Attachment

PCB Emission Calculations For the 242-A Evaporator

In support of the "Application for Risk-Based Disposal for Polychlorinated Biphenyls --Hanford 200 Area Liquid Waste Processing Facilities, Appendix 1" DOE/RL-2002-002

February 2002

(This page intentionally left blank)

This attachment contains detailed calculations regarding PCB emissions that would be emitted from the Evaporator stack. The initial feed concentration is set at 0.2 mg/L of AroClor 1016. Additional information regarding emission rates is contained in Section A.2.3 of Appendix 1.

Mass Balance/ Operating Data CA-1



 $Q_{airleak1} := 1 \frac{ft^3}{min}$ (SCFM) (from Safety Analysis Report based on dip tube and leakage)

Converting Qairleak1 to mol/min

$$Q_{airleak1molar} := \frac{Q_{airleak1} \cdot \left(28.317 \frac{L}{ft^3}\right)}{22.4 \frac{L}{mol}}$$

 $Q_{airleak1molar} = 1.264 \frac{mol}{min}$

Converting $Q_{airleak1}$ to kg/min

$$Q_{airleak 1 mass} \coloneqq \frac{Q_{airleak 1 molar} \left(29 \frac{gm}{mol}\right)}{1000 \frac{gm}{kg}}$$

$$Q_{airleak 1 mass} \equiv 0.0367 \frac{kg}{mol}$$

 $airleak1mass = 0.036 / \frac{1}{min}$

Feed: Flow is 60 gal/min with SpG = 1.02 (from Campaign 01-01)

$$Q_{1\text{mass}} \coloneqq 60 \frac{\text{gal}}{\text{min}} \cdot \left(3.785 \frac{\text{L}}{\text{gal}}\right) \cdot \left(1.020 \frac{\text{kg}}{\text{L}}\right)$$
$$Q_{1\text{mass}} = 231.642 \frac{\text{kg}}{\text{min}}$$

Assume 18gm/mol

$$Q_{1 \text{molar}} := Q_{1 \text{mass}} \cdot \frac{\left(1000 \frac{\text{gm}}{\text{kg}}\right)}{18 \frac{\text{gm}}{\text{mol}}}$$
$$Q_{1 \text{molar}} = 12869 \frac{\text{mol}}{\text{min}}$$

Boiloff: Waste Volume Reduction from Campaign 01-01 boiloff was 81%

boiloff₁ :=
$$(0.81) \cdot 60 \frac{\text{gal}}{\text{min}}$$

boiloff₁ = $48.6 \frac{\text{gal}}{\text{min}}$

This has a SpG of 1.0

Converting boiloffto kg/min

boiloff₂ := (boiloff₁)
$$\cdot \left(3.785 \frac{L}{gal}\right) \cdot \left(1.0 \frac{kg}{L}\right)$$

boiloff₂ = 183.951 $\frac{kg}{min}$

Converting boiloffto mol/min

boiloff₃ :=
$$\frac{\text{boiloff}_2 \cdot \left(1000 \frac{\text{gm}}{\text{kg}}\right)}{18 \frac{\text{gm}}{\text{mol}}}$$

boiloff₃ =
$$10220 \frac{\text{mol}}{\text{min}}$$

Application for Risk-Based Disposal Approval for Polychlorinated Biphenyls Hanford Site Liquid Waste Processing Facilities

$Q_3 = boiloff + Q_{airleak}$

 $Q_{3mass} := boiloff_2 + Q_{airleak1mass}$

 $Q_{3mass} = 183.988 \frac{kg}{min}$

 $Q_{3molar} := boiloff_3 + Q_{airleak1molar}$

 $Q_{3molar} = 1.022 \times 10^4 \frac{mol}{min}$

 $Q_2 := Q_{1molar} - boiloff_3$

 $Q_2 = 2.649 \times 10^3 \, \frac{\text{mol}}{\text{min}}$

Mass Balance Operating Data EC-1



 Q_{3mass} = 184 kg/min, which is 0.0367 kg/min dry air ($Q_{airleak1mass}$)

 Q_5 is dry air and moisture; at 40 °C, there 0.0491 kg H₂O/kg dry air (Perry's 6th Ed., Table 12-1). The moisture is therefore 0.0367 kg/min(0.0491 kg H₂O/kg dry air) = 1.80x10⁻³ kgH₂O/min

The molar H_2O flow is then (1.80x10⁻³ kg H_2O /min) (1000gm/kg)/(18gm/mol)=0.100 mol H_2O /min

$$Q_5 := Q_{airleak1mass} + 1.80 \, 10^{-3} \, \frac{\text{kg}}{\text{min}}$$

 $Q_5 = 0.0385 \frac{\text{kg}}{\text{min}}$

 $Q_{5molar} := Q_{airleak1molar} + 0.100 \frac{mol}{min}$

$$Q_{5molar} = 1.364 \frac{mol}{min}$$

 $Q_4 = Q_3 - Q_5$

$$Q_{4mass} := Q_{3mass} - Q_5$$

$$Q_{4mass} = 183.949 \frac{\text{kg}}{\text{min}}$$

 $Q_{4molar} := Q_{3molar} - Q_{5molar}$

$$Q_{4molar} = 1.022 \times 10^4 \frac{mol}{min}$$

Balance/Operating Data E-C2



 Q_5 = 0.0385 kg/min and consists of 0.0367 kg/min air and 1.80x10 ⁻³ kg/min of H₂O Q_5 = 1.364 mol/min and consists of 1.264 mol/min air and 0.100mol/min of H ₂O

Inbleed: Inbleed in mol/min

$$Q_{inbleed1molar} := \frac{Q_{inbleed1} \cdot \left(28.317 \frac{L}{ft^3}\right)}{22.4 \frac{L}{mol}}$$

 $Q_{inbleed1molar} = 31.604 \frac{mol}{min}$

Inbleed in kg/min

$$Q_{\text{inbleed1mass}} := \frac{Q_{\text{inbleed1molar}} \left(29 \frac{\text{gm}}{\text{mol}}\right)}{1000 \frac{\text{gm}}{\text{kg}}}$$

$$Q_{inbleed1mass} = 0.917 \frac{kg}{min}$$

Steam: Steam in kg/min

$$Q_{\text{steam1mass}} \coloneqq Q_{\text{steam1}} \cdot \left(3.785 \frac{L}{\text{gal}}\right) \cdot \left(1.0 \frac{\text{kg}}{\text{L}}\right)$$

 $Q_{steam1mass} = 4.656 \frac{kg}{min}$

Convert to mol/min:

$$Q_{\text{steam1molar}} := \frac{Q_{\text{steam1mass}} \cdot \left(1000 \frac{\text{gm}}{\text{kg}}\right)}{18 \frac{\text{gm}}{\text{mol}}}$$

 $Q_{steam1molar} = 258.642 \frac{mol}{min}$

 $Q_{6mass} := Q_5 + Q_{inbleed1mass} + Q_{steam1mass}$

 $Q_{6mass} = 5.611 \frac{kg}{min}$

Q_{6molar} := Q_{5molar} + Q_{steam1molar} + Q_{inbleed1molar}

 $Q_{6molar} = 291.61 \frac{mol}{min}$

 Q_8 is the dry air and moisture at 50 °C (assumed), there is 0.0868 kg H₂O/kg dry air (from Perry's 6th Ed., Table 12-1. The total dry air is 0.0367 kg/min + 0.917 kg/min = 0.954 kg/min. The moisture is therefore 0.954kg/min(0.0868)=0.0828 kgH2O/min.

The molar H2O flow is:

 $Molar_{H2Oflow} := \frac{0.0828 \frac{kg}{min} \cdot 1000 \frac{gm}{kg}}{18 \frac{gm}{mol}}$

 $Molar_{H2Oflow} = 4.6 \frac{mol}{min}$

 $Q_8 = dryair + moisture$

$$Q_{8mass} := 0.954 \frac{\text{kg}}{\text{min}} + 0.0828 \frac{\text{kg}}{\text{min}}$$

 $Q_{8mass} = 1.037 \frac{\text{kg}}{\text{min}}$

Q_{8molar} := Q_{airleak1molar} + Q_{inbleed1molar} + Molar_{H2Oflow}

 $Q_{8molar} = 37.468 \frac{mol}{min}$

 $Q_7 = Q_6 - Q_8$

 $Q_{7mass} := Q_{6mass} - Q_{8mass}$

 $Q_{7mass} = 4.574 \frac{kg}{min}$

 $Q_{7molar} := Q_{6molar} - Q_{8molar}$

$$Q_{7\text{molar}} = 254.142 \frac{\text{mol}}{\text{min}}$$

Mass Balance / Operating Data EC-3



This balance is the same as EC-2 except that there is no air inbleed.

 $Q_{steam2} := 1.23 \cdot \frac{gal}{min}$

 $Q_{8 \text{ (mass)}}$ = 1.04 kg/min and is 0.954 kg/min air and 0.083 kg/min H $_2$ O $Q_{8 \text{ (molar)}}$ = 37.5 mol/min and is 32.9 mol/min air and 4.60 mol/minH $_2$ O

 $Q_{\text{steam1mass}} = 4.656 \frac{\text{kg}}{\text{min}}$

 $Q_{steam1molar} = 258.642 \frac{mol}{min}$

 $Q_{9mass} := Q_{8mass} + Q_{steam1mass}$

$$Q_{9mass} = 5.692 \frac{\text{kg}}{\text{min}}$$

 $Q_{9molar} := Q_{8molar} + Q_{steam1molar}$

 $Q_{9molar} = 296.11 \frac{mol}{min}$

Q₁₁ is dry air + moisture. Since no additional dry air was added, and the operating temperature is unchanged, the quantity of water is unchanged.

 $Q_{11mass} := Q_{8mass}$

 $Q_{11mass} = 1.037 \frac{kg}{min}$

$Q_{11molar} := Q_{8molar}$

 $Q_{11molar} = 37.468 \frac{mol}{min}$

 $Q_{10} = Q_9 - Q_{11}$

 $Q_{10mass} \coloneqq Q_{9mass} - Q_{11mass}$

$$Q_{10mass} = 4.656 \frac{\text{kg}}{\text{min}}$$

 $Q_{10molar} := Q_{9molar} - Q_{11molar}$

 $Q_{10molar} = 258.642 \frac{mol}{min}$

Mass Balance/Operating Data C-100 Tank



C-100 tank receives condensate from EC-1, EC-2 & EC-3. It also has two air additions. Dip Tube (DT) air sparges through the liquid and is fully saturated. Air inleakage enters the top and is unsaturated.



Application for Risk-Based Disposal Approval for Polychlorinated Biphenyls Hanford Site Liquid Waste Processing Facilities

$$Q_{airleakmol} := \frac{150 \frac{\text{ft}^3}{\text{min}} \cdot \left(28.317 \frac{\text{L}}{\text{ft}^3}\right)}{22.4 \frac{\text{L}}{\text{mol}}}$$

$$Q_{airleakmol} = 189.62 \frac{\text{mol}}{\text{min}}$$

$$Q_{airleakmass} := \frac{189.62 \frac{\text{mol}}{\text{min}} \cdot \left(29 \cdot \frac{\text{gm}}{\text{mol}}\right)}{1000 \frac{\text{gm}}{\text{kg}}}$$

$$Q_{airleakmass} = 5.499 \frac{\text{kg}}{\text{min}}$$

$$Q_{12mass} := Q_{4mass} + Q_{7mass} + Q_{10mass}$$

 $Q_{12mass} = 193.178 \frac{\text{kg}}{\text{min}}$

(approximately 51gpm)

 $Q_{12molar} := Q_{4molar} + Q_{7molar} + Q_{10molar}$

 $Q_{12molar} = 1.073 \times 10^4 \frac{mol}{min}$

 Q_{14} is the airleakage ($Q_{airleak}$) plus the dip tube air (Q_{DT}) + moisture from diptube air. At 45°C, there is 0.0654 kg H₂O/kg air (Perry's 6th Ed., Table 12-1). kgH₂O in diptube air = 0.0654 kg H₂O/kg(3.67x10⁻³ kg/min) = 2.4x10⁻⁴ kg/min mol H₂O in diptube air = (2.40x10⁻⁴ kg/min) (1000 gm/kg)/(18 gm/mol) = 1.33x10⁻² mol/min

Mass water := $2.4 \cdot 10^{-4} \cdot \frac{\text{kg}}{\text{min}}$

$$Mol_{water} := \frac{Mass_{water} \cdot \left(1000 \frac{gm}{kg}\right)}{18 \frac{gm}{mol}}$$

 $Mol_{water} = 0.0133 \frac{mol}{min}$

 $Q_{14mass} := Q_{airleakmass} + Q_{DTmass} + Mass_{water}$

$$Q_{14mass} = 5.5 \frac{kg}{min}$$

 $Q_{14molar} := Q_{airleakmol} + Q_{DTmolar} + Mol_{water}$

$$Q_{14\text{molar}} = 189.76 \frac{\text{mol}}{\text{min}}$$

 $Q_{13mass} := Q_{12mass} + Q_{airleakmass} + Q_{DTmass} - Q_{14mass}$

 $Q_{13mass} = 193.178 \frac{kg}{min}$

 $Q_{13molar} := Q_{12molar} + Q_{airleakmol} + Q_{DTmolar} - Q_{14molar}$

 $Q_{13molar} = 10732.17 \frac{mol}{min}$

Mass Balance/Operating Vessel Vent



 $\mathsf{Q}_{\text{airbleed}}$ is 370 SCFM (based of flow testing performed during HEPA filter efficiency test).

$$Q_{airbleedmol} \coloneqq \frac{370 \frac{\text{ft}^3}{\text{min}} \cdot \left(28.317 \frac{\text{L}}{\text{ft}^3}\right)}{22.4 \frac{\text{L}}{\text{mol}}}$$

$$Q_{airbleedmol} = 467.736 \frac{\text{mol}}{\text{min}}$$

$$Q_{airbleedmos} \coloneqq \frac{Q_{airbleedmot} \left(29 \frac{\text{gm}}{\text{mol}}\right)}{1000 \frac{\text{gm}}{\text{kg}}}$$

$$Q_{airbleedmass} \coloneqq 13.56 \frac{\text{kg}}{\text{min}}$$

$$Q_{ventmass} \coloneqq Q_{11mass} + Q_{14mass} + Q_{airbleedmass}$$

$$Q_{ventmass} \equiv 20.104 \frac{\text{kg}}{\text{min}}$$

$$Q_{ventmol} \coloneqq Q_{11molar} + Q_{14molar} + Q_{airbleedmol}$$

$$Q_{ventmol} \coloneqq 694.97 \frac{\text{mol}}{\text{min}}$$

Hanford Site Liquid Waste Processing Facilities

Application for Risk-Based Disposal Approval for Polychlorinated Biphenyls

February 2002

Volumetric flow at STP

Volumetric flow:=
$$\frac{\text{Qventmol} \cdot \left(22.4 \frac{\text{L}}{\text{mol}}\right)}{1000 \frac{\text{L}}{\text{m}^3}}$$
Volumetric flow=
$$15.567 \frac{\text{m}^3}{\text{min}}$$

(approxim. 550 SCFM)

Henry's Law

This is an example of how the Henry's Law constant is corrected for different operating temperatures. The example is for Aroclor 1016 at 50°C.

Henry's Law constants are given in a variety of units. The U.S. Army Corps of Engineers gives constants in units "atm-m ³/mol", while Sanders gives units of "mol/dm³-atm", where 1m = 10 dm. The unit used in this PCB analysis is "atm", which is corrected for the molarity of the solution.

The U.S. Army Corps of Engineers gives a Henry's Law constant of 3.3x10⁻⁴ atm-m³/mol. To convert this to mol/dm³-atm (for use with temperature correction factor from Sander):

Convert to dm:

$$dm := 1m \cdot 10^{-1}$$

$$K_{H1} := K_H \cdot \left(\frac{1m}{10dm}\right)^3$$

$$K_{H1} = 3.03 \frac{mol}{dm^3 \cdot atm}$$

A temperature correction factor is given in Sander:

$$K_{\text{HT}} = K_{\text{H}} \cdot e^{\left[\frac{-\Delta \text{solnH}}{R} \cdot \left(\frac{1}{T} - \frac{1}{T_{\text{ref}}}\right)\right]}$$

 $\frac{-\Delta solnH}{R}$ is given in Sander. An average of +7400 is used for Aroclor 1016

$$\mathbf{K}_{50} := \mathbf{K}_{H1} \cdot \mathbf{e}^{\left[7400 \cdot \left[\left(\frac{1}{50+273}\right) - \left(\frac{1}{25+273}\right)\right]\right]}$$

$$K_{50} = 0.443 \frac{\text{mol}}{\text{dm}^3 \cdot \text{atm}}$$

To convert this to atm, use equation from Sander (which uses the solution molarity, which is the same as water molarity):

$$K_{\rm H}\left(\frac{\rm mol}{\rm dm^3 \cdot atm}\right) \cdot {\rm H}(\rm atm) = 55.3$$

$$H(atm) = \frac{55.3}{K_{H}\left(\frac{mol}{dm^{3} \cdot atm}\right)}$$

 $H(atm) := 126 \cdot atm$

Note that the ambient value is :

$$\frac{55.3}{3.03} = 18.251$$
 atm

242-A EVAP CA-1



x: mol fraction PCB, liquid phase y: mol fraction PCB, gas phase

 $x_1Q_1+y_{airleak1}Q_{airleak1} = y_3Q_3+x_2Q_2$

y_{airleak1}=0 (no PCB in air)

Calculate x_1Q_1 (molar feed rate of PCB)

Feed rate = 60 gal/min

Feed PCB conc. = 0.2 μ g/L Feed density = 1.02 kg/L

Feed PCB massflow Q_{1(mass)} = 231.6kg/min Q_{1(molar)} = 12869 mol/min

$$\mu := 1 \cdot 10^{-6}$$

Feed_{conc} :=
$$0.2 \frac{\mu \cdot g}{L}$$

Feed_{density} :=
$$1.02 \frac{\text{kg}}{\text{L}}$$

$$PCB_{conc} := \frac{Feed_{conc}}{Feed_{density}}$$

$$PCB_{conc} = 0.196 \frac{\mu \cdot g}{kg}$$

$$Q_{1\text{mass}} \coloneqq 231.6 \frac{\text{kg}}{\text{min}}$$

$$PCB_{\text{rate}} \coloneqq \frac{(PCB_{\text{conc}}) \cdot (Q_{1\text{mass}})}{\left(1000000 \frac{\mu \cdot g}{\text{gm}}\right)}$$

$$PCB_{\text{rate}} = 4.541 \times 10^{-5} \frac{\text{gm}}{\text{min}}$$

Converting to mol/min

$$Q_{1molar} := 12869 \frac{mol}{min}$$

$$PCB_{rate2} \coloneqq \frac{PCB_{rate}}{258 \cdot \frac{gm}{mol}}$$
$$PCB_{rate2} = 1.76 \times 10^{-7} \frac{mol}{min}$$

$$PCB_{rate2} = x_1Q_1$$

$$x_1 = x_1Q_1/Q_1$$

$$x_1 := \frac{PCB_{rate2}}{Q_{1molar}}$$

$$x_1 = 1.368 \times 10^{-11} \quad (unitless)$$

P := 60 torr (from operating data)

Converting to atmospheres

$$P_{atm} := \frac{60torr}{760\frac{torr}{atm}}$$

 $P_{atm}=0.079atm$

 $H_1 := 126atm$ (at 50°C) (See section on Henry's Law)

$$\mathrm{Q}_2 \coloneqq 2650 \frac{mol}{min}$$

$$Q_3 := 10221 \frac{\text{mol}}{\text{min}}$$

Henry's Law:

$$y_3P = x_2H$$
 or $x_2 = y_3P/H$
 $x_1Q_1 = x_2Q_2+y_3Q_3$
 $x_1Q_1 = y_3(PQ_2/H + Q_3)$

$$y_{3} := \frac{x_{1} \cdot Q_{1molar}}{\left(\frac{P_{atm} \cdot Q_{2}}{H_{1}} + Q_{3}\right)}$$

$$y_3 = 1.722 \times 10^{-11}$$

$$PCB_{vent} := y_3 \cdot Q_3$$

(PCB to vent)

$$PCB_{vent} = 1.76 \times 10^{-7} \frac{\text{mol}}{\text{min}}$$

Massrate := PCB_{vent} $\cdot \left(258 \frac{\text{gm}}{\text{mol}}\right)$

Massrate = $4.54 \times 10^{-5} \frac{\text{gm}}{\text{min}}$ $x_2 := \frac{y_3 \cdot P_{\text{atm}}}{H_1}$ $x_2 = 1.08 \times 10^{-14}$ PCB_{slurry} := $x_2 \cdot Q_2$ PCB_{slurry} = $2.86 \times 10^{-11} \frac{\text{mol}}{\text{min}}$ Slurrymassflow := PCB_{slurry} · $\left(258 \frac{\text{gm}}{\text{mol}}\right)$ Slurrymassflow = $7.38 \times 10^{-9} \frac{\text{gm}}{\text{min}}$ (PCB to slurry)

 $DF := \frac{x_1 \cdot Q_{1 \text{ molar}}}{x_2 \cdot Q_2}$

DF = 6156.74

%volatized := $\frac{y_3 \cdot Q_3}{x_1 \cdot Q_{1molar}} \cdot 100$

%volatized = 99.984%

EC-1 Condenser



Define Temperature Unit

 $degC \equiv 1$

Kelvin to Celsius:	c(k) := (k - 273.15)	c(293.15) = 20 degC
Celsius to Kelvin:	$k(c) := (c + 273.15) \cdot K$	k(20) = 293.15K

Solve similar to CA-1 using mass balance and Henry's Law.

$$y_{3} \cdot Q_{3} = x_{4} \cdot Q_{4} + y_{5} \cdot Q_{5}$$

$$y_{3} := 1.72 \cdot 10^{-11}$$

$$Q_{3} := 1022 \cdot \frac{\text{mol}}{\text{min}}$$

$$y_{3} \cdot Q_{3} = 1.76 \times 10^{-7} \cdot \frac{\text{mol}}{\text{min}}$$

$$Q_{4} := 10219 \cdot \frac{\text{mol}}{\text{min}}$$

$$Q_{5} := 1.364 \cdot \frac{\text{mol}}{\text{min}}$$

$$P := 0.105 \text{atm}$$

$$P := 0.105 \text{atm}$$

$$T := c(313.15)$$

$$T = 40 \text{ degC}$$

$$H := 61 \cdot \text{atm}$$

$$At \ 40^{\circ}\text{C}.$$

As before:

$$y_5 := \frac{y_3 \cdot Q_3}{\left(\frac{P \cdot Q_4}{H} + Q_5\right)}$$
 $y_5 = 9.28 \times 10^{-9}$

$$mw := 258 \frac{gm}{mol}$$
Molecular weight $y_5 \cdot Q_5 = 1.27 \times 10^{-8} \frac{mol}{min}$ PCB mol rate, vent. $y_5 \cdot Q_5 \cdot mw = 3.26 \times 10^{-6} \frac{gm}{min}$ PCB mas rate, vent.

 $x_4 = 1.6 \times 10^{-11}$

DF = 1.08

%volatalized = 7.2%

$$x_4 := \frac{y_5 \cdot P}{H}$$

 $x_4 \cdot Q_4 = 1.63 \times 10^{-7} \frac{\text{mol}}{\text{min}}$ PCB mol rate, condensate. $x_4 \cdot Q_4 \cdot \text{mw} = 4.21 \times 10^{-5} \frac{\text{gm}}{\text{min}}$ PCB mass rate, condensate.

$$DF := \frac{y_3 \cdot Q_3 \cdot mw}{x_4 \cdot Q_4 \cdot mw}$$

%volatalized := $\frac{y_5 \cdot Q_5 \cdot mw}{y_3 \cdot Q_3 \cdot mw}$

$$ppm_{vol} := y_5 \cdot 10^6$$
 $ppm_{vol} = 9.28 \times 10^{-3}$

EC-2 Condenser



Define Temperature Unit

 $degC \equiv 1$

Kelvin to Celsius:	c(k) := (k - 273.15)	$c(293.15) = 2 \times 10^1 \text{ degC}$
Celsius to Kelvin:	$k(c) := (c + 273.15) \cdot K$	$k(20) = 2.93 \times 10^2 \mathrm{K}$

Solve similar to previous examples.

As before:

$$y_8 = \frac{y_6 \cdot Q_6}{\left(\frac{P \cdot Q_7}{H} + Q_8\right)}$$
 and $x_7 = \frac{y_8 \cdot P}{H}$

P := 0.61 atm Assumption that J-EC1-1 pulls 70% of the vacuum. It is the larger jet.

 $T := c(323.15) T = 5 \times 10^{1} degC Assumption$ $H := 126 atm At 50^{\circ}C.$ $y_{5} := 9.28 \cdot 10^{-9}$ $Q_{5} := 1.364 \frac{mol}{min}$ $y_{5} \cdot Q_{5} = 1.27 \times 10^{-8} \frac{mol}{min}$ $Q_{6} := 292 \cdot \frac{mol}{min}$ $Q_{7} := 254 \frac{mol}{min}$

 $y_{steam1} := 0$

 $Q_8 := 37.5 \cdot \frac{\text{mol}}{\text{min}}$ $y_6 \cdot Q_6 = y_5 \cdot Q_5 + y_{inbleed1} \cdot Q_{inbleed1} + y_{steam1} \cdot Q_{steam1}$ $y_{inbleed1} := 0$ $y_6 := \frac{y_5 \cdot Q_5}{O_6}$ $y_6 = 4.33 \times 10^{-11}$ Note that $y_5 \cdot Q_5 = y_6 \cdot Q_6 = 1.27 \times 10^{-8} \frac{\text{mol}}{10^{-8}}$ min $mw := 258 \cdot \frac{gm}{mol}$ Molecular weight $y_6 \cdot Q_6 \cdot mw = 3.27 \times 10^{-6} \frac{gm}{min}$ Mass Flow $y_8 := \frac{y_6 \cdot Q_6}{\left(\frac{P \cdot Q_7}{H} + Q_8\right)}$ $y_8 = 3.27 \times 10^{-10}$ $x_7 := \frac{y_8 \cdot P}{H}$ $x_7 = 1.58 \times 10^{-12}$ Vent $y_8 \cdot Q_8 = 1.23 \times 10^{-8} \frac{\text{mol}}{\text{min}}$ Molar Flow $y_8 \cdot Q_8 \cdot mw = 3.16 \times 10^{-6} \text{ gm}$ Mass Flow **Condensate** $x_7 \cdot Q_7 = 4.02 \times 10^{-10} \frac{\text{mol}}{\text{min}}$ Molar Flow $x_7 \cdot Q_7 \cdot mw = 1.04 \times 10^{-7} \frac{gm}{min}$ Mass Flow $DF := \frac{y_6 \cdot Q_6 \cdot mw}{x_7 \cdot Q_7 \cdot mw}$ = Feed Cond $DF = 3.15 \times 10^{1}$ %volatalized := $\frac{y_8 \cdot Q_8 \cdot mw}{y_6 \cdot Q_6 \cdot mw} = \frac{Vent}{Feed}$ %volatalized = 97%

EC-3 Condenser



Define Temperature Unit

 $degC \equiv 1$

Kelvin to Celsius:	c(k) := (k - 273.15)	c(293.15) = 20 degC
Celsius to Kelvin:	$k(c) := (c + 273.15) \cdot K$	k(20) = 293.15K

Equations are identical to EC-2.

$$y_{11} = \frac{y_9 \cdot Q_9}{\left(\frac{P \cdot Q_{10}}{H} + Q_{11}\right)}$$
 and $x_{10} = \frac{y_{11} \cdot P}{H}$

- P := 0.9 & the matrix and the matrix P := 0.9 and P := 0.9
- T := c(323.15) T = 50 degC
- H := 126 atm At 50°C.

 $y_8 := 3.27 \cdot 10^{-10}$

 $Q_8 := 37.5 \cdot \frac{\text{mol}}{\text{min}}$

$$y_8 \cdot Q_8 = 1.23 \times 10^{-8} \frac{\text{mol}}{\text{min}}$$

$$Q_9 := 293 \cdot \frac{\text{mol}}{\text{min}}$$

$$Q_{10} \coloneqq 258 \cdot \frac{\text{mol}}{\text{min}}$$

$$Q_{11} := 37.5 \cdot \frac{\text{mol}}{\text{min}}$$

 $y_9 \cdot Q_9 = y_8 \cdot Q_8 + y_{steam2} \cdot Q_{steam2}$ $y_{steam2} := 0$ $y_9 := \frac{y_8 \cdot Q_8}{Q_9}$ $y_9 = 4.19 \times 10^{-11}$ $mw := 258 \cdot \frac{gm}{mol}$ Molecular weight Note that $y_8 \cdot Q_8 = y_9 \cdot Q_9 = 1.23 \times 10^{-8} \frac{\text{mol}}{10^{-8}}$ $y_{11} := \frac{y_9 \cdot Q_9}{\left(\frac{P \cdot Q_{10}}{H} + Q_{11}\right)}$ $y_{11} = 3.1 \times 10^{-10}$ $\mathbf{x}_{10} \coloneqq \frac{\mathbf{y}_{11} \cdot \mathbf{P}}{\mathbf{H}}$ $x_{10} = 2.41 \times \ 10^{-12}$ Feed $y_9 \cdot Q_9 = 1.23 \times 10^{-8} \frac{\text{mol}}{\text{mol}}$ Molar Flow $y_9 \cdot Q_9 \cdot mw = 3.16 \times 10^{-6} \frac{gm}{min}$ Mass Flow Vent $y_{11} \cdot Q_{11} = 1.16 \times 10^{-8} \frac{\text{mol}}{10^{-8}}$ Molar Flow min $y_{11} \cdot Q_{11} \cdot mw = 3 \times 10^{-6} \frac{gm}{r}$ Mass Flow min Condensate $x_{10} \cdot Q_{10} = 6.23 \times 10^{-10} \frac{\text{mol}}{\text{min}}$ Molar Flow $x_{10} \cdot Q_{10} \cdot mw = 1.61 \times 10^{-7} \frac{gm}{min}$ Mass Flow $DF := \frac{y_9 \cdot Q_9 \cdot mw}{x_{10} \cdot Q_{10} \cdot mw}$ = Feed Cond DF = 19.7 %volatalized := $\frac{y_{11} \cdot Q_{11} \cdot mw}{y_9 \cdot Q_9 \cdot mw} = \frac{Vent}{Feed}$ %volatalized = 94.9%

C-100 Diptubes



Kelvin to Celsius:c(k) := (k - 273.15) $c(293.15) = 20 \deg C$ Celsius to Kelvin: $k(2\emptyset) = (298.25K \cdot 15) \cdot K$

The model of C-100 is in two parts: a diffusion emission and a diptube emission. The diptube emission is similar to others using Henry's Law.

$$x_{12} \cdot Q_{12} = x_4 \cdot Q_4 + x_7 \cdot Q_7 + x_{10} \cdot Q_{10}$$

Molar Flow

$$x4_{Q4} := 1.63 \cdot 10^{-7} \cdot \frac{\text{mol}}{\text{min}}$$

$$x7_{Q7} := 4.02 \cdot 10^{-10} \cdot \frac{\text{mol}}{\text{min}}$$

$$x10_{Q.10} := 6.23 \cdot 10^{-10} \cdot \frac{\text{mol}}{\text{min}}$$

$$x12_{Q12} := x4_{Q4} + x7_{Q7} + x10_{Q.10}$$

$$x12_{Q12} = 1.64 \times 10^{-7} \frac{\text{mol}}{\text{min}}$$

Mass Flow

$$mw := 258 \cdot \frac{gm}{mol}$$

$$x 12_{Q12} \cdot mw = 4.23 \times 10^{-5} \frac{gm}{min}$$
Molecular weight

Model the Diptubes

P := 0.98atm
 From Campaign 2001-01.

 T := c(318.15)
 T = 45 degC
 From Campaign 2001-01.

 H := 88 atm
 At 45°C.

$$Q_{DTin} := 0.126 \frac{mol}{min}$$
 Air

 $Q_{DTin} \cdot 0.0291 \frac{kg}{mol} = 3.67 \times 10^{-3} \frac{kg}{min}$
 Mass Rate

Calculate the moisture to add to DT_{air} . At 45 °C, from Perry's, there is 0.0654 (kg H₂O)/(kg air). Moisture is 3.67x10⁻³ kg/min (0.0654 (kg H₂O)/(kg air) = 2.4x10⁻⁴ kg H₂O/min. This converts to (molar):

moisture :=
$$\frac{2.4 \ 10^{-4} \cdot \frac{\text{kg}}{\text{min}}}{18 \cdot \frac{\text{gm}}{\text{mol}}}$$
 moisture = $0.0133 \frac{\text{mol}}{\text{min}}$
 $Q_{\text{DTout}} := Q_{\text{DTin}} + \text{moisture}$ $Q_{\text{DTout}} = 0.139 \frac{\text{mol}}{\text{min}}$

 $Q_{13} := 10731 \cdot \frac{\text{mol}}{\text{min}}$

 $y_{DTout} = 1.37 \times 10^{-9}$

$$y_{DTout} \coloneqq \frac{x12_{Q12}}{\left(\frac{P \cdot Q_{13}}{H} + Q_{DTout}\right)}$$

Vent

$$y_{DTout} \cdot Q_{DTout} = 1.91 \times 10^{-10} \frac{mol}{min}$$
 Molar Flow

 $y_{DTout} \cdot Q_{DTout} \cdot mw = 4.93 \times 10^{-8} \frac{gm}{min}$ Mass Flow

$$x_{13} := \frac{y_{DTout} \cdot P}{H}$$
 $x_{13} = 1.53 \times 10^{-11}$

Condensate to LERF

$x_{13} \cdot Q_{13} = 1.64 \times 10^{-7} \frac{\text{mol}}{\text{min}}$		Molar Flow
$x_{13} \cdot Q_{13} \cdot mw = 4.23 \times 10^{-5} \frac{gm}{min}$		Mass Flow
$DF := \frac{x_{12}Q_{12}}{x_{13} \cdot Q_{13}}$	= Feed rate Cond rate	DF = 1.0012

%volatalized :=
$$\frac{\text{y}_{DTout} \cdot \text{Q}_{DTout} \cdot \text{mw}}{\text{x}_{12}\text{Q}_{12} \cdot \text{mw}} = \frac{\text{Vent rate}}{\text{Feed rate}}$$
 %volatalized = 0.12%

c(293.15) = 20 degC

C-100 Diffusion

Define Units

 $degC \equiv 1$

Kelvin to Celsius: Celsius to Kelvin:

k(2))=(298.25K.15)·K

c(k) := (k - 273.15)

 $\operatorname{scfm} = \frac{\operatorname{ft}^3}{\min}$

 $\mu g \equiv \frac{gm}{10^6}$

The diffusion rate is given by $m = J \cdot A$

Where: m = mass rate (gm/min) J = Diffusion flux (gm/cm² sec)A = Surface Area

J is determined by the formula $J = K \cdot \left(c - \frac{c_{air}}{H}\right)$

Where: K = overall transfer rate (cm/sec) c = concentration in liquid (gm/cm³) c_{air} = concentration in air (gm/cm³) H = Henry's law (dimensionless version)

K is determined by the formula $K = \frac{k_g \cdot k_l}{k_g + k_l \cdot H}$

Where: k_{q} = gas phase diffusion (cm/sec) k₁ = liquid phase diffusion (cm/sec) H = Henry's law (dimensionless version)

The gas diffusion is the velocity in the vapor space (since airflow is much greater than natural diffusion). The liquid phase is determined by the formula:

$$k_l = \sqrt{\frac{D \cdot v}{h}}$$

Where:

v =

h = height of liquid in tank

D is determined by the correlation $D = \frac{13.2610^{-5}}{\mu^{1.14} \cdot v^{0.589}}$

Where: μ = viscosity (cp) v = specific molar volume, 247.3 cm³/mol

D = diffusion (cm²/sec)

The calculation consists of the following steps:

- 1) Calculate k_g using air velocity in tank
- 2) Calculate D using assumed viscosity
- 3) Calculate k₁ using a water velocity, D and h
- 4) Calculate K from k_g and k_I
- 5) Calculate J from K (assume $c_{air} = 0$)
- 6) Calculate m from J and tank surface area (A)
- 1) For air velocity, use airflow in tank divided by surface area, A.

$$d := 4.3 \text{ m}$$
Tank diameter per RCRA permit.

$$A := \frac{\pi}{4} \cdot d^2$$

$$A = 1.45 \times 10^5 \text{ cm}^2$$
airflow := 150 scfm
airflow = 7.08 \times 10^4 \frac{\text{cm}^3}{\text{sec}}
Air inleakage
$$k_g := \frac{\text{airflow}}{A}$$

$$k_g = 0.487 \frac{\text{cm}}{\text{sec}}$$
Air velocity
$$\mu := 0.641 \text{ cP}$$
At 45°C for H₂O (Literature)
$$v := 247.3 \frac{\text{cm}^3}{\text{mol}}$$

$$D := \frac{13.2610^{-5}}{\mu^{1.14} \cdot v^{0.589}} \cdot \frac{\text{cm}^2}{\text{sec}}$$

$$D = 8.57 \times 10^{-6} \frac{\text{cm}^2}{\text{sec}}$$

Application for Risk-Based Disposal Approval for Polychlorinated Biphenyls Hanford Site Liquid Waste Processing Facilities

2)

- 3) v: the volumetric flow divided by the surface area; there is no agitation in the tank.
 - $\begin{array}{ll} Q_{12}\coloneqq 193 \cdot \frac{kg}{\min} & \text{Mass flow into the tank} \\ \rho \coloneqq 1.0 \cdot \frac{kg}{L} & \text{Density of this flow} \\ \text{volumetric}_{flow}\coloneqq \frac{Q_{12}}{\rho} & \text{volumetric}_{flow} = 3.22 \times 10^3 \frac{\text{cm}^3}{\text{sec}} \\ \nu \coloneqq \frac{\text{volumetric}_{flow}}{A} & \nu = 0.0222 \frac{\text{cm}}{\text{sec}} \\ h \coloneqq 7.5 \cdot \text{ft} & h = 229 \text{cm} & \text{From operating experience at 50\% level.} \\ k_l \coloneqq \sqrt{\frac{D \cdot \nu}{h}} & k_l = 2.88 \times 10^{-5} \frac{\text{cm}}{\text{sec}} \end{array}$
- 4) Convert H to dimensionless: [H(dimensionless) = H (mol/dm³.atm)· (RT)]
 - $R := 0.08206 \frac{L \cdot atm}{mol \cdot K}$ $T := 318 \cdot K \qquad 45^{\circ}C$ $H := 3.0 \cdot \frac{mol}{L \cdot atm} \cdot R \cdot T \qquad H = 78$ $k_1 \cdot k_2 = 0$

$$K := \frac{k_l \cdot k_g}{k_g + \frac{k_l}{H}} \qquad \qquad K = 2.88 \times 10^{-5} \frac{\text{cm}}{\text{sec}}$$

Note that K is approximately equal to k₁. This means liquid phase diffusion is limiting.

5) Assume $c_{air}/H \ll c$, so J = Kc.

Determine c (concentration in liquid (gm/cm³)

$$x12_{Q12} := 1.64 \times 10^{-7} \cdot \frac{\text{mol}}{\text{min}}$$
PCB molar flow rate
$$mw := 258 \cdot \frac{\text{gm}}{\text{mol}}$$

$$x12_{Q12} \cdot mw = 4.23 \times 10^{-5} \frac{\text{gm}}{\text{min}}$$
PCM mass flow rate

volumetric
flow =
$$3.22 \times 10^3 \frac{\text{cm}^3}{\text{sec}}$$
Calculated in step 3 above. $c := \frac{x12_{Q12} \cdot \text{mw}}{\text{volumetric}_{flow}}$ $c = 2.19 \times 10^{-10} \frac{\text{gm}}{\text{cm}^3}$ $J := \text{K} \cdot \text{c}$ $J = 6.32 \times 10^{-15} \frac{\text{gm}}{\text{cm}^2 \cdot \text{sec}}$ $m := J \cdot \text{A}$ $m = 5.51 \times 10^{-8} \frac{\text{gm}}{\text{min}}$

Compare this with liquid mass rate of 4.24x10⁻⁵ gm/min.

$$DF := \frac{x12Q_{12} \cdot mw}{x12Q_{12} \cdot mw - m} \qquad DF = 1.0013$$

%volatalized :=
$$\frac{\text{m}}{(\text{x12}_{\text{Q12}} \cdot \text{mw})}$$
 %volatalized = 0.13%

Combined Dip Tube and Diffusion

6)

DipTubevent massrate :=
$$4.94 \, 10^{-8} \cdot \frac{\text{gm}}{\text{min}}$$

Combined_{DTDiffusion} := m + DipTubevent_{massrate}

Combined_{DTDiffusion} = $1.04 \times 10^{-7} \frac{\text{gm}}{\text{min}}$

 $\text{LERF}_{\text{rate}} = 4.22 \times 10^{-5} \frac{\text{gm}}{\text{min}}$

 $Liquid_{conc} = 2.19 \times 10^{-7} \frac{gm}{L}$

 $\text{LERF}_{\text{rate}} := (x 1 2_{Q12} \cdot \text{mw}) - \text{Combined}_{\text{DTDiffusion}}$

$$Liquid_{conc} := \frac{x12Q_{12} \cdot mw}{\frac{Q_{12}}{\rho}}$$

$$Liquid_{conc} = 0.22 \frac{\mu g}{L}$$

to LERF

$$C100_{ventconc} := \frac{Combined_{DTDiffusion}}{airflow} \qquad C100_{ventconc} = 2.46 \times 10^{-14} \frac{gm}{cm^3}$$

C-100 Vent Concentration

$$vent_{conc} := \frac{Combined_{DTDiffusion}}{airflow} \qquad vent_{conc} = 2.46 \times 10^{-14} \frac{gm}{cm^3}$$

Note: In step 5 assumed c _{air}/H << c.

 $c_{air} := 2.46 \, 10^{-14}$

 $\frac{c_{air}}{H} = 3.2 \times 10^{-16} \text{ which is } << 2.19 \times 10^{-10} \text{ gm/cm}^3.$

 $DF_{total} := \frac{x12_{Q12} \cdot mw}{(x12_{Q12} \cdot mw) - Combined_{DTDiffusion}}$

 $DF_{total} = 1.0025$

%volatalized := $\frac{\text{Combined}_{\text{DTDiffusion}}}{(x12_{\text{Q12}} \cdot \text{mw})}$

%volatalized = 0.25%



Application for Risk-Based Disposal Approval for Polychlorinated Biphenyls Hanford Site Liquid Waste Processing Facilities

min

min

 $EC123_{\text{overheads}} := 2.98 \, 10^{-6} \cdot \frac{\text{gm}}{\text{m}}$

 $EC123_{condensate} := 4.2410^{-5} \cdot \frac{gm}{10^{-5}}$

$\% EC123_{overheads} := \frac{EC123_{overheads}}{EC123_{feed}}$	%EC123 _{overheads} = 7%
$C100_{\text{feed}} := 4.24 10^{-5} \cdot \frac{\text{gm}}{\text{min}}$	
$C100_{vent} := 1.05 \cdot 10^{-7} \cdot \frac{gm}{min}$	
$C100_{\text{condesate}} := 4.23 \cdot 10^{-5} \cdot \frac{\text{gm}}{\text{min}}$	
$\%C100_{vent} := \frac{C100_{vent}}{C100_{condesate}}$	%C100 _{vent} = 0.25%

 $\text{Vessel}_{\text{vent}} = 3.08 \times 10^{-6} \frac{\text{gm}}{\text{min}}$

 $Vessel_{vent} = 5.14 \times 10^{-8} \text{ gm}$

 $CA1_{slurry\%} = 0.016\%$

 $\%_{cond} = 93\%$

To Vessel Vent

 $Vessel_{vent} := EC123_{overheads} + C100_{vent}$

Determine % slurry, condesate, vent

$$CA1_{slurry\%} := \frac{CA1_{slurry}}{CA1_{feedrate}}$$

$$%_{\text{cond}} \coloneqq \frac{\text{C100}_{\text{condesate}}}{\text{CA1}_{\text{feedrate}}}$$

$$\%_{\text{vent}} \coloneqq \frac{\text{Vessel}_{\text{vent}}}{\text{CA1}_{\text{feedrate}}}$$
 $\%_{\text{vent}} = 6.8\%$

Calculate slurry, condesate and vent concentrations

feed_{flow} :=
$$60 \cdot \frac{\text{gal}}{\text{min}}$$

Condensate Flow = boiloff + steam jet flow

Slurry flow = feed - boiloff

Boiloff is 81% (Campaign 01-01)

Slurry
flow := feed
flow (1 - 0.81)Slurry
flow = 11.4 $\frac{gal}{min}$ Condensate
flow := feed
flow := feed
flow $0.81 + (1.23 + 1.23) \cdot \frac{gal}{min}$ Condensate
flow = $51 \frac{gal}{min}$ Slurry
conc := $\frac{CA1_{slurry}}{Slurry_{flow}}$ Slurry
conc = $1.71 \times 10^{-4} \frac{\mu g}{L}$ Condensate
conc := $\frac{C10Q_{condesate}}{Condensate flow}$ Condensate
conc = $0.22 \frac{\mu g}{L}$

Note that the concentration of PCB in the PC is greater than the feed. This is because about 90% of the PCB is in the PC, but only 80% of the volume.

Vesselvent flow :=
$$550 \frac{\text{ft}^3}{\text{min}}$$
 from annual flow checks
Vent_{conc} := $\frac{\text{Vessel}_{\text{vent}}}{\text{Vesselvent}_{\text{flow}}}$ Vent_{conc} = $0.198 \frac{\mu g}{m^3}$