Rizzo, Jonathan

From: Emery, Michael (DEC) <michael.emery@dec.ny.gov>
Sent: Thursday, April 27, 2017 9:15 AM
To: Szalda, Bryan
Cc: Carlacci, Alfred (DEC); Rizzo, Jonathan
Subject: CWM tables
Attachments: Tables (4-26-17).xlsx

Hi Bryan,
Here are the tables for your review.
Mike

CWM - estimated emissions SLF 1-6 stand pipes (select chemicals). Based on table 6 in report 7 (March 2017

Green shaded cells are for data input, the rest are calculations

Compounds	CAS Number	VOC	HAP	Mol. Weight	Density	Leachate Conc.	Leachate Conc.	Chemical Equation	Is there a benzene ring?	# Carbon Atoms	# Hydrogen Atoms	# Oxygen Atoms	# Chloride Atoms	# Fluorine Atoms	# Sulfur Atoms	# Bromine Atoms	# Nitrogen Atoms	Atomic Diffusion Volume for Da [3] Calculation	Gas Diffusion Coefficient Da Numerator	Gas Diffusion Coefficient Da Denominator	Gas Diffusion Coefficient Da [4]	Gas Diffusion Coefficient Da [4]	Atomic Volume for D_l Calculation [5]	Liquid Diffusion Coefficient D_l	Liquid Diffusion Coefficient D_l [5]	Schmidt Number S_c [7]	Reynolds Number R_e [7]	Sherwood Number S_h [7]	Total Surface Area [8]	Char. Length [9]	k_g [7]	k_l [7]	$1/K_{OL}$ [7]	K_{OL} [7]	DEC Henry's Constant [10] (used in these calc's)	CWM Henry's Constant	K_{OG} [7]	DEC Emissions	CWM Emissions from application (March 2017)	DEC Emissions	CWM Emissions	DEC Emissions	CWM Emissions	VOC Emissions	HAP Emissions	Difference compared to CWM (lb/yr value)	Larger Emission Rate (lb/yr)	Difference due to:
				(g/mol)	(g/cm3)	(ug/L)	(ug/m3)		(y/n)													(cm3/s)	(m3/h)	(cm3/mol)	(cm2/sec)	(m2/h)					(m3)	(m)	(m/h)	(m/h)						(ug/hr)	(ug/hr)	(lb/hr)	(lb/hr)	(lb/yr)	(lb/yr)	(lb/yr)	(lb/yr)		(CWM or DEC)	
Colounm #				1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	40	41	42	43	44
Acetone	000067-64-1			58.08	0.7845	740000	740,000,000	C_3H_6O	n	3	6	1	0					66.86	4.7223071	45.93655736	0.1028006	3.70E-02	74.03	1.14E-05	4.10E-06	1.60	24,815.5	122.362	6.77	2.60	1.740407	6.06E-03	526.46	1.90E-03	1.59E-03	1.59E-03	1.19E+00	9515981.37	9490000.00	2.0979E-02	2.09E-02	183.77545	183.25	-	-	0.3%	DEC	
Aroclor 1242 [1,*]	053469-21-9	X	X	291.98	1.441	2810	2,810,000	C12H6Cl4	y	12	6	0	4					267.68	4.0436239	83.97289809	0.0481539	1.73E-02	202.62	8.00E-06	2.88E-06	3.42	24,815.5	157.556	6.77	2.60	1.049723	5.07E-03	205.98	4.85E-03	*1.07E-01*	2.13E-02	4.54E-02	92357.66	67600.00	2.0361E-04	1.49E+04	1.7836385	1.31	1.7836385	1.7836385	36.2%	DEC	Henry's constant & ?
Aroclor 1254	11097-69-1	X	X	326.42	1.38	795	795,000	C12H5Cl5	y	12	5	0	5					285.2	4.0243049	86.51450744	0.046516	1.67E-02	236.54	8.00E-06	2.88E-06	3.54	24,815.5	159.384	6.77	2.60	1.025781	5.07E-03	206.19	4.85E-03	*1.07E-01*	8.20E-02	4.53E-02	26103.33	21300.00	5.7547E-05	4.70E-05	0.5041152	0.41	0.5041152	0.5041152	23.0%	DEC	Henry's constant & ?
Aroclor 1260 [1]	011096-82-5	X	X	360.86	1.593	690	690,000	C12H4Cl6	y	12	4	0	6					302.72	4.0086052	88.98968723	0.0450457	1.62E-02	226.53	8.00E-06	2.88E-06	3.65	24,815.5	161.099	6.77	2.60	1.004051	5.07E-03	206.38	4.85E-03	*1.07E-01*	1.89E-01	4.53E-02	22634.07	18400.00	4.9899E-05	4.05E-05	0.4371159	0.35	0.4371159	0.4371159	24.9%	DEC	Henry's constant
2,4-Dimethylphenol [1]	000105-67-9	X		122.16	0.965	2600	2,600,000	$C_8H_{10}O$	y	8	10	1	0					137.08	4.290049	62.01679208	0.0691756	2.49E-02	126.59	8.69E-06	3.13E-06	2.38	24,815.5	139.635	6.77	2.60	1.336459	5.29E-03	9,314.04	1.07E-04	8.20E-05	8.20E-05	1.31E+00	1889.83	145000.00	4.1663E-06	3.02E-06	0.036497	0.03	0.036497	-	21.7%	DEC	Henry's constant
4-Methylphenol [1]	000106-44-5	X	X	108.14	1.034	1700	1,700,000	C_7H_8O	y	7	8	1	0					116.62	4.3430738	57.83004093	0.0751007	2.70E-02	104.58	1.00E-05	3.60E-06	2.19	24,815.5	135.862	6.77	2.60	1.411722	5.67E-03	22,039.06	4.54E-05	3.24E-05	3.25E-05	1.40E+00	522.21	5150.00	1.1513E-06	1.14E-05	0.0100851	0.10	0.0100851	0.0100851	89.9%	CWM	
Phenol [1]	000108-95-2	X	X	94.113	1.072	140000	140,000,000	C_6H_6O	y	6	6	1	0					96.16	4.4109839	53.29486913	0.0827656	2.98E-02	87.79	9.10E-06	3.28E-06	1.99	24,815.5	131.531	6.77	2.60	1.506215	5.41E-03	40,915.82	2.44E-05	1.63E-05	1.63E-05	1.50E+00	23164.63	22800.00	5.1069E-05	5.03E-05	0.4473623	0.44	0.4473623	0.4473623	1.7%	DEC	
Total																																															

CWM Re = 24,813.80
DEC Re = 24,815.48
Using Re = 24,815.48

Italicized Henry's consents are different than CWM's

hrs/yr = 8760

DEC SUM	3.22	3.18
CWM SUM	2.64	2.61
DEC PCB	2.72	
CWM PCB	2.07	

34% Percent differnce for PCBs

	CWM	GHD	Difference
PCB's (lb/yr)	2.725	2.07	31.6%

Henry Constant references - NJ table (used by DEC), which are similar to EPA values at 20C,

EPA website - https://www3.epa.gov/ceampubl/learn2model/part-two/onsite/esthenry.html

Column # notes

Footnote numbers are from CWM/GHD table and note used here

1 Molecular weight, density and chemical equation are from Pubchem.ncbi.nlm.nih.gov, except as noted below

1 Molecular weight and chemical equation are from Sigma-Aldrich.com for 2,4-Dimethylpheno

Density is from www.guidechem.com for Aroclor 1242,
Density os from www.worldofchemicals.com for Aroclor 1260.

1 Aroclor 1242 is 2,2',3,4'-Tetrachlorobiphenyl in the PubChem database.

1 Aroclor 1260 is 2,2',3,3',4,4'-hexachlorobiphenyl in the PubChem database.
Density

4 1 L = 0.001 m^3 and 1000 L = 1 m^3

6 The presence of a benzene ring (Aromatic or heterocyclic ring) is part of the Atomic diffusion Voume calculation

15 Following the steps in USEPA Paper *"Overall Mass Transfer Coefficient for Pollutants Emissions from Small Water Pools under Simulated Indoor Environmental Conditions" (2002), (Attachment 3 in report 8)*

example for Phenol:

22 Calculate the Schmidt number using equation (13)
Sc = μ/ρD_a
Where
Sc = Schmidts number
μ = viscosity of air (g/m/h) =

μ (Pa s) =	1.98E-05	where 1 Pa s = 1 kg/(m s) = 3.6E06 g/(m h), and 1 Pa = 1 kg/(m*s^2)
1 Pa s = 1 kg/(m s) =	3.60E+06	
μ (g/m h)) =	**71.39**	g/(m h), the example in the EPA paper used 66.8 g/m/h

ρ = density of air (g/m^3) @ 68 F (20 C) & 1 atm = 1205 g/m3, Engineering ToolBox.com (http://www.engineeringtoolbox.com/air-properties-d_156.html) - [EPA example uses 1180 g/m3]

ρ (g/m^3) =	**1205**	1205	71.39

Da = diffusivity in air (m^2/h) - See Fuller and Chapter 11 print out.

15 Calculate the Diffusion Volume, follow example from Chapter 11 of Michigan University,
The diffusion volume for a component is calculated by multipling the number of atoms, say carbon, by the Atomic and Structural Diffusion Volume Increments for each atom in Table D-1 of chapter 11

Ex H20 = (2 x 1.98) + (1 x 5.48) = 9.44
From table D-1 Special Atomic Diffusion Voumes of Chapter 11 from U of Michigar

Carbon	16.5
Hydrogen	1.98
Oxygen	5.48
Chlorine	19.5
Benzene ring	-20.2

18 Calculate Gas diffusivite (Gas diffusion coefficient) following the method in Chapter 11 of U of Michigan book
$Di = (10^{-3} T^{1.75} ((1/M_A)+(1/M_B))^{0.5}) / (P ((\Sigma V_A)^{1/3} + (\Sigma V_B)^{1/3})^{2.5})$
Where:
D_i = diffusivity of compound, cm^2/s
T = Temperature, K (use 20 C (68 F)), where $T_K = T_C + 273.15$

T (K) =	293.15	Assumed CWM used 20C

M_A = molecular weight of air, provided in U of Michigan example

M_A =	29.0

M_B = molecular weight of compound, column 1
P = total pressure, atm (use 1 atm)

P (atm) =	1

V_A = sum of the diffusion volume for air (use 20.1 as provided in Chapter 11 of U of M document)

V_A =	20.1

V_B = sum of the diffusion volume for compound, column 14
Calculate the gas diffusion for phenol:

Phenol MW =	94.113	
Phenol Diffusion volume =	96.16	
16 Numerator =	4.410983892	4.410983892 check
17 Denominator =	53.29486913	53.29486913
18 Di (cm2/s) =	0.082765639	
19 Di (m2/h) =	0.02979563	CWM value
19 Di = Da (m2/h) =	2.98E-02	2.98E-02

20 Calculate Atomic Volume (cm3/mol)
Atomic Volume = atomic weight/density
Where:
Atomic weight = molecuar weight

Phenol Atomic weight (g/mol) =	94.113	
Density (g/cm3) =	1.072	Density from Pubchem.ncbi.nlm.nigh.gov, use close to 20 C density as possible
Atomic Volume (cm3/mol) =	**87.7920**	CWM used 103.4

CWM provided =	103.4
DEC provided =	87.792
Using =	**87.792**

21 D_l, Determine the Liquid Diffusion Coefficient D_l

Phenol diffusion coefficent in water (cm2/sec) =	9.10E-06	from *Chemical Properties for Calculation of Impact to Groundwater Soil Remediation Standards* pdf file, from NJ
Convert to m2/hr		
D_l (m2/hr) =	3.276E-06	CWM used 3.55E-06

23 Schmidt Number S_c = μ/ρDa

Equ. 13 in "Overall Mass Transfer Coefficient for Pollution Emission from Small Water Pools Under Simulated Indoor Environmental Conditions", December 2002

Where:

μ, viscosity of air (g/(m h)) =	71.39
ρ density of air (g/m^3) =	1205
Di air diffusion coefficent (Da in table) (m2/h) =	0.0298
Sc =	1.988 CWM = 1.9

24 Reynolds Number $R_e = (L w \rho)/\mu$ — Equ. 14 in "Overall Mass Transfer Coefficient for Pollution Emission from Small Water Pools Under Simulated Indoor Environmental Conditions", December 2002, (wind speed assumed ot be 11.8 mph

Where:

L = characteristic length (m) calculated from the square root of the source area, L (m) = $A^{0.5}$

26 Area of pond, A (m2) = 6.77 Provided by CWM

27 L (m) = 2.602

air velocity (miles/h) = 0.35110 Wind speed not provided. By trial and error, CWM used ~0.3511 mph

Convert to mph to meters/hr, where 1 mile = 1609.34 meters

w , air velocity (meters/h) = 565.04

ρ air density (g/m^3) = 1205

μ viscosity of air (g/(m h) = 71.39

24 Re = **24,815.48**

CWM =	24,813.80
DEC =	24,815.48
using =	**24,815.48**

25 Sherwood number, $Sh = 0.664\ S_c^{1/3}\ R_e^{0.5}$ — Equ. 11 in "Overall Mass Transfer Coefficient for Pollution Emission from Small Water Pools Under Simulated Indoor Environmental Conditions", December 2002,

Where:

Sc = 1.988

Re = 24,815.48

Sh = 131.53 CWM = 129.6

28 K_G (m/h) --> derive from $Sh = (K_L L)/D_a$ ---> $K_G = (S_h\ D_a) / L$

Where:

Sh = 131.531

Da = Di (m2/h)= 0.0298

L (m) = 2.602

K_G (m/h) = 1.5062 CWM used 1.48

KL	
0.005411817	0.0056
3.28E-06	

29 Calculate K_c, $K_c = 2.99(D_i \text{^} 0.5)$ — Equ. 18 in "Overall Mass Transfer Coefficient for Pollution Emission from Small Water Pools Under Simulated Indoor Environmental Conditions", December 2002

D_i (m2/hr) = 3.276E-06

K_c (m/h) = 5.412E-03 CWM used 5.63E-03

31 Calculate KOL, where 1/KOL = (1/KL) + (1/KGH) — Equ. 3 in "Overall Mass Transfer Coefficient for Pollution Emission from Small Water Pools Under Simulated Indoor Environmental Conditions", December 2002

K_L = 5.41E-03

K_G = 1.5062

32 H, Henry's constant (unitless) = **1.63E-05** from *Chemical Properties for Calculation of Impact to Groundwater Soil Remediation Standards* pdf file, from NJ

30 1/KOL = 40915.8215

31 KOL = 2.44404E-05 CWM used 2.41E-05

H, Henry's constant for Phenol (unitless) = GSI environmenatal	2.47E-05
NJ reference matchs	1.63E-05

34 $K_{OG} = K_{OL}/H$, where K_{OG} is the overall gas phase mass transer coefficeint

KOL = 2.44404E-05

H = 0.0000163

KOG = 1.499412477 CWM used 1.48

35 Emissions , E (R in equ 2) (ug/h) = S x KOG x CL x H

Where:

S is the source area, A (m2) = 6.77

K_{OG} (m/h) = 1.499412477

C_L, pollutant concentration in the liguid (ug/m3) = 140000000 (phenol)

H, Henry's Constant = 0.0000163

E (R in equ) (ug/h) = 23,164.63 CWM reported 22,800

37 convert to lb/hr, where 1 ug = 2.2046E-09 lb

E (lb/h) = 5.10688E-05 CWM reported 5.03E-05

39 Convet to lb/yr, where 1 yr (hr) = 8760

E (lb/yr) = 0.447362254 CWM reported 0.44 lb/yr

CWM - estimated emissions from stormwater detention basin (RMU-2 contact stormwater), Table 6 in Report 8 (March 2017)

Green shaded cells are for data input, the rest are calculations.

Compounds	CAS Number	VOC	HAP	Mol. Weight	Density	Leachate Conc.	Leachate Conc.	Chemical Equation	Is there a benzene ring?	# Carbon Atoms	# Hydrogen Atoms	# Oxygen Atoms	# Chloride Atoms	# Fluorine Atoms	# Sulfur Atoms	# Bromine Atoms	# Nitrogen Atoms	Atomic Diffusion Volume for Da [3] Calculation	Gas Diffusion Coefficient Da Denominator	Gas Diffusion Coefficient Da Numerator	Gas Diffusion Coefficient Da [4]	Gas Diffusion Coefficient Da [4]	Atomic Volume for D_l Calculation [5]	Liquid Diffusion Coefficient D_l	Liquid Diffusion Coefficient D_l [6]	Schmidt Number S_c [7]	Reynolds Number R_e [7]	Sherwood Number S_h [7]	Total Surface Area [8]	Char. Length [9]	k_g [7]	k_l [7]	$1/K_{OL}$ [7]	K_{OL} [7]	DEC Henry's Constant [10] (used in these calc's)	CWM Henry's Constant	K_{OG} [7]	DEC Emissions	CWM Emissions from application (March 2017)	DEC Emissions	CWM Emissions	DEC Emissions	CWM Emissions	VOC Emissions	HAP Emissions	Difference compared to CWM (lb/yr value)	Larger Emission Rate (lb/yr)	Difference due to:
				(g/mol)	(g/cm3)	(ug/L)	(ug/m3)		(y/n)												(cm^2/s)	(m^2/h)	(cm^3/mol)	(cm2/sec)	(m^2/h)				(m^2)	(m)	(m/h)	(m/h)					(m/h)	(ug/hr)	(ug/hr)	(lb/hr)	(lb/hr)	(lb/yr)	(lb/yr)	(lb/yr)	(lb/yr)			(CWM or DEC)	
Column #				1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45
Acetone	000067-64-1			58.08	0.7845	0.5	500	C_3H_6O	n	3	6	1	0					66.86	4.7223	45.9366	0.10280	3.70E-02	74.03	1.14E-05	4.10E-06	1.60	5,048,549.3	1745.295	248.07	15.75	4.100907	6.06E-03	318.46	3.14E-03	1.59E-03	1.59E-03	1.97E+00	389.49	396.00	8.5867E-07	8.73E-07	0.0075219	0.0076477	-	-	1.6%	CWM	
Aroclor 1242 [1,*]	053469-21-9	X	X	291.98	1.441	0.5	500	C12H6Cl4	y	12	6	0	4					267.68	4.0436	83.9729	0.04815	1.73E-02	202.62	8.00E-06	2.88E-06	3.42	5,048,549.3	2247.278	248.07	15.75	2.473454	5.07E-03	200.85	4.98E-03	*1.07E-01*	2.13E-02	4.65E-02	617.54	487.00	1.3614E-06	1.07E-06	0.0119261	0.0094051	0.0119261	0.0119261	26.8%	DEC	Henry's constant & ?
Aroclor 1260 [1]	011096-82-5	X	X	360.86	1.593	0.5	500	C12H4Cl6	y	12	4	0	6					302.72	4.0086	88.9897	0.04505	1.62E-02	226.53	8.00E-06	2.88E-06	3.65	5,048,549.3	2297.821	248.07	15.75	2.365839	5.07E-03	201.03	4.97E-03	*1.07E-01*	1.89E-01	4.65E-02	617.01	502.00	1.3603E-06	1.11E-06	0.0119159	0.0096948	0.0119159	0.0119159	22.9%	DEC	Henry's constant & ?
2,4-Dimethylphenol [1]	000105-67-9	X		122.16	0.965	0.5	500	$C_8H_{10}O$	y	8	10	1	0					137.08	4.2900	62.0168	0.06918	2.49E-02	126.59	8.69E-06	3.13E-06	2.38	5,048,549.3	1991.665	248.07	15.75	3.149087	5.29E-03	4,061.68	2.46E-04	*8.20E-05*	3.90E-03	3.00E+00	30.54	446.00	6.7324E-08	9.83E-07	0.0005898	0.0086133	0.0005898	-	93.2%	CWM	Henry's constant
4-Methylphenol [1]	000106-44-5	X	X	108.14	1.034	0.5	500	C_7H_8O	y	7	8	1	0					116.62	4.3431	57.8300	0.07510	2.70E-02	104.58	1.00E-05	3.60E-06	2.19	5,048,549.3	1937.847	248.07	15.75	3.326431	5.67E-03	9,454.74	1.06E-04	*3.24E-05*	2.11E-08	3.26E+00	13.12	0.01	2.8922E-08	1.94E-11	0.0002534	1.696E-07	0.0002534	0.0002534	149317.0%	DEC	Henry's constant
Phenol [1]	000108-95-2	X	X	94.113	1.072	0.5	500	C_6H_6O	y	6	6	1	0					96.16	4.4110	53.2949	0.08277	2.98E-02	87.79	9.10E-06	3.28E-06	1.99	5,048,549.3	1876.077	248.07	15.75	3.549082	5.41E-03	17,470.85	5.72E-05	1.63E-05	1.63E-05	3.51E+00	7.10	7.16	1.5652E-08	1.58E-08	0.0001371	0.0001383	0.0001371	0.0001371	0.8%	CWM	
Total																																															

CWM Re = 5,288,426.50
DEC Re = 5,048,549.30
Using Re = 5,048,549.3

hrs/yr = 8760

DEC SUM	0.025	0.0242
CWM SUM	0.030	0.0200
Difference	17.3%	21.2%

	DEC	CWM	difference
PCB totals	0.023842	0.0191	25%

Italicized Henry's consents are different than CWM's

Henry's consents in pink box are a factor of at least 2 different than CWM's

Henry Constant references - NJ table (used by DEC), which are similar to EPA values at 20C,
EPA website - https://www3.epa.gov/ceampubl/learn2model/part-two/onsite/esthenry.html

Column # notes

Footnote numbers are from CWM/GHD table and note used here.

1 Molecular weight, density and chemical equation are from Pubchem.ncbi.nlm.nih.gov, except as noted below.

1 Molecular weight and chemical equation are from Sigma-Aldrich.com for 2,4-Dimethylphenol
Density is from www.guidechem.com for Aroclor 1242,
Density os from www.worldofchemicals.com for Aroclor 1260.

1 Aroclor 1242 is 2,2',3,4'-Tetrachlorobiphenyl in the PubChem database.

1 Aroclor 1260 is 2,2',3,3',4,4'-hexachlorobiphenyl in the PubChem database.
Density

4 1 L = 0.001 m^3 and 1000 L = 1 m^3

6 The presence of a benzene ring (Aromatic or heterocycliec ring) is part of the Atomic diffusion Voume calculation.

15 Following the steps in USEPA Paper *"Overall Mass Transfer Coefficient for Pollutants Emissions from Small Water Pools under Simulated Indoor Environmental Conditions" (2002), (Attachment 3 in report 8)*

example for Phenol:

23 Calculate the Schmidt number using equation (13):
$Sc = \mu/\rho D_a$
Where
Sc = Schmidts number
μ = viscosity of air (g/m/h) =

μ (Pa s) =	1.98E-05	where 1 Pa s = 1 kg/(m s) = 3.6E06 g/(m h), and 1 Pa = 1 kg/(m*s^2)
1 Pa s = 1 kg/(m s) =	3.60E+06	
μ (g/(m h)) =	71.39	g/(m h), the example in the EPA paper used 66.8 g/m/h

ρ = density of air (g/m^3) @ 68 F (20 C) & 1 atm = 1205 g/m3, Engineering ToolBox.com (http://www.engineeringtoolbox.com/air-properties-d_156.html) - [EPA example uses 1180 g/m3]

ρ (g/m^3) =	1205

D_a = diffusivity in air (m^2/h) - See Fuller and Chapter 11 print out.

15 Calculate the Diffusion Volume, follow example from Chapter 11 of Michigan University
The diffusion volume for a component is calculated by multipling the number of atoms, say carbon, by the Atomic and Structural Diffusion Volume Increments for each atom in Table D-1 of chapter 11

Ex H20 = (2 x 1.98) + (1 x 5.48) = 9.44
From table D-1 Special Atomic Diffusion Voumes of Chapter 11 from U of Michigan

Carbon	16.5
Hydrogen	1.98
Oxygen	5.48
Chlorine	19.5
Benzene ring	-20.2

18 Calculate Gas diffusivite (Gas diffusion coefficient) following the method in Chapter 11 of U of Michigan book.
$Di = (10^{-3} T^{1.75} ((1/M_A)+(1/M_B))^{0.5}) / (P ((\Sigma V_A)^{1/3} + ((\Sigma V_B)^{1/3})^2))$
Where:
D_i = diffusivity of compound, cm2/s

T = Temperature, K (use 20 C (68 F)) T (K) =	293.15	
M_A = molecular weight of air M_A =	29.0	
M_B = molecular weight of compound, column 1		
P = total pressure, atm (use 1 atm) P (atm) =	1	
V_A = sum of the diffusion volume for air (use 20.1 as provided in Chapter 11 of U of M document) V_A =	20.1	
V_B = sum of the diffusion volume for compound, column 14		
Calculate the gas diffusion for phenol:		
Phenol MW =	94.113	
Phenol Diffusion volume =	96.16	
16 Numerator =	4.410983892	4.410983892 check
17 Denominator =	53.29486913	53.29486913
18 Di (cm2/s) =	0.082765639	
19 Di (m2/h) =	0.02979563	CWM value
19 Di = Da (m2/h) =	2.98E-02	2.98E-02

20 Calculate Atomic Volume (cm3/mol)
Atomic Volume = atomic weight/density
Where:
Atomic weight = molecuar weight

Phenol Atomic weight (g/mol) =	94.113		
Density (g/cm3) =	1.072	Density from Pubchem.ncbi.nlm.nigh.gov, use close to 20 C density as possible.	
Atomic Volume (cm3/mol) =	**87.7920**	CWM used 103.4	CWM provided = 103.4
			DEC calc = 87.792
			Using = **87.792**

21 D_L, Determine the Liquid Diffusion Coefficient D_L

Phenol diffusion coefficent in water (cm2/sec) =	9.10E-06	from *Chemical Properties for Calculation of Impact to Groundwater Soil Remediation Standards* pdf file, from NJ
Convert to m2/hr		
22 D_L (m2/hr) =	3.276E-06	CWM used 3.55E-06

23 Schmidt Number $S_c = \mu/\rho Da$ — Equ. 13 in "Overall Mass Transfer Coefficient for Pollution Emission from Small Water Pools Under Simulated Indoor Environmental Conditions", December 2002

Where:

μ, viscosity of air (g/(m h)) =	71.39	
ρ density of air (g/m^3) =	1205	
Di air diffusion coefficent (Da in table) (m2/h) =	0.0298	
Sc =	1.988	CWM = 1.9

24 Reynolds Number $R_e = (L\upsilon\rho)/\mu$ — Equ. 14 in "Overall Mass Transfer Coefficient for Pollution Emission from Small Water Pools Under Simulated Indoor Environmental Conditions", December 2002, (wind speed assumed ot be 11.8 mph

Where:

L = characteristic length (m) calculated from the square root of the source area, L (m) = $A^{0.5}$

26	Area of pond, A (m2) =	248.07	
27	L (m) =	15.750	
	air velocity (miles/h) =	11.8	(assumed 11.8 mph, per CWM) - 11.8 mph is used in the TANKS or AP-42 TANKS documents for Buffalo, NY

Convert to mph to meters/hr, where 1 mile = 1609.34 meters

	υ , air velocity (meters/h) =	18,990.21	
	ρ air density (g/m^3) =	1205	
	μ viscosity of air (g/(m h) =	71.39	
	Re =	**5,048,549.30**	CWM = 5,288,426.50
			DEC = 5,048,549.30
			using = 5,048,549.30

25 Sherwood number, $Sh = 0.664\, S_c^{1/3} R_e^{0.5}$ — Equ. 11 in "Overall Mass Transfer Coefficient for Pollution Emission from Small Water Pools Under Simulated Indoor Environmental Conditions", December 2002,

Where:

Sc =	1.988	
Re =	5,048,549.30	
Sh =	1876.08	CWM = 1891.8

28 K_G (m/h) --> derive from $Sh = (K_G L)/D_a$ ---> $K_G = (S_h\, D_a) / L$

Where:

Sh =	1876.077		KL	
Da = Di (m2/h)=	0.0298		0.005411817	0.0056
L (m) =	15.750		3.78E-06	
K_G (m/h) =	3.5491	CWM used 3.58		

29 Calculate K_c, $K_c = 2.99(D_i \text{^} 0.5)$ — Equ. 18 in "Overall Mass Transfer Coefficient for Pollution Emission from Small Water Pools Under Simulated Indoor Environmental Conditions", December 2002

D_i (m2/hr) =	3.276E-06	
K_c (m/h) =	5.412E-03	CWM used 5.63E-03

31 Calculate KOL, where 1/KOL = (1/KL) + (1/KGH) — Equ. 3 in "Overall Mass Transfer Coefficient for Pollution Emission from Small Water Pools Under Simulated Indoor Environmental Conditions", December 2002

K_L =	5.41E-03	
K_G =	3.5491	
32 H, Henry's constant (unitless) =	**1.63E-05**	from *Chemical Properties for Calculation of Impact to Groundwater Soil Remediation Standards* pdf file, from NJ
30 1/KOL =	17470.85259	
31 KOL =	5.72382E-05	CWM used 5.77E-05

H, Henry's constant for Phenol (unitless) =	GSI environmenatal	2.47E-05
	NJ reference matchs	1.63E-05

34 $K_{OG} = K_{OL}/H$, where K_{OG} is the overall gas phase mass transer coefficeint

KOL =	5.72382E-05	
H =	0.0000163	
KOG =	3.511545468	CWM used 3.54

35 Emissions , E (R in equ 2) (ug/h) = S x KOG x CL x H

Where:

S is the source area, A (m2) =	248.07	
K_{OG} (m/h) =	3.511545468	
C_L, pollutant concentration in the liguid (ug/m3) =	500	(phenol)
H, Henry's Constant =	0.0000163	
E (R in equ) (ug/h) =	7.099539037	CWM reported 7.16

37 convert to lb/hr, where 1 ug = 2.2046E-09 lb

E (lb/h) =	1.56516E-08	CWM reported 1.58E-08

39 Convet to lb/yr, where 1 yr (hr) = 8760

E (lb/yr) =	0.000137108	CWM reported 0.00 lb/yr, not helpful in verifying the hours used.

Comparision for Phenol emission calcuation:	ug/hr	lb/yr (8760 hr)
Calculated by CWM/GHD	7.16	1.58E-08
Calculated by DEC	7.0995	1.57E-08