not completely nitrifying (and thus, have nitrite ion in effluent), it is commonly found that chlorination to the breakpoint cannot be achieved at normal chlorine dose rates.

To ensure a free chlorine residual, good practice is to chlorinate beyond the breakpoint, so that the required chlorine dose is several times the ammonia concentration. However, effluents sometimes contain so much reductant that breakpoint chlorination would be prohibitively expensive, and in such cases, you should attempt to determine the cause. If there are high concentrations of nitrite, this would indicate a need for a change in operational practices. For effluents containing high ammonia concentrations, chlorination is commonly taken to the point of maximum combined available chlorine.

Once chlorine has been added to the water, the chlorine residual depends on the dose (concentration added), and the time elapsed after the administration of the dose. Continuous chlorination systems are usually designed with a chlorine contact chamber to hold the chlorinated effluent for a set time interval (eg. 30 or 60 minutes) before discharge to receiving waters.

2.0 Scope

This method applies to the measurement of free and total chlorine residual in environmental waters and wastewaters with chlorine in the range of 0.1 to 1.0 mg/L. This method is not suitable for highly coloured waters, as intense colours might interfere with the colour comparison.

3.0 Principle

Chlorine concentrations are determined by colorimetry, using a colour comparator apparatus. The colourimetric reagent, Diethyl-P-Phenylene Diamine (DPD), turns pink-red upon reaction with chlorine, and is available in the following tablet forms:

- No. 1 DPD tablets will determine free available chlorine;
- No. 1 and No. 2 DPD combined will determine free chlorine, plus monochloramine; and
- No. 4 DPD, (or No. 1 and No. 3 DPD combined) will determine total chlorine.

Kits normally supplied contain only No. 1 and No. 3 tablets, and are used for free and total chlorine.

The comparator has two cells that are filled with the water to be tested. To one cell, the correct amount of reagent is added. This causes a colour to develop according to the concentration of chlorine. A coloured filter, having several segments of different colours (representing a series of chlorine concentrations), is placed over the other cell. The intensity of colour that develops during the test is compared directly to the

colours seen through the filters. The filter that matches most closely with the colour developed during the test is selected as representing the chlorine concentration of the sample.

4.0 Procedure

4.1 Collect sample

Collect sample using a clean sampling beaker or sample container, and rinse this container between samples.

4.2 Prepare comparator

- Insert the chlorine colour comparator disc into the comparator so that the numbered standards face you. If necessary, adjust the translucent spacer to suit the size of the cells used.
- Place the cell containing the treated sample (the one with the reagent) in the right compartment, and the cell containing untreated sample in the left compartment.

4.3 Measure free chlorine

- Flush two 10mL moulded cells with sample, and leave a few drops of sample in the cells.
- Fill one cell to the 10mL mark with sample, and place in the left compartment of the comparator.
- To the other cell, add one DPD No. 1 tablet and allow to disintegrate, or gently crush with a stirring rod while supporting the cell.
- Fill the cell with sample to the 10mL mark, mix with the stirring rod, and place the cell in the right compartment of the comparator.
- Hold the comparator so that it is illuminated, and look through the cells.
- Rotate the colour disc until the colour of the left cell matches the colour of the right cell.
- Record the number shown on the disk as free chlorine.

4.4 Measure total chlorine

- Add a DPD No. 3 tablet to the coloured liquid in the right cell, and mix to dissolve.
- Allow to stand for two minutes.
- Rotate the disc until the colours match.
- Record the number shown on the disk as total residual chlorine.

5.0 Troubleshooting

No adjustment of the test equipment is possible. Maintenance involves keeping the cells and colour filters scrupulously clean. Any that become permanently marked will need to be replaced. Residues on cell walls from previous tests can give false high readings.

6.0 Calculations

If required, subtract the free residual chlorine value $[Cl]_{\text{free residual}}$ from the total residual chlorine value $[Cl]_{\text{total residual}}$ to find the combined residual chlorine value $[Cl]_{\text{combined residual}}$. This figure should be reported to the NPI as chlorine emissions to water. A sample calculation is shown at example .

7.0 Precision

Under field conditions, the precision of measurement is $\pm 0.1 \text{ mg/L}$

Example 2. Estimation of Combined Residual Chlorine Emissions to Water

$[Cl]_{\text{combined residual}}$	=	$[Cl]_{\text{total residual}} - [Cl]_{\text{free residual}}$
	=	0.5 mg/L
OpHrs of STP (24hrs * 365 dys)	=	8760 hr/yr
Flow rate (A)	=	2800 kL/day
Annual emissions of chlorine	=	$E_{\text{kpy,Cl}}$
$E_{\text{kpy,Cl}}$	=	$EF_{\text{Cl}} * A * \text{OpHrs}$
	=	$(0.5 * 10^{-6}) (2800 * 1000) / 24 * 8760$
	=	511 kg Cl/yr

APPENDIX II

Estimating Emissions to Air

Listed below are EETs that may be useful for estimating emissions to air from sewage and wastewater treatment facilities. Some of the techniques can also be used for estimating emissions to land and water.

1.0 Engineering Calculations

Theoretical equations can be used to calculate air emissions from wastewater treatment facilities. 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. It is important to realise that these calculations have to be performed for each individual NPI-listed substance found in the wastewater.

The rate of volatilisation of substances in wastewater can be determined 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 emission of interest. These overall mass transfer coefficients are then used to calculate emission rates in grams per second, that can then be used to determine emissions per year for NPI reporting purposes.

Figure 1 is a flow diagram to assist in determining the appropriate combination of emission equations for estimating VOC emissions from various types of wastewater treatment, storage, and collection systems. Tables 4 and 5 present the emission equations and definitions respectively.

VOCs vary in their volatility. The emission equations presented in this appendix can be used for organic compounds of high, medium, and low volatility. 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. The volatility of VOCs is categorised below:

High volatility	$HLC > 10^{-3} \text{ atm-m}^3/\text{gmol}$
Medium volatility	$10^{-3} > HLC > 10^{-5} \text{ atm-m}^3/\text{gmol}$
Low volatility	$HLC < 10^{-5} \text{ atm-m}^3/\text{gmol}$

The design and arrangement of collection, treatment, and storage systems are facility-specific, therefore the most accurate emissions from wastewater treatment operations will come from actual tests at a facility (eg. direct measurement of emissions from openings). In the event that actual data is unavailable, the emission equations provided can be used.

Emission equations should be given site-specific information whenever it is available, as the most extensive characterisation of an actual system will produce the most accurate estimates from an emissions model.

Using the Flow Diagram and Equations for Estimating VOC Emissions

Step 1 - Using Figure 1 and Tables 4 and 5.

Trace through Figure 1 to determine the correct equations to use for your process.

Figure 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/non-aerated systems;
- biologically active systems;
- oil film layer systems; and
- surface impoundment flowthrough, or disposal (or fate management).

In flowthrough systems, wastewater is treated and subsequently discharged to a subsequent sewage treatment facility, or a receiving body of water such as a river or stream. In general, municipal wastewater treatment facilities and industrial wastewater treatment facilities are both classified as flowthrough systems.

Disposal systems, also referred to as fate management systems, on the other hand, do not discharge any wastewater.

Step 2 - Using the Equations

The numbers in Figure 1 under the columns for K_p , K_g , K_{oil} , K_D , K and N refer to the appropriate equations in Table 4. Definitions for all parameters in these equations are given in Table 5. This table also supplies the units that must be used for each parameter, with codes to help locate input values. If the parameter is coded with:

A - a site-specific value is required;

B - requires a site-specific parameter, but defaults are available;

C - the parameter can be obtained from literature data. Table 10 contains a list of approximately 150 chemicals and their physical properties that are needed to calculate emissions from wastewater using the correlations in Table 4; and

D - these are calculated values.

Assumption

All emission systems presented in Figure 1 imply a completely mixed, or uniform wastewater concentration system.

To estimate an emission rate (N), the first step is to calculate individual gas-phase, and liquid-phase mass transfer coefficients (K_g and K_l respectively), using the appropriate equations. The individual coefficients are then used to calculate the overall mass transfer coefficient, K. Exceptions to this procedure are the calculation of the 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 emission rates (N).

This process must be repeated for each different constituent in the wastewater for which you are determining emissions.

Step 3 - Calculating Annual Emissions

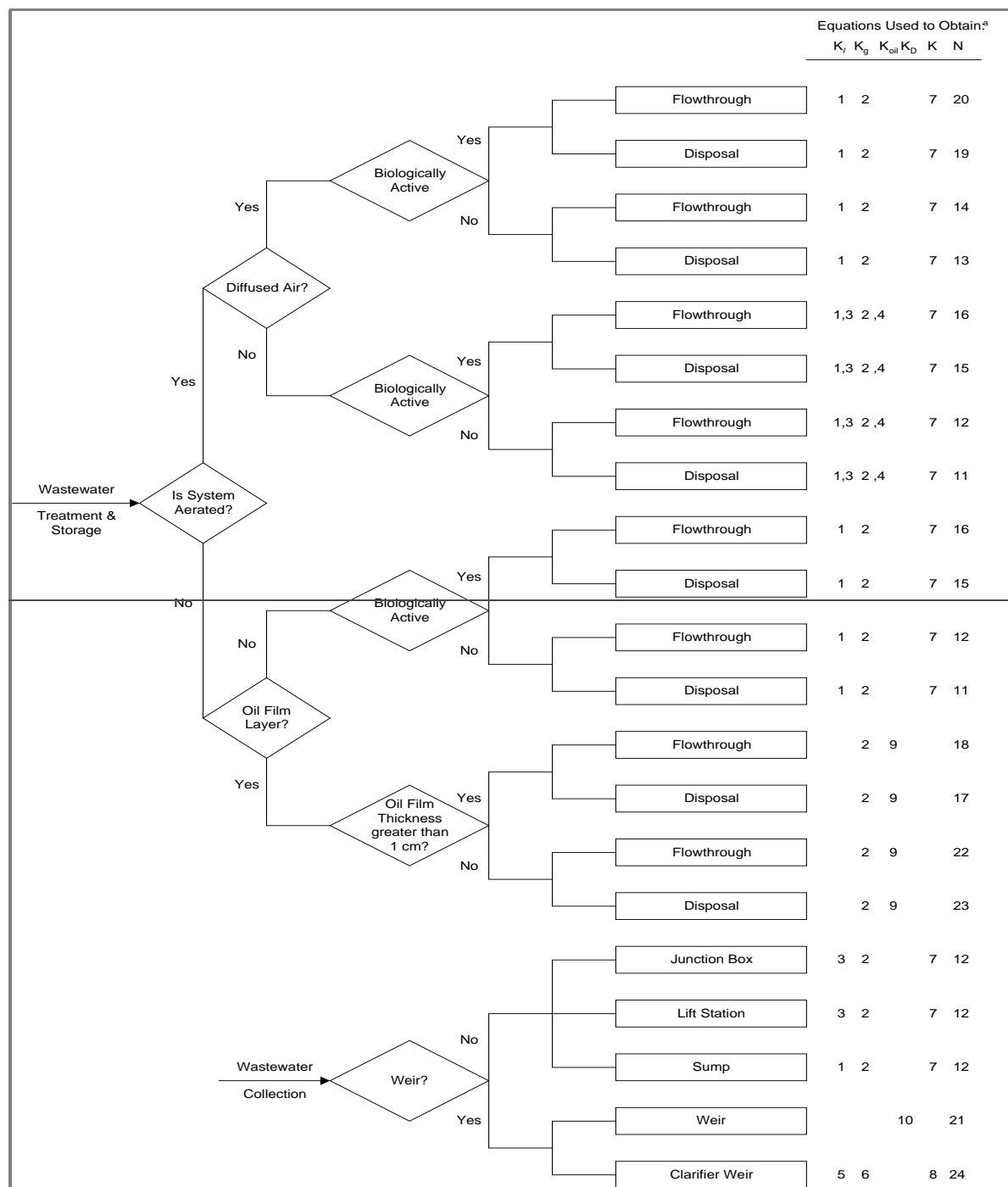
Once the emission rates (N) have been calculated, the next step is to determine emissions on an annual basis. This is achieved using the following equation.

$$E = N * OpHrs * 10^{-6} * 3600 \quad (1)$$

where :

E	=	annual emissions, tonne/yr
N	=	emissions rate, g/sec
OpHrs	=	operating time per year, hr/yr
10^{-6}	=	conversion factor, tonne/g
3600	=	conversion factor, sec/hr

The annual emission that is obtained can then be used as an emission estimate for NPI reporting purposes.



Numbered equations are present in Table 1

- K_l = Individual liquid phase mass transfer coefficient, m/s
 K_g = Individual gas-phase mass transfer coefficient, m/s
 K_{oil} = Overall mass transfer coefficient in the oil phase, m/s
 K_D = Volatilisation - reaeration theory mass transfer coefficient
 K = Overall mass transfer coefficient, m/s
 N = Emissions, g/s

Figure 1. Flow Diagram for Estimating VOC Emissions from Wastewater Collection, Treatment, and Storage

Source: USEPA, AP-42, Section 4.3, 1991.

Table 4. Mass Transfer Correlations and Emission Equations

Equation Number	Equation
1.	<p>Individual liquid (K_l) and gas (K_g) phase mass transfer coefficients</p> $K_l \text{ (m/s)} = (2.78 * 10^{-6}) (D_w/D_{\text{ether}})^{2/3}$ <p>For: $0 < U_{10} < 3.25 \text{ m/s}$ and all F/D ratios</p> $K_l \text{ (m/s)} = [(2.605 * 10^{-9})(F/D) + (1.277 * 10^{-7})] (U_{10})^2 (D_w/D_{\text{ether}})^{2/3}$ <p>For: $U_{10} > 3.25 \text{ m/s}$ and $14 < F/D < 51.2$</p> $K_l \text{ (m/s)} = (2.61 * 10^{-7}) (U_{10})^2 (D_w/D_{\text{ether}})^{2/3}$ <p>For: $U_{10} > 3.25 \text{ m/s}$ and $F/D > 51.2$</p> $K_l \text{ (m/s)} = 1.0 * 10^{-6} + 144 * 10^{-4} (U^*)^{2.2} (Sc_L)^{-0.5}; U^* < 0.3$ $K_l \text{ (m/s)} = 1.0 * 10^{-6} + 34.1 * 10^{-4} U^* (Sc_L)^{-0.5}; U^* > 0.3$ <p>For: $U_{10} > 3.25 \text{ m/s}$ and $F/D < 14$</p> <p>where:</p> $U^* \text{ (m/s)} = (0.01)(U_{10})(6.1 + 0.63(U_{10}))^{0.5}$ $Sc_L = \mu_L / (\rho_L D_w)$ $F/D = 2 (A/\pi)^{0.5}$
2.	$K_g \text{ (m/s)} = (4.82 * 10^{-3})(U_{10})^{0.78} (Sc_G)^{-0.67} (d_e)^{-0.11}$ <p>where: $Sc_G = \mu_a / (\rho_a D_a)$</p> $d_e \text{ (m)} = 2 (A/\pi)^{0.5}$
3.	$K_l \text{ (m/s)} = [(8.22 * 10^{-9})(J)(\text{POWER})(1.024)^{(T-20)} * (O_l)(10^6)(MW_L)/(V a_v \rho_L)](D_w/D_{O2,w})^{0.5}$ <p>where: $(\text{POWER}) \text{ (hp)} = (\text{total power to aerators})(V)$</p> <p>$V a_v \text{ (ft}^2\text{)} = (\text{fraction of area agitated})(A)$</p>
4.	$K_g \text{ (m/s)} = (1.35 * 10^{-7})(Re)^{1.42} (P)^{0.4} (Sc_G)^{0.5} (Fr)^{-0.21} (D_a MW_a / d)$ <p>where: $Re = d^2 w \rho_a / \mu_a$</p> <p>$P = [(0.85)(\text{POWER})(550 \text{ (ft-lb}_f\text{/s-hp)})/N_f] g_c / (\rho_L (d^*)^5 w^3)$</p> <p>$Sc_G = \mu_a / (\rho_a D_a)$</p> <p>$Fr = (d^*) w^2 / g_c$</p>

Table 4. Mass Transfer Correlations and Emission Equations (cont')

Equation Number	Equation
5.	$K_l \text{ (m/s)} = (f_{\text{air},l})(Q)/[3600 \text{ s/min } (h_c)(\pi d_c)]$ <p>where: $f_{\text{air},l} = 1 - 1/r$ $r = \exp[0.77(h_c)^{0.623} (Q/\pi d_c)^{0.66} (D_w/D_{O_2,w})^{0.66}]$</p>
6.	$K_g \text{ (m/s)} = 0.001 + (0.0462(U^*)(Sc_G)^{-0.67})$ <p>where: $U^* \text{ (m/s)} = [6.1 + (0.63)(U_{10})]^{0.5} (U_{10}/100)$ $Sc_G = \mu_a/(\rho_a D_a)$</p> <p>Overall mass transfer coefficients for water (K) and oil (K_{oil}) phases and for weirs (K_D)</p>
7.	$K = (K_l \text{ Keq } K_g)/(Keq \text{ } K_g + K_l)$ <p>where: $Keq = H/(RT)$</p>
8.	$K \text{ (m/s)} = [[MW_L/(K_{lPL} * (100\text{cm/m}))] + [MW_a/K_g \rho_a H^* 55 \text{ } 555 * (100\text{cm/m})]]^{-1} MW_L/[(100\text{cm/m})\rho_L]$
9.	$K_{\text{oil}} = K_g \text{ Keq}_{\text{oil}}$ <p>where: $Keq_{\text{oil}} = P^* \rho_a MW_{\text{oil}}/(\rho_{\text{oil}} MW_a P_o)$</p>
10.	$K_D = 0.16h (D_w/D_{O_2,w})^{0.75}$ <p>Air Emissions (N)</p>
11.	$N(\text{g/s}) = (1 - Ct/Co) V \text{ } Co/t$ <p>where: $Ct/Co = \exp[-KA \text{ } t/V]$</p>
12.	$N(\text{g/s}) = KC_L A$ <p>where: $C_L \text{ (g/m}^3\text{)} = Q \text{ } Co/(KA + Q)$</p>
13.	$N(\text{g/s}) = (1 - Ct/Co) V \text{ } Co/t$ <p>where: $Ct/Co = \exp[-(KA + KeqQ_a)t/V]$</p>

Table 4. Mass Transfer Correlations and Emission Equations (cont')

Equation Number	Equation
14.	$N(g/s) = (KA + Q_a K_{eq})C_L$ <p>where: $C_L(g/m^3) = QCo/(KA + Q + Q_a K_{eq})$</p>
15.	$N(g/s) = (1-Ct/Co) KA/(KA + K_{max} b_i V/K_s) V Co/t$ <p>where: $Ct/Co = \exp[-K_{max} b_i t/K_s - KA t/V]$</p>
16.	$N(g/s) = K C_L A$ <p>where: $C_L(g/m^3) = [-b + (b^2 - 4ac)^{0.5}]/(2a)$</p> <p>and:</p> $a = KA/Q + 1$ $b = K_s(KA/Q + 1) + K_{max} b_i V/Q - Co$ $c = -K_s Co$
17.	$N(g/s) = (1-Ct_{oil}/Co_{oil})V_{oil} Co_{oil}/t$ <p>where: $Ct_{oil}/Co_{oil} = \exp[-K_{oil} t/D_{oil}]$</p> <p>and:</p> $Co_{oil} = Kow Co/[1 - FO + FO(Kow)]$ $V_{oil} = (FO)(V)$ $D_{oil} = (FO)(V)/A$
18.	$N(g/s) = K_{oil} C_{L,oil} A$ <p>where: $C_{L,oil}(g/m^3) = Q_{oil} C_{oil}/(K_{oil} A + Q_{oil})$</p> <p>and:</p> $Co_{oil} = Kow Co/[1 - FO + FO(Kow)]$ $Q_{oil} = (FO)(Q)$
19.	$N(g/s) = (1-Ct/Co)(KA + Q_a K_{eq})/(KA + Q_a K_{eq} + K_{max} b_i V/K_s) V * Co/t$ <p>where: $Ct/Co = \exp[-(KA + K_{eq}Q_a)t/V - K_{max} b_i t/K_s]$</p>

Table 4. Mass Transfer Correlations and Emission Equations (cont')

Equation Number	Equation
20.	$N(g/s) = (KA + Q_a K_{eq})C_L$ <p>where: $C_L(g/m^3) = [-b + (b^2 - 4ac)^{0.5}]/(2a)$</p> <p>and: $a = (KA + Q_a K_{eq})/Q + 1$ $b = K_s[(KA + Q_a K_{eq})/Q + 1] + K_{max} b_i$ $V/Q - C_o$ $c = -K_s C_o$</p>
21.	$N(g/s) = (1 - \exp[-K_D])Q C_o$
22.	$N(g/s) = K_{oil} C_{L,oil} A$ <p>where: $C_{L,oil}(g/m^3) = Q_{oil}(C_{oil}^*)/(K_{oil} A + Q_{oil})$</p> <p>and: $C_{oil}^* = C_o/FO$ $Q_{oil} = (FO)(Q)$</p>
23.	$N(g/s) = (1 - Ct_{oil}/C_{oil}^*)(V_{oil})(C_{oil}^*)/t$ <p>where: $Ct_{oil}/C_{oil}^* = \exp[-K_{oil} t/D_{oil}]$</p> <p>and: $C_{oil}^* = C_o/FO$ $V_{oil} = (FO)(V)$ $D_{oil} = (FO)(V)/A$</p>
24.	$N(g/s) = (1 - \exp[-K \pi d_c h_c/Q])Q C_o$

Table 5. Parameter Definitions for Mass Transfer Correlations and Emission Equations

Parameter	Definition	Units	Code ^a
A	Waste water surface area	m 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	A,B
d [*]	Impeller diameter	ft	B
D _a	Diffusivity of constituent in air	cm ² /s	B
d _c	Clarifier diameter	m	B
d _e	Effective diameter	m	D
D _{ether}	Diffusivity of ether in water	cm ² /s	(8.5 * 10 ⁻⁶) ^b
D _{O2,w}	Diffusivity of oxygen in water	cm ² /s	(2.4 * 10 ⁻⁵) ^b
D _{oil}	Oil film thickness	m	B
D _w	Diffusivity of constituent in water	cm ² /s	C
f _{air,l}	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	Gravitational constant (a conversion factor)	lb _m -ft/s ² -lb _f	32.17

Table 5. Parameter Definitions for Mass Transfer Correlations and Emission Equations (cont')

Parameter	Definition	Units	Code ^a
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 the constituent	atm-m ³ /gmol	C
J	Oxygen transfer rating of the 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	Volatilisation-reaeration theory mass transfer coefficient	dimensionless	D
K_{eq}	Equilibrium constant or partition coefficient (concentration in gas phase/concentration in liquid phase)	dimensionless	D
$K_{eq_{oil}}$	Equilibrium constant or partition coefficient (concentration in gas phase/concentration in oil phase)	dimensionless	D
K_g	Gas phase mass transfer coefficient	M/sec	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
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^*	Vapour pressure of the constituent	atm	C
P_o	Total pressure	atm	A
POWER	Total power to aerators	hp	B
Q	Volumetric flowrate	m ³ /s	A
Q_a	Diffused air flowrate	m ³ /s	B
Q_{oil}	Volumetric flowrate 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

Table 5. Parameter Definitions for Mass Transfer Correlations and Emission Equations (cont')

Parameter	Definition	Units	Code ^a
Sc _G	Schmidt number on gas side	dimensionless	D
Sc _L	Schmidt number on liquid side	dimensionless	D
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	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	1.2 * 10 ⁻³
ρ _L	Density of water	g/cm ³	1 ^b
ρ _{oil}	Density of oil	g/m ³	B
μ _a	Viscosity of air	g/cm-s	(1.8 * 10 ⁻⁴) ^b
μ _L	Viscosity of water	g/cm-s	(8.93 * 10 ⁻³) ^b

^a Code:

A = Site-specific parameter

B = Site-specific parameter. For default values, see Table 6.

C = Parameter can be obtained from Tables 10 & 11. These represent chemical properties at 25°C.

D = Calculated value.

^b Reported values at 25°C.

Table 6. Site-Specific Default Parameters

Default Parameter	Definition	Default Value
General		
T	Temperature of water	298 K
U_{10}	Wind speed	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) (for activated sludge)	0.75 hp/1000 ft ³ (V) 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
V_a	Turbulent surface area (for aerated treatment system) (for activated sludge)	0.24 (A) 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 flowrate	0.0004(V) m ³ /s
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 flowrate 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	0.001

Table 6. Site-Specific Default Parameters (cont')

Default Parameter	Definition	Default Value
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	28.5 m
h	Weir height	1.8 m
h _c	Clarifier weir height	0.1 m

1.2 Mass Balance

A mass balance identifies the quantity of substance going in and out of an entire facility, process, or piece of equipment. Emissions can be calculated as the difference between input and output of each listed substance.

Accumulation or depletion of the substance within the equipment should be accounted for in your calculation.

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

1.3 Emission Models

Some emission models may be based on measured or empirical values. The computer model can be based on theoretical equations that have been calibrated using actual data. 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 wastewater treatment system configuration, the properties of the specific compounds present in the wastewater streams, and the emission estimation approaches used in the model algorithms.

Because of the complexity involved in using manual calculations, computer programs are available that incorporate these equations to estimate emissions from wastewater treatment facilities.

Included with this Manual is a copy of WATER8, which can be used to estimate air emissions of NPI-listed substances.

WATER8

This is a publicly available computer model developed by the USEPA that models the fate of organic compounds in various wastewater treatment units. WATER8 contains such features as the ability to link treatment units to form a treatment system, the ability to recycle among units, and the ability to generate and save site-specific data for a very large number of chemicals. The mathematical equations used to calculate emissions in this model are those outlined in Table 1.

Downloading from USEPA

The WATER8 model is also publicly available on the Clearinghouse for Inventories and Emission Factors (CHIEF) bulletin board system at the USEPA. The web address is:

www.epa.gov/ttn/chief/software.html

1. Locate USEPA web site according to above address
2. Site will open and list various programs. Click on "WATER8" in top box display.
3. Once you have clicked on "WATER8" in the box display, you will see a list of Water8/Chemdat 8 Files. Under "File Name" in the table presented you will see "water8.zip". This zipped file contains the Water8 Model, Manual and various other documents. You have to download this zipped file to access the Model and Manual.
4. Double click on the "water8.zip" file. A message will appear which will ask you if you wish to save this file to disk or open it then and there. Select "save file" to download to disk (Ensure you have disk in your a or b drive of your computer, unless you are saving to the hard drive.)
5. This file you have downloaded is a zipped (zip) file and hence needs to be unzipped. If you use Microsoft Windows you may already have the "WINZIP" program which will enable you to unzip the file. A 30-day evaluation version of "WINZIP" is available on the Internet. Or you could use PKUNZIP as recommended in Water8 "readme.txt" or "readme.1st".
6. If you have the WINZIP program, open it and under File select "Wizard". You select the Wizard because you have to unzip the water8.zip file and the

Wizard guides you through the necessary steps to achieve this.

7. The first screen you will see tells a little of what WINZIP is capable of. Select "Next".

8. The next screen asks you to select the zipped file you wish to unzip. Select "Search" below the window display and instruct WINZIP to search the disk you have downloaded the file onto (a or b drive of your computer). Once listed, highlight the "water8 zip" file and select the "Next" button. Immediately select "Unzip Now" on next screen. Files will unzip in a matter of seconds and will be displayed.

9. A list of ~50 files will now be displayed. Scroll through the list and you will find the Water8.exe file (Water8 Model) and Water8.man file (Water8 Manual).

10. Double click on Water8.exe file. You should now be in Water8 Model.

11. Once you have followed all of the above steps and the water8.zip file has been unzipped, you may now save only the Water8.exe and water8.man files. To do this select one of the files and use right hand cursor of mouse to send file to floppy disk or wherever you would like it to be sent.

It is important to remember that you must unzip the water8.zip file in order to access the Model and Manual. When you first open WINZIP you can select Open Archive and select the water8.zip file you have saved onto disk. All of the documents contained within the zipped file will be listed. However when you go to open the Water8.exe file you will see the message "File not found at address..." This is because the water8.zip file has not yet been unzipped.

Using WATER8

Contained on the floppy disk that accompanies this manual are the following two files:

Water8.exe : this file contains the Water program

Water8.man : this file is the Water8 user's manual, in WordPerfect 5.1.

It is essential to read the user's manual before attempting to use WATER8. Most word processing packages (eg Microsoft Word, Word Perfect) should open the file Water8.man.

The **WATER8** package apparently runs faster in DOS or Windows 98 or earlier versions of Windows than in Windows NT. Results can be printed on an Epson clone printer, but "Postscript printers are not supported. You may wish to divert the

printer input to a disk file and use a word processor that supports your postscript printer for the printing”.

Step 1

- Put the diskette containing Water8.exe and Water8.man into the A disk drive.
- Open the file either through DOS or through Windows.
- A graphics-based title screen will appear.
- Press any key to clear the title screen. A MAIN menu will be displayed next, and the program will automatically load the compound data from the master compound file.

Step 2

- Use the arrow keys to highlight COMPOUND on the MAIN menu and then [ENTER] to obtain the COMPOUND OPTIONS LIST. Use the cursor keys to highlight “Tag compounds in Waste”, then press [ENTER] to view a list of compounds.
- Follow the directions on the screen to select compounds from the list in the existing data base. Tag all compounds in the waste for which emission estimates are to be made. For the sample case, tag benzene and phenol. [Pg Up] [Pg Dn] are helpful to review the list of compounds. Press [SPACE BAR] to return to the Compound Option List. Press [ESC] to return to the main menu.
- Use the cursor keys to highlight UNIT on the MAIN menu, then press [ENTER] to obtain “UNIT OPTIONS”. Use the cursor keys to select “specify wastewater treatment system”, then press [ENTER] to review or modify the operating parameters of the treatment system.
- You will see a wastewater treatment system worksheet. You can specify the units for the treatment train on this worksheet. For the sample case, press [F3] and you will see a pop-up menu that has the name of the units supported by WATER8. Select “activated sludge” and press [ENTER] to obtain a secondary data input screen on the right of your worksheet. This secondary data input screen contains default values. Use the arrow keys to move to the data input for activated sludge. Enter data for your system, overwriting the default values. **For the sample case, the covered flag remains at [0] rather than [1] because the unit does not have a cover.** Press [ESC] to return to the main menu.
- Upon returning to the MAIN menu, use the arrow keys to highlight UNIT and press [ENTER], then use the arrow keys to highlight “specify waste constituent concentrations”. Press [ENTER]. Type in the concentration of each selected compound, then press [ESC] to return to the MAIN menu. For the sample case, enter 2 for benzene and 1 for phenol, erase additional characters with the [SPACE BAR], and then press [ESC] to return to the MAIN menu.
- Upon returning to the MAIN menu, use the arrow keys to highlight UNIT and press [ENTER], then use the arrow keys to highlight “specify system default parameters”. Press [ENTER]. Type in the flow rate to the treatment plant in the correct data entry location. **For the sample case, the flow rate is [0.1].** Enter the wind speed and the temperature also. For the sample case, the default values given are 447 cm/s and 25°C. Press [ESC] to return to the MAIN menu.
- When you return to the MAIN menu, use the arrow keys to highlight “details of wastewater treatment of a compound” under the “view” submenu. Press [ENTER]. There will be an automatic data check. Confirm your data entries by pressing [ENTER], or change the data entry by editing the value now. After the data check is completed, a menu will be displayed with a list of compounds. Select [BENZENE]. Emissions estimates for your selected compound will be shown on screen. Press any key to move to the next screen when viewing the results of

calculations. When you have finished with this procedure, you will return automatically to the MAIN menu.

- Upon returning to the MAIN menu, use the arrow keys to highlight PRINT if you desire to have a printout of these results. Press [ENTER], then use the arrow keys to highlight the type of report that you wish to print. For the sample case, move the cursor to “print wastewater treatment report”. Press [ENTER], then a caution message will prompt you for the readiness of the printer. Hit the [Right] key and press [ENTER] to initiate the printing.
- The program will automatically return to the MAIN menu. If you wish to save the current selection, use the arrow keys to select FILE and press [ENTER]. Highlight “save current case study” and press [ENTER]. Next, highlight “save in a new file”. Press [ENTER]. Type the name of your file and press [ENTER].
- To terminate the WATER8 program, highlight QUIT on the MAIN menu and press [ENTER], then highlight “exit program” and press [ENTER].

The user’s manual provides additional explanations on how to use WATER8.

1.4 Gas-Phase Measurements

Measuring air emissions from the 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 measure emissions using standard measurement techniques.

1.5 Emission Factors

An emission factor is a tool that is used to estimate emissions to the environment. It relates the quantity of substances emitted from a source, to some common activity associated with those emissions. Emission factors are obtained from US, European, and Australian sources, and are usually expressed as the weight of a substance emitted, divided by the unit weight or volume of wastewater discharged from the whole process, or from an individual unit operation.

The VOCs and their concentrations present in wastewater vary from plant to plant, and with time at a given plant. Because of these variations, the only way accurate estimates of emissions can be obtained is by continuous source and air modelling. Such monitoring is both physically and economically impractical. Therefore, emission factors are developed that relate the amount of a VOC emitted, to individual processes and operations.

The emission factors used to estimate air emissions are defined as the fraction of the total unit, or process-influent mass loading, removed from a process through

volatilisation. Influent mass loading rates are determined by monitoring the influent stream flow rates and species concentrations. Mass emission rates from unit operations and processes are determined by measuring offgas concentrations and flow rates where possible. Emissions from covered units are measured at vents. Flux chambers are typically used to measure emissions from uncovered units. Emissions at weirs, drop junctions, meters, screens, and similar devices are estimated as the difference in upstream, and downstream liquid concentrations.

Emission rates are estimated for individual steps in a treatment process by the application of Equation (1).

$$E_{i,unit} = EF_{i,unit} Q_{in} C_i \quad (1)$$

where:

$$\begin{aligned} E_{i,unit} &= \text{mass emission rate for volatile organic compound species i, g/day} \\ EF_{i,unit} &= \text{emission factor of species i for the unit, g/g} \\ Q_{in} &= \text{liquid volumetric flow rate into the unit, m}^3/\text{day} \\ C_i &= \text{influent liquid concentration of volatile organic compound species i, g/m}^3 \end{aligned}$$

The emission factors below have been developed in a Pooled Emissions Estimation Program (PEEP) by the USA.

Table 7. Estimated VOC Emissions from Headworks Consisting of Bar Screens, Pumps, and Nonaerated Grit Chambers at a 300 000 m³/d Facility ^a

Compound	Influent Concentration µg/L	Influent Mass Rate kg/day	Mass Emission Rate kg/day	Emission Factor kg/kg of wastewater	Emission Factor Rating
Dichloromethane	19	2 097	29	0.014	U
Chloroform	28	3 091	43	0.014	U
Benzene	2	221	14	0.063	U

^a James M. Montgomery in *Toxic Air Emissions from Wastewater Treatment Facilities*, 1995

Table 8. Emissions from Aerated Grit Chambers at a 270 000m³/d Facility with Airflow Rate of 64 m³/min. ^{a, b}

Compound	Influent Concentration μg/L	Effluent Concentration μg/L	Influent Air Concentration ppbv	Effluent Air Concentration ppbv	Emission Factor kg/kg of wastewater r
Dichlorometha	39	38	20.5	110.5	0.026
Chloroform	8	7	0.0	225	0.125
Benzene	60	56	24.5	500.0	0.067

^a James M. Montgomery, 1990 in *Toxic Air Emissions from Wastewater Treatment Facilities*, 1995

^b Emission Factor Rating - U

ppbv is parts per billion volume

Table 9. Summary of Pooled Emission Estimation Program and Environment Canada Emission Factors for Physical Unit Operations

NPI-Listed Substance	Aerated Grit Chambers		Sedimentation ^a		Tertiary Filtration ^a	
	PEEP	Environment Canada ^b	Primary	Secondary	Quiescent	Backwash
Benzene	0.032	0.011	0.39 ^c	0.0 ^c	0.00085 ^c	0.0 ^c
Chloroform	0.0037	0.0029	0.0	0.0021	0.00055	0.11
Tetrachloroethylene	0.0068	0.0023	0.0	0.0008	0.0027 ^c	1.0
Styrene	0.0013 ^c	Neg	0.0039 ^c	0.0 ^c	0.00085 ^c	0.0 ^c
Trichloroethylene	0.010	0.0021	0.034	0.00083 ^c	0.0027 ^c	0.11 ^c
Toluene	0.0013	0.0070	0.0039	0.0 ^c	0.00085	0.0 ^c
Xylenes	0.00025	0.0057	0.0039 ^c	0.0 ^c	0.00085 ^c	0.0 ^c
Formaldehyde	Neg	Neg	Neg	Neg	0.35	Neg

^a James M. Montgomery, 1990 in *Toxic Air Emissions from Wastewater Treatment Facilities*, 1995

^b Bell et al., 1988 in *Toxic Air Emissions from Wastewater Treatment Facilities*, 1995

^c Extrapolated values, *Toxic Air Emissions from Wastewater Treatment Facilities*, 1995

Extrapolated values are based on the mean emission factor values for compounds with satisfactory concentration values. In making the extrapolations the compounds were grouped as non-halogenated, and halogenated. Emission factors can also be determined for aerated grit chambers, and diffused aeration activated sludge processes.

Emission Factor Rating - U

All units are kg of pollutant per kg of wastewater

APPENDIX III

Table 10. SIMS Chemical Property Data File (Part 1)

Chemical Name	CASR Number	Molecular Weight	Vapour 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 (cm ² /s)
ACETALDEHYDE	75-07-0	44.00	760	9.50E-04	1.41E-04	0.124
ACETIC ACID	64-19-7	60.05	15.4	6.27E-01	1.20E-04	0.113
ACETIC ANHYDRIDE	108-24-7	102.09	5.29	5.91E-05	9.33E-05	0.235
ACETONE	67-64-1	58.00	266	2.50E-04	1.14E-04	0.124
ACETONITRILE	75-05-8	41.03	90	5.80E-05	1.66E-04	0.128
ACROLEIN	107-02-8	56.10	244.2	5.66E-04	1.22E-04	0.105
ACRYLAMIDE	79-06-1	71.09	0.012	5.20E-09	1.06E-04	0.097
ACRYLIC ACID	79-10-7	72.10	5.2	1.00E-06	1.06E-04	0.098
ACRYLONITRILE	107-13-1	53.10	114	8.80E-04	1.34E-04	0.122
ADIPIC ACID	124-04-9	146.14	0.0000225	5.00E-10	6.84E-05	0.0659
ALLYL ALCOHOL	107-18-6	58.10	23.3	1.80E-04	1.14E-04	0.114
AMINOPHENOL(-O)	95-55-6	109.12	0.511	3.67E-05	8.64E-05	0.0774
AMINOPHENOL(-P)	123-30-8	109.12	0.893	1.97E-04	2.39E-05	0.0774
AMMONIA	7664-41-7	17.03	7470	3.28E-03	6.93E-04	0.259
AMYL ACETATE(-N)	628-37-8	130.18	5.42	4.64E-03	1.20E-05	0.064
ANILINE	62-53-3	93.10	1	2.60E-05	8.30E-05	0.07
BENZENE	71-43-2	78.10	95.2	5.50E-02	9.80E-05	0.088
BENZO(A)ANTHRACENE	56-55-3	228.30	0.0000001	1.38E-08	9.00E-05	0.051
BENZO(A)PYRENE	50-32-8	252.30	0.00568	1.38E-08	9.00E-05	0.043
CRESYLIC ACID	1319-77-3	108.00	0.3	1.70E-05	8.30E-05	0.074

Table 10. SIMS Chemical Property Data File (Part 1) cont'

Chemical Name	CASR Number	Molecular Weight	Vapour 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 (cm ² /s)
CROTONALDEHYDE	4170-30-0	70.09	30	1.54E-05	1.02E-04	0.0903
CUMENE (ISOPROPYLBENZENE)	98-82-8	120.20	4.6	1.46E-01	7.10E-05	0.065
CYCLOHEXANE	110-82-7	84.20	100	1.37E-01	9.10E-05	0.0839
CYCLOHEXANOL	108-93-0	100.20	1.22	4.47E-05	8.31E-05	0.214
CYCLOHEXANONE	108-94-1	98.20	4.8	4.13E-05	8.62E-05	0.0784
DI-N-OCTYL PHTHALATE	117-84-0	390.62	0	1.37E-00	4.10E-05	0.0409
DIBUTYLPHTHALATE	84-74-2	278.30	0.00001	2.80E-06	7.90E-05	0.0438
DICHLORO(-2)BUTENE (1,4)	764-41-0	125.00	2.87	2.59E-03	8.12E-05	0.0725
DICHLOROBENZENE (1,2) (-O)	95-50-1	147.00	1.5	1.94E-02	7.90E-05	0.069
DICHLOROBENZENE (1,3) (-M)	541-73-1	147.00	2.28	3.61E-02	7.90E-05	0.069
DICHLOROBENZENE (1,4) (-P)	106-46-7	147.00	1.2	1.60E-02	7.90E-05	0.069
DICHLORODIFLUOROMETHANE	75-71-8	120.92	5000	4.01E-00	1.00E-04	0.0001
DICHLOROETHANE (1,1)	75-34-3	99.00	234	5.54E-02	1.05E-04	0.0914
DICHLOROETHANE (1,2)	107-06-2	99.00	80	1.20E-02	9.90E-05	0.104
DICHLOROETHYLENE (1,2)	156-54-2	96.94	200	3.19E-01	1.10E-04	0.0935
DICHLOROPHENOL (2,4)	120-83-2	163.01	0.1	4.80E-05	7.60E-05	0.0709
DICHLOROPHENOXY ACETIC ACID (2,4)	94-75-7	221.00	290	6.21E-01	6.49E-05	0.0588
DICHLOROPROPANE (1,2)	78-87-5	112.99	40	2.30E-02	8.70E-05	0.0782
DIETHYL (N,N) ANILIN	91-66-7	149.23	0.00283	5.74E-07	5.87E-05	0.0513
DIETHYL PHTHALATE	84-66-2	222.00	0.003589	1.11E-01	5.80E-06	0.0542
DIMETHYL FORMAMIDE	68-12-2	73.09	4	1.92E-04	1.03E-04	0.0939
DIMETHYL HYDRAZINE (1,1)	57-14-7	60.10	157	1.24E-03	1.09E-04	0.106

Table 10. SIMS Chemical Property Data File (Part 1) cont'

Chemical Name	CASR Number	Molecular Weight	Vapour 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 (cm ² /s)
DIMETHYL PHTHALATE	131-11-3	194.20	0.000187	2.15E-05	6.30E-05	0.0586
DIMETHYLBENZ(A)ANTHRACENE	57-97-6	256.33	0	2.70E-09	4.98E-05	0.0461
DIMETHYLPHENOL (2,4)	105-67-9	122.16	0.0573	9.21E-03	8.40E-05	0.0712
DINITROBENZENE(-M)	99-56-0	168.10	0.05	2.20E-04	7.64E-05	0.279
DINITROTOLUENE(2,4)	121-14-2	182.10	0.0051	4.07E-05	7.06E-05	0.203
DIOXANE (1,4)	123-91-1	88.20	37	2.31E-04	1.02E-04	0.229
DIOXIN	NOCAS2	322.00	0	8.12E-04	5.60E-05	0.104
DIPHENYLAMINE	122-39-4	169.20	0.00375	2.78E-05	6.31E-05	0.058
EPICHLOROHYDRIN	106-89-8	92.50	17	3.23E-04	9.80E-05	0.086
ETHANOL	64-17-5	46.10	50	3.03E-04	1.30E-04	0.123
ETHANOLAMINE(MONO-)	141-43-5	61.09	0.4	3.22E-06	1.14E-04	0.107
ETHYL ACRYLATE	140-88-5	100.00	40	3.50E-03	8.60E-05	0.077
ETHYL CHLORIDE	75-00-3	64.52	1200	1.40E-01	1.15E-04	0.271
ETHYL-(2)PROPYL-(3) ACROLEIN	645-62-5	92.50	17	3.23E-04	9.80E-05	0.086
ETHYLACETATE	141-78-6	88.10	100	1.28E-03	9.66E-05	0.0732
ETHYLBENZENE	100-41-4	106.20	10	6.44E-02	7.80E-05	0.075
ETHYLENEOXIDE	75-21-8	44.00	1250	1.42E-03	1.45E-04	0.104
ETHYLETHER	60-29-7	74.10	520	6.80E-03	9.30E-05	0.074
FORMALDEHYDE	50-00-0	30.00	3500	5.76E-04	1.98E-04	0.178

Table 10. SIMS Chemical Property Data File (Part 1) cont'

Chemical Name	CASR Number	Molecular Weight	Vapour 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 (cm ² /s)
FORMIC ACID	64-18-6	46.00	42	7.00E-06	1.37E-05	0.079
FREONS		120.92	5000	4.01E-00	1.00E-04	0.104
FURAN	110-00-9	68.08	596	5.34E-02	1.22E-04	0.104
FURFURAL	96-01-1	96.09	2	8.11E-04	1.04E-04	0.0872
HEPTANE (ISO)	142-82-5	100.21	66	1.84E+01	7.11E-05	0.187
HEXACHLOROBENZENE	118-74-1	284.80	1	6.80E-03	5.91E-05	0.0542
HEXACHLOROBUTADIENE	87-68-3	260.80	0.15	2.56E-01	6.20E-05	0.0561
HEXACHLOROCYCLOPENTADIENE	77-47-4	272.80	0.081	1.60E-01	6.16E-05	0.0561
HEXACHLOROETHANE	67-72-1	237.00	0.65	2.49E-05	6.80E-05	0.00249
HEXANE(-N)	100-54-3	86.22	150	1.22E-00	7.77E-05	0.2
HEXANOL(-1)	111-27-3	102.18	0.812	1.82E-04	7.53E-05	0.059
HYDROCYCANIC ACID	74-90-8	27.00	726	4.65E-06	1.82E-04	0.197
HYDROFLUORIC ACID	7664-39-3	20.00	900	2.37E-03	3.30E-04	0.388
HYDROGEN SULFIDE	7783-06-4	34.10	15200	2.30E-01	1.61E-04	0.176
ISOPHORONE	78-59-1	138.21	0.439	5.76E-04	6.76E-05	0.0623
METHANOL	67-56-1	32.00	114	2.70E-05	1.64E-04	0.15
METHYL ACETATE	79-20-9	74.10	235	1.02E-03	1.00E-04	0.104
METHYL CHLORIDE	74-87-3	50.50	3830	8.14E-02	6.50E-05	0.126
METHYL ETHYL KETONE	78-93-3	72.10	100	4.35E-04	9.80E-05	0.0808
METHYL ISOBUTYL KETONE	108-10-1	100.20	15.7	4.95E-04	7.80E-05	0.075

Table 10. SIMS Chemical Property Data File (Part 1) cont'

Chemical Name	CASR Number	Molecular Weight	Vapour 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 (cm ² /s)
METHYL METHACRYLATE	80-62-6	100.10	39	6.60E-04	8.60E-05	0.077
METHYL STYRENE (ALPHA)	98-83-9	118.00	0.076	5.91E-02	1.14E-04	0.264
METHYLENE CHLORIDE	75-09-2	85.00	438	3.19E-02	1.17E-04	0.101
MORPHOLINE	110-91-8	87.12	10	5.73E-04	9.60E-05	0.091
NAPHTHALENE	91-20-3	128.20	0.23	1.18E-02	7.50E-05	0.059
NITROANILINE (-O)	88-74-4	138.14	0.003	5.00E-06	8.00E-05	0.073
NITROBENZENE	98-95-3	123.10	0.3	1.31E-04	8.60E-05	0.076
PENTACHLOROBENZENE	608-93-5	250.34	0.0046	7.30E-02	6.30E-05	0.057
PENTACHLOROETHANE	76-01-7	202.30	4.4	2.10E-00	7.30E-05	0.066
PENTACHLOROPHENOL	87-86-5	266.40	0.00099	2.80E-05	6.10E-05	0.056
PHENOL	108-95-2	94.10	0.34	4.54E-06	9.10E-05	0.082
PHOSGENE	75-44-5	98.92	1390	1.71E-00	1.12E-05	0.108
PHTHALIC ACID	100-21-0	166.14	121	1.32E-01	6.80E-05	0.064
PHTHALIC ANHYDRIDE	85-44-9	148.10	0.0015	9.00E-06	8.60E-00	0.071
PICOLINE (-2)	108-99-6	93.12	10.4	1.27E-03	9.60E-05	0.075
POLYCHLORINATED BIPHENYLS	1336-36-3	290.00	0.00185	4.00E-03	1.00E-04	0.104
PROPANOL (ISO)	71-23-8	60.09	42.8	1.50E-03	1.04E-04	0.098
PROPIONALDEHYDE	123-38-6	58.08	300	1.15E-02	1.14E-04	0.102
PROPYLENE GLYCOL	57-55-6	76.1	0.3	1.50E-05	1.02E-04	0.093
PROPYLENE OXIDE	75-66-9	58.10	525	1.34E-02	1.00E-04	0.104
PYRIDINE	110-86-1	79.10	20	2.36E-04	7.60E-05	0.091
RESORCINOL	108-46-3	110.11	0.00026	1.88E-07	8.70E-05	0.078

Table 10. SIMS Chemical Property Data File (Part 1) cont'

Chemical Name	CASR Number	Molecular Weight	Vapour 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 (cm ² /s)
STYRENE	100-42-5	104.20	7.3	2.61E-02	8.00E-05	0.071
TETRACHLOROETHANE(1,1,1,2)	630-20-6	167.85	6.5	2.00E-02	7.90E-05	0.071
TETRACHLOROETHANE(1,1,2,2,)	79-34-5	167.85	6.5	3.80E-03	7.90E-05	0.071
TETRACHLOROETHYLENE	127-18-4	165.83	19	2.90E-01	8.20E-05	0.072
TETRAHYDROFURAN	109-99-9	72.12	72.1	4.90E-04	1.05E-04	0.098
TOLUENE	109-88-3	92.40	30	6.68E-02	8.60E-05	0.087
TOLUENE DIISOCYANATE (2,4)	584-84-9	174.16	0.08	8.30E-05	6.20E-05	0.061
TRICHLORO(1,1,2)TRIFLUOROETHANE	76-13-1	187.38	300	4.35E-00	8.20E-05	0.078
TRICHLOROBENZENE(1,2,4)	120-82-1	181.50	0.18	1.42E-02	7.70E-05	0.0676
TRICHLOROBUTANE(1,2,3)		161.46	4.39	4.66E+01	7.20E-05	0.066
TRICHLOROETHANE(1,1,1)	71-55-6	133.40	123	4.92E-02	8.80E-05	0.078
TRICHLOROETHANE(1,1,2)	79-00-5	133.40	25	7.42E-03	8.80E-05	0.078
TRICHLOROETHYLENE	79-01-6	131.40	75	9.10E-02	9.10E-05	0.079
TRICHLOROFLUOROMETHANE	75-69-4	137.40	796	5.83E-01	9.70E-05	0.087
TRICHLOROPHENOL(2,4,6)	88-06-2	197.46	0.0073	1.77E-04	7.50E-05	0.0661
TRICHLOROPROPANE(1,1,1)		147.43	3.1	2.90E-01	7.90E-05	0.071
TRICHLOROPROPANE(1,2,3)	96-18-4	147.43	3	2.80E-01	7.90E-05	0.071

Table 10. SIMS Chemical Property Data File (Part 1) cont'

Chemical Name	CASR Number	Molecular Weight	Vapour Pressure At 25°C (mm Hg)	Henry's Law Constant At 25°C (atm.m³/mol)	Diffusivity Of Chemical In Water At 25°C (cm²/s)	Diffusivity Of Chemical In Air At (cm²/s)
UREA	57-13-6	60.06	6.69	2.64E-03	1.37E-04	0.122
VINYL ACETATE	108-05-4	86.09	115	6.20E-03	9.20E-05	0.085
VINYL CHLORIDE	75-01-4	62.50	2660	8.60E-01	1.23E-04	0.106
VINYLDENE CHLORIDE	75-35-4	97.00	591	1.50E-01	1.04E-04	0.09
XYLENE(-M)	1330-20-7	106.17	8	5.20E-02	7.80E-05	0.07
XYLENE(-O)	95-47-6	106.17	7	5.27E-02	1.00E-04	0.087

Table 11. SIMS Chemical Property Data File (Part 2)

Chemical Name	Antoine's Equation Vapour Pressure Coefficient A	Antoine's Equation Vapour Pressure Coefficient B	Antoine's Equation Vapour 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	2.29E-04	419.0542	2.69153
ACETIC ACID	7.387	1533.313	222.309	3.89E-05	14.2857	0.48978
ACETIC ANHYDRIDE	7.149	1444.718	199.817	2.69E-05	1.9323	1
ACETONE	7.117	1210.595	229.664	3.61E-06	1.1304	0.57544
ACETONITRILE	7.119	1314.4	230	4.25E-05	152.6014	0.45709
ACROLEIN	2.39	0	0	2.17E-05	22.9412	0.81283
ACRYLAMIDE	11.2932	3939.877	273.16	4.25E-05	56.2388	6.32182
ACRYLIC ACID	5.652	648.629	154.683	2.69E-05	54.7819	2.04174
ACRYLONITRILE	7.038	1232.53	222.47	5.00E-05	24	0.12023
ADIPIC ACID	0	0	0	2.69E-05	66.9943	1.20226
ALLYL ALCOHOL	0	0	0	4.89E-05	3.9241	1.47911
AMINOPHENOL(-O)	0	0	0	4.25E-05	68.1356	3.81533
AMINOPHENOL(-P)	-3.357	699.157	-331.343	4.25E-05	68.1356	3.81533
AMMONIA	7.5547	1002.711	247.885	4.25E-05	15.3	1
AMYL ACETATE (-N)	0	0	0	2.69E-05	16.1142	51.10801
ANILINE	7.32	1731.515	206.049	1.97E-05	.3381	7.94328
BENZENE	6.905	1211.033	220.79	5.28E-05	13.5714	141.25375
BENZO(A)ANTHRACENE	6.9824	2426.6	156.6	8.64E-05	1.7006	407380.2778
BENZ(A)PYRENE	9.2455	3724.363	273.16	8.64E-05	1.2303	954992.58602
BENZYL CHLORIDE	0	0	0	4.93E-05	17.5674	199.52623
BIS(2-CHLOROETHYL)ETHER	0	0	0	2.99E-05	20.0021	38.01894
BIS(2-CHLOROISOPROPYL)ETHER	0	0	0	2.99E-05	8.3382	380.1894
BIS(2-ETHYLHEXYL)PHTHALATE	0	0	0	2.14E-06	2.2	199526.2315
BROMOFORM	0	0	0	2.99E-05	10.653	199.52623

Table 11. SIMS Chemical Property Data File (Part 2) cont'

Chemical Name	Antoine's Equation Vapour Pressure Coefficient A	Antoine's Equation Vapour Pressure Coefficient B	Antoine's Equation Vapour Pressure Coefficient C	Maximum Biodegradation Rate Constant (g/g Biomass-s)	Half Saturation Constant (g/m ³)	Octanol-Water Partition Coefficient At 25°C
BROMOMETHANE	0	0	0	2.99E-05	30.4422	12.58925
BUTADIENE-(1,3)	6.849	930.546	238.854	4.25E-05	15.3	74.32347
BUTANOL (ISO)	7.4743	1314.19	186.55	2.17E-05	70.9091	5.62341
BUTANOL-(1)	7.4768	1362.39	178.77	2.17E-05	70.9091	5.62341
BUTYL BENZYL PHTHALATE	0	0	0	8.64E-05	14.1364	60255.95861
CARBON DISULFIDE	6.942	1169.11	241.59	4.25E-05	5.8175	1
CARBON TETRACHLORIDE	6.934	1242.43	230	4.17E-06	1	524.80746
CHLORO(-P)CRESOL(-M)	0	0	0	2.99E-05	5.2902	1258.92541
CHLOROACETALDEHYDE	0	0	0	2.99E-05	49.838	3.4405
CHLOROBENZENE	6.978	1431.05	217.55	1.08E-06	.039	316.22777
CHLOROFORM	6.493	929.44	196.03	8.17E-06	3.7215	91.20108
CHLORONAPHTHALENE-(2)	0	0	0	2.99E-05	2.167	13182.56739
CHLOROPRENE	6.161	783.45	179.7	3.00E-05	6.3412	1
CRESOL(-M)	7.508	1856.36	199.07	6.45E-05	1.3653	93.32543
CRESOL(-O)	6.911	1435.5	165.16	6.33E-05	1.34	95.49926
CRESOL (-P)	7.035	1511.08	161.85	6.45E-05	1.3653	87.09636
CRESYLIC ACID	0	0	0	4.17E-05	15	1
CROTONALDEHYDE	0	0	0	2.69E-05	27.6285	12.36833
CUMENE (ISOPROPYLBENZENE)	6.963	1460.793	207.78	8.65E-05	16.5426	1
CYCLOHEXANE	6.841	1201.53	222.65	4.25E-05	15.3	338.0687
CYCLOHEXANOL	6.255	912.87	109.13	2.69E-05	18.0816	37.74314
CYCLOHEXANONE	7.8492	2137.192	273.16	3.19E-05	41.8921	6.45654
DI-N-OCTYL PHTHALATE	0	0	0	8.30E-07	0.02	141253.7
DIBUTYLPHTHALATE	6.639	1744.2	113.59	1.11E-06	0.4	158489.31925

Table 11. SIMS Chemical Property Data File (Part 2) cont'

Chemical Name	Antoine's Equation Vapour Pressure Coefficient A	Antoine's Equation Vapour Pressure Coefficient B	Antoine's Equation Vapour Pressure Coefficient C	Maximum Biodegradation Rate Constant (g/g Biomass-s)	Half Saturation Constant (g/m ³)	Octanol-Water Partition Coefficient At 25°C
DICHLORO(-2)BUTENE(1,4)	0	0	0	2.99E-05	9.8973	242.1542
DICHLOROBENZENE(1,2) (-O)	.176	0	0	6.94E-06	4.3103	2398.83292
DICHLOROBENZENE(1,3) (-M)	0	0	0	1.78E-05	2.7826	2398.83292
DICHLOROBENZENE(1,4) (-P)	.079	0	0	1.78E-05	2.7826	2454.70892
DICHLORODIFLUOROMETHANE	0	0	0	2.99E-05	12.0413	144.54398
DICHLOROETHANE(1,1)	0	0	0	2.99E-05	4.6783	61.6595
DICHLOROETHANE(1,2)	7.025	1272.3	222.9	5.83E-06	2.1429	61.6595
DICHLOROETHYLENE(1,2)	6.965	1141.9	231.9	2.99E-05	6.3294	1
DICHLOROPHENOL (2,4)	0	0	0	6.94E-05	7.5758	562.34133
DICHLOROPHENOXY ACETIC ACID (2,4)	0	0	0	2.99E-05	14.8934	82.61445
DICHLOROPROPANE(1,2)	6.98	1380.1	22.8	4.72E-05	12.1429	1
DIETHYL (N,N) ANILIN	7.466	1993.57	218.5	4.25E-05	27.0047	43.57596
DIETHYL PHTHALATE	0	0	0	7.35E-06	1.28	1412.537
DIMETHYL FORMAMIDE	6.928	1400.87	196.43	4.25E-05	15.3	1
DIMETHYL HYDRAZINE(1,1)	7.408	1305.91	225.53	4.25E-05	15.3	1
DIMETHYL PHTHALATE	4.522	700.31	51.42	6.11E-06	0.7097	74.13102
DIMETHYLBENZ(A)ANTHRACENE	0	0	0	8.64E-05	0.3377	28680056.33087
DIMETHYLPHENOL(2,4)	0	0	0	2.97E-05	2.2766	263.0268
DINITROBENZENE (-M)	4.337	229.2	-137	4.25E-05	29.9146	33.28818
DINITROTOLUENE (2,4)	5.798	1118	61.8	4.25E-05	19.5233	102.3293
DIOXANE (1,4)	7.431	1554.68	240.34	2.69E-05	24.7001	16.60956
DIOXIN	12.88	6465.5	273	3.00E-05	6.3412	1
DIPHENYLAMINE	0	0	0	5.28E-05	8.4103	1659.58691

Table 11. SIMS Chemical Property Data File (Part 2) cont'

Chemical Name	Antoine's Equation Vapour Pressure Coefficient A	Antoine's Equation Vapour Pressure Coefficient B	Antoine's Equation Vapour Pressure Coefficient C	Maximum Biodegradation Rate Constant (g/g Biomass-s)	Half Saturation Constant (g/m ³)	Octanol-Water Partition Coefficient At 25°C
EPICHLOROHYDRIN	8.2294	2086.816	273.16	3.00E-05	6.3412	1.07152
ETHANOL	8.321	1718.21	237.52	2.44E-05	9.7778	0.47863
ETHANOLAMINE(MONO-)	7.456	1577.67	173.37	4.25E-05	223.0321	0.16865
ETHYL ACRYLATE	7.9645	1897.011	273.16	2.69E-05	39.4119	4.85667
ETHYL CHLORIDE	6.986	1030.01	238.61	2.99E-05	22.8074	26.91535
ETHYL-(2)PROPYL-(3)ACROLEIN	0	0	0	4.25E-05	15.3	1
ETHYLACETATE	7.101	1244.95	217.88	4.88E-05	17.58	1
ETHYLBENZENE	6.975	1424.255	213.21	1.89E-05	3.2381	1412.53754
ETHYLENEOXIDE	7.128	1054.54	237.76	1.17E-05	4.6154	0.50003
ETHYLETHER	6.92	1064.07	228.8	2.69E-05	17.1206	43.57596
FORMALDEHYDE	7.195	970.6	244.1	1.39E-05	20	87.09636
FORMIC ACID	7.581	1699.2	260.7	2.69E-05	161.3977	0.1191
FREONS	0	0	0	3.00E-05	6.3412	1
FURAN	6.975	1060.87	227.74	2.69E-05	14.1936	71.37186
FURFURAL	6.575	1198.7	162.8	2.69E-05	18.0602	37.86047
HEPTANE (ISO)	6.8994	1331.53	212.41	4.25E-05	15.3	1453.372
HEXACHLOROBENZENE	0	0	0	2.99E-05	0.6651	295120.92267
HEXACHLOROBUTADIENE	0.824	0	0	3.00E-05	6.3412	5495.408
HEXACHLOROCYCLOPENTADIENE	0	0	0	3.00E-05	0.3412	9772.372
HEXACHLOROETHANE	0	0	0	2.99E-05	3.3876	4068.32838
HEXANE(-N)	6.876	1171.17	224.41	4.25E-05	15.3	534.0845
HEXANOL(-1)	7.86	1761.26	196.66	2.69E-05	15.2068	59.52851
HYDROCYANIC ACID	7.528	1329.5	260.4	2.69E-05	1.9323	1
HYDROFLUORIC ACID	7.217	1268.37	273.87	2.69E-05	1.9323	1

Table 11. SIMS Chemical Property Data File (Part 2) cont'

Chemical Name	Antoine's Equation Vapour Pressure Coefficient A	Antoine's Equation Vapour Pressure Coefficient B	Antoine's Equation Vapour Pressure Coefficient C	Maximum Biodegradation Rate Constant (g/g Biomass-s)	Half Saturation Constant (g/m ³)	Octanol-Water Partition Coefficient At 25°C
HYDROGEN SULFIDE	7.614	885.319	250.25	2.99E-05	6.3294	1
ISOPHORONE	0	0	0	4.25E-05	25.6067	50.11872
METHANOL	7.897	1474.08	229.13	5.00E-05	90	0.19953
METHYL ACETATE	7.065	1157.63	219.73	5.52E-05	159.2466	0.81283
METHYL CHLORIDE	7.093	948.58	249.34	2.99E-05	14.855	83.17638
METHYL ETHYL KETONE	6.9742	1209.6	216	5.56E-06	10	1.90546
METHYL ISOBUTYL KETONE	6.672	1168.4	191.9	2.06E-06	1.6383	23.98833
METHYL METHACRYLATE	8.409	2050.5	274.4	2.69E-05	109.2342	0.33221
METHYL STYRENE (ALPHA)	6.923	1486.88	202.4	8.64E-05	11.12438	2907.589
METHYLENE CHLORIDE	7.409	1325.9	252.6	6.11E-05	54.5762	17.78279
MORPHOLINE	7.7181	1745.8	235	4.25E-05	291.9847	0.08318
NAPHTHALENE	7.01	1733.71	201.86	1.18E-04	42.47	1
NITROANILINE (-O)	8.868	336.5	273.16	4.25E-05	22.8535	67.6083
NITROBENZENE	7.115	1746.6	201.8	3.06E-05	4.7826	69.1831
PENTACHLOROBENZENE	0	0	0	2.99E-05	0.4307	925887.02902
PENTACHLOROETHANE	6.74	1378	197	2.99E-05	0.4307	925887.02902
PENTACHLOROPHENOL	0	0	0	3.61E-04	38.2353	102329.29923
PHENOL	7.133	1516.79	174.95	2.69E-04	7.4615	28.84032
PHOSGENE	6.842	941.25	230	4.25E-05	70.8664	3.4405
PHTHALIC ACID	0	0	0	2.69E-05	34.983	6.64623
PHTHALIC ANHYDRIDE	8.022	2868.5	273.16	4.89E-05	3.9241	0.23988
PICOLINE(-2)	7.032	1415.73	211.63	4.25E-05	44.8286	11.48154
POLYCHLORINATED BIPHENYLS	0	0	0	5.28E-05	20	1
PROPANOL (ISO)	8.117	1580.92	219.61	4.17E-05	200	0.69183

Table 11. SIMS Chemical Property Data File (Part 2) cont'

Chemical Name	Antoine's Equation Vapour Pressure Coefficient A	Antoine's Equation Vapour Pressure Coefficient B	Antoine's Equation Vapour Pressure Coefficient C	Maximum Biodegradation Rate Constant (g/g Biomass-s)	Half Saturation Constant (g/m ³)	Octanol-Water Partition Coefficient At 25°C
PROPIONALDEHYDE	16.2315	2659.02	-44.15	2.69E-05	39.2284	4.91668
PROPYLENE GLYCOL	8.2082	2085.9	203.5396	2.69E-05	109.3574	0.33141
PROPYLENE OXIDE	8.2768	1656.884	273.16	4.89E-05	3.9241	1
PYRIDINE	7.041	1373.8	214.98	9.73E-05	146.9139	4.46684
RESORCINOL	6.9243	1884.547	186.0596	2.69E-05	35.6809	6.30957
STYRENE	7.14	1574.51	224.09	8.64E-05	282.7273	1445.43977
TETRACHLOROETHANE (1,1,1,2)	6.898	1365.88	209.74	2.99E-05	6.3294	1
TETRACHLOROETHANE(1,1,2,2)	6.631	1228.1	179.9	1.72E-05	9.1176	363.07805
TETRACHLOROETHYLENE	6.98	1386.92	217.53	1.72E-05	9.1176	398.10717
TETRAHYDROFURAN	6.995	1202.29	226.25	2.69E-05	20.3702	27.58221
TOLUENE	6.954	1344.8	219.48	2.04E-04	30.6167	489.77882
TOLUENE DIISOCYANATE(2,4)	0	0	0	4.25E-05	15.3	1
TRICHLORO(1,1,2)TRIFLUOROETHANE	6.88	1099.9	227.5	2.99E-05	3.3876	4068.32838
TRICHLOROBENZENE(1,2,4)	0	0	0	2.99E-05	2.4495	9549.92586
TRICHLOROBUTANE(1,2,3)	0	0	0	3.00E-05	6.3412	1450901.06626
TRICHLOROETHANE(1,1,1)	8.643	2136.6	302.8	9.72E-06	4.7297	309.02954
TRICHLOROETHANE(1,1,2)	6.951	1314.41	209.2	9.72E-06	4.7297	1
TRICHLOROETHYLENE	6.518	1018.6	192.7	1.08E-05	4.4318	194.98446
TRICHLOROFLUOROMETHANE	6.884	1043.004	236.88	3.00E-05	6.3412	338.8441
TRICHLOROPHENOL (2,4,6)	0	0	0	4.25E-05	58.8462	4897.78819
TRICHLOROPROPANE(1,1,1)	0	0	0	2.99E-05	10.7719	193.7827
TRICHLOROPROPANE(1,2,3)	6.903	788.2	243.23	2.99E-05	10.7719	193.7827
UREA	0	0	0	4.25E-05	4.8169	4068.32838
VINYL ACETATE	7.21	1296.13	226.66	2.69E-05	31.8363	8.51722

Table 11. SIMS Chemical Property Data File (Part 2) cont'

Chemical Name	Antoine's Equation Vapour Pressure Coefficient A	Antoine's Equation Vapour Pressure Coefficient B	Antoine's Equation Vapour Pressure Coefficient C	Maximum Biodegradation Rate Constant (g/g Biomass-s)	Half Saturation Constant (g/m ³)	Octanol-Water Partition Coefficient At 25°C
VINYL CHLORIDE	3.425	0	0	3.00E-05	6.3412	1.14815
VINYLDENE CHLORIDE	6.972	1099.4	237.2	3.00E-05	6.3412	1
XYLENE(-M)	7.009	1426.266	215.11	8.64E-05	14.0094	1584.89319
XYLENE(-O)	6.998	1474.679	213.69	1.13E-05	22.8569	891.25094

Example 3: Using Engineering Equations to Estimate Air Emissions

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 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 Numbers from Table 4
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 you have determined the appropriate emission model, 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 = $0.0623 \text{ m}^3/\text{s}$
D = Wastewater depth = 1.97 m
A = Wastewater surface area = $17,652 \text{ m}^2$
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 6, but where available, site-specific values should be used. For this facility, all available general and bio-treatment system defaults from Table 6 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 of aerators = 0.75 hp/1,000 ft ³ (V)
O_t	=	Oxygen transfer correction factor = 0.83
Va_v	=	Turbulent surface areas = 0.24 (A)
d	=	Impeller diameter = 61 cm
d^*	=	Impeller diameter = 2 ft
w	=	Rotational speed of impeller = 126 rad/s
N_1	=	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 10. Water, air, and other property values are given in Table 5.

A. Benzene (from Table 10)

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

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

ρ_a	=	Density of air = $1.2 * 10^{-3}$ g/cm ³
ρ_L	=	Density of water = 1 g/cm ³
μ_a	=	Viscosity of air = $1.81 * 10^{-4}$ g/cm-s
$D_{O_2,w}$	=	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 -ft/lb _f -s ²
R	=	Universal gas constant = $8.21 * 10^{-5}$ (atm-m ³ /gmol/K)

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.

Turbulent area of impoundment - Equations (3) and (4) from Table 4.

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

$$K_l(\text{m/s}) = [(8.22 * 10^{-9})(J)(\text{POWR})(1.024)^{(T-20)} \\ (O_i)(10^6)\text{MW}_L/(\text{Va}_v * \rho_L)](D_w/D_{O_2,W})^{0.5}$$

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):

$$\begin{aligned} \text{POWR (hp)} &= 0.75 \text{ hp}/1,000 \text{ ft}^3(\text{V}) \\ \text{V} &= \text{wastewater volume, m}^3 \\ \text{V (m}^3\text{)} &= (\text{A})(\text{D}) = (17,652 \text{ m}^2)(1.97\text{m}) \\ \text{V} &= 34,774 \text{ m}^3 \\ \text{POWR} &= (0.75 \text{ hp}/1,000 \text{ ft}^3)(\text{ft}^3/0.028317 \text{ m}^3) \\ &= (34,774 \text{ m}^3) \\ &= 921 \text{ hp} \end{aligned}$$

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

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

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

$$\begin{aligned} K_l(\text{m/s}) &= [(8.22 * 10^{-9})(3 \text{ lb O}_2/\text{hp-hr})(921 \text{ hp}) * \\ & (1.024)^{(25-20)}(0.83)(10^6)(18 \text{ g/gmol})/ \\ & ((45,576 \text{ ft}^2)(1 \text{ g/cm}^3))]* \\ & [(9.8 * 10^{-6} \text{ cm}^2/\text{s})/(2.4 * 10^{-5} \text{ cm}^2/\text{s})]^{0.5} \\ &= (0.00838)(0.639) \\ K_l &= 5.35 * 10^{-3} \text{ m/s} \end{aligned}$$

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

$$K_g(\text{m/s}) = (1.35 * 10^{-7})(\text{Re})^{1.42}(\text{P})^{0.4}(\text{Sc}_g)^{0.5}(\text{Fr})^{-0.21}(\text{D}_a\text{MW}_a/d)$$

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:

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

2. Calculate power number, P:

$$\begin{aligned} P &= [(0.85)(\text{POWR})(550 \text{ ft-lb}_f/\text{s-hp})/N_i] g_c / (P_L (d^5 w^3)) \\ N_i &= \text{POWR}/0.75 \text{ hp (default presented in III)} \\ P &= (0.85)(75\text{hp})(\text{POWR}/\text{POWR})(550 \text{ ft-lb}_f/\text{s-hp}) * \\ &\quad (32.17 \text{ lb}_m\text{-ft}/\text{lb}_f\text{-s}^2) / [(62.4 \text{ lb}_m/\text{ft}^3)(2 \text{ ft})^5 (126 \text{ rad/s})^3] \\ &= 2.8 * 10^{-4} \end{aligned}$$

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

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

4. Calculate Froude number, Fr:

$$\begin{aligned} \text{Fr} &= (d^3 w^2) / g_c \\ &= (2 \text{ ft})(126 \text{ rad/s})^2 / (32.17 \text{ lb}_m\text{-ft}/\text{lb}_f\text{-s}^2) \\ &= 990 \end{aligned}$$

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

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

Quiescent surface area of impoundment - Equations 1 and 2 from Table 4.

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 U₁₀ > 3.25 m/s and F/D > 51.2 use the following:

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

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

$$K_g = (4.82 * 10^{-3})(U_{10})^{0.78}(Sc_G)^{-0.67}(d_e)^{-0.11}$$

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 :
 $Sc_G = \mu_a / (\rho_a D_a) = 1.71$ (same as for turbulent impoundments)
2. Calculate the effective diameter, d_e :

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

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 4).

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

$$\begin{aligned}K_T \text{ (m/s)} &= (K_l Keq K_g) / (Keq K_g + K_l) \\Keq &= H/RT \\&= (0.0055 \text{ atm}\cdot\text{m}^3/\text{gmol}) / [(8.21 * 10^{-5} \text{ atm}\cdot\text{m}^3/\text{gmol}\cdot^\circ\text{K})(298^\circ\text{K})] \\&= 0.225 \\K_T \text{ (m/s)} &= (5.35 * 10^{-3} \text{ m/s})(0.225)(0.109) / [(0.109 \text{ m/s})(0.225) + (5.35 * 10^{-6} \text{ m/s})] \\K_T &= 4.39 * 10^{-3} \text{ m/s}\end{aligned}$$

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

$$\begin{aligned}K_Q \text{ (m/s)} &= (K_l Keq K_g) / (Keq K_g + K_l) \\&= (5.74 * 10^{-6} \text{ m/s})(0.225)(6.24 * 10^{-3} \text{ m/s}) / [(6.24 * 10^{-3} \text{ m/s})(0.225) + (5.74 * 10^{-6} \text{ m/s})] \\&= 5.72 * 10^{-6} \text{ m/s}\end{aligned}$$

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

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

VII. Calculate VOC Emissions For An Aerated Biological Flowthrough Impoundment

Equation (16) from Table 4:

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

where:

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

and:

$$\begin{aligned}
 a &= (KA/Q) + 1 \\
 b &= K_s((KA/Q) + 1) + K_{max} b_i V/Q - C_o \\
 c &= -K_s C_o
 \end{aligned}$$

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

1. Calculate a:

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

2. Calculate b:

($V = 34,774 \text{ m}^3$ from V):

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

3. Calculate c:

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

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:

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