EMISSIONS OF SELECTED VOC COMPOUNDS FROM THE USE OF LAUNDRY AND DISHWASHING PRODUCTS

Prepared for

The Soap and Detergent Association

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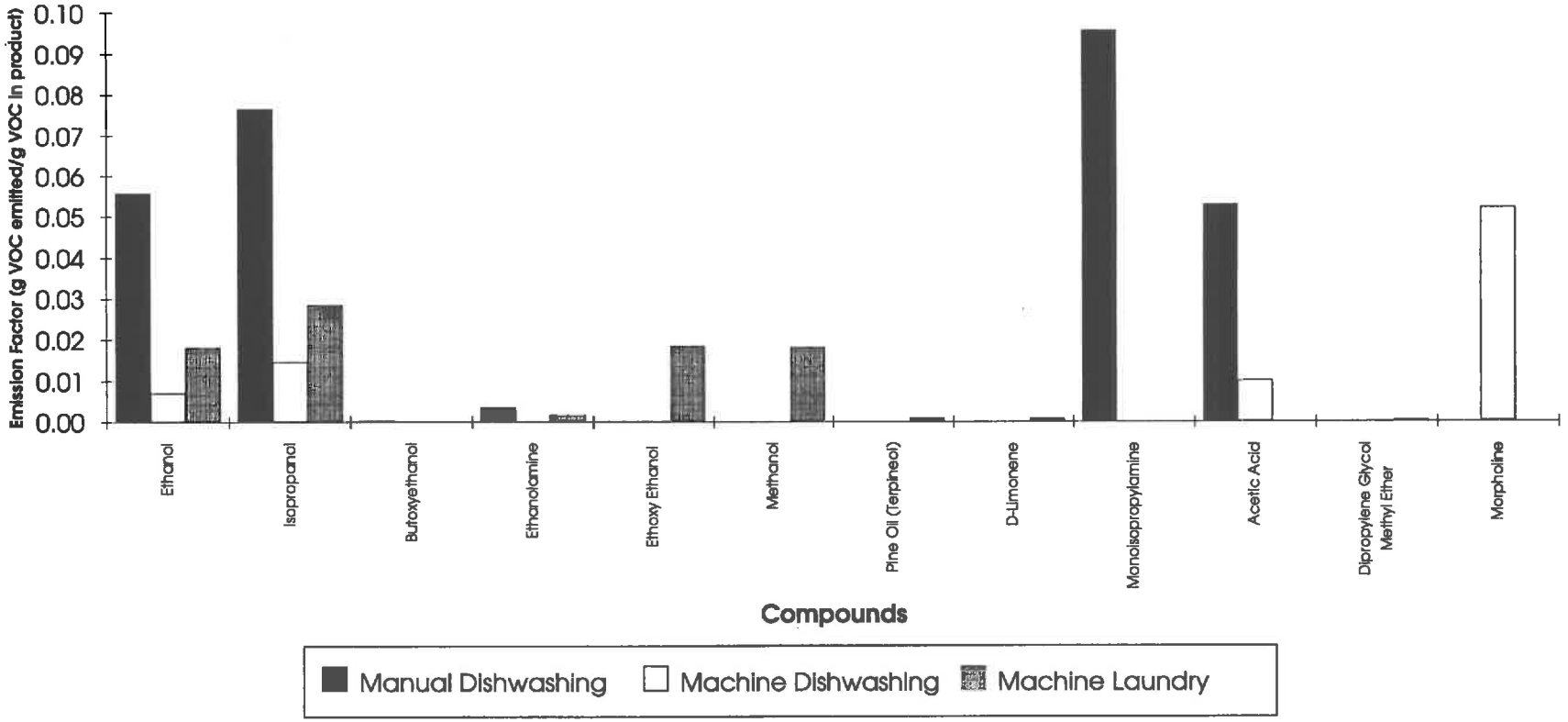
Executive Summary

The Soap and Detergent Association (SDA) retained CH2M HILL to assess the potential emissions from the use of various volatile organic compounds (VOC) in laundry and dishwashing products disposed into wastewater treatment systems. Using methodologies developed by the Environmental Protection Agency (EPA) and followed in previous studies for SDA, an analysis was conducted regarding the potential emissions from 12 VOC species, including ethanol, known to be used in consumer detergent products.

Figure ES-1 shows the predicted emission factors for each VOC species corresponding to the types of products in which they are used. Average overall emission factors for hard dishwashing, machine dishwashing, and laundry product VOCs are approximately 0.05, 0.02, and 0.01, respectively. Using the results of this study as well as national usage of VOCs in laundry and dishwashing products, an estimate of annual emissions of the 12 study VOC species from these products can be derived.

The results of this study indicate that the bulk of VOCs used in laundry and dishwashing products are not emitted to the atmosphere. This result is reasonable because the VOC species used in these products are generally both nonvolatile and biodegradable. Therefore, the primary fate of the VOC species is biological degradation at the publicly owned treatment works (POTW) and discharge of the remaining VOC to WWTP receiving waters.

Figure ES-1. Overall Emission Factors for Cleaning Product VOC's



Note: Some compounds are not applicable to product category (See Table 4)

Section 1
Introduction

The Environmental Protection Agency (EPA), in developing regulations for the Clean Air Act Amendments (CAAA) of 1990, is considering the regulation of volatile organic compounds (VOCs) in consumer products.

In order to develop a national inventory of VOC emissions from consumer and commercial products, as required under the CAAA, EPA conducted a survey of manufacturers in which each manufacturer was asked to self report the types and annual quantities of volatile organic materials used within its product formulations. Cleaning product manufacturers reported a wide variety of organic material use within the product categories of laundry and dishwashing products.

SDA has previously studied the emissions potential from the use of VOC in its members' products (CH2M HILL, 1992) for the purposes of evaluating EPA's Draft Report to Congress on "Volatile Organic Compound Emissions for Consumer and Commercial Products" (1990). CH2M HILL subsequently prepared a 1991 evaluation of "Ethanol Emissions from Wastewater Collection and Treatment Systems" for SDA's use in rule development negotiations with the California Air Resources Board (CARB). Additionally, two studies of the potential in-home emissions were conducted by the University of California at Berkeley in 1989. These studies focused on the emissions from the use of liquid detergents during hand dishwashing and machine clothes washing.

In this study, SDA has retained CH2M HILL to conduct further emissions analysis on a select list of VOC species contained in EPA's survey results. The analysis follows the methods used in the previous SDA study conducted by CH2M HILL (1992) but expands the analysis from ethanol to include a list of 11 other compounds. The methodology used is briefly discussed in Section 2. The results of the analysis are presented in Section 3.

Section 2
Methodology

This study of an expanded list of compounds uses the methodologies of previous studies to provide consistency of results and to adhere to emissions estimation methodologies used by EPA. The approach to estimating emissions closely follows that used by EPA in the Surface Impoundment Modeling System (SIMS) model (1990). Some model variations have been implemented, as recommended in the 1992 CH2M HILL study/ review of EPA's Draft Report to Congress.

Selection of List of Compounds

Using EPA's survey, SDA staff further evaluated the reported chemicals to screen out those not considered to be reportable VOCs according to definitions utilized in EPA's survey. A list of 12 highest volume reported VOCs was developed based upon the reported annual mass of use in laundry and dishwashing products. The list of compounds addressed in this study is contained in Table 1 (Appendix A).

Development of Physico-Chemical Database

Using the short list of compounds, a literature review was undertaken to develop the basic physico-chemical parameters needed to apply the SIMS equations. The list of physico-chemical parameters of interest in SIMS is:

- Molecular Weight
- Henry's Law Constant
- Liquid Phase Diffusion Coefficient
- Gas Phase Diffusion Coefficient
- Biological Degradation Rate Constants

It was anticipated that many of the compounds on the list would prove difficult in terms of available literature information. Also, as is generally the case, the values from different sources can be highly variable. Review of available sources of information resulted in the database shown in Table 1 (see Appendix A). References are shown in Appendix B.

In developing the database, preference was given to EPA values contained in Appendix B of the SIMS documentation. While additional, more refined data may be available, use of EPA values promotes acceptability of the analysis. Should emission estimates for any given VOC species be considered significant, a further, more detailed evaluation of the Table 1 values could be conducted. As indicated in Table 1, the data gathering effort resulted in some data gaps. To fill these gaps and complete this analysis, several approximations have been made.

D-Limonene

A Henry's Law constant for d-limonene was not found in the literature reviewed. For the purposes of this assessment, a value was assigned, based upon the similarity of the compound and its vapor pressure to terpineol.

Dipropylene Glycol Methyl Ether

Little information was available in the literature reviewed for this compound. For the purposes of analysis, values for a Henry's Law constant and a gas/liquid diffusion coefficient were assigned, based on similarity of structure and vapor pressure to butoxyethanol.

Biodegradation Rate Constants

EPA's SIMS model requires input of two values for the calculation of biodegradation in activated sludge units. They are:

- The half saturation biorate constant (g/m^3)
- The maximum biorate concentration (g/g-s)

Data on biological degradation for common VOC species are often difficult to obtain and generally subject to great uncertainty. For many of the VOC species in this study, little or no data were available. To gather available data, EPA's databases in the SIMS and WATER7 models were used (EPA 1990a and EPA 1990b). SIMS provided values for the half saturation constant for 6 of the 12 study compounds. The value of the remaining six compounds was conservatively assumed to be equal to the lowest value observed for the six compounds for which data is available. This results in low estimates of biodegradation, and therefore, conservative (high) values for air emissions.

The maximum biorate constant was obtained for the same six compounds from the database in WATER7. A unit conversion was made and the values were used here. The same approach as above was used to fill in data for compounds that were not in the database.

Estimation of In-Home Emissions

As mentioned in Section 1, UC Berkeley conducted extensive studies on the emissions of ethanol from in-home use of liquid detergents. These studies resulted in publication of emission factors in units of grams emitted per gram used. Values were given for normal use and for high agitation use.

For the purposes of this study, it has been assumed that these studies, which were based on simulations of household laundering and dishwashing, were applicable to commercial uses of these products as well as household uses.

Section 3
Discussion of Results

Following the methodology outlined above, a series of spreadsheets was developed to complete the analysis of emissions of select VOCs during use of cleaning products. Appendix A contains printouts of these spreadsheets. Table 2 in Appendix A contains the emissions estimation calculations for POTW emissions, following EPA's SIMS approach. Table 3 in Appendix A presents the compound-specific emission factors calculated for each POTW unit process, as well as the overall POTW emission factor for each compound. Table 4 in Appendix A summarizes the calculated emission factors resulting from the use of laundry and dishwashing products for the 12 compounds in this study, as well as ethanol.

Table 4 also presents an overall VOC species emission factor that accounts for the losses in each mechanism and can be used to derive quickly estimates of emissions for each species. Also shown are average emission factors derived by arithmetically averaging the 12 species shown in Table 4. This provides an emission factor for each category of product that can be used to extrapolate for other species of similar nature that were not studied here.

Figure ES-1 graphically presents the in-home and POTW emission factors for each of the 12 study compounds. From this presentation, it is clear that some compounds are emitted (on a g/g basis) at rates greater than ethanol. The emission factors reported for ethanol are very similar to those reported in earlier studies (Wooley, et al., 1990; CH2M HILL, 1991), confirming that the approach used in this study is appropriate for these types of compounds.

The derivations of emission factors in this study are based on several assumptions that will result in a conservative (high) estimate of emissions. Assumptions include:

- No biological or chemical degradation of any of the 12 VOC species was assumed, except in processes designed for biological treatment.

- No adsorption mechanisms for the 12 VOC species were accounted for, either in the collection system or POTW.

The results of this study indicate that the bulk of VOCs used in laundry and dishwashing products are not emitted to the atmosphere. This result is reasonable because the VOC species used in these products are generally both nonvolatile and biodegradable. Therefore, the primary fate of the VOC species is biological degradation at the publicly owned treatment works (POTW) and discharge of the remaining VOC to WWTP receiving waters.

Appendix A
SPREADSHEET CALCULATIONS

Table 1
Summary of Physico-Chemical Properties
Soap and Detergent Association - Supplemental Study

CAS #	Name	Molecular Weight	Vapor Pressure (mm Hg)	Henry's Constant (atm-m3/M)	Liquid Diffusivity (cm2/s)	Gas Diffusivity (cm2/s)	Half Saturation Biorate Conc. (g/m^3)	WATER7 Biorate Const. (mg/g-hr)	Maximum Biorate Const. (g/g-s)	Reference
64175	Ethanol	46.07	40	6.29E-06	1.30E-05	0.123	9.78	8.8	2.44E-06	See Line-by-line references in MODEL.XLS
67630	Isopropanol	60.1	32	8.07E-06	9.90E-06	0.12	200.00	15.00	4.17E-06	
111762	Butoxyethanol (Ethylene glycol monobutyl ether)	118.18	0.88	2.08E-08	6.60E-06	0.09	**9.78**	**8.80**	2.44E-06	
141435	Ethanolamine	61.09	0.4	3.20E-07	1.20E-05	0.11	223.00	9.70	2.69E-06	
110805	Ethoxy Ethanol (Ethylene glycol monoethyl ether)	90	5.4	6.89E-06	8.16E-06	0.10	**9.78**	**8.80**	2.44E-06	
67561	Methanol	32	114	5.19E-06	1.64E-05	0.15	90.00	18.00	5.00E-06	
	Pine Oil (Terpineol)	154	<1	3.55E-07	6.15E-06	0.06	**9.78**	**8.80**	2.44E-06	
	D-Limonene	136.23	1.92	**3.00E-07**	5.11E-06	0.07	**9.78**	**8.80**	2.44E-06	
75310	Monoisopropylamine	59.11	569.6	1.12E-05	9.70E-06	0.12	**9.78**	**8.80**	2.44E-06	
64197	Acetic Acid	60.05	15.4	5.58E-06	1.20E-05	0.11	14.00	14.00	3.89E-06	
34950948	Dipropylene Glycol Methyl Ether	148.23	0.01	**1.00E-07**	**5.00E-06**	**0.10**	**9.78**	**8.80**	2.44E-06	
110918	Morpholine	87.12	10	5.73E-05	9.60E-06	0.09	291.00	9.70	2.69E-06	

Note: Values shown in italics are assumed based on similarity with other compounds in the study.

Note: Values shown in bold are conservatively assumed to be equal to the lowest biological rate values observed from the other compounds.

Table 2											
Modeling of VOC Fate in WWTPs											
Soap and Detergent Association - Supplemental Study											
		Ethanol		**Isopropanol**		**Butoxyethanol**		**Ethanolamine**		**Ethoxyethanol**	
Process	**Variable**	**Value**	**Ref #**	**Value**	**Ref #**	**Value**	**Ref #**	**Value**	**Ref #**	**Value**	**Ref #**
Basic Physical/Chemical Constants											
	Dw, Diffusivity in Water, cm^2/sec	1.30E-05	8	9.90E-06	13	6.60E-06	13	1.20E-05	8	8.16E-06	8
	Da, Diffusivity in Air, cm^2/sec	0.123	8	0.12	13	0.09	13	0.11	8	0.10	8
	Do2w, Diffusivity in Water of Oxygen, cm^2/sec	2.40E-05	7	2.40E-05	7	2.40E-05	7	2.40E-05	7	2.40E-05	7
	Dether, Diffusivity in Water of Ether, cm^2/sec	8.50E-06	7	8.50E-06	7	8.50E-06	7	8.50E-06	7	8.50E-06	7
	H, Henry's Law Constant, atm-m^3/gmol	6.29E-06	14	8.07E-06	16	2.08E-08	8	3.20E-07	8	6.89E-06	8
	R, Universal Gas Constant, atm-m^3/gmol-K	8.21E-05	7	8.21E-05	7	8.21E-05	7	8.21E-05	7	8.21E-05	7
	pl, Density (liquid), g/cm^3	1		1		1		1		1	
	ul, Viscosity (liquid), g/cm-s	8.93E-03	10	8.93E-03	10	8.93E-03	10	8.93E-03	10	8.93E-03	10
	pa, Density (air), g/cm^3	1.20E-03	10	1.20E-03	10	1.20E-03	10	1.20E-03	10	1.20E-03	10
	ua, Viscosity (air), g/cm-s	1.81E-04	10	1.81E-04	10	1.81E-04	10	1.81E-04	10	1.81E-04	10
	T, Temperature (liquid), K	298	10	298	10	298	10	298	10	298	10
	T, Temperature (liquid), C	25	10	25	10	25	10	25	10	25	10
	MW, Molecular Weight, g/gmol	46.07	8	60.1	15	118.18	8	61.09	8	90	8
	Scg, Schmidt Number (gas) (Scg=ua/(pa*Da)	1.23	3	1.26	3	1.77	3	1.33	3	1.49	3
	Scl, Schmidt Number (liquid) (Scl=ul/(pl*Dw)	686.92	3	902.02	3	1354.06	3	744.17	3	1094.50	3
	Q, Total Flow Rate, mgd	32	1	32	1	32	1	32	1	32	1
	Q, Total Flow Rate, m^3/sec	1.40	1	1.40	1	1.40	1	1.40	1	1.40	1
	bi, Biomass Concentration, g/m^3	4000	2	4000	2	4000	2	4000	2	4000	2
	Ks, Half Saturation Biorate Concentration, g/m^3	**9.78**	**8**	**200.00**	**8**	**9.78**	**Calc'd**	**223.00**	**8**	**9.78**	**Calc'd**
	Kmax, Maximum Biorate Constant, g/g-s	**2.44E-06**	**8**	**4.17E-06**	**20**	**2.44E-06**	**Calc'd**	**2.69E-06**	**20**	**2.44E-06**	**Calc'd**

Table 2											
Modeling of VOC Fate in WWTPs											
Soap and Detergent Association - Supplemental Study											
		Ethanol		**Isopropanol**		**Butoxyethanol**		**Ethanolamine**		**Ethoxyethanol**	
Process	**Variable**	**Value**	**Ref #**	**Value**	**Ref #**	**Value**	**Ref #**	**Value**	**Ref #**	**Value**	**Ref #**
Lift Station	A, Surface Area, m^2	94.67	1	94.67	1	94.67	1	94.67	1	94.67	1
	D, Depth, m	5.54	1	5.54	1	5.54	1	5.54	1	5.54	1
	V, Volume, m^3	524.35	1	524.35	1	524.35	1	524.35	1	524.35	1
	De, Effective Diameter, m (De=(4*A/PI)^0.5)	10.98	3	10.98	3	10.98	3	10.98	3	10.98	3
	Ci, Influent Concentration, g/m^3	2.31		2.31		2.31		2.31		2.31	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	0.4		0.4		0.4		0.4		0.4	
	POWR, Aerator Power, hp	13.82	10	13.82	10	13.82	10	13.82	10	13.82	10
	J, Aerator Oxygen Transfer Rate, lb/hp-hr	3	10	3	10	3	10	3	10	3	10
	Ot, Oxygen Transfer Coefficient	0.83	10	0.83	10	0.83	10	0.83	10	0.83	10
	Vav, Aerator Turbulent Surface Area, m^2	94.67	2	94.67	2	94.67	2	94.67	2	94.67	2
	Kg, Gas Phase Mass Transfer Coefficient, m/s	0.0015806	3	0.00155467	3	0.00123647	3	0.0014933	3	0.0013851	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)										
	Kl, Liquid Phase Mass Transfer Coefficient, m/s	0.11	3	0.13	3	0.21	3	0.15	3	0.18	3
	(Kl=(8.22E-9*J*POWR*1.024^(T-20)*Ot*1E6*MW/(Vav*pl))*(Dw/Do2w)^0.5										
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	2.57E-04	3	3.30E-04	3	8.50E-07	3	1.31E-05	3	2.82E-04	3
	K, Overall Mass Transfer Coefficient, m/sec	4.06E-07	3	5.13E-07	3	1.05E-09	3	1.95E-08	3	3.90E-07	3
	(1/K = 1/Kl + 1/(Kg * Keq))										
	Co, Effluent Concentration, g/m^3 (Co=Q*Ci/(K*A+Q))	2.31	3	2.31	3	2.31	3	2.31	3	2.31	3
	E, Emission Rate, g/yr (E=K*A*Co*86400*365)	2802.54	3	3536.60	3	7.25	3	134.71	3	2690.17	3
	EF, Emission Factor, g/g (EF=E/(Ci*Q*82400*365))	2.88E-05		3.63E-05		7.44E-08		1.38E-06		2.76E-05	

Table 2

Modeling of VOC Fate in WWTPs

Soap and Detergent Association - Supplemental Study

Process	Variable	Ethanol		Isopropanol		Butoxyethanol		Ethanolamine		Ethoxyethanol	
		Value	Ref #	Value	Ref #	Value	Ref #	Value	Ref #	Value	Ref #
Barscreen	A, Surface Area, m^2	3.79	1	3.79	1	3.79	1	3.79	1	3.79	1
	D, Depth, m	1.08		1.08		1.08		1.08		1.08	
	V, Volume, m^3	4.08	1	4.08	1	4.08	1	4.08	1	4.08	1
	De, Effective Diameter, m (De=(4*A/PI)^0.5)	2.20	3	2.20	3	2.20	3	2.20	3	2.20	3
	Ci, Influent Concentration, g/m^3	2.31		2.31		2.31		2.31		2.31	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	0.4		0.4		0.4		0.4		0.4	
	b, Escape Coefficient, m^-1	0.1	11	0.1	11	0.1	11	0.1	11	0.1	11
	theta, Detention time, hr	1.03E-04	11	1.03E-04	11	1.03E-04	11	1.03E-04	11	1.03E-04	11
	z, Headloss through Screen, m	0.135	11	0.135	11	0.135	11	0.135	11	0.135	11
	n, Diffusivity Ratio Exponent	0.75	11	0.75	11	0.75	11	0.75	11	0.75	11
	vel, Liquid Velocity, ft/sec (vel=Q*D/V)	2.52	10	2.52	10	2.52	10	2.52	10	2.52	10
	Kg, Gas Phase Mass Transfer Coefficient, m/s	0.00188673	3	0.00185577	3	0.00147595	3	0.00178252	3	0.00165336	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)										
	Kl, Liquid Phase Mass Transfer Coefficient, m/s		5		5		5		5		5
	Kla=((b*z)/theta)*(Dw/Do2w)^n	82.934194		67.6086883		49.8525312		78.1019808		58.479522	
	Kl=Kla/D/3600	0.02139176		0.01743875		0.01285879		0.02014535		0.015084	
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	2.57E-04	3	3.30E-04	3	8.50E-07	3	1.31E-05	3	2.82E-04	3
	K, Overall Mass Transfer Coefficient, m/sec	4.85E-07	3	6.12E-07	3	1.25E-09	3	2.33E-08	3	4.66E-07	3
	(1/K = 1/Kl + 1/(Kg * Keq))										
	Co, Effluent Concentration, g/m^3 (Co=Q*Ci/(K*A+Q))	2.31	3	2.31	3	2.31	3	2.31	3	2.31	3
	E, Emission Rate, g/yr (E=K*A*Co*86400*365)	133.81	3	168.86	3	0.35	3	6.43	3	128.44	3
	EF, Emission Factor, g/g (EF=E/(Ci*Q*82400*365))	1.3738E-06		1.7336E-06		3.5539E-09		6.6032E-08		1.3187E-06	

Table 2											
Modeling of VOC Fate in WWTPs											
Soap and Detergent Association - Supplemental Study											
		Ethanol		**Isopropanol**		**Butoxyethanol**		**Ethanolamine**		**Ethoxyethanol**	
Process	**Variable**	**Value**	**Ref #**	**Value**	**Ref #**	**Value**	**Ref #**	**Value**	**Ref #**	**Value**	**Ref #**
Grit Chamber	N, Number of Tanks	4	1	4	1	4	1	4	1	4	1
	Qa, Diffused Air Flow Rate, m^3/sec	0.11	1	0.11	1	0.11	1	0.11	1	0.11	1
	A, Surface Area, m^2	426.04	1	426.04	1	426.04	1	426.04	1	426.04	1
	D, Depth, m	2.31	1	2.31	1	2.31	1	2.31	1	2.31	1
	V, Volume, m^3	983.16	1	983.16	1	983.16	1	983.16	1	983.16	1
	De, Effective Diameter, m (De=(4*A/PI)^0.5)	11.65	3	11.65	3	11.65	3	11.65	3	11.65	3
	Ci, Influent Concentration, g/m^3	2.31		2.31		2.31		2.31		2.31	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	4.47	2	4.47	2	4.47	2	4.47	2	4.47	2
	Us, Surface Velocty, m/sec (U*=0.01*U*(6.1+0.63*U)^0.5)	0.13	3	0.13	3	0.13	3	0.13	3	0.13	3
	HRT, Hydraulic Residence Time, sec	701.25		701.25		701.25		701.25		701.25	
	Kg, Gas Phase Mass Transfer Coefficient, m/s	1.03E-02	3	1.01E-02	3	8.07E-03	3	9.75E-03	3	9.04E-03	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)										
	Kl, Liquid Phase Mass Transfer Coefficient, m/s	7.54E-06	3	6.71E-06	3	5.66E-06	3	7.29E-06	3	6.18E-06	3
	(Kl=1E-6+144E-4*Us^2.2*Scl^-0.5)										
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	2.57E-04	3	3.30E-04	3	8.50E-07	3	1.31E-05	3	2.82E-04	3
	K, Overall Mass Transfer Coefficient, m/sec	1.96E-06	3	2.23E-06	3	6.85E-09	3	1.25E-07	3	1.80E-06	3
	(1/K = 1/Kl + 1/(Kg * Keq))										
	E, Emission Rate, g/yr	63011.78	3	72009.24	3	219.81	3	3998.11	3	58289.19	3
	E=(K*A+Qa*Keq)*Q*Ca/(K*A+Q+Qa*Keq)*86400*365										
	EF, Emission Factor, g/g (EF=E/(Ci*Q*82400*365))	6.47E-04		7.39E-04		2.26E-06		4.10E-05		5.98E-04	
	Co, Effluent Concentration, g/m^3	2.3099	3	2.3098	3	2.3100	3	2.3100	3	2.3099	3
	Co=Ci-E/(Q*82400*365)										

Table 2
Modeling of VOC Fate in WWTPs
Soap and Detergent Association - Supplemental Study

		Ethanol		Isopropanol		Butoxyethanol		Ethanolamine		Ethoxyethanol	
Process	Variable	Value	Ref #	Value	Ref #	Value	Ref #	Value	Ref #	Value	Ref #
Primary Clarifier-	N, Number of Tanks	6	1	6	1	6	1	6	1	6	1
Quiescent	A, Surface Area, m^2	4459.17	1	4459.17	1	4459.17	1	4459.17	1	4459.17	1
	D, Depth, m	4.31	1	4.31	1	4.31	1	4.31	1	4.31	1
	V, Volume, m^3	19208.74	1	19208.74	1	19208.74	1	19208.74	1	19208.74	1
	De, Effective Diameter, m (De=(4*A/PI)^0.5)	30.77	3	30.77	3	30.77	3	30.77	3	30.77	3
	Cl, Influent Concentration, g/m^3	2.31		2.31		2.31		2.31		2.31	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	4.47	2	4.47	2	4.47	2	4.47	2	4.47	2
	Kg, Gas Phase Mass Transfer Coefficient, m/s (Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)	9.27E-03	3	9.12E-03	3	7.25E-03	3	8.76E-03	3	8.13E-03	3
	Kl, Liquid Phase Mass Transfer Coefficient, m/s (Kl=2.611E-7*(U^2*(Dw/Dether)^0.67	6.94E-06	3	5.78E-06	3	4.40E-06	3	6.57E-06	3	5.08E-06	3
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	2.57E-04	3	3.30E-04	3	8.50E-07	3	1.31E-05	3	2.82E-04	3
	K, Overall Mass Transfer Coefficient, m/sec (1/K = 1/Kl + 1/(Kg * Keq))	1.77E-06	3	1.98E-06	3	6.16E-09	3	1.13E-07	3	1.58E-06	3
	Co, Effluent Concentration, g/m^3 (Co=Q*Cl/(K*A+Q))	2.2969	3	2.2954	3	2.3100	3	2.3092	3	2.2983	3
	E, Emission Rate, g/yr (E=K*A*Co*86400*365)	573068.16	3	638623.33	3	2000.60	3	36573.26	3	509806.02	3
	EF, Emission Factor, g/g (EF=E/(Cl*Q*82400*365))	5.88E-03		6.56E-03		2.05E-05		3.75E-04		5.23E-03	

Table 2

Modeling of VOC Fate in WWTPs

Soap and Detergent Association - Supplemental Study

Process	Variable	Ethanol Value	Ethanol Ref #	Isopropanol Value	Isopropanol Ref #	Butoxyethanol Value	Butoxyethanol Ref #	Ethanolamine Value	Ethanolamine Ref #	Ethoxyethanol Value	Ethoxyethanol Ref #
Primary Clarifier-Weir	N, Number of Tanks	6	1	6	1	6	1	6	1	6	1
	D, Depth, m	4.31	1	4.31	1	4.31	1	4.31	1	4.31	1
	V, Volume, m^3	1499.78	1	1499.78	1	1499.78	1	1499.78	1	1499.78	1
	Ci, Influent Concentration, g/m^3	2.2969		2.2954		2.3100		2.3092		2.2983	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	4.47	2	4.47	2	4.47	2	4.47	2	4.47	2
	De, Effective Diameter, m	0.60		0.60		0.60		0.60		0.60	
	Z, Weir Height, m	0.60	1	0.60	1	0.60	1	0.60	1	0.60	1
	qi, Discharge per meter of Weir Width, m^2/sec	2.42E-03	1	2.42E-03	1	2.42E-03	1	2.42E-03	1	2.42E-03	1
	WL, Total Weir Area, m^2	348.16	1	348.16	1	348.16	1	348.16	1	348.16	1
	Di, Diameter of Clarifier, m	30.77	1	30.77	1	30.77	1	30.77	1	30.77	1
	HRT, Hydraulic Residence Time, sec	1069.74254		1069.74254		1069.74254		1069.74254		1069.74254	
	r voc, VOC Deficit Ratio	1.00001226	5	1.00001	5	1.00000737	5	1.00001155	5	1.00000865	5
	r voc=EXP(0.042*Z^0.872*(qi/3600)^0.509*(Dw/Do2w)^0.75)										
	Kg, Gas Phase Mass Transfer Coefficient, m/s	1.43E-02	3	1.41E-02	3	1.12E-02	3	1.35E-02	3	1.25E-02	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)										
	Kl, Liquid Phase Mass Transfer Coefficient, m/s	4.94E-08	5	4.03E-08	5	2.97E-08	5	4.65E-08	5	3.48E-08	5
	(Kl=(1-1/r voc)*qi/Z)										
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	2.57E-04	3	3.30E-04	3	8.50E-07	3	1.31E-05	3	2.82E-04	3
	K, Overall Mass Transfer Coefficient, m/sec	4.87E-08	3	3.99E-08	3	7.20E-09	3	3.68E-08	3	3.45E-08	3
	(1/K = 1/Kl + 1/(Kg * Keq))										
	Co, Effluent Concentration, g/m^3 (Co=Q*Ci/(K*WL+Q))	2.2969	3	2.2954	3	2.3100	3	2.3091	3	2.2983	3
	E, Emission Rate, g/yr (E=K*WL*Co*86400*365)	1228.69	3	1005.70	3	182.66	3	933.29	3	869.99	3
	EF, Emission Factor, g/g (EF=E/(Ci*Q*82400*365))	2.65E-06		2.17E-06		3.94E-07		2.02E-06		1.88E-06	

Table 2
Modeling of VOC Fate in WWTPs
Soap and Detergent Association - Supplemental Study

		Ethanol		Isopropanol		Butoxyethanol		Ethanolamine		Ethoxyethanol	
Process	Variable	Value	Ref #	Value	Ref #	Value	Ref #	Value	Ref #	Value	Ref #
Activated Sludge-Aeration	N, Number of Tanks	25	1	25	1	25	1	25	1	25	1
	Qa, Diffused Air Flow Rate, m^3/sec	3.19	1	3.19	1	3.19	1	3.19	1	3.19	1
	A, Surface Area, m^2	35502.96	1	35502.96	1	35502.96	1	35502.96	1	35502.96	1
	D, Depth, m	4.62	1	4.62	1	4.62	1	4.62	1	4.62	1
	V, Volume, m^3	163859.81	1	163859.81	1	163859.81	1	163859.81	1	163859.81	1
	De, Effective Diameter, m (De=(4*A/PI)^0.5)	42.53	3	42.53	3	42.53	3	42.53	3	42.53	3
	Ci, Influent Concentration, g/m^3	2.30		2.30		2.31		2.31		2.30	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	4.47	2	4.47	2	4.47	2	4.47	2	4.47	2
	F/D, Fetch to Depth Ratio	108.33		108.33		108.33		108.33		108.33	
	HRT, Hydraulic Residence Time, sec	27309.97		27309.97		27309.97		27309.97		27309.97	
	Kg, Gas Phase Mass Transfer Coefficient, m/s	8.95E-03	3	8.80E-03	3	7.00E-03	3	8.45E-03	3	7.84E-03	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)										
	Kl, Liquid Phase Mass Transfer Coefficient, m/s	6.94E-06	3	5.78E-06	3	4.40E-06	3	6.57E-06	3	5.08E-06	3
	(Kl=2.611E-7*(U^2*(Dw/Dether)^0.67										
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	2.57E-04	3	3.30E-04	3	8.50E-07	3	1.31E-05	3	2.82E-04	3
	K, Overall Mass Transfer Coefficient, m/sec	1.73E-06	3	1.93E-06	3	5.94E-09	3	1.09E-07	3	1.54E-06	3
	(1/K = 1/Kl + 1/(Kg * Keq))										
	VOC Biodegradation Rate Coefficients										
	a=(K*A+Qa*Keq)/Q+1	1.04	12	1.05	12	1.00	12	1.00	12	1.04	12
	b=Ks*((K*A+Qa*Keq)/Q+1))+(V/Q)*Kmax*bl-Ca	1150.92	12	2157.86	12	1152.56	12	1483.28	12	1152.95	12
	c=-Ks*Ci	-22.46	12	-459.08	12	-22.59	12	-514.94	12	-22.48	12
	Co, Effluent Concentration, g/m^3	0.0213		0.2344		0.0196		0.3490		0.0211	
	Co=(-b+(b^2-4*a*c)^0.5/2*a										
	E, Emission Rate(w/o biodegradation), g/yr	39791.17		491032.76		126.03		40966.87		35191.67	
	E=K*A*Co+Qa*Keq*Co										
	EF, Emission Factor, g/g (EF=E/(Ci*Q*82400*365))	4.09E-04		5.04E-03		1.29E-06		4.21E-04		3.61E-04	

Table 2
Modeling of VOC Fate in WWTPs
Soap and Detergent Association - Supplemental Study

		Ethanol		Isopropanol		Butoxyethanol		Ethanolamine		Ethoxyethanol	
Process	Variable	Value	Ref #	Value	Ref #	Value	Ref #	Value	Ref #	Value	Ref #
Activated Sludge-Weir	N, Number of Tanks	25	1	25	1	25	1	25	1	25	1
	Ci, Influent Concentration, g/m^3	0.0213	1	0.2344	1	0.0196	1	0.3490	1	0.0211	1
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	4.47	2	4.47	2	4.47	2	4.47	2	4.47	2
	De, Effective Diameter, m	0.62		0.62		0.62		0.62		0.62	
	Z, Weir Height, m	0.62	1	0.62	1	0.62	1	0.62	1	0.62	1
	qi, Discharge per meter of Weir Width, m^2/sec	6.08E-03		6.08E-03		6.08E-03		6.08E-03		6.08E-03	
	WL, Total Weir Area, m^2	142.01	1	142.01	1	142.01	1	142.01	1	142.01	1
	r voc, VOC Deficit Ratio	1.0000	5	1.0000	5	1.0000	5	1.0000	5	1.0000	5
	r voc=EXP(0.042*Z^0.872*(qi/3600)^0.509*(Dw/Do2w)^0.75)										
	Kg, Gas Phase Mass Transfer Coefficient, m/s	1.43E-02	3	1.40E-02	3	1.12E-02	3	1.35E-02	3	1.25E-02	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)										
	Kl, Liquid Phase Mass Transfer Coefficient, m/s	1.98E-07	5	1.61E-07	5	1.19E-07	5	1.86E-07	5	1.39E-07	5
	(Kl=(1-1/r voc)*qi/Z)										
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	2.57E-04	3	3.30E-04	3	8.50E-07	3	1.31E-05	3	2.82E-04	3
	K, Overall Mass Transfer Coefficient, m/sec	1.87E-07	3	1.56E-07	3	8.78E-09	3	9.05E-08	3	1.34E-07	3
	(1/K = 1/Kl + 1/(Kg * Keq))										
	Co, Effluent Concentration, g/m^3 (Co=Q*Ci/(K*WL+Q))	0.0213	3	0.2344	3	0.0196	3	0.3490	3	0.0211	3
	E, Emission Rate, g/yr (E=K*WL*Co*86400*365)	17.87	3	163.40	3	0.77	3	141.47	3	12.65	3
	EF, Emission Factor, g/g (EF=E/(Ci*Q*82400*365))	1.83E-07		1.68E-06		7.92E-09		1.45E-06		1.30E-07	

Table 2
Modeling of VOC Fate in WWTPs
Soap and Detergent Association - Supplemental Study

Process	Variable	Ethanol Value	Ethanol Ref #	Isopropanol Value	Isopropanol Ref #	Butoxyethanol Value	Butoxyethanol Ref #	Ethanolamine Value	Ethanolamine Ref #	Ethoxyethanol Value	Ethoxyethanol Ref #
Secondary Clar.	N, Number of Tanks	25	1	25	1	25	1	25	1	25	1
Quiescent	A, Surface Area, m^2	15049.70	1	15049.70	1	15049.70	1	15049.70	1	15049.70	1
	D, Depth, m	4.62	1	4.62	1	4.62	1	4.62	1	4.62	1
	V, Volume, m^3	69460.17	1	69460.17	1	69460.17	1	69460.17	1	69460.17	1
	De, Effective Diameter, m (De=(4*A/PI)^0.5)	27.69	3	27.69	3	27.69	3	27.69	3	27.69	3
	Ci, Influent Concentration, g/m^3	0.0213		0.2344		0.0196		0.3490		0.0211	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	4.47	2	4.47	2	4.47	2	4.47	2	4.47	2
	Kg, Gas Phase Mass Transfer Coefficient, m/s (Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)	9.38E-03	3	9.23E-03	3	7.34E-03	3	8.86E-03	3	8.22E-03	3
	Kl, Liquid Phase Mass Transfer Coefficient, m/s (Kl=2.611E-7*(U^2*(Dw/Dether)^0.67))	6.94E-06	3	5.78E-06	3	4.40E-06	3	6.57E-06	3	5.08E-06	3
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	2.57E-04	3	3.30E-04	3	8.50E-07	3	1.31E-05	3	2.82E-04	3
	K, Overall Mass Transfer Coefficient, m/sec (1/K = 1/Kl + 1/(Kg * Keq))	1.79E-06	3	1.99E-06	3	6.23E-09	3	1.14E-07	3	1.59E-06	3
	Co, Effluent Concentration, g/m^3 (Co=Q*Ci/(K*A+Q))	0.0209	3	0.2295	3	0.0196	3	0.3486	3	0.0207	3
	E, Emission Rate, g/yr (E=K*A*Co*86400*365)	17738.08	3	217116.45	3	57.97	3	18846.89	3	15633.03	3
	EF, Emission Factor, g/g (EF=E/(Ci*Q*82400*365))	1.82E-04		2.23E-03		5.95E-07		1.93E-04		1.60E-04	

Table 2											
Modeling of VOC Fate in WWTPs											
Soap and Detergent Association - Supplemental Study											
		Ethanol		**Isopropanol**		**Butoxyethanol**		**Ethanolamine**		**Ethoxyethanol**	
Process	**Variable**	**Value**	**Ref #**	**Value**	**Ref #**	**Value**	**Ref #**	**Value**	**Ref #**	**Value**	**Ref #**
Secondary Clar.	N, Number of Tanks	25	1	25	1	25	1	25	1	25	1
Weir	D, Depth, m	4.62	1	4.62	1	4.62	1	4.62	1	4.62	1
	Cl, Influent Concentration, g/m^3	0.0209		0.2295		0.0196		0.3486		0.0207	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	4.47	2	4.47	2	4.47	2	4.47	2	4.47	2
	De, Effective Diameter, m	30.77	3	30.77	3	30.77	3	30.77	3	30.77	3
	Z, Weir Height, m	0.60	1	0.60	1	0.60	1	0.60	1	0.60	1
	qi, Discharge per meter of Weir Width, m^2/sec	5.80E-04	1	5.80E-04	1	5.80E-04	1	5.80E-04	1	5.80E-04	1
	WL, Total Weir Area, m^2	1450.68	1	1450.68	1	1450.68	1	1450.68	1	1450.68	1
	Dl, Diameter of Clarifier, m	30.77	1	30.77	1	30.77	1	30.77	1	30.77	1
	r voc, VOC Deficit Ratio	1.0000000	5	1.0000000	5	1.0000001	5	1.0000000	5	1.0000000	5
	r voc=EXP(0.042*Z^0.872*(qi/3600)^0.509*(Dw/Do2w)^0.75)										
	Kg, Gas Phase Mass Transfer Coefficient, m/s	9.27E-03	3	9.12E-03	3	7.25E-03	3	8.76E-03	3	8.13E-03	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)										
	Kl, Liquid Phase Mass Transfer Coefficient, m/s	8.13E-13	5	7.49E-13	5	5.69E-11	5	6.43E-12	5	8.88E-13	5
	(Kl=(1-1/r voc)*qi/Z)										
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	2.57E-04	3	3.30E-04	3	8.50E-07	3	1.31E-05	3	2.82E-04	3
	K, Overall Mass Transfer Coefficient, m/sec	8.13E-13	3	7.49E-13	3	5.63E-11	3	6.43E-12	3	8.88E-13	3
	(1/K = 1/Kl + 1/(Kg * Keq))										
	Co, Effluent Concentration, g/m^3 (Co=Q*Cl/(K*WL+Q))	0.0209	3	0.2295	3	0.0196	3	0.3486	3	0.0207	3
	E, Emission Rate, g/yr (E=K*WL*Co*86400*365)	7.77E-04	3	7.87E-03	3	5.05E-02	3	1.03E-01	3	8.42E-04	3
	EF, Emission Factor, g/g (EF=E/(Cl*Q*82400*365))	7.98E-12		8.08E-11		5.19E-10		1.05E-09		8.64E-12	

Table 2											
Modeling of VOC Fate in WWTPs											
Soap and Detergent Association - Supplemental Study											
		Methanol		**Pine Oil (terpineol)**		**D-Limonene**		**Isopropylamine**		**Acetic Acid**	
Process	**Variable**	**Value**	**Ref #**	**Value**	**Ref #**	**Value**	**Ref #**	**Value**	**Ref #**	**Value**	**Ref #**
Lift Station	A, Surface Area, m^2	94.67	1	94.67	1	94.67	1	94.67	1	94.67	1
	D, Depth, m	5.54	1	5.54	1	5.54	1	5.54	1	5.54	1
	V, Volume, m^3	524.35	1	524.35	1	524.35	1	524.35	1	524.35	1
	De, Effective Diameter, m (De=(4*A/Pi)^0.5)	10.98	3	10.98	3	10.98	3	10.98	3	10.98	3
	Ci, Influent Concentration, g/m^3	2.31		2.31		2.31		2.31		2.31	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	0.4		0.4		0.4		0.4		0.4	
	POWR, Aerator Power, hp	13.82	10	13.82	10	13.82	10	13.82	10	13.82	10
	J, Aerator Oxygen Transfer Rate, lb/hp-hr	3	10	3	10	3	10	3	10	3	10
	Ot, Oxygen Transfer Coefficient	0.83	10	0.83	10	0.83	10	0.83	10	0.83	10
	Vav, Aerator Turbulent Surface Area, m^2	94.67	2	94.67	2	94.67	2	94.67	2	94.67	2
	Kg, Gas Phase Mass Transfer Coefficient, m/s	0.00180537	3	0.000955174	3	0.00107408	3	0.00154597	3	0.0014933	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)										
	Kl, Liquid Phase Mass Transfer Coefficient, m/s	0.09	3	0.26	3	0.21	3	0.13	3	0.14	3
	(Kl=(8.22E-9*J*POWR*1.024^(T-20)*Ot*1E6*MW/(Vav*pl))										
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	2.12E-04	3	1.45E-05	3	1.23E-05	3	4.58E-04	3	4.58E-04	3
	K, Overall Mass Transfer Coefficient, m/sec	3.83E-07	3	1.39E-08	3	1.32E-08	3	7.08E-07	3	6.84E-07	3
	(1/K = 1/Kl + 1/(Kg * Keq))										
	Co, Effluent Concentration, g/m^3 (Co=Q*Ci/(K*A+Q))	2.31	3	2.31	3	2.31	3	2.31	3	2.31	3
	E, Emission Rate, g/yr (E=K*A*Co*86400*365)	2641.27	3	95.59	3	90.83	3	4880.78	3	4714.51	3
	EF, Emission Factor, g/g (EF=E/(Ci*Q*82400*365))	2.71E-05		9.81E-07		9.33E-07		5.01E-05		4.84E-05	

Table 2											
Modeling of VOC Fate in WWTPs											
Soap and Detergent Association - Supplemental Study											
		Methanol		**Pine Oil (terpineol)**		**D-Limonene**		**Isopropylamine**		**Acetic Acid**	
Process	**Variable**	**Value**	**Ref #**	**Value**	**Ref #**	**Value**	**Ref #**	**Value**	**Ref #**	**Value**	**Ref #**
Barscreen	A, Surface Area, m^2	3.79	1	3.79	1	3.79	1	3.79	1	3.79	1
	D, Depth, m	1.08		1.08		1.08		1.08		1.08	
	V, Volume, m^3	4.08	1	4.08	1	4.08	1	4.08	1	4.08	1
	De, Effective Diameter, m (De=(4*A/PI)^0.5)	2.20	3	2.20	3	2.20	3	2.20	3	2.20	3
	Ci, Influent Concentration, g/m^3	2.31		2.31		2.31		2.31		2.31	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	0.4		0.4		0.4		0.4		0.4	
	b, Escape Coefficient, m^-1	0.1	11	0.1	11	0.1	11	0.1	11	0.1	11
	theta, Detention time, hr	1.03E-04	11	1.03E-04	11	1.03E-04	11	1.03E-04	11	1.03E-04	11
	z, Headloss through Screen, m	0.135	11	0.135	11	0.135	11	0.135	11	0.135	11
	n, Diffusivity Ratio Exponent	0.75	11	0.75	11	0.75	11	0.75	11	0.75	11
	vel, Liquid Velocity, ft/sec (vel=Q*D/V)	2.52	10	2.52	10	2.52	10	2.52	10	2.52	10
	Kg, Gas Phase Mass Transfer Coefficient, m/s	0.00215503	3	0.001140169	3	0.0012821	3	0.00184539	3	0.00178252	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)										
	Kl, Liquid Phase Mass Transfer Coefficient, m/s		5		5		5		5		5
	Kla=((b*z)/theta)*(Dw/Do2w)^n	98.7208759		47.30776717		41.1891622		66.5817054		78.1019808	
	Kl=Kla/D/3600	0.02546372		0.0122024		0.01062419		0.01717385		0.02014535	
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	2.12E-04	3	1.45E-05	3	1.23E-05	3	4.58E-04	3	4.58E-04	3
	K, Overall Mass Transfer Coefficient, m/sec	4.57E-07	3	1.65E-08	3	1.57E-08	3	8.45E-07	3	8.16E-07	3
	(1/K = 1/Kl + 1/(Kg * Keq))										
	Co, Effluent Concentration, g/m^3 (Co=Q*Ci/(K*A+Q))	2.31	3	2.31	3	2.31	3	2.31	3	2.31	3
	E, Emission Rate, g/yr (E=K*A*Co*86400*365)	126.11	3	4.56	3	4.34	3	233.03	3	225.10	3
	EF, Emission Factor, g/g (EF=E/(Ci*Q*82400*365))	1.2947E-06		4.68563E-08		4.4526E-08		2.3924E-06		2.3109E-06	

Table 2
Modeling of VOC Fate in WWTPs
Soap and Detergent Association - Supplemental Study

		Methanol		Pine Oil (terpineol)		D-Limonene		Isopropylamine		Acetic Acid	
Process	Variable	Value	Ref #	Value	Ref #	Value	Ref #	Value	Ref #	Value	Ref #
Primary Clarifier-	N, Number of Tanks	6	1	6	1	6	1	6	1	6	1
Quiescent	A, Surface Area, m^2	4459.17	1	4459.17	1	4459.17	1	4459.17	1	4459.17	1
	D, Depth, m	4.31	1	4.31	1	4.31	1	4.31	1	4.31	1
	V, Volume, m^3	19208.74	1	19208.74	1	19208.74	1	19208.74	1	19208.74	1
	De, Effective Diameter, m (De=(4*A/PI)^0.5)	30.77	3	30.77	3	30.77	3	30.77	3	30.77	3
	CI, Influent Concentration, g/m^3	2.31		2.31		2.31		2.31		2.31	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	4.47	2	4.47	2	4.47	2	4.47	2	4.47	2
	Kg, Gas Phase Mass Transfer Coefficient, m/s	1.06E-02	3	5.60E-03	3	6.30E-03	3	9.07E-03	3	8.76E-03	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)										
	Kl, Liquid Phase Mass Transfer Coefficient, m/s	8.10E-06	3	4.20E-06	3	3.71E-06	3	5.70E-06	3	6.57E-06	3
	(Kl=2.611E-7*(U^2*(Dw/Dether)^0.67										
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	2.12E-04	3	1.45E-05	3	1.23E-05	3	4.58E-04	3	4.58E-04	3
	K, Overall Mass Transfer Coefficient, m/sec	1.76E-06	3	7.98E-08	3	7.57E-08	3	2.40E-06	3	2.49E-06	3
	(1/K = 1/Kl + 1/(Kg * Keq))										
	Co, Effluent Concentration, g/m^3 (Co=Q*CI/(K*A+Q))	2.2970	3	2.3094	3	2.3094	3	2.2923	3	2.2916	3
	E, Emission Rate, g/yr (E=K*A*Co*86400*365)	568233.55	3	25906.01	3	24582.78	3	774348.19	3	802703.12	3
	EF, Emission Factor, g/g (EF=E/(CI*Q*82400*365))	5.83E-03		2.66E-04		2.52E-04		7.95E-03		8.24E-03	

Table 2

Modeling of VOC Fate in WWTPs

Soap and Detergent Association - Supplemental Study

Process	Variable	Methanol		Pine Oil (terpineol)		D-Limonene		Isopropylamine		Acetic Acid	
		Value	Ref #	Value	Ref #	Value	Ref #	Value	Ref #	Value	Ref #
Primary Clarifier-Weir	N, Number of Tanks	6	1	6	1	6	1	6	1	6	1
	D, Depth, m	4.31	1	4.31	1	4.31	1	4.31	1	4.31	1
	V, Volume, m^3	1499.78	1	1499.78	1	1499.78	1	1499.78	1	1499.78	1
	Ci, Influent Concentration, g/m^3	2.2970		2.3094		2.3094		2.2923		2.2916	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	4.47	2	4.47	2	4.47	2	4.47	2	4.47	2
	De, Effective Diameter, m	0.60		0.60		0.60		0.60		0.60	
	Z, Weir Height, m	0.60	1	0.60	1	0.60	1	0.60	1	0.60	1
	qi, Discharge per meter of Weir Width, m^2/sec	2.42E-03	1	2.42E-03	1	2.42E-03	1	2.42E-03	1	2.42E-03	1
	WL, Total Weir Area, m^2	348.16	1	348.16	1	348.16	1	348.16	1	348.16	1
	Di, Diameter of Clarifier, m	30.77	1	30.77	1	30.77	1	30.77	1	30.77	1
	HRT, Hydraulic Residence Time, sec	1069.74254		1069.742545		1069.74254		1069.74254		1069.74254	
	r voc, VOC Deficit Ratio	1.0000146	5	1.000006994	5	1.00000609	5	1.00000984	5	1.00001155	5
	r voc=EXP(0.042*Z^0.872*(qi/3600)^0.509*(Dw/Do2w)^0..										
	Kg, Gas Phase Mass Transfer Coefficient, m/s	1.63E-02	3	8.64E-03	3	9.72E-03	3	1.40E-02	3	1.35E-02	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)										
	Kl, Liquid Phase Mass Transfer Coefficient, m/s	5.88E-08	5	2.82E-08	5	2.45E-08	5	3.96E-08	5	4.65E-08	5
	(Kl=(1-1/r voc)*qi/Z)										
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	2.12E-04	3	1.45E-05	3	1.23E-05	3	4.58E-04	3	4.58E-04	3
	K, Overall Mass Transfer Coefficient, m/sec	5.78E-08	3	2.30E-08	3	2.03E-08	3	3.94E-08	3	4.62E-08	3
	(1/K = 1/Kl + 1/(Kg * Keq))										
	Co, Effluent Concentration, g/m^3 (Co=Q*Ci/(K*WL+Q))	2.2970	3	2.3094	3	2.3094	3	2.2923	3	2.2916	3
	E, Emission Rate, g/yr (E=K*WL*Co*86400*365)	1457.56	3	583.16	3	515.67	3	991.52	3	1161.22	3
	EF, Emission Factor, g/g (EF=E/(Ci*Q*82400*365))	3.15E-06		1.26E-06		1.11E-06		2.14E-06		2.51E-06	

Table 2
Modeling of VOC Fate in WWTPs
Soap and Detergent Association - Supplemental Study

Process	Variable	Methanol		Pine Oil (terpineol)		D-Limonene		Isopropylamine		Acetic Acid	
		Value	Ref #	Value	Ref #	Value	Ref #	Value	Ref #	Value	Ref #
Activated Sludge-Aeration	N, Number of Tanks	25	1	25	1	25	1	25	1	25	1
	Qa, Diffused Air Flow Rate, m^3/sec	3.19	1	3.19	1	3.19	1	3.19	1	3.19	1
	A, Surface Area, m^2	35502.96	1	35502.96	1	35502.96	1	35502.96	1	35502.96	1
	D, Depth, m	4.62	1	4.62	1	4.62	1	4.62	1	4.62	1
	V, Volume, m^3	163859.81	1	163859.81	1	163859.81	1	163859.81	1	163859.81	1
	De, Effective Diameter, m (De=(4*A/PI)^0.5)	42.53	3	42.53	3	42.53	3	42.53	3	42.53	3
	CI, Influent Concentration, g/m^3	2.30		2.31		2.31		2.29		2.29	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	4.47	2	4.47	2	4.47	2	4.47	2	4.47	2
	F/D, Fetch to Depth Ratio	108.33		108.33		108.33		108.33		108.33	
	HRT, Hydraulic Residence Time, sec	27309.97		27309.97		27309.97		27309.97		27309.97	
	Kg, Gas Phase Mass Transfer Coefficient, m/s	1.02E-02	3	5.41E-03	3	6.08E-03	3	8.75E-03	3	8.45E-03	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)										
	Kl, Liquid Phase Mass Transfer Coefficient, m/s	8.10E-06	3	4.20E-06	3	3.71E-06	3	5.70E-06	3	6.57E-06	3
	(Kl=2.611E-7*(U^2*(Dw/Dether)^0.67										
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	2.12E-04	3	1.45E-05	3	1.23E-05	3	4.58E-04	3	4.58E-04	3
	K, Overall Mass Transfer Coefficient, m/sec	1.71E-06	3	7.70E-08	3	7.31E-08	3	2.35E-06	3	2.44E-06	3
	(1/K = 1/Kl + 1/(Kg * Keq))										
	VOC Biodegradation Rate Coefficients										
	a=(K*A+Qa*Keq)/Q+1	1.04	12	1.00	12	1.00	12	1.06	12	1.06	12
	b=Ks*((K*A+Qa*Keq)/Q+1))+(V/Q)*Kmax*bi-Ca	2431.45	12	1152.58	12	1152.58	12	1828.44	12	1832.94	12
	c=-Ks*CI	-206.73	12	-22.59	12	-22.59	12	-22.42	12	-32.08	12
	Co, Effluent Concentration, g/m^3	0.0926		0.0197		0.0197		0.0138		0.0198	
	Co=(-b+(b^2-4*a*c)^0.5/2*a										
	E, Emission Rate(w/o biodegradation), g/yr	171076.03		1645.52		1558.38		35256.03		52285.78	
	E=K*A*Co+Qa*Keq*Co										
	EF, Emission Factor, g/g (EF=E/(CI*Q*82400*365))	1.76E-03		1.69E-05		1.60E-05		3.62E-04		5.37E-04	

Table 2

Modeling of VOC Fate in WWTPs

Soap and Detergent Association - Supplemental Study

Process	Variable	Methanol		Pine Oil (terpineol)		D-Limonene		Isopropylamine		Acetic Acid	
		Value	Ref #	Value	Ref #	Value	Ref #	Value	Ref #	Value	Ref #
Activated Sludge-Weir	N, Number of Tanks	25	1	25	1	25	1	25	1	25	1
	Ci, Influent Concentration, g/m^3	0.0926	1	0.0197	1	0.0197	1	0.0138	1	0.0198	1
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	4.47	2	4.47	2	4.47	2	4.47	2	4.47	2
	De, Effective Diameter, m	0.62		0.62		0.62		0.62		0.62	
	Z, Weir Height, m	0.62	1	0.62	1	0.62	1	0.62	1	0.62	1
	qi, Discharge per meter of Weir Width, m^2/sec	6.08E-03		6.08E-03		6.08E-03		6.08E-03		6.08E-03	
	WL, Total Weir Area, m^2	142.01	1	142.01	1	142.01	1	142.01	1	142.01	1
	r voc, VOC Deficit Ratio	1.0000	5	1.0000	5	1.0000	5	1.0000	5	1.0000	5
	r voc=EXP(0.042*Z^0.872*(qi/3600)^0.509*(Dw/Do2w)^0.:										
	Kg, Gas Phase Mass Transfer Coefficient, m/s	1.63E-02	3	8.62E-03	3	9.69E-03	3	1.39E-02	3	1.35E-02	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)										
	Kl, Liquid Phase Mass Transfer Coefficient, m/s	2.35E-07	5	1.13E-07	5	9.81E-08	5	1.59E-07	5	1.86E-07	5
	(Kl=(1-1/r voc)*qi/Z)										
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	2.12E-04	3	1.45E-05	3	1.23E-05	3	4.58E-04	3	4.58E-04	3
	K, Overall Mass Transfer Coefficient, m/sec	2.20E-07	3	5.93E-08	3	5.37E-08	3	1.55E-07	3	1.81E-07	3
	(1/K = 1/Kl + 1/(Kg * Keq))										
	Co, Effluent Concentration, g/m^3 (Co=Q*Ci/(K*WL+Q))	0.0926	3	0.0197	3	0.0197	3	0.0138	3	0.0198	3
	E, Emission Rate, g/yr (E=K*WL*Co*86400*365)	91.35	3	5.22	3	4.73	3	9.56	3	15.99	3
	EF, Emission Factor, g/g (EF=E/(Ci*Q*82400*365))	9.38E-07		5.36E-08		4.86E-08		9.82E-08		1.64E-07	

Table 2

Modeling of VOC Fate in WWTPs

Soap and Detergent Association - Supplemental Study

Process	Variable	Methanol		Pine Oil (terpineol)		D-Limonene		Isopropylamine		Acetic Acid	
		Value	Ref #	Value	Ref #	Value	Ref #	Value	Ref #	Value	Ref #
Secondary Clar.	N, Number of Tanks	25	1	25	1	25	1	25	1	25	1
Quiescent	A, Surface Area, m^2	15049.70	1	15049.70	1	15049.70	1	15049.70	1	15049.70	1
	D, Depth, m	4.62	1	4.62	1	4.62	1	4.62	1	4.62	1
	V, Volume, m^3	69460.17	1	69460.17	1	69460.17	1	69460.17	1	69460.17	1
	De, Effective Diameter, m (De=(4*A/PI)^0.5)	27.69	3	27.69	3	27.69	3	27.69	3	27.69	3
	Ci, Influent Concentration, g/m^3	0.0926		0.0197		0.0197		0.0138		0.0198	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	4.47	2	4.47	2	4.47	2	4.47	2	4.47	2
	Kg, Gas Phase Mass Transfer Coefficient, m/s (Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)	1.07E-02	3	5.67E-03	3	6.38E-03	3	9.18E-03	3	8.86E-03	3
	Kl, Liquid Phase Mass Transfer Coefficient, m/s (Kl=2.611E-7*(U^2*(Dw/Dether)^0.67))	8.10E-06	3	4.20E-06	3	3.71E-06	3	5.70E-06	3	6.57E-06	3
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	2.12E-04	3	1.45E-05	3	1.23E-05	3	4.58E-04	3	4.58E-04	3
	K, Overall Mass Transfer Coefficient, m/sec (1/K = 1/Kl + 1/(Kg * Keq))	1.78E-06	3	8.07E-08	3	7.66E-08	3	2.42E-06	3	2.51E-06	3
	Co, Effluent Concentration, g/m^3 (Co=Q*Ci/(K*A+Q))	0.0909	3	0.0197	3	0.0197	3	0.0134	3	0.0192	3
	E, Emission Rate, g/yr (E=K*A*Co*86400*365)	76580.34	3	752.68	3	714.11	3	15429.44	3	22919.86	3
	EF, Emission Factor, g/g (EF=E/(Ci*Q*82400*365))	7.86E-04		7.73E-06		7.33E-06		1.58E-04		2.35E-04	

Table 2

Modeling of VOC Fate in WWTPs

Soap and Detergent Association - Supplemental Study

Process	Variable	Methanol		Pine Oil (terpineol)		D-Limonene		Isopropylamine		Acetic Acid	
		Value	Ref #	Value	Ref #	Value	Ref #	Value	Ref #	Value	Ref #
Secondary Clar.	N, Number of Tanks	25	1	25	1	25	1	25	1	25	1
Weir	D, Depth, m	4.62	1	4.62	1	4.62	1	4.62	1	4.62	1
	Ci, Influent Concentration, g/m^3	0.0909		0.0197		0.0197		0.0134		0.0192	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	4.47	2	4.47	2	4.47	2	4.47	2	4.47	2
	De, Effective Diameter, m	30.77	3	30.77	3	30.77	3	30.77	3	30.77	3
	Z, Weir Height, m	0.60	1	0.60	1	0.60	1	0.60	1	0.60	1
	qi, Discharge per meter of Weir Width, m^2/sec	5.80E-04	1	5.80E-04	1	5.80E-04	1	5.80E-04	1	5.80E-04	1
	WL, Total Weir Area, m^2	1450.68	1	1450.68	1	1450.68	1	1450.68	1	1450.68	1
	Di, Diameter of Clarifier, m	30.77	1	30.77	1	30.77	1	30.77	1	30.77	1
	r voc, VOC Deficit Ratio	1.0000000	5	1.0000000	5	1.0000000	5	1.0000000	5	1.0000000	5
	r voc=EXP(0.042*Z^0.872*(qi/3600)^0.509*(Dw/Do2w)^0.										
	Kg, Gas Phase Mass Transfer Coefficient, m/s	1.06E-02	3	5.60E-03	3	6.30E-03	3	9.07E-03	3	8.76E-03	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)										
	Kl, Liquid Phase Mass Transfer Coefficient, m/s	8.18E-13	5	8.33E-12	5	8.66E-12	5	6.48E-13	5	6.30E-13	5
	(Kl=(1-1/r voc)*ql/Z)										
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	2.12E-04	3	1.45E-05	3	1.23E-05	3	4.58E-04	3	4.58E-04	3
	K, Overall Mass Transfer Coefficient, m/sec	8.18E-13	3	8.33E-12	3	8.66E-12	3	6.48E-13	3	6.30E-13	3
	(1/K = 1/Kl + 1/(Kg * Keq))										
	Co, Effluent Concentration, g/m^3 (Co=Q*Ci/(K*WL+Q))	0.0909	3	0.0197	3	0.0197	3	0.0134	3	0.0192	3
	E, Emission Rate, g/yr (E=K*WL*Co*86400*365)	3.40E-03	3	7.49E-03	3	7.79E-03	3	3.98E-04	3	5.55E-04	3
	EF, Emission Factor, g/g (EF=E/(Ci*Q*82400*365))	3.49E-11		7.69E-11		7.99E-11		4.09E-12		5.70E-12	

Table 2					
Modeling of VOC Fate in WWTPs					
Soap and Detergent Association - Supplemental Study					
		Dipropylene Glycol Methyl Ether		**Morpholine**	
Process	**Variable**	**Value**	**Ref #**	**Value**	**Ref #**
Basic Physical/Chemical Constants					
	Dw, Diffusivity in Water, cm^2/sec	5.00E-06	Assumed	9.60E-06	8
	Da, Diffusivity in Air, cm^2/sec	0.1	Assumed	0.09	8
	Do2w, Diffusivity in Water of Oxygen, cm^2/sec	2.40E-05	7	2.40E-05	7
	Dether, Diffusivity in Water of Ether, cm^2/sec	8.50E-06	7	8.50E-06	7
	H, Henry's Law Constant, atm-m^3/gmol	1.00E-07	Assumed	5.73E-05	8
	R, Universal Gas Constant, atm-m^3/gmol-K	8.21E-05	7	8.21E-05	7
	pl, Density (liquid), g/cm^3	1		1	
	ul, Viscosity (liquid), g/cm-s	8.93E-03	10	8.93E-03	10
	pa, Density (air), g/cm^3	1.20E-03	10	1.20E-03	10
	ua, Viscosity (air), g/cm-s	1.81E-04	10	1.81E-04	10
	T, Temperature (liquid), K	298	10	298	10
	T, Temperature (liquid), C	25	10	25	10
	MW, Molecular Weight, g/gmol	148.23	18	87.12	8
	Scg, Schmidt Number (gas) (Scg=ua/(pa*Da)	1.51	3	1.66	3
	Scl, Schmidt Number (liquid) (Scl=ul/(pl*Dw)	1786.00	3	930.21	3
	Q, Total Flow Rate, mgd	32	1	32	1
	Q, Total Flow Rate, m^3/sec	1.40	1	1.40	1
	bl, Biomass Concentration, g/m^3	4000	2	4000	2
	Ks, Half Saturation Biorate Concentration, g/m^3	**9.78**	**Calc'd**	**291.00**	**8**
	Kmax, Maximum Biorate Constant, g/g-s	**2.44E-06**	**Calc'd**	**2.69E-06**	**20**

Table 2					
Modeling of VOC Fate in WWTPs					
Soap and Detergent Association - Supplemental Study					
		Dipropylene Glycol Methyl Ether		**Morpholine**	
Process	**Variable**	**Value**	**Ref #**	**Value**	**Ref #**
Lift Station	A, Surface Area, m^2	94.67	1	94.67	1
	D, Depth, m	5.54	1	5.54	1
	V, Volume, m^3	524.35	1	524.35	1
	De, Effective Diameter, m (De=(4*A/PI)^0.5)	10.98	3	10.98	3
	CI, Influent Concentration, g/m^3	2.31		2.31	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	0.4		0.4	
	POWR, Aerator Power, hp	13.82	10	13.82	10
	J, Aerator Oxygen Transfer Rate, lb/hp-hr	3	10	3	10
	Ot, Oxygen Transfer Coefficient	0.83	10	0.83	10
	Vav, Aerator Turbulent Surface Area, m^2	94.67	2	94.67	2
	Kg, Gas Phase Mass Transfer Coefficient, m/s	0.001375896	3	0.00129165	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)				
	Kl, Liquid Phase Mass Transfer Coefficient, m/s	0.23	3	0.19	3
	(Kl=(8.22E-9*J*POWR*1.024^(T-20)*Ot*1E6*MW/(Vav*pl))				
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	4.09E-06	3	2.34E-03	3
	K, Overall Mass Transfer Coefficient, m/sec	5.62E-09	3	3.03E-06	3
	(1/K = 1/Kl + 1/(Kg * Keq))				
	Co, Effluent Concentration, g/m^3 (Co=Q*CI/(K*A+Q))	2.31	3	2.31	3
	E, Emission Rate, g/yr (E=K*A*Co*86400*365)	38.79	3	20859.05	3
	EF, Emission Factor, g/g (EF=E/(CI*Q*82400*365))	3.98E-07		2.14E-04	

Table 2					
Modeling of VOC Fate in WWTPs					
Soap and Detergent Association - Supplemental Study					
		Dipropylene Glycol Methyl Ether		**Morpholine**	
Process	**Variable**	**Value**	**Ref #**	**Value**	**Ref #**
Barscreen	A, Surface Area, m^2	3.79	1	3.79	1
	D, Depth, m	1.08		1.08	
	V, Volume, m^3	4.08	1	4.08	1
	De, Effective Diameter, m (De=(4*A/Pi)^0.5)	2.20	3	2.20	3
	Ci, Influent Concentration, g/m^3	2.31		2.31	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	0.4		0.4	
	b, Escape Coefficient, m^-1	0.1	11	0.1	11
	theta, Detention time, hr	1.03E-04	11	1.03E-04	11
	z, Headloss through Screen, m	0.135	11	0.135	11
	n, Diffusivity Ratio Exponent	0.75	11	0.75	11
	vel, Liquid Velocity, ft/sec (vel=Q*D/V)	2.52	10	2.52	10
	Kg, Gas Phase Mass Transfer Coefficient, m/s	0.001642375	3	0.00154181	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)				
	Kl, Liquid Phase Mass Transfer Coefficient, m/s		5		5
	Kla=((b*z)/theta)*(Dw/Do2w)^n	40.50453187		66.0662321	
	Kl=Kla/D/3600	0.010447598		0.01704089	
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	4.09E-06	3	2.34E-03	3
	K, Overall Mass Transfer Coefficient, m/sec	6.71E-09	3	3.61E-06	3
	(1/K = 1/Kl + 1/(Kg * Keq))				
	Co, Effluent Concentration, g/m^3 (Co=Q*Ci/(K*A+Q))	2.31	3	2.31	3
	E, Emission Rate, g/yr (E=K*A*Co*86400*365)	1.85	3	995.76	3
	EF, Emission Factor, g/g (EF=E/(Ci*Q*82400*365))	1.90127E-08		1.0223E-05	

Table 2					
Modeling of VOC Fate in WWTPs					
Soap and Detergent Association - Supplemental Study					
		Dipropylene Glycol Methyl Ether		**Morpholine**	
Process	**Variable**	**Value**	**Ref #**	**Value**	**Ref #**
Grit Chamber	N, Number of Tanks	4	1	4	1
	Qa, Diffused Air Flow Rate, m^3/sec	0.11	1	0.11	1
	A, Surface Area, m^2	426.04	1	426.04	1
	D, Depth, m	2.31	1	2.31	1
	V, Volume, m^3	983.16	1	983.16	1
	De, Effective Diameter, m (De=(4*A/PI)^0.5)	11.65	3	11.65	3
	Cl, Influent Concentration, g/m^3	2.31		2.31	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	4.47	2	4.47	2
	Us, Surface Velocty, m/sec (U*=0.01*U*(6.1+0.63*U)^0.5)	0.13	3	0.13	3
	HRT, Hydraulic Residence Time, sec	701.25		701.25	
	Kg, Gas Phase Mass Transfer Coefficient, m/s	8.98E-03	3	8.43E-03	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)				
	Kl, Liquid Phase Mass Transfer Coefficient, m/s	5.06E-06	3	6.62E-06	3
	(Kl=1E-6+144E-4*Us^2.2*Scl^-0.5)				
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	4.09E-06	3	2.34E-03	3
	K, Overall Mass Transfer Coefficient, m/sec	3.65E-08	3	4.96E-06	3
	(1/K = 1/Kl + 1/(Kg * Keq))				
	E, Emission Rate, g/yr	1165.27	3	173080.62	3
	E=(K*A+Qa*Keq)*Q*Ca/(K*A+Q+Qa*Keq)*86400*365				
	EF, Emission Factor, g/g (EF=E/(Cl*Q*82400*365))	1.20E-05		1.78E-03	
	Co, Effluent Concentration, g/m^3	2.3100	3	2.3093	3
	Co=Cl-E/(Q*82400*365)				

Table 2					
Modeling of VOC Fate in WWTPs					
Soap and Detergent Association - Supplemental Study					
		Dipropylene Glycol Methyl Ether		**Morpholine**	
Process	**Variable**	**Value**	**Ref #**	**Value**	**Ref #**
Primary Clarifier-	N, Number of Tanks	6	1	6	1
Quiescent	A, Surface Area, m^2	4459.17	1	4459.17	1
	D, Depth, m	4.31	1	4.31	1
	V, Volume, m^3	19208.74	1	19208.74	1
	De, Effective Diameter, m (De=(4*A/PI)^0.5)	30.77	3	30.77	3
	Ci, Influent Concentration, g/m^3	2.31		2.31	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	4.47	2	4.47	2
	Kg, Gas Phase Mass Transfer Coefficient, m/s	8.07E-03	3	7.58E-03	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)				
	Kl, Liquid Phase Mass Transfer Coefficient, m/s	3.66E-06	3	5.66E-06	3
	(Kl=2.611E-7*(U^2*(Dw/Dether)^0.67				
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	4.09E-06	3	2.34E-03	3
	K, Overall Mass Transfer Coefficient, m/sec	3.27E-08	3	4.29E-06	3
	(1/K = 1/Kl + 1/(Kg * Keq))				
	Co, Effluent Concentration, g/m^3 (Co=Q*Ci/(K*A+Q))	2.3098	3	2.2782	3
	E, Emission Rate, g/yr (E=K*A*Co*86400*365)	10621.04	3	1374916.48	3
	EF, Emission Factor, g/g (EF=E/(Ci*Q*82400*365))	1.09E-04		1.41E-02	

Table 2					
Modeling of VOC Fate in WWTPs					
Soap and Detergent Association - Supplemental Study					
		Dipropylene Glycol Methyl Ether		**Morpholine**	
Process	**Variable**	**Value**	**Ref #**	**Value**	**Ref #**
Primary Clarifier-	N, Number of Tanks	6	1	6	1
Weir	D, Depth, m	4.31	1	4.31	1
	V, Volume, m^3	1499.78	1	1499.78	1
	Ci, Influent Concentration, g/m^3	2.3098		2.2782	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	4.47	2	4.47	2
	De, Effective Diameter, m	0.60		0.60	
	Z, Weir Height, m	0.60	1	0.60	1
	ql, Discharge per meter of Weir Width, m^2/sec	2.42E-03	1	2.42E-03	1
	WL, Total Weir Area, m^2	348.16	1	348.16	1
	Dl, Diameter of Clarifier, m	30.77	1	30.77	1
	HRT, Hydraulic Residence Time, sec	1069.742545		1069.74254	
	r voc, VOC Deficit Ratio	1.000005988	5	1.00000977	5
	r voc=EXP(0.042*Z^0.872*(ql/3600)^0.509*(Dw/Do2w)^0.:				
	Kg, Gas Phase Mass Transfer Coefficient, m/s	1.24E-02	3	1.17E-02	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)				
	Kl, Liquid Phase Mass Transfer Coefficient, m/s	2.41E-08	5	3.93E-08	5
	(Kl=(1-1/r voc)*ql/Z)				
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	4.09E-06	3	2.34E-03	3
	K, Overall Mass Transfer Coefficient, m/sec	1.64E-08	3	3.93E-08	3
	(1/K = 1/Kl + 1/(Kg * Keq))				
	Co, Effluent Concentration, g/m^3 (Co=Q*Ci/(K*WL+Q))	2.3097	3	2.2782	3
	E, Emission Rate, g/yr (E=K*WL*Co*86400*365)	414.89	3	982.46	3
	EF, Emission Factor, g/g (EF=E/(Ci*Q*82400*365))	8.96E-07		2.12E-06	

Table 2					
Modeling of VOC Fate in WWTPs					
Soap and Detergent Association - Supplemental Study					
		Dipropylene Glycol Methyl Ether		**Morpholine**	
Process	**Variable**	**Value**	**Ref #**	**Value**	**Ref #**
Activated Sludge-	N, Number of Tanks	25	1	25	1
Aeration	Qa, Diffused Air Flow Rate, m^3/sec	3.19	1	3.19	1
	A, Surface Area, m^2	35502.96	1	35502.96	1
	D, Depth, m	4.62	1	4.62	1
	V, Volume, m^3	163859.81	1	163859.81	1
	De, Effective Diameter, m (De=(4*A/PI)^0.5)	42.53	3	42.53	3
	Ci, Influent Concentration, g/m^3	2.31		2.28	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	4.47	2	4.47	2
	F/D, Fetch to Depth Ratio	108.33		108.33	
	HRT, Hydraulic Residence Time, sec	27309.97		27309.97	
	Kg, Gas Phase Mass Transfer Coefficient, m/s	7.79E-03	3	7.31E-03	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)				
	Kl, Liquid Phase Mass Transfer Coefficient, m/s	3.66E-06	3	5.66E-06	3
	(Kl=2.611E-7*(U^2*(Dw/Dether)^0.67				
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	4.09E-06	3	2.34E-03	3
	K, Overall Mass Transfer Coefficient, m/sec	3.16E-08	3	4.25E-06	3
	(1/K = 1/Kl + 1/(Kg * Keq))				
	VOC Biodegradation Rate Coefficients				
	a=(K*A+Qa*Keq)/Q+1	1.00	12	1.11	12
	b=Ks*((K*A+Qa*Keq)/Q+1))+(V/Q)*Kmax*bl-Ca	1152.57	12	1583.56	12
	c=-Ks*Ci	-22.59	12	-662.96	12
	Co, Effluent Concentration, g/m^3	0.0196		0.5185	
	Co=(-b+(b^2-4*a*c)^0.5/2*a				
	E, Emission Rate(w/o biodegradation), g/yr	669.33		2471768.70	
	E=K*A*Co+Qa*Keq*Co				
	EF, Emission Factor, g/g (EF=E/(Ci*Q*82400*365))	6.87E-06		2.54E-02	

Table 2					
Modeling of VOC Fate in WWTPs					
Soap and Detergent Association - Supplemental Study					
		Dipropylene Glycol Methyl Ether		**Morpholine**	
Process	**Variable**	**Value**	**Ref #**	**Value**	**Ref #**
Activated Sludge-	N, Number of Tanks	25	1	25	1
Weir	Cl, Influent Concentration, g/m^3	0.0196	1	0.5185	1
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	4.47	2	4.47	2
	De, Effective Diameter, m	0.62		0.62	
	Z, Weir Height, m	0.62	1	0.62	1
	ql, Discharge per meter of Weir Width, m^2/sec	6.08E-03		6.08E-03	
	WL, Total Weir Area, m^2	142.01	1	142.01	1
	r voc, VOC Deficit Ratio	1.0000	5	1.0000	5
	r voc=EXP(0.042*Z^0.872*(ql/3600)^0.509*(Dw/Dc2w)^0.:				
	Kg, Gas Phase Mass Transfer Coefficient, m/s	1.24E-02	3	1.17E-02	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)				
	Kl, Liquid Phase Mass Transfer Coefficient, m/s	9.65E-08	5	1.57E-07	5
	(Kl=(1-1/r voc)*ql/Z)				
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	4.09E-06	3	2.34E-03	3
	K, Overall Mass Transfer Coefficient, m/sec	3.33E-08	3	1.57E-07	3
	(1/K = 1/Kl + 1/(Kg * Keq))				
	Co, Effluent Concentration, g/m^3 (Co=Q*Cl/(K*WL+Q))	0.0196	3	0.5185	3
	E, Emission Rate, g/yr (E=K*WL*Co*86400*365)	2.92	3	363.43	3
	EF, Emission Factor, g/g (EF=E/(Cl*Q*82400*365))	3.00E-08		3.73E-06	

Table 2					
Modeling of VOC Fate in WWTPs					
Soap and Detergent Association - Supplemental Study					
		Dipropylene Glycol Methyl Ether		**Morpholine**	
Process	**Variable**	**Value**	**Ref #**	**Value**	**Ref #**
Secondary Clar.	N, Number of Tanks	25	1	25	1
Quiescent	A, Surface Area, m^2	15049.70	1	15049.70	1
	D, Depth, m	4.62	1	4.62	1
	V, Volume, m^3	69460.17	1	69460.17	1
	De, Effective Diameter, m (De=(4*A/PI)^0.5)	27.69	3	27.69	3
	Ci, Influent Concentration, g/m^3	0.0196		0.5185	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	4.47	2	4.47	2
	Kg, Gas Phase Mass Transfer Coefficient, m/s	8.17E-03	3	7.67E-03	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)				
	Kl, Liquid Phase Mass Transfer Coefficient, m/s	3.66E-06	3	5.66E-06	3
	(Kl=2.611E-7*(U^2*(Dw/Dether)^0.67))				
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	4.09E-06	3	2.34E-03	3
	K, Overall Mass Transfer Coefficient, m/sec	3.31E-08	3	4.30E-06	3
	(1/K = 1/Kl + 1/(Kg * Keq))				
	Co, Effluent Concentration, g/m^3 (Co=Q*Ci/(K*A+Q))	0.0196	3	0.4956	3
	E, Emission Rate, g/yr (E=K*A*Co*86400*365)	308.06	3	1012279.31	3
	EF, Emission Factor, g/g (EF=E/(Ci*Q*82400*365))	3.16E-06		1.04E-02	

Table 2					
Modeling of VOC Fate in WWTPs					
Soap and Detergent Association - Supplemental Study					
		Dipropylene Glycol Methyl Ether		**Morpholine**	
Process	**Variable**	**Value**	**Ref #**	**Value**	**Ref #**
Secondary Clar.	N, Number of Tanks	25	1	25	1
Weir	D, Depth, m	4.62	1	4.62	1
	Ci, Influent Concentration, g/m^3	0.0196		0.4956	
	U, Wind Speed 10 Meters Above Liquid Surface, m/sec	4.47	2	4.47	2
	De, Effective Diameter, m	30.77	3	30.77	3
	Z, Weir Height, m	0.60	1	0.60	1
	qi, Discharge per meter of Weir Width, m^2/sec	5.80E-04	1	5.80E-04	1
	WL, Total Weir Area, m^2	1450.68	1	1450.68	1
	Di, Diameter of Clarifier, m	30.77	1	30.77	1
	r voc, VOC Deficit Ratio	1.0000000	5	1.0000000	5
	r voc=EXP(0.042*Z^0.872*(qi/3600)^0.509*(Dw/Do2w)^0.7				
	Kg, Gas Phase Mass Transfer Coefficient, m/s	8.07E-03	3	7.58E-03	3
	(Kg=4.82E-3*U^0.78*Scg^-0.67*De^-0.11)				
	Kl, Liquid Phase Mass Transfer Coefficient, m/s	1.63E-11	5	4.19E-13	5
	(Kl=(1-1/r voc)*qi/Z)				
	Keq, Equilibrium Partition Coefficient (Keq=H/RT)	4.09E-06	3	2.34E-03	3
	K, Overall Mass Transfer Coefficient, m/sec	1.62E-11	3	4.19E-13	3
	(1/K = 1/Kl + 1/(Kg * Keq))				
	Co, Effluent Concentration, g/m^3 (Co=Q*Ci/(K*WL+Q))	0.0196	3	0.4956	3
	E, Emission Rate, g/yr (E=K*WL*Co*86400*365)	1.46E-02	3	9.51E-03	3
	EF, Emission Factor, g/g (EF=E/(Ci*Q*82400*365))	1.50E-10		9.76E-11	

Table 3

Summary of Calculated Emission Factors

Soap and Detergent Association - Supplemental Study

Units = g/g

Chemical	CAS Number	Lift Station	Bar-Screens	Aerated Grit	Primary Clarifier Quiescent	Primary Clarifier Weir	Activated Sludge Surface	Activated Sludge Weir	Secondary Clarifier Quiescent	Secondary Clarifier Weir	Total
Ethanol	64175	2.8772E-05	1.3738E-06	6.47E-04	5.88E-03	2.65E-06	4.09E-04	1.83E-07	1.82E-04	7.98E-12	7.15E-03
Isopropanol	67630	3.63E-05	1.7336E-06	7.39E-04	6.56E-03	2.17E-06	5.04E-03	1.68E-06	2.23E-03	8.08E-11	1.46E-02
Butoxyethanol (Ethylene glycol monobutyl ether	111762	7.44E-08	3.5539E-09	2.26E-06	2.05E-05	3.94E-07	1.29E-06	7.92E-09	5.95E-07	5.19E-10	2.52E-05
Ethanolamine	141435	1.38E-06	6.6032E-08	4.10E-05	3.75E-04	2.02E-06	4.21E-04	1.45E-06	1.93E-04	1.05E-09	1.04E-03
Ethoxy Ethanol (Ethylene glycol monoethyl ether	110805	2.76E-05	1.3187E-06	5.98E-04	5.23E-03	1.88E-06	3.61E-04	1.30E-07	1.60E-04	8.64E-12	6.39E-03
Methanol	67561	2.71E-05	1.2947E-06	6.31E-04	5.83E-03	3.15E-06	1.76E-03	9.38E-07	7.86E-04	3.49E-11	9.04E-03
Pine Oil (Terpineol)	na	9.81E-07	4.6856E-08	2.96E-05	2.66E-04	1.26E-06	1.69E-05	5.36E-08	7.73E-06	7.69E-11	3.23E-04
D-Limonene	?	9.33E-07	4.4526E-08	2.80E-05	2.52E-04	1.11E-06	1.60E-05	4.86E-08	7.33E-06	7.99E-11	3.06E-04
Monoisopropylamine	75310	5.01E-05	2.3924E-06	9.07E-04	7.95E-03	2.14E-06	3.62E-04	9.82E-08	1.58E-04	4.09E-12	9.43E-03
Acetic Acid	64197	4.84E-05	2.3109E-06	9.20E-04	8.24E-03	2.51E-06	5.37E-04	1.64E-07	2.35E-04	5.70E-12	9.99E-03
Dipropylene Glycol Methyl Ether	34950948	3.98E-07	1.9013E-08	1.20E-05	1.09E-04	8.96E-07	6.87E-06	3.00E-08	3.16E-06	1.50E-10	1.32E-04
Morpholine	110918	2.14E-04	1.0223E-05	1.78E-03	1.41E-02	2.12E-06	2.54E-02	3.73E-06	1.04E-02	9.76E-11	5.19E-02

Table 4
Summary of Emission Factors for Cleaning Product VOCs
Soap and Detergent Association - Supplemental Study

		EF During Product Use					Overall EF		
Compounds	CAS #	EF for Manual Dishwashing (g/g)	EF for Machine Dishwashing (g/g) (*)	EF for Machine Laundry (g/g)	EF for WWTP (g/g)		Manual Dishwashing (g/g)	Machine Dishwashing (g/g)	Machine Laundry (g/g)
Ethanol	64175	0.05	0	1.10E-02	7.15E-03		5.58E-02	7.15E-03	1.81E-02
Isopropanol	67630	0.06	0	1.41E-02	1.46E-02		7.66E-02	1.46E-02	2.85E-02
Butoxyethanol	111762	0.00	na	3.64E-05	2.52E-05		1.87E-04	na	6.15E-05
Ethanolamine	141435	0.00	na	5.60E-04	1.04E-03		3.53E-03	na	1.59E-03
Ethoxy Ethanol	110805	na	na	1.20E-02	6.39E-03		na	na	1.84E-02
Methanol	67561	na	na	9.08E-03	9.04E-03		na	na	1.80E-02
Pine Oil (Terpineol)	na	na	na	6.21E-04	3.23E-04		na	na	9.43E-04
D-Limonene	?	na	na	5.25E-04	3.06E-04		na	na	8.30E-04
Monoisopropylamine	75310	0.09	na	na	9.43E-03		9.59E-02	na	na
Acetic Acid	64197	0.04	0	na	9.99E-03		5.30E-02	9.99E-03	na
Dipropylene Glycol Methyl Ether	34950948	na	na	1.75E-04	1.32E-04		na	na	3.07E-04
Morpholine	110918	na	0	na	5.19E-02		na	5.19E-02	na
Average		4.09E-02	0.00E+00	5.35E-03	9.19E-03		4.75E-02	2.09E-02	9.64E-03

na - not applicable because VOC species not used in this application.

* - Note that EF for Machine dishwashing is assumed to be zero because system is closed.

Appendix B
REFERENCES

Appendix B
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