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ENGINEERING DATA TRANSMITTAL

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1	1	Cog. Eng. - M. W. Bowman	M.W. Bowman	6-13-96	R1-51						
1	1	Cog. Mgr. - D. Alison	D Alison	6-13-96	R1-51						
1	1	Env. - D. D. Bachand	MW Bowman for DDB per cc:mail	6-13-96	R1-51						
1	1	Evap. Proj. Eng. - B. H. Von Bargen	Brian Von Bargen	6/17/96	R1-43						

18. Mark Bowman Signature of EDT Originator Date 6-13-96	19. Authorized Representative for Receiving Organization Date	20. D Alison 6-13-96 Cognizant Manager Date	21. DOE APPROVAL (if required) Ctrl. No. ☐ Approved ☐ Approved w/comments ☐ Disapproved w/comments

Organic Emission Calculations for the 242-A Evaporator Vessel Vent System

M. W. Bowman
Westinghouse Hanford Company, Richland, WA 99352
U.S. Department of Energy Contract DE-AC06-87RL10930

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Abstract: This document contains historical calculations originally published in the *242-A Evaporator Dangerous Waste Permit Application*, DOE/RL-90-42, Rev 0. They are being released as a supporting document, along with brief explanatory information, to be used as a reference in Rev 1 of the permit application and in other supporting documents, such as the 242-A Evaporator Data Quality Objectives.

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JUN 21 1996
②
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Approved for Public Release

RECORD OF REVISION	(1) Document Number WHC-SD-WM-ES-380	Page 1 of 1

(2) Title
Organic Emission Calculations for the 242-A Evaporator Vessel Vent System

CHANGE CONTROL RECORD

(3) Revision	(4) Description of Change - Replace, Add, and Delete Pages	Authorized for Release	
		(5) Cog. Engr.	(6) Cog. Mgr. Date
Rev 0 RS	(7) Initial Release, EDT #615281, release on June 20, 1996.	N/A	N/A

A-7320-005 (08/91) WEF168

ORGANIC EMISSION CALCULATIONS
FOR THE 242-A EVAPORATOR
VESSEL VENT SYSTEM

WHC-SD-WM-ES-380

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1.0 INTRODUCTION

The 242-A Evaporator is a Treatment Storage or Disposal (TSD) unit which performs distillation of wastes with organic levels greater than 10 ppm. For such facilities, the requirements in 40 CFR 264 (EPA 1995) Subpart AA limiting vessel vent organic emissions apply.

Section 264.1032 of Subpart AA (EPA 1995) requires either 1) organic emissions from all affected vents not exceed 1.4 kg/hr (3 lbs/hr) and 2.8 Mg/yr (3.1 tons/yr), or 2) organic emissions from all affected vents are reduced by 95%. The Hanford Site has chosen to limit organic emissions for the entire site to less than 1.4 kg/hr (3 lbs/hr) and 2.8 Mg/yr (3.1 tons/yr), applied to all TSD units where Subpart AA is applicable.

Subpart AA states that engineering calculations or performance tests can be used to determine vessel vent organic emissions. At the 242-A Evaporator, engineering calculations are used to establish organic concentration limits on the waste which is processed.

To ensure the limits of Subpart AA are not exceeded, organics limits are established for the waste feed solution. If organic concentrations in the feed are below these established limits, the waste can be processed without exceeding an organic emission rate of 0.64 kg/hr (1.4 lbs/hr), which is less than the regulatory limit of 1.4 kg/hr (3 lbs/hr) to account for continuous operating time and potential emissions from other Hanford Site TSD units. The feed limits are based on equilibrium calculation models given in Appendix B. A brief discussion of the calculations is included here.

The equilibrium values in Appendix B can also be used to develop calculations of the amount of organic emissions during 242-A Evaporator campaigns. These calculations are given in Appendix C, along with emission calculations for campaigns 94-1 and 94-2.

Waste processed at the 242-A Evaporator does not exceed 10% organic by weight, so the requirements of 40 CFR 264 Subpart BB do not apply. The waste is mixed waste and is therefore exempted from the requirements in 40 CFR 264, Subpart CC.

2.0 ASSUMPTIONS USED IN THE ENGINEERING CALCULATIONS

There are two ventilation streams which combine to form the vessel vent stream for the 242-A Evaporator: the ventilation stream from the vapor-liquid separator (evaporator vessel), C-A-1, and the ventilation stream from condensate collection tank, TK-C-100. The vapor in the ventilation stream leaving C-A-1 is material boiled away in the evaporation process. The vapor passes through three condensers, E-C-1, E-C-2 and E-C-3, arranged in series. Water and organics condense to form process condensate which flows into TK-C-100. The ventilation stream leaving TK-C-100 is vapor drawn from the tank's vapor space, which is maintained under vacuum for contamination control.

The calculations for acetone in Appendix A show that organic emissions from TK-C-100 are about 1,000 times greater than those from C-A-1. The C-A-1 emissions are low because the vapor passes through three condensers in series, each removing about 90% of the organics. Tank TK-C-100 off-gas does not pass through the condensers before discharge.

The following assumptions were used in the calculations:

1. The maximum allowable emission rate of organics is 0.71 lbs/hr, which was determined by dividing the annual emissions limit of 3.1 tons/yr by the total hours in the year (assuming continuous operation). After the calculations were completed, the maximum allowable emission rate was adjusted to 1.4 lbs/hr (see below) and the feed limits were adjusted proportionately.

2. The emissions from vapor-liquid separator, C-A-1, are insignificant in comparison to emissions from TK-C-100 and are ignored in calculating the total 242-A Evaporator volatile organic emissions. The calculations for acetone in Appendix A show that emissions from TK-C-100 are about 1,000 times greater than those from C-A-1. The C-A-1 emissions are low because the vapor passes through three condensers, E-C-1, E-C-2, and E-C-3, in series with each removing about 90% of the organics. Tank TK-C-100 off-gas does not pass through the condensers before discharge.

3. The vapors exiting C-A-1 and TK-C-100 are in equilibrium with the aqueous solution (process condensate). This assumption maximizes the calculated organic emissions from the system.

4. The concentration of organics given in the Stream Specific Report are representative and can be used for determining activity coefficients. The maximum concentrations in the Stream Specific Report are multiplied by ten to provide an additional degree of conservatism to the calculations.

5. The following plant conditions are used:
    1) The flowrate exiting TK-C-100 is 150 ft3/min.
    2) The pressure in TK-C-100 is 750 mm Hg.
    3) The temperature in TK-C-100 is 75°C (348°K). (Note - organic emissions are very temperature sensitive. 75°C is conservative - the typical operating temperature is around 40°C).

3.0 DESCRIPTION OF ENGINEERING CALCULATIONS

Engineering calculations for organic emissions are based on the vapor-liquid equilibrium equation:

$$y_i P_T = x_i \gamma_i P_i^* \qquad \text{Equation 1}$$

where:
y_i = vapor phase mole fraction of constituent i
P_T = total system vapor pressure (750 mm Hg in TK-C-100)
x_i = liquid phase (process condensate) mole fraction of constituent i
γ_i = liquid phase activity coefficient for constituent i
P^*_i = vapor pressure of pure constituent i at system temperature

The following engineering calculations were performed in Appendix B for each constituent:

1. The value of the activity coefficient, γ_i, is determined using correlation parameters available in literature and the concentration of the constituent in the process condensate given in the Stream Specific Report.

2. Vapor pressure, P^*_i, is determined based on empirical evaluations available in literature for each constituent and the temperature in TK-C-100.

3. The vapor phase mole fraction, y_i, is calculated using Equation 1. The values for the liquid phase mole fraction, x_i, are determined using the concentration of the constituent in the Stream Specific Report.

4. Using the vapor phase mole fraction, y_i, calculated in Step 3, the TK-C-100 emission rates are determined using the flowrate and molecular weight of the constituent.

5. Steps 1 - 4 are repeated for the average concentration, maximum concentration, and ten times the maximum concentration in the Stream Specific Report. The calculations are also repeated for 15, 30, 45, 60, and 75°C. The results for each constituent are printed in tables in Appendix B.

6. Given the maximum emission rate determined in Step 5 (which occurs at ten times the maximum concentration of the constituent in the Stream Specific Report and 75°C), a process condensate concentration limit is determined from the ratio of the calculated maximum emission rate and the emission limit of 0.71 lbs/hr.

7. The process condensate concentration limit is converted to a limit in the waste feed by addition of a correction factor "(R-1)/R", which adjusts the limits based on the campaign's planned boiloff rate (R is the ratio of feed flowrate to slurry flowrate). A typical operational value for R is two, i.e., the feed flowrate into the 242-A Evaporator is twice the slurry flowrate out. In this case, (R-1)/R is one-half, and the feed concentration limits are halved (e.g., twice as restrictive).

The feed tank limits are given in Appendix B for each constituent.

The limits calculated in Appendix B are based on an organic emission limit of 0.32 kg/hr (0.71 lbs/hr), which assumes continuous operation 365 days per year. After these calculations were completed, the *242-A Evaporator/Liquid Effluent Retention Facility Data Quality Objectives* (DQO, WHC 1995) determined that 365 days continuous operation per year is not a reasonable assumption. Six months (182 days) of operation each year was determined to be more realistic because the 242-A Evaporator must shut down during the year for time-consuming activities such as maintenance outages, candidate feed tank analysis, and establishing transfer routes for staging waste in the DSTs. The total operating time for the two campaigns in 1994 was 86 days. For this reason, the DQO analysis establishes the maximum allowable vessel vent organic emission, based on six months of operations, at 0.64 kg/hr (1.4 lbs/hr).

Table 1 gives the feed tank limits for 0.32 kg/hr (0.71 lbs/hr) and 0.64 kg/hr (1.4 lbs/hr) for each constituent given in Appendix B. The DQO analyzed the likelihood of these constituents being present in the feed and established limits for five compounds and required analysis for four addition compounds. The limits are presented in Table 2 and are included in the DQO and the Waste Analysis Plan.

The limits in Table 2 use the "sum-of-the-fractions" technique: a ratio of each contituent to its limit is determined; the sum of these ratios must be less than one for the waste to be acceptable for processing. Use of the "sum-of-the-fractions" technique allows separate limits to be established for each contituent while still meeting a total organic emission limit.

4.0 DETERMINING EMISSIONS FROM EVAPORATOR OPERATIONS

Using the information provided in Appendix B, it is possible to determine the vessel vent organic emission rate based on the organic concentrations in the 242-A Evaporator feed. The equation for emission is:

$$\dot{m}=\sum \dot{m}_i=\sum y_i\,(MW_i)\,n_{100} \qquad \text{Equation 2}$$

where:
$\dot{m}$ = total mass flowrate of organics in vessel vent stream
$\dot{m}_i$ = mass flowrate of constituent i in vessel vent stream
y_i = vapor phase mole fraction of constituent i
MW_i = molecular weight of constituent i
n_{100} = total mole flowrate in vessel vent stream

Substituting the value for y_i in equation 1 (above):

$$\dot{m}=\sum \dot{m}_i=\sum x_i\gamma_i\frac{P_i^*}{P_T}\,(MW_i)\,n_{100} \qquad \text{Equation 3}$$

where:
$\dot{m}$ = total mass flowrate of organics in vessel vent stream
$\dot{m}_i$ = mass flowrate of constituent i in vessel vent stream
x_i = liquid phase (process condensate) mole fraction of constituent i
γ_i = liquid phase activity coefficient for constituent i
P^*_i = vapor pressure of pure constituent i at system temperature
P_T = total system vapor pressure
MW_i = molecular weight of constituent i
n_{100} = total molar flowrate in vessel vent stream

The value of the liquid phase mole fraction in the process condensate, x_i, can be determined from the waste feed concentration by conservatively assuming the entire quantity of the organic constituent in the feed is transferred to the process condensate. Using flowsheet values for calculating the mole flowrate, n_{100}, and system vapor pressure, P_T, the following equation is derived in Appendix C:

$$\dot{m}_i(kg/hr) = 0.322\gamma_i P_i^*(atm) X_{Fi}(g/l) \qquad \text{Equation 4}$$

where:
$\dot{m}_i$ = mass flowrate of constituent i in vessel vent stream, kg/hr
γ_i = liquid phase activity coefficient for constituent i
P^*_i = vapor pressure of pure constituent i at system temperature, atm
X_{Fi} = feed concentration of constituent i, g/l

The value $0.322\gamma_i P^*_i$ can be determined using the values in Appendix B. This number, given for each compound in Table 1, serves as a "partition factor" for converting feed concentration or organic emission rate. This partition factor also represents the relative volatility of the compound. The greater the value of partition factor, the more volatile the compound.

The organic emissions can be determined by totalling the product of partition factor for each component and its concentration in the candidate feed tanks. Sample calculations for 242-A Evaporator Campaigns 94-1 and 94-2 are given in Appendix C.

5.0 REFERENCES

EPA 1995, 40 CFR 264, *Standards for Owners and Operators of Hazardous Waste Treatment, Storage, and Disposal Facilities.* Code of Federal Regulations, as amended.

WHC 1995, Von Bargen, B. H., *242-A Evaporator/Liquid Effluent Retention Facility Data Quality Objectives*, WHC-SD-WM-DQO-014, Rev 1. Westinghouse Hanford Company, Richland Washington.

APPENDIX A REFERENCES:

Pierotti, G. J., Deal, C. H., and Derr, E. L., "Activity Coefficients and Molecular Structure", *Ind. Eng. Chem.*, Vol 51, No. 1, pg 95 - 102, 1959.

Prausnitz, J. M., Lichtenthaler, R. N., and de Azevedo, E. G., *Molecular Thermodynamics of Fluid-Phase Equilibria*, Prentice-Hall, Inc., Englewood Cliffs, NJ, 1969.

Schreiber, L. B, and Eckert, C. A., "Use of Infinite Dilution Activity Coefficients with Wilson's Equation", *Ind. Eng. Chem., Process Des. Development*, Vol. 10, No. 4, pg 572 - 576, 1971.

APPENDIX B REFERENCES:

Felder, R. M., and Rousseau, R. W., *Elementary Principles of Chemical Processes*, John Wiley & Sons, Inc., New York, NY, 1978.

Prausnitz, J. M., Lichtenthaler, R. N., and de Azevedo, E. G., *Molecular Thermodynamics of Fluid-Phase Equilibria*, Prentice-Hall, Inc., Englewood Cliffs, NJ, 1986.

Reid, R. C., Prausnitz, J. M., and Poling, B. E., *The Properties of Gases and Liquids*, 4th edition, McGraw-Hill, Inc., New York, NY, 1987.

APPENDIX C REFERENCE:

DOE 1991, *242-A Evaporator Dangerous Waste Permit Application*, DOE/RL-90-42, Rev 0. U. S. Department of Energy, Richland Operations Office, Richland, WA.

TABLE 1

DATA FROM VESSEL VENT EMISSION CALCULATIONS

Constituent	MW_i (g/mol)	γ_i	P^*_i (atm)	Limit for 0.7 lb/hr (mg/L)	Limit for 1.4 lb/hr (mg/L)	Partition Factor: $0.322\gamma_i P^*_i$	Page No.
Acetone	58.1	11.5	1.82	87.2	174.4	6.74 X_{Fi}	B-10
Benzyl Alcohol	108	2.03E+3	4.99E-3	182	364	3.26 X_{Fi}	B-22
Butanal	72.1	96.9	0.997	18.8	37.6	31.1 X_{Fi}	B-35
1-Butanol	74.1	48.1	0.169	226	452	2.62 X_{Fi}	B-49
2-Butanone (Methyl Ethyl Ketone)	72.1	37.1	0.854	58.0	116	10.2 X_{Fi}	B-61
2-Butoxyethanol	118	592	0.0327	95.2	190.4	6.23 X_{Fi}	B-73
3,5-Dimethylpyridine	107	356	0.0403	129	258	4.62 X_{Fi}	B-87
Ethoxytriethylene glycol	178	7.39E+3	7.03E-4	355	710	1.67 X_{Fi}	B-109
2-Hexanone	100	437	0.100	41.6	83.2	14.1 X_{Fi}	B-123
Hexone (Methyl Isobutyl Ketone)	100	437	0.257	16.4	32.8	36.2 X_{Fi}	B-137
2-Pentanone	86.2	126	0.406	36.1	72.2	16.5 X_{Fi}	B-150
Phenol	94.1	370	0.0156	320	640	1.86 X_{Fi}	B-162

TABLE 1 (continued)

Constituent	MW_i (g/mol)	γ_i	P^*_i (atm)	Limit for 0.7 lb/hr (mg/L)	Limit for 1.4 lb/hr (mg/L)	Partition Factor: $0.322\gamma_i P^*_i$	Page No.
2-Propanol	60.1	10.0	0.743	247	494	2.39 X_{Fi}	B-174
Pyridine	79.1	11.5	0.263	609	1218	0.974 X_{Fi}	B-186
Tetrahyrofuran	72.1	96.6	1.32	14.4	28.8	41.1 X_{Fi}	B-206
Tetradecane	198	1.0	1.28E-3	1.43E+6	2.86E+6	4.12E-4 X_{Fi}	B-218
Tributyl Phosphate	266	1.0	0.181	1.01E+4	2.02E+4	5.82E-2 X_{Fi}	B-230
Tridecane	184	1.0	3.15E-3	5.84E+5	1.17E+6	1.01E-3 X_{Fi}	B-241

MW_i: molecular weight of component i (gm/mol)
γ_i: activity coefficient (dimensionless)
P^*_i: vapor pressure of pure component i (atm)
Limit for 0.7 lb/h: limit in (mg/L) for component i so organic emissions do not exceed 0.7 lb/hr
Limit for 1.4 lb/h: limit in (mg/L) for component i so organic emissions do not exceed 1.4 lb/hr
Partition Factor: $0.322\gamma_i P^*_i$: a factor for converting waste feed concentration of component i, X_{Fi}, in gm/l to vessel vent emissions in kg/hr
Page No: page number in Appendix B giving emission calculations.

TABLE 2

Candidate Feed Tank Limits for Vessel Vent Organic Discharge
(based on 1.4 lbs/hr limit)

Feed Constituent	Limit (mg/L)[1,2,3]
Acetone	174.4 x (R-1)/R
1-Butanol	452 x (R-1)/R
2-Butoxyethanol	190.4 x (R-1)/R
2-Butanone	116 x (R-1)/R
Tri-Butyl Phosphate	2.030 E+4 x (R-1)/R
2-Hexanone[3]	83.2 x (R-1)/R
2-Pentanone[3]	72.1 x (R-1)/R
Methyl Isobutyl Ketone[3]	32.8 x (R-1)/R
Tetrahydrofuran[3]	28.8 x (R-1)/R

[1] The limits are applied using the sum of the fraction technique:

$$\sum_{n=1}^{i} \left(\frac{Conc_n}{LIMIT_n} \right) \leq 1$$

where i is the number of organic constituents detected in analysis of the waste feed tank.

[2] R is the ratio of feed flowrate to slurry flowrate (typically R = 2).

[3] The DQO (WHC 1995) has not established limits for hexanone, pentanone, methyl isobutyl ketone and tetrahydrofuran, pending collection of additional data. If additional data determines that limits should be established for these constituents, the limits given would be the included in the DQO.

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APPENDIX A

ORGANIC EMISSION CALCULATIONS DISCUSSION AND COMPARISON TO MEASURED VALUES

Appendix A contains vapor-liquid equilibrium and mass balance calculations, performed by Westinghouse Environmental and Geotechnical Services, Inc., used to model the quantity of volatile organic compounds discharged from the 242-A Evaporator. Appendix A was included as Appendix 3E of the *242-A Evaporator Dangerous Waste Permit Application*, Revision 0 (DOE-RL 1992). Appendix A includes:

- Methodology for determining vapor-liquid equilibrium
- Calculations of vapor-liquid equilibrium for acetone and a comparision between calculated values for acetone and experimental values from literature
- Calculations of acetone concentrations and emissions from average, maximum and 10 X maximum concentrations in the process condensate
- Calculations of maximum acetone concentration in the process condensate so that 3.0 lb/hr is not exceeded in the vessel vent
- Calculations of maximum acetone concentration in the feed stream to ensure the slurry product is acceptable for land disposal
- Technical documentation used in performing the calculations.

Westinghouse Environmental & Geotechnical Services, Inc.

CALCULATION WORKSHEET

Page No. 1 of 30
Job No. 89-5060-ES Client/Project 242-A Part-B
Title: ORGANIC Emissions 242-A
Date: 8-90 by WG Richmond
Checked: Jon Perry 3/[illegible] by Jon Perry

Subject: Vapor Phase organic Emissions 242-A

Objective: Calculate Vapor Phase Organic Emissions From 242-A Vessel Vent System ~~and~~ Based On Condensate Composition Data and Vapor-liquid Equilbrium of acetone-water at Exit Conditions

1) Calculation of VLE

Ref A

- model VLE Using wilsons Equation For Activity coef
  ref Prausnitz Et al "Molecular Thermodynamics of Fluid Phase Equilibria" EQ 6.11-1-5 pp 234-237

Ref B

- and Determine Coefficents using technique described by Schreiber et al in USE of Infinite Dilution activity coefficents with wilsons Equation Ind Eng Chem Proc Des Dev V 10 #4, 1971 pp 572-576

Ref C

- Determine Infinite Dilution activity coefficents as described in:

  Activity Coef & Molecular Structure G J Pierotti et al Ind & Eng Chem V 51 #1, Jan 1959 pp 95-102 as updated by RC Reid et al The properties of Gases and liquids pp 290-296

Westinghouse Environmental & Geotechnical Services, Inc.

CALCULATION WORKSHEET

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Job No. 89-5010-ES Client/Project 242-A EVAP
Title: Emissions 242-A
Date: 8-90 by WB Richard
Checked: 3/8/91 by J. Perry

Ref D

Component Vapor Pressures

From RC Reid etal, Properties of liquids and gases pp 656-732

EQuations USED and Assumptions/SAMPlE Calculation

Vapor liquid EQuilibrium

$$P_t Y_i = X_i \gamma_i P_i$$

P_t - Total system vapor pressure

Y_i - Vapor Phase mol Fraction

X_i - liquid Phase mol Fraction

γ_i - Activity Coef liquid Phase

P_i - Vapor Pressure Component in Pure Phase at system Temperature

$$\ln \gamma_1 \overset{\gamma}{=} -\ln(X_1 + \Lambda_{12} X_2) + X_2 \left[\frac{\Lambda_{12}}{X_1 + \Lambda_{12} X_2} - \frac{\Lambda_{21}}{\Lambda_{21} X_1 + X_2} \right]$$

$$\ln \gamma_2 = -\ln(X_2 + \Lambda_{21} X_1) - X_1 \left[\frac{\Lambda_{12}}{X_1 + \Lambda_{12} X_2} - \frac{\Lambda_{21}}{\Lambda_{21} X_1 + X_2} \right]$$

Westinghouse Environmental
& Geotechnical Services, Inc.

CALCULATION WORKSHEET

Page No. 3 of 30
Job No. 89-5010-ES Client/Project 242-A
Title: Emissions 242-A
Date: 8-90 by WERichard
Checked: 3/8/91 by J. Perry

4) The AQueous Fraction of the Process Condensate is Essentially Pure water.

Basis: 1) Condensate results from Distillation
2) Analysis presented in stream specific Report WHC-SP-0342 Add 15

Equations

VLE: $P_t Y_i = X_i \gamma_i P_i$ Eq 1

Y_i - Vapor Phase mol fraction

X_i - liquid Phase mol fraction

γ_i liquid

P_t - Total System Pressure

P_i - Pure Component Vapor Pressure at system Temperature

Activity Coefficents -

$$\ln \gamma_1 = -\ln(x_1 + \Lambda_{12} X_2) + X_2 \left[\frac{\Lambda_{12}}{x_1 + \Lambda_{12} X_2} - \frac{\Lambda_{21}}{\Lambda_{21} x_1 + X_2} \right]$$

REF A
6.11-2

$$\ln \gamma_2 = -\ln(X_2 + \Lambda_{21} X_1 - X_1 \left[\frac{\Lambda_{12}}{X_1 + \Lambda_{12} X_2} - \frac{\Lambda_{21}}{\Lambda_{21} X_1 + X_2} \right]$$

REF A
6.11-3

Westinghouse Environmental
& Geotechnical Services, Inc.

CALCULATION WORKSHEET

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Job No. 89-5010-ES Client/Project 242-A

Title: Emissions 242-A

Date: 8-90 by WG Richnand

Checked: 3/8/91 by J Perry

Calculation of Λ_{2} & Λ_{12}

$\ln \gamma_1^{\infty} = -\ln(\Lambda_{12}) - \Lambda_{21} + 1$ Ref C 8-10.25

$\ln \gamma_2^{\infty} = -\ln(\Lambda_{21}) - \Lambda_{12} + 1$ Ref C 8-10.26

Where γ_1^{∞} & γ_2^{∞} are infinite Dilution activity Coefficents

let 1 Be Acetone & 2 Be Water

acetone

$\log \gamma_1^{\infty} = \alpha + \epsilon N_1 + \zeta\left(\frac{1}{N_1'} + \frac{1}{N_1''}\right) + \eta(N_1 - N_2)^2$ Ref C pp 298

$N_1 = 3$ $N_1' = 2$ $N_1'' = 2$

water – Ref C pp 295 (C)

$\log \gamma_2^{\infty} = \alpha + \epsilon N_2 + \zeta\left(\frac{1}{N_2'} + \frac{1}{N_2''} + \frac{1}{N_2'''}\right) + \theta\left(\frac{1}{N_1'} + \frac{1}{N_1''}\right)$

$N_2' = N_2'' = N_2''' = 0$ $N_1' = 2$ $N_1'' = 2$

Where:

N_1, N_2 – Total Number of Carbon Atoms ~~in~~ in molecules 1 & 2

N', N'', N''' – Number of Carbon atoms in respective Branches

and $\alpha, \epsilon, \zeta, \eta, \theta$ are as given in Table 8-17 Ref C

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Checked: 7/8/91 by J Peng

Table 8-17 REF C Provides Values for $\alpha, \epsilon, \zeta, \eta, \theta$ at 25, 60, and 100 °C upon Plotting all are found to have a linear relationship with temperature. To facilitate Calculations at Varying temperatures the three Values were regressed to give Equations for the adjustable parameters as a function of temperature. The Values used and the corresponding regression coefficients are given below:

Parameter = mT + b (T in Kelvin)

ACETone	25 °C 298 K	60 °C 333 K	100 °C 373 K	m	b
α	-1.475	-1.040	-0.621	1.1365E-2	-4.8484
ϵ	0.622	0.583	0.517	-1.4059E-3	1.044513
ζ	0.500	0.330	0.200	-3.9822E-3	1.676059
η	0	0	0	0	0
Water					
α	1.857	1.493	1.231	-8.3041E-3	4.306119
ϵ	0	0	0	0	0
ζ	0	0	0	0	0
θ	-1.019	-0.73	-0.557	6.117×10^{-3}	-2.816

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Job No. 90-5440-ES Client/Project 242-A & VAP

Title: Emissions 242-A

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Checked: 3/8/91 by J Perry

Calculation of P_i (APPENDIX A Ref C)
(pp 656 - 732)

ACETONE

$$\ln(P_{v1}/P_{c1}) = (1-x)^{-1}[Ax + Bx^{1.5} + Cx^3 + Dx^6]$$

$$x = 1 - T/T_{c1}$$

$P_{c1} = 47.0$ Bar A = -7.45514 C = -2.4396

$T_{c1} = 508.1$ K B = 1.20200 D = -3.35590

Valid From 259 K TO 508.1 K

WATER

$$\ln(P_2/P_{c2}) = (1-x)^{-1}[Ax + Bx^{1.5} + Cx^3 + Dx^6]$$

$$x = 1 - T/T_{c2}$$

A = -7.76451 C = -2.77580

$P_{c2} = 221.2$ Bar

$T_{c2} = 647.2$ K B = 1.45838 D = -1.23303

Valid ⇒ 275 K TO 647.2 K

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Sample Calculation

let $x_1 = 0.1$ (acetone concentration)

let T = 45°C ⇒ 378 K

1) Calculate Infinite Dilution activity Coefficents

ACETONE

$$\log(\gamma_{\phi}^{\infty}) = \alpha + \epsilon N_1 + \zeta\left(\frac{1}{N_1'} + \frac{1}{N_1''}\right) + \eta(N_1 - N_2)^2$$

$N_1 = 3 \quad N_1' = 2 \quad N_1'' = 2$

$\alpha = 1.7365E\text{-}2(318) - 4.8484 \quad = -1.2326$

$\epsilon = -1.4059E\text{-}3(318) + 1.044513 \quad = 0.59723$

$\zeta = -3.9822E\text{-}3(318) + 1.676059 \quad = 0.409122$

$\eta = 0 \quad = 0$

$$\log(\gamma_1^{\infty}) = -1.2326 + 0.59723(3) + 0.409122\left(\frac{1}{2} + \frac{1}{2}\right) =$$

$\gamma_1^{\infty} = 9.2934$

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WATER

$$\log(\gamma_2^{\infty}) = \alpha + \epsilon N_2 + \zeta\left(\frac{1}{N_2'} + \frac{1}{N_2''} + \frac{1}{N_2'''}\right) + \theta\left(\frac{1}{N_1'} + \frac{1}{N_1''}\right)$$

$\alpha = -8.3041E-3(318) + 4.30612 = 1.6642$

$\epsilon = 0 \qquad = 0$

$\zeta = 0 \qquad = 0$

$\theta = 6.117E-3(318) - 2.816 = -0\ 8.705\times10^{-1}$

$\log(\gamma_2^{\infty}) = 1.6642 + 0(\ ) + 0(\ )\ 0.9152\left(\frac{1}{2} + 1/2\right)$

$\gamma_2^{\infty} = 6.255$

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2) Calculate Λ_{12} & Λ_{21}

$$\ln \gamma_1^{\infty} = -\ln(\Lambda_{12}) - \Lambda_{21} + 1$$

$$\ln \gamma_2^{\infty} = -\ln(\Lambda_{21}) - \Lambda_{12} + 1$$

$$\ln(9.2934) = -\ln(\Lambda_{12}) - \Lambda_{21} + 1$$

$$\ln(5.6106) = -\ln(\Lambda_{21}) - \Lambda_{12} + 1$$

$\Lambda_{12} = 0.2058$ $\Lambda_{21} = 0.3537$

3) Calculate γ_1 & γ_2

$$\ln \gamma_1 = -\ln(x_1 + \Lambda_{12} x_2) + x_2 \left[\frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{\Lambda_{21} x_1 + x_2} \right]$$

$$\ln \gamma_1 = -\ln(0.1) + 0.2058 (0.9) + 0.9 \left[\frac{0.2058}{0.1 + 0.2058(0.9)} - \frac{0.3537}{.3537\,(0.1) + 0.9} \right]$$

$$\ln \gamma_1 = 1.56$$

$$\gamma_1 = 4.776$$

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Calculate γ_2

$$\ln \gamma_2 = -\ln(x_2 + \Lambda_{21} x_1) - x_1 \left[\frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{\Lambda_{21} x_1 + x_2} \right]$$

$$\ln \gamma_2 = -\ln(0.9 + 0.3537\,(0.1)) - 0.1 \left[\frac{0.2058}{0.1 + 0.2058(0.9)} - \frac{0.3537}{0.3537(0.1) + .09} \right]$$

$$\ln \gamma_2 = .032$$

$$\gamma_2 = 1.033$$

4) Calculate P_1 & P_2

$$\ln(P_1/P_{c1}) = (1-x)^{-1}\left[Ax + Bx^{1.5} + Cx^3 + Dx^6\right]$$

$$x = 1 - T/T_{c1} = 1 - 318/508.1 = 0.374$$

$$\ln(P_1/47.0) = 2.67\left[-7.45514(0.374) + 1.202(0.374)^{1.5} + -2.4396(0.374)^3 + 3.35590(0.374)^6\right]$$

$$\ln(P_1/47.0) = -4.2304$$

$$P_1 = 0.68366 \text{ Bar} = 512.79 \text{ mmHg}$$

Similarly: $P_2 = 71.97$ mmHg

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Calculate Y_1 ; Y_2 $T = 45°C$

$X_1 = 0.1$ $X_2 = 0.9$

$P_1 = 0.68366$ Bar $P_2 = 0.09595$ Bar

$\gamma_1 = 4.776$ $\gamma_2 = 1.033$

$Y_1 P = \gamma_1 x_1 P_1 = (4.776)(0.1)(0.68366) = 0.327$

$Y_2 P = \gamma_2 x_2 P_2 = (1.033)(0.9)(0.09595) = 8.92E-2$

$Y_1 P + Y_2 P = 4.16E-1$

$P(Y_1 + Y_2) = 0.416$ But $Y_1 + Y_2 = 1$ so $P = 0.416$

$Y_1 = 0.786$ $Y_2 = 0.214$

Similar Calculations Have been conducted for comparison with Tabulated Values (attached) and Graphs Prepared For comparison.

Data From 25°C Constant Temperature (Fig 1-4)
(Curve marked M Is measured, P-Predicted D-Difference)

Data From 1 ATM Constant Pressure (Fig 5-6)
M- measured P-Predicted D-Difference)

These Figures Verify modelling Used as they show small deviations

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Litterature Data ACETONE WATER System.

SYSTEM 32C

REFERENCE 17

(A) Acetone C_3H_6O (B) Water H_2O

Mole % in Liquid (A)	Mole % in Vapor (A)	Temp. °C	Pressure mm. Hg.
0.0	0.0	25.00	23.7
1.936	52.34		50.1
2.89	62.12		61.8
4.495	71.68		81.3
5.556	75.91		91.9
9.39	83.51		126.1
9.51	84.16		126.6
13.10	86.18		144.3
14.7	87.68		150.6
17.91	87.82		159.8
26.54	88.56		176.1
35.38	89.54		184.4
58.08	91.58		199.1
78.52	94.21		213.5
100.0	100.0		229.6

SYSTEM 32A

REFERENCE 167

(A) Acetone C_3H_6O (B) Water H_2O

Mole % in Liquid (A)	Mole % in Vapor (A)	Temp. °C	Pressure mm. Hg.
1.0	33.5	87.8	760
2.3	46.2	83.0	
4.1	58.5	76.5	
12.0	75.6	66.2	
26.4	80.2	61.8	
30.0	80.9	61.1	
44.4	83.2	60.0	
50.6	83.7	59.7	
53.8	84.0	59.5	
60.9	84.7	58.9	
66.1	86.0	58.5	
79.3	90.0	57.4	
85.0	91.8	57.1	

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Measured Values vs. Predicted Values Acetone-Water 25oC

Liquid (MF)	Predicted Vapor (MF)	Measured Vapor (MF)	Difference
0.000	0.000	0.000	0.000
.019	.576	.523	.052
.029	.658	.621	.037
.045	.735	.717	.018
.056	.765	.759	.006
.094	.824	.835	-.011
.095	.825	.842	-.016
.131	.851	.862	-.011
.147	.859	.877	-.018
.179	.870	.878	-.008
.265	.888	.886	.003
.354	.899	.895	.003
.581	.917	.916	.001
.785	.939	.942	-.003
1.000	1.000	1.000	0.000

Measured Values vs. Predicted Values Acetone-Water 25oC

Liquid (MF)	Predicted (mm Hg)	Measured (mm Hg)	Difference (mm Hg)
0.000	23.8	23.7	.1
.019	54.5	50.1	4.4
.029	66.8	61.8	5
.045	84.4	81.3	3.1
.056	94.2	91.9	2.3
.094	120.9	126.1	-5.2
.095	121.6	126.6	-5
.131	138.2	144.3	-6.1
.147	143.9	150.6	-6.7
.179	153.3	159.8	-6.5
.265	169.5	176.1	-6.6
.354	179.4	184.4	-5
.581	195.5	199.1	-3.6
.785	210.2	213.5	-3.3
1.000	231.1	229.6	1.5

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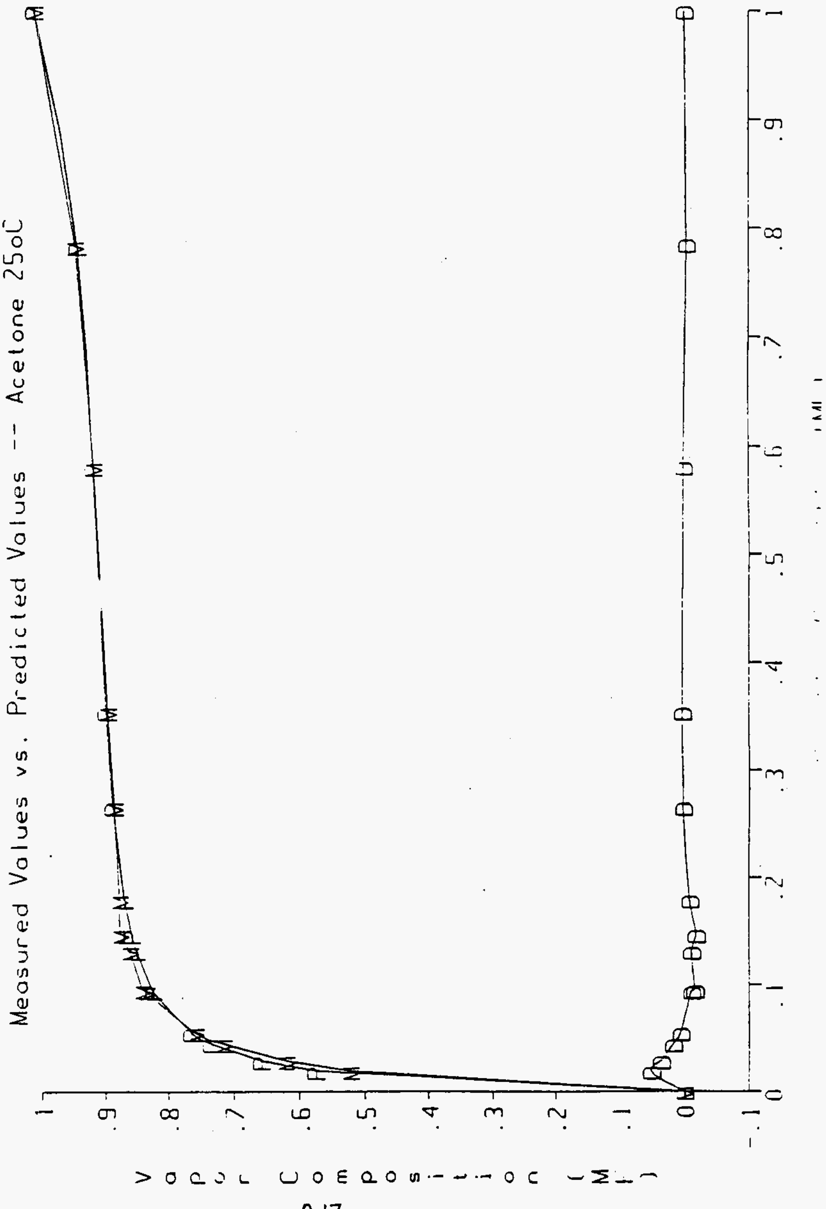
Measured Values vs. Predicted Values Acetone-Water 1 ATM

Liquid (MF)	Predicted Vapor (MF)	Measured Vapor (MF)	Difference
.010	.324	.335	-.011
.023	.502	.462	.040
.041	.621	.585	.036
.120	.773	.756	.017
.264	.832	.802	.030
.300	.839	.809	.030
.444	.859	.832	.027
.506	.867	.837	.030
.538	.871	.840	.031
.609	.881	.847	.034
.661	.889	.860	.029
.793	.915	.900	.015
.850	.930	.918	.012

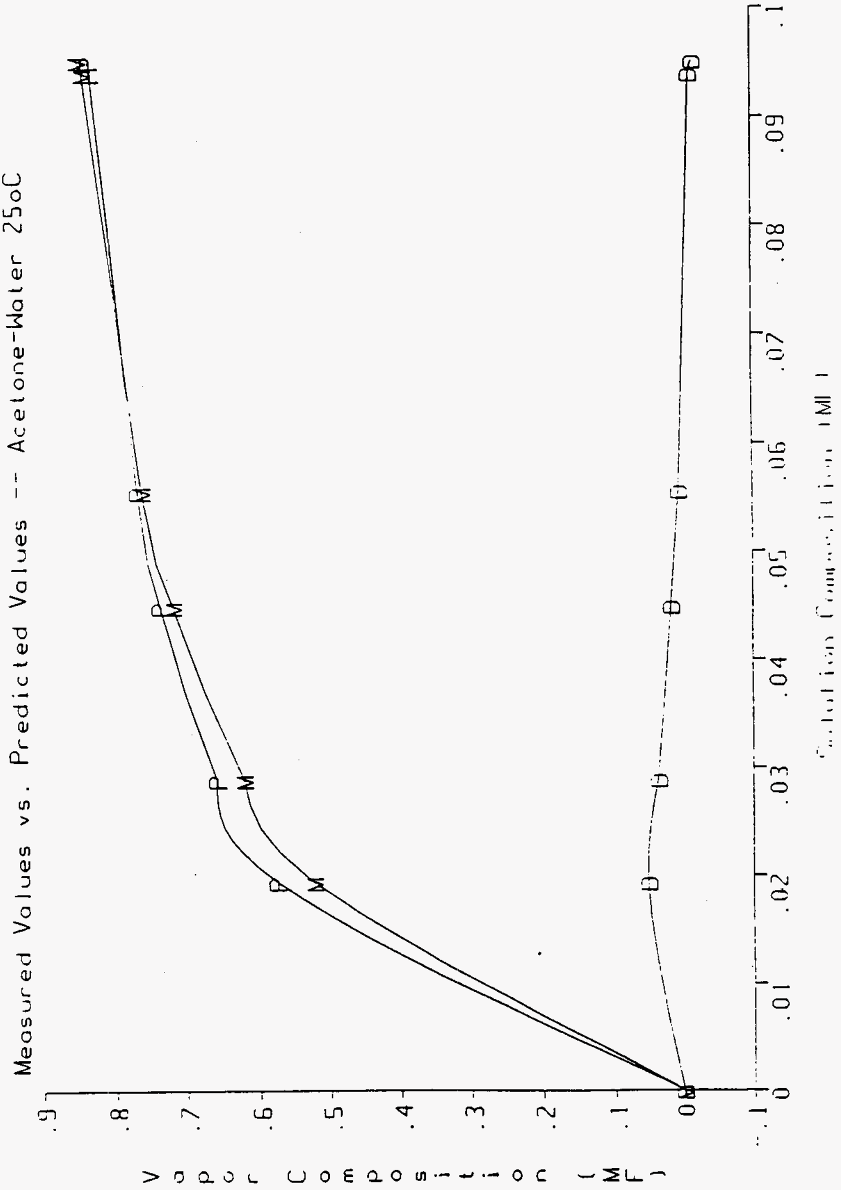
Measured Values vs. Predicted Values Acetone-Water 1 ATM

Liquid (MF)	Predicted (mm Hg)	Measured (mm Hg)	Difference (mm Hg)
.010	692.3	760	-67.7
.023	753	760	-7
.041	733.4	760	-26.6
.120	715.5	760	-44.5
.264	715.4	760	-44.6
.300	711.2	760	-48.8
.444	722.2	760	-37.8
.506	728.6	760	-31.4
.538	730.8	760	-29.2
.609	731.8	760	-28.2
.661	733.8	760	-26.2
.793	739.1	760	-20.9
.850	746.7	760	-13.3

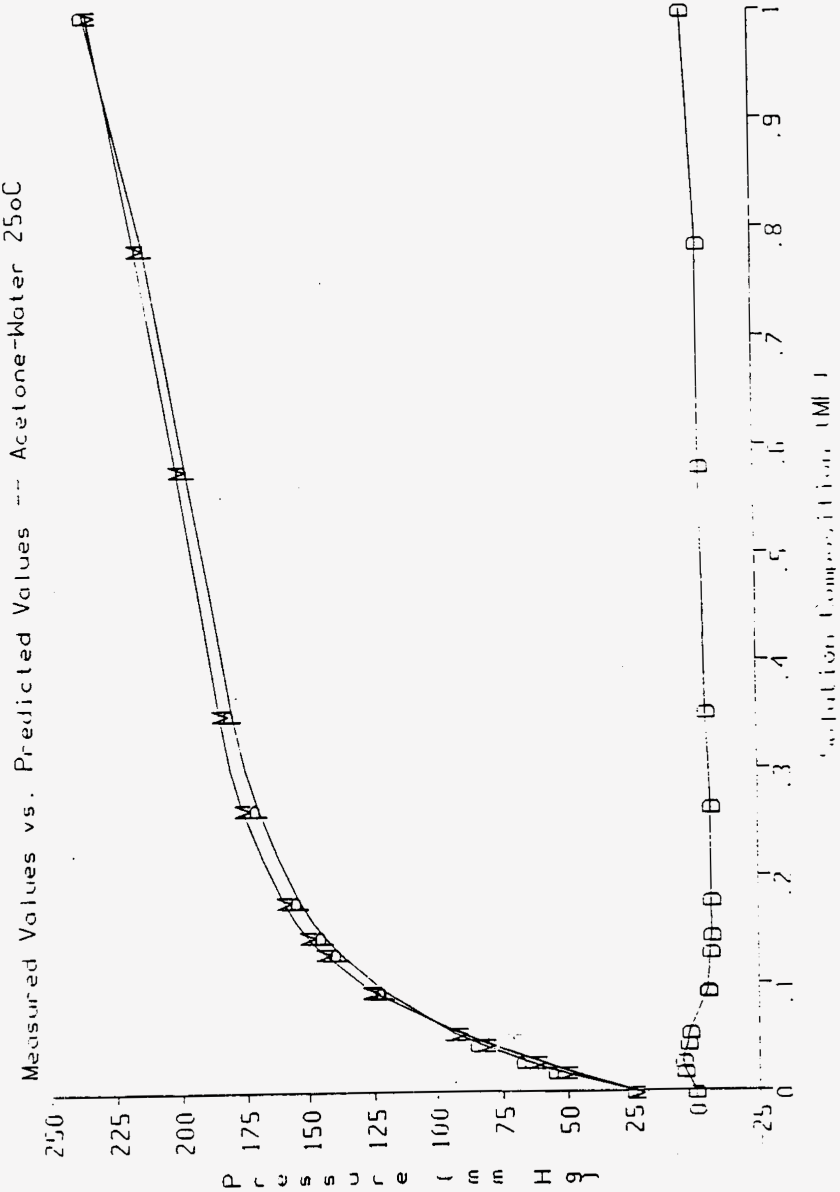
15-30


Measured Values vs. Predicted Values -- Acetone 25oC
Vapor Composition (Ml)
(Ml)
1
.9
.8
.7
.6
.5
.4
.3
.2
.1
0
-.1
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1
M
D
P

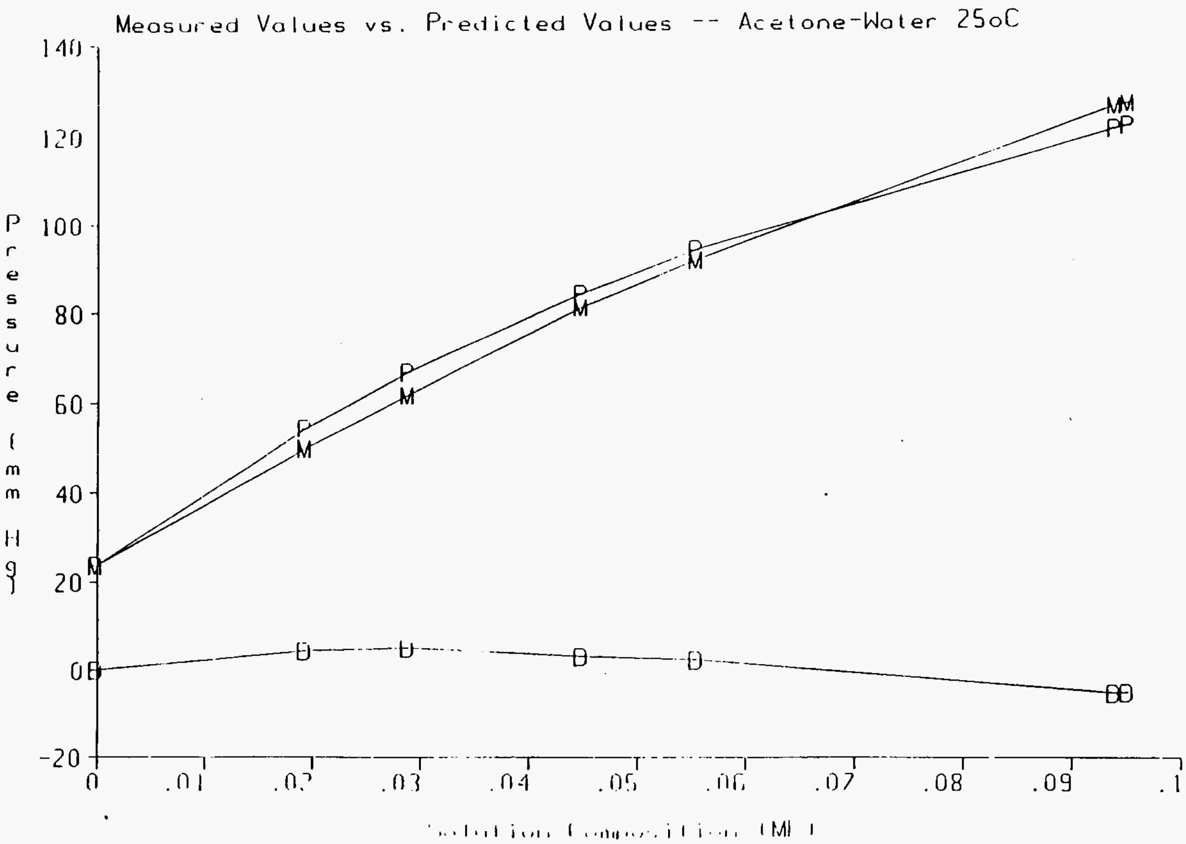
16-


Measured Values vs. Predicted Values -- Acetone-Water 25oC
Vapor Composition (MF)
Solution Composition (MF)
-.1
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
0
.01
.02
.03
.04
.05
.06
.07
.08
.09
.1
M
P
D

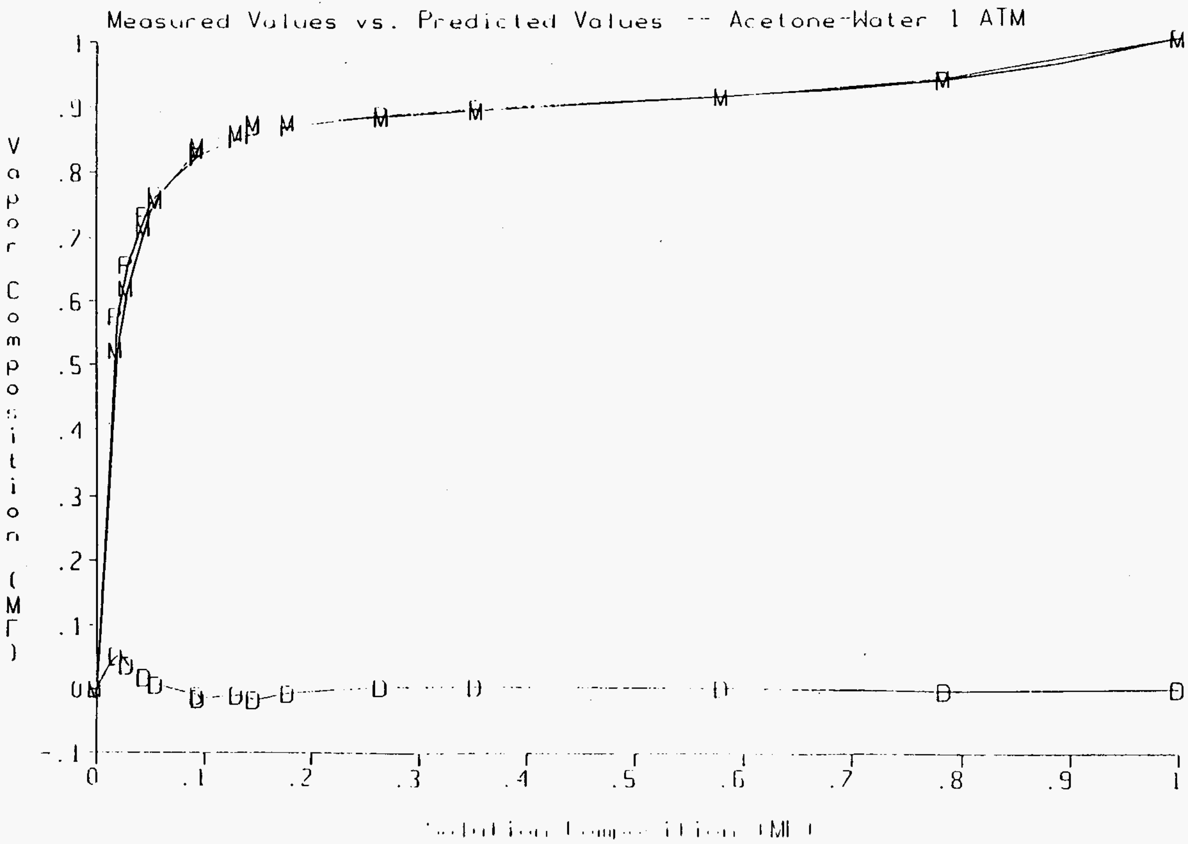
17 ;0

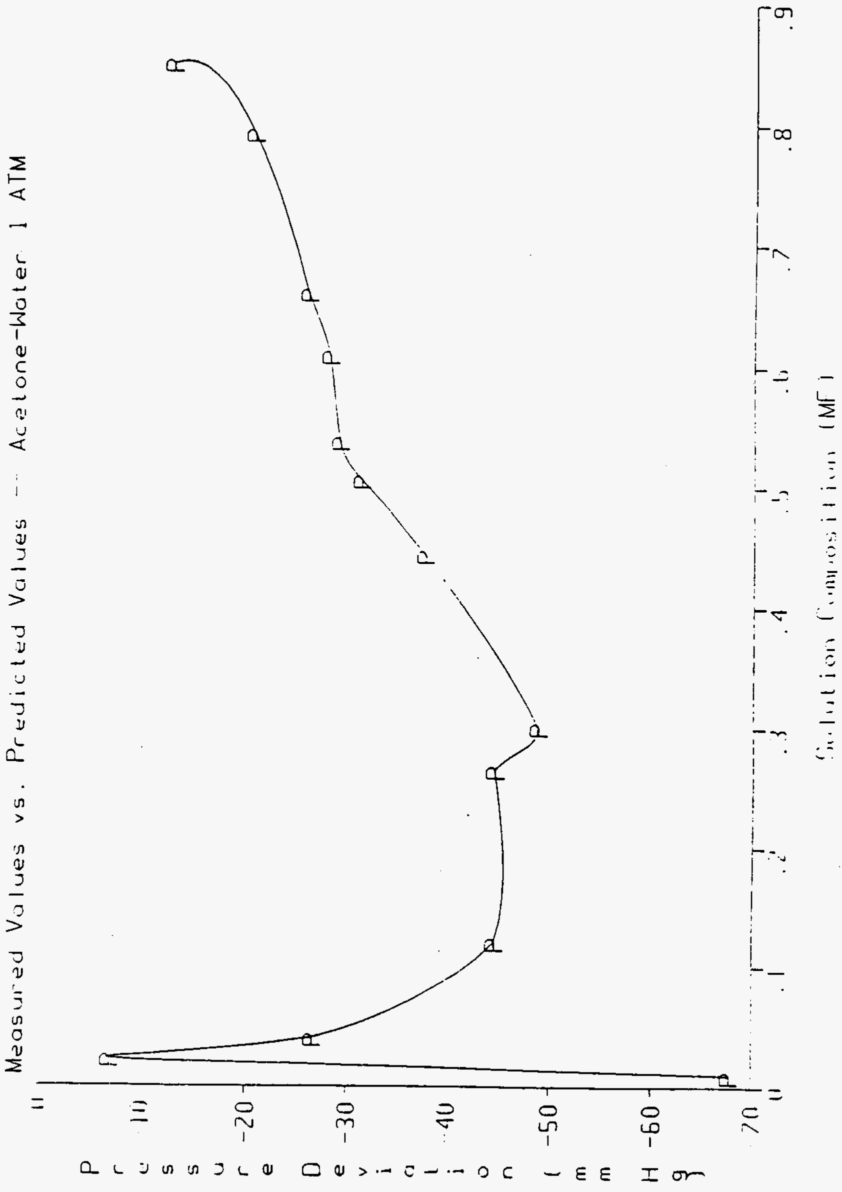

Measured Values vs. Predicted Values -- Acetone-Water 25oC
Pressure (mm Hg)
250
225
200
175
150
125
100
75
50
25
0
-25
Solution Composition (Mf)
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1
M
D

18- C


Measured Values vs. Predicted Values -- Acetone-Water 25oC
Pressure (mm Hg)
140
120
100
80
60
40
20
0
-20
0
.01
.02
.03
.04
.05
.06
.07
.08
.09
.1
Solution Composition (MF)
M
P
D
MM
PP
DD

19 30


Measured Values vs. Predicted Values -- Acetone-Water 1 ATM
Vapor Composition (MF)
Solution Composition (MF)
1
.9
.8
.7
.6
.5
.4
.3
.2
.1
0
-.1
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1
M
P
D


Measured Values vs. Predicted Values -- Acetone-Water 1 ATM
Pressure Deviation (mm Hg)
0
10
-20
-30
-40
-50
-60
70
Solution Composition (MF)
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
P
P
P
P
P
P
P
P
P
P
P
P

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Now That method and model for Equilibrium Calculations Has been Established we now need to model the evaporator system.

The Relevant stream In-flows and out flows and a general Flow Diagram are provided on Page 22.

Calculation method - Approach

Prepare 3 Cases:

Case I - Average Conditions

Case II - Highest observed Conditions

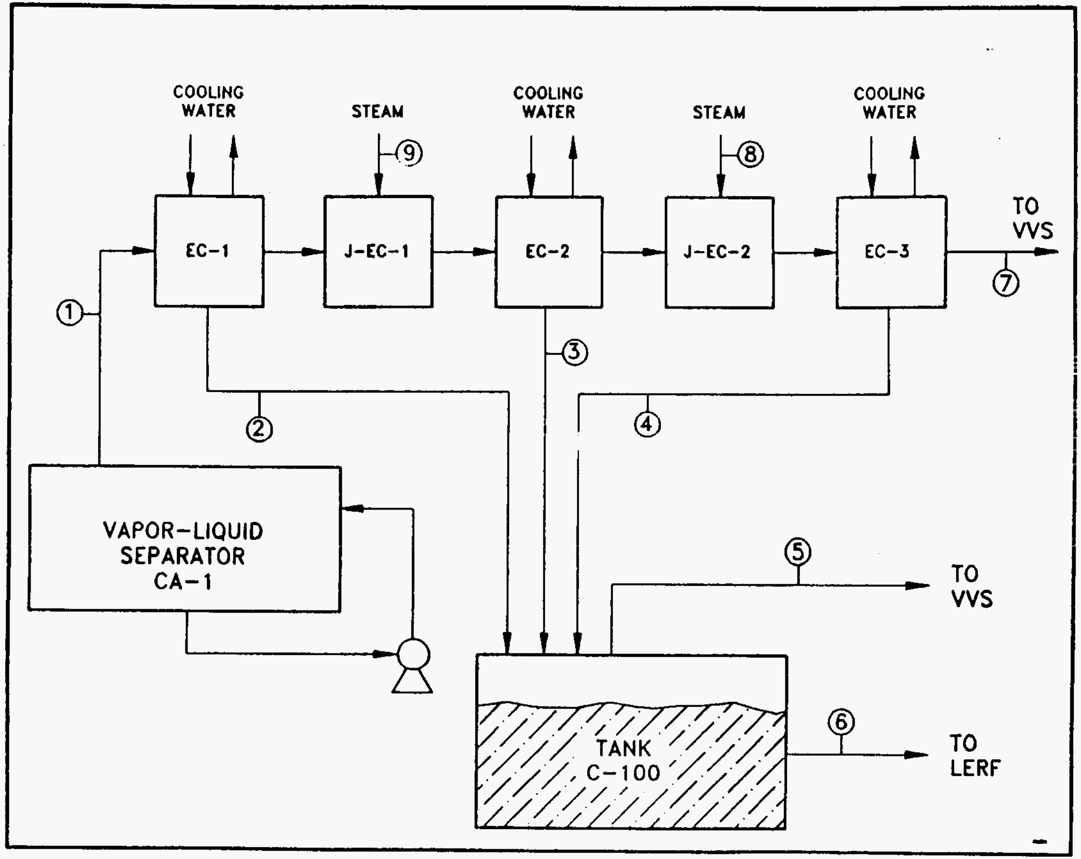
Case III - 10x Highest observed conditions

Evaluate Each Case for air Emissions from EC-3 ! C-100

Approach

① Calculate Vapor Phase concentration in Condenser EC-1 assuming Equilibrium with Process condensate at condenser temperature (use 5 Temperatures 15°C, 30°C, 45°C, 60°C, 75°C)

Take Process condensate Composition From stream specific Report


COOLING WATER
STEAM
⑨
COOLING WATER
STEAM
⑧
COOLING WATER
EC-1
J-EC-1
EC-2
J-EC-2
EC-3
TO VVS
⑦
①
③
②
④
VAPOR-LIQUID SEPARATOR CA-1
⑤
TO VVS
TANK C-100
⑥
TO LERF

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② Calculate Equilbrium of this phase with a condensate at the same temperature used in ① and assuming a pressure of 400 mm Hg.

Basis for Pressure Assumption -

EC-1 operates at ~60 Torr

EC-3 operates at ~ 750 Torr

Assume EC-2 splits the difference ~400 Torr

Balance of Vapor Phase in EC-2 & EC-3 is Air

③ Calculate Equilbrium in EC-3 as in step 2 with pressure = 750 Torr (6" wt)

Note: This approach is Conservative as it does not consider the water added by the steam jets which will serve to Further reduce Vapor phase concentrations and corresponding Emmissions

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by	JPerry

Average Process condensate Composition =

980 ppb acetone = 3.042E-7 MF Acetone

max Process Cond Composition

5,100 ppb Acetone = 1.583E-6 MF Acetone

10x Process Condensate Composition

51,000 ppb Acetone = 1.58E-5 MF Acetone

Condensor EC-1 Equilibrium Concentrations

Temperature	Condensate (MF)	Vapor (MF)	Pressure (mm Hg)
15	3.042E-7	2.622E-5	12.8
15	1.583E-6	1.364E-4	12.8
15	1.583E-5	1.362E-3	12.8
30	3.042E-7	2.269E-5	31.9
30	1.583E-6	1.181E-4	31.9
30	1.583E-5	1.179E-3	31.9
45	3.042E-7	2.014E-5	72
45	1.583E-6	1.048E-4	72
45	1.583E-5	1.047E-3	72
60	3.042E-7	1.829E-5	149.6
60	1.583E-6	9.515E-5	149.6
60	1.583E-5	9.505E-4	149.7
75	3.042E-7	1.694E-5	289.4
75	1.583E-6	8.812E-5	289.4
75	1.583E-5	8.804E-4	289.6

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Condensor EC-2 Equilibrium Concentration

T (°C)	x1 Condensate (MF)	y1 Vapor (MF)
15	1E-7	2.735E-7
15	4.929E-7	1.348E-6
15	6.857E-7	1.875E-6
30	8.786E-7	5.181E-6
30	1.071E-6	6.315E-6
30	1.264E-6	7.453E-6
45	1.457E-6	1.723E-5
45	1.65E-6	1.952E-5
45	1.843E-6	2.18E-5
60	2.036E-6	4.546E-5
60	2.229E-6	4.977E-5
60	2.421E-6	5.406E-5
75	2.614E-6	1.046E-4
75	2.807E-6	1.124E-4
75	3E-6	1.201E-4

Condensor EC-3 Equilibrium Concentrations

Temperature	Condensate (MF)	Vapor (MF)
15	4.005E-10	5.967E-10
15	2.11E-9	3.105E-9
15	2.11E-8	3.105E-8
30	4.056E-10	1.285E-9
30	2.11E-9	6.689E-9
30	2.11E-8	6.689E-8
45	4.056E-10	2.577E-9
45	2.11E-9	1.341E-8
45	2.11E-8	1.341E-7
60	4.056E-10	4.862E-9
60	2.11E-9	2.53E-8
60	2.11E-8	2.53E-7
75	4.056E-10	8.711E-9
75	2.11E-9	4.533E-8
75	2.11E-8	4.532E-7

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Title: 242-A Emission

Date: 8-90 by Richmond

Checked: 3/8/91 by J Perry

Now that Exit air Concentrations are known Calculate emissions Based on Flow Rate

Flow Rate from EC-3 has been measured as 55 CFM at -6" wb For conservatism use 50 CFM at -6" wb

Assuming Ideal Gas Law.

pressure correct

Temp correct

$$\frac{50\ ft^3}{min} \times \frac{28.317\ l}{ft^3} \times \frac{60\ min}{hr} \times \frac{750\ mmHg}{760\ mmHg} \times \frac{298}{T} \times \frac{1\ mol}{22.4\ l}$$

$$= \frac{1{,}114{,}584.7}{T}\ \frac{mol}{hr}\ \text{emission}$$

Given concentration from Previous Calculations and Temperature Use

$$\frac{\#\ organic}{hr} = \frac{mol}{hr} \times \text{mol fraction acetone} \times 1\ \frac{58\ g\ Acetone}{mol\ Acetone} \times \frac{1\ lb\ Acetone}{454\ g\ Acetone}$$

$$= \frac{1{,}114{,}584.7}{T} \times Y_1 \times 0.1277 = \#\ \text{acetone organic} = \frac{142{,}391.9\ Y_1}{T}$$

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CALCULATION WORKSHEET

Page No. 27 of 30
Job No. 89-5010-E Client/Project 242-A wHr
Title: 242-A Emissions
Date: 8-90 by Richmond
Checked: 3/8/91 by J Perry

Vessel Vent System Emissions

Temperature (oC)	Vapor (MF)	VVS Organic Emission (lb/hr)
15	5.967E-10	2.8E-7
15	3.105E-9	1.5E-6
15	3.105E-8	1.5E-5
30	1.285E-9	6E-7
30	6.689E-9	3.1E-6
30	6.689E-8	3.1E-5
45	2.577E-9	1.2E-6
45	1.341E-8	6E-6
45	1.341E-7	6E-5
60	4.862E-9	2.1E-6
60	2.53E-8	1.1E-5
60	2.53E-7	1.1E-4
75	8.711E-9	3.6E-6
75	4.533E-8	1.9E-5
75	4.532E-7	1.9E-4

Note: These calculations Indicate that under No reasonable Conditions are emissions from the Vessell Vent system ever even close to the 3#/hr Emission limit or the 3.08 Ton/yr limit ~~from~~ Even assuming 100% operating time.

$$1.9E-4\ \text{lb/hr} \times \frac{24\ \text{hr}}{\text{day}} \times \frac{365.25\ \text{day}}{\text{yr}} \times \frac{1\ \text{Ton}}{2000\#} = 8.33E-4\ \text{Ton/yr}$$

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CALCULATION WORKSHEET

Page No. 28 of 30
Job No. 89-5210-ES Client/Project 242-A WHP
Title: 242-A Emissions
Date: 8-90 by Richmond
Checked: 3/8/91 by JPerry

Calculate Emissions From C-100

Use same method as for Vessel Vent system.

Except Flow Rate for stream is 150 CFM 6" WG

Per previous measurements

so Emissions are Given by:

$$\frac{150\ ft^3}{min} \times \frac{28.317\ \ell}{ft^3} \times \frac{60\ min}{hr} \times \frac{750\ mmHg}{760\ mmHg} \times \frac{298}{T} \times \frac{1\ mol}{22.414\ \ell} \times Y \times \frac{58\ g}{mol} \times$$

$$\frac{1\ lb}{454\ g} = \#\ acetone/hr = \cancel{40}\ 4.27E5/T\ (Y)$$

Vessel Vent System Emissions

Temperature (oC)	Condensate (MF)	C-100 Vapor (MF)
15	3.042E-7	4.475E-7
15	1.583E-6	2.329E-6
15	1.583E-5	2.329E-5
30	3.042E-7	9.642E-7
30	1.583E-6	5.017E-6
30	1.583E-5	5.017E-5
45	3.042E-7	1.933E-6
45	1.583E-6	1.006E-5
45	1.583E-5	1.006E-4
60	3.042E-7	3.647E-6
60	1.583E-6	1.898E-5
60	1.583E-5	1.897E-4
75	3.042E-7	6.534E-6
75	1.583E-6	3.4E-5
75	1.583E-5	3.4E-4

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CALCULATION WORKSHEET

Page No. 29 of 30
Job No. 89-540-ES Client/Project 242-AWMP
Title: 242-A Emissions
Date: 8-90 by Richmond
Checked: 3/8/91 by J Perry

Vessel Vent System Emissions

Temperature (oC)	Condensate (MF)	C-100 Organic Emission (lb/hr)
15	3.042E-7	6.6E-4
15	1.583E-6	3.5E-3
15	1.583E-5	3.5E-2
30	3.042E-7	1.4E-3
30	1.583E-6	7.1E-3
30	1.583E-5	7.1E-2
45	3.042E-7	2.6E-3
45	1.583E-6	1.4E-2
45	1.583E-5	1.4E-1
60	3.042E-7	4.7E-3
60	1.583E-6	2.4E-2
60	1.583E-5	2.4E-1
75	3.042E-7	8E-3
75	1.583E-6	4.2E-2
75	1.583E-5	4.2E-1

These calculations indicate that the major contributors to Organic Emissions is the C-100 Tank They also indicate that under all reasonable conditions Organic Emissions will be less than 3#/hour of 3.01 Tons/year Even at 100% operating time

Approach to setting limits

1) Determine condensate composition for Emissions = 3#/hr and 3.01 Ton/yr at C-100 ASD spec.

Temperature limit (160°F) = 71°C

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CALCULATION WORKSHEET

Page No. 30 of 30

Job No. 89-5040 Client/Project 242-A WAP

Title: 242-A Emissions

Date: 8-90 by WG Richmond

Checked: 3/8/91 by J Perry

Using Previous methods

For 3.0 #/hr Emissions: $3.0 = \frac{4.27E5}{T}[Y_1]$

$\frac{\text{\# Acetone}}{\text{Hr}} = 1.29E3\ (Y_1)$

$Y_1 = 2.42E-3$ mol Fraction Acetone in Vapor

$x_1 = 1.31E-4$ mF = 423,000 PPB

For 3.01 Ton/year = 6.863E-1 #/hr

$= 6.867E-1 = 1.24E+3\ (Y_1)$

$Y_1 = 6.097E-4$ mol Fraction in Vapor

$X_1 = 3.00E-5$ mF = 97,000 ppb

Atlantic Richfield Hanford Company

Date: November 11, 1975

To: G. T. Dukelow

From: J. H. Palmer, 2-2507

Subject: QUALITY ASSURANCE DOP TEST 242-S BUILDING
STACK NO. 296-S-19

	Pent.	Eff. %
Primary filter	.002	99.998
Secondary Filter	.003	99.997
Overall	.003	99.997

Primary filter D/P	.3" w.g.
Secondary filter D/P	.27" w.g.
Pre-filter D/P	.35" w.g.
Fan Inlet pressure	-8.00" w.g.
Stack air flow	384 cfm.
Flow from C-100-1K	75 cfm.
Flow from E-C-3 condenser	2 cfm.
flow from in bleed valve	196 cfm.

C-100 tank	Dry Bulb	Wet Bulb	RH
	75° F	72° F	90%
Room Temperature	72° F	59° F	45%

Required filter efficiency for system is 99.95% tested with 100% DOP base.

JHP:sd

cc: HY Cleaver
WP Ingalls
L Mauws
V Petty
KR Price
RA Zinsli

Atlantic Richfield Hanford Company

Date: November 12, 1975

To: G. T. Dukelow

From: J. H. Palmer, 2-2507

Subject: QUALITY ASSURANCE DOP TEST - 242-S BUILDING
STACK NO. 296-5-18

K-1-15-1	DOP Pent.	Eff. %
	.003	99.997%
K-1-15-2	.003	99.997%

Stack flow 19,020 cfm.

Pre-filter K-1-15-1	D/P	.48" w.g.
Primary K-1-6-1	D/P	2.20" w.g.
Secondary K-1-6-3	D/P	.80" w.g.

Pre-filter K-1-15-2	D/P	.48" w.g.
Primary K-1-6-2	D/P	2.78" w.g.
Secondary K-1-6-4	D/P	.80" w.g.

	Dry	Wet	RH
Exhaust stack temperature	68° F	56° F	45%
Ambient temperature	50° F	44° F	61%

System meets requirements of 99.95% Efficiency.
Tested with 40% DOP base.

JHP:sd

cc: HY Cleaver
WP Ingalls
V Petty
KR Price
RA Zinsli

Atlantic Richfield Hanford Company

Date: November 15, 1975

To: J. J. Fitzpatrick

From: J. H. Palmer, Z-2507

Subject: 702-A

Discharge after filters 5,304 cfm.
Wet 86 Dry 129
Ambient 42 53

Inlet before filters 5,153 cfm.
Wet 65 Dry 64

JHP:sd

cc: PE Alley
GT Dukelow
DL Merrick

54-6000-084 (9-70)

J17.10.2

Atlantic Richfield Hanford Company

Date: November 17, 1975

To: G. T. Dukelow

From: J. H. Palmer, 2-2507

Subject: 242-S VESSEL VENT SYSTEM - STACK NO. 296-S-19

Flow at inbleed valve	196 cfm.
Flow from C-100 tank	63 cfm.
Flow from E-C-3 condenser	50 cfm.
Fan discharge static	.3" w.g.
Fan inlet static	6.6" w.g.
Stack flow second floor	368 cfm.
Stack flow third floor	427 cfm.

JHP:sd

cc: HY Cleaver
V Petty
L Mauws

.6000-084 (9-70)

Atlantic Richfield Hanford Company

Date: November 11, 1975

To: G. T. Dukelow

From: J. H. Palmer, 2-2507

Subject: QUALITY ASSURANCE DOP TEST - BUILDING 242-S
STACK NO. 296-S-18

	Penetration	Eff. %
Tank vent filter	.003	99.997

Filter D/P .02" w.g.
Air Flow 2 cfm.

100% DOP base used for test.

System meet required standards of 99.95% Efficiency.

JHP:sd

cc: HY Cleaver
D [illegible]

Westinghouse Environmental & Geotechnical Services, Inc.

CALCULATION WORKSHEET

Page No. 1 of 12
Job No. 89-5010-ES Client/Project WHC
Title: 242-A Volatile Organic Removal
Date: Sept 90 by WE Richmond
Checked: 3/8/91 by J. Perry

Calculation Purpose

modelling 242-A Evaporator as a stirred tank or mixed Reactor Determine the maximum Feed concentration of Organics such that the slurry Product will have an organic content less than the Health Based limits used by EPA To Review Delisting Petitions. (These limits and their Bases are Provided as an attachment to these calculations) It Should be noted that the Feed concentration limits will be a Function of the Feed Rate, Slurry Rate Evaporator operating Temprature and waste Volume Reduction or Condensate Rate.

Westinghouse Environmental & Geotechnical Services, Inc.

CALCULATION WORKSHEET

Page No. 2 of 12
Job No. 89-5010-ES Client/Project WHC
Title: 242-A Volatile Organic Removal
Date: Sept 90 by WG Richmond
Checked: 3/8/91 by J. Perry

Assumptions

1) The Evaporator is adequately modelled as a stirred Tank or mixed reactor

Basis:
Facts - source Chapter 4 sec 4.1 - 4.2.3.1.2

- Evaporator operation recirculates the Tank at an approximate rate of 14,000 gal/min (52,500 l/min)
- The Evaporator Vapor liquid Seperator has a normal operating volume of 22,500 - 25,000 gallons (84,400 - 94,000 l).
- Typical Feed Rates are 90 - 140 gpm (337 - 525 l/min)
- Typical Slurry Rates are from 32 - 110 gpm (120 - 412 l/min)
- Typical Process condensate Rates are 20-60gpm (75 - 225 l/min)

Interpretation

1) Tank is well mixed as Entire Volume is recirculated Every 1.6 - 1.8 minutes and Feed is added and product withdrawn from the recirculation line and Feed/slurry rates are less than 1% of total operating volume.

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CALCULATION WORKSHEET

Page No. 3 of 12
Job No. 89-5010-ES Client/Project WHC
Title: 242-A Volatile Organic Removal
Date: Sept 90 by WG Richmond
Checked: 3/8/91 by JPerry

VLE Assumptions

1) Assume Evaporation solution is Pure water with organic contamination

Basis

This is a conservative Assumption [that is projected removal of organics will be lower than that actually observed] as the vapor will contain a greater Fraction water than would be actually found due to the decrease in water vapor pressure which would result from the presence of disolved salts.

2) model VLE as in APPENDIX 3E

(see Appendix 3E for assumptions Bases)

- use Wilsons EQn for modelling VLE
- Determine activity Coefficents by Schrieber et al and G J Pierotti et al.
  Ind Eng Proc Des Dev V10 #4 1971 pp572ff
  Ind Eng Chem V51 #1, 1959, pp95ff
- Vapor Pressures From Ried etc al. pp 656-732
- Ideal Vapor Phase

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CALCULATION WORKSHEET

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Job No. 89-5070-ES Client/Project WHC
Title: 242-A Volatile Organic Removal
Date: Sept 90 by WG Richmond
Checked: 3/8/91 by JPerry

Since Evaporator is modelled as a continous stirred tank the following mass balance applies

$$\text{In flow} - \text{out Flow} = \text{accumulation}$$

$$\text{In flow} - [\text{Condensate Flow} + \text{Slurry Flow}] = \text{accumulation}$$

Therefore ~~for~~ the individual component balances are,

$$\left[(F_{in} C_F) - (F_{Cond} C_C) - (F_{slurry} C_s)\right] = \frac{d}{dt}\left((C_p) V_p\right)$$

__Where__

F_{in} = Feed Flow

C_F = Feed concentration

F_{Cond} = condensate Flow rate

C_C = Condensate Concentration

F_{slurry} = slurry Flow

C_s = slurry Concentrat

V_p = Volume of VLS

C_p = concentration in VLS

VLS = Vapor Liquid Separator

But at steady state

$$C_p = C_s \quad \text{and} \quad \frac{d}{dt} C_p V_p \neq 0 \quad x_i$$

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CALCULATION WORKSHEET

Page No. 5 of 12
Job No. 89-5010-ES Client/Project WHC
Title: 242-A Volatile Organic Removal
Date: Sept 90 by WG Richmond
Checked: 3/8/91 by J Perry

So mass balance Reduces to:

$$F_{in} C_F = F_{cond} C_C + F_{slurry} C_S$$

combining with overall mass Balance

$$F_{in} = F_{cond} + F_{slurry}$$

Rearrange:

$$F_{in} - F_{slurry} = F_{cond}$$

$$F_{in} C_F = (F_{in} - F_{slurry}) C_C + F_{slurry} C_S$$

or

$$\frac{F_{in}}{F_{slurry}} C_F - \left[\frac{F_{in} - F_{slurry}}{F_{slurry}}\right] C_C = C_S$$

$$\frac{F_{in}}{F_{slurry}} C_F - \left(\frac{F_{in}}{F_{slurry}} - 1\right) C_C = C_S$$

let $\frac{F_{in}}{F_{slurry}} = R$ (Ratio of Feed to Product mass Rates)

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CALCULATION WORKSHEET

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Job No. 89-50.10-ES Client/Project WHC
Title: 242-A Volatile Organic Removal
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Checked: 3/8/91 by J Perry

$$R C_f - (R-1) C_c = C_s$$

$$R C_f + (1-R) C_c = C_s \quad (1)$$

∴ Given: C_s – Slurry Concentration
R – Feed To Product Ratio = F_{in}/F_{prod}

where we can calculate C_c by Vapor liq EQ and C_F by EQ 1.

Appropriate Values for C_s are the Health Based Levels (HBL) or Treatment standards for LDR waste – Values and sources shown below all values in mg/L (sources attached)

Chemical	HBL	LDR STD
Acetone	4	0.05
n-Butyl Alchol		5.0
IsoButanol		5.0
MEK	2.0	0.05
MIBK	5×10^{-3}	0.05

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CALCULATION WORKSHEET

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Job No. 89-50 10-ES Client/Project WHC
Title: 242-A Volatile Organic Removal
Date: Sept 90 by WG Richmond
Checked: 3/8/91 by J. Perry

- Therefore to Determine feed Concentration limit use the following method

1) select concentration limit for constituent

2) Determine operating temperature

3) calculate Condensate concentration using VLE Assuming Vapor is in Equilibrium at limiting concentration

4) Using Equation (1) Calculate feed concentration limit as Function of R.

Sample: Constituent = Acetone

limit concentration = 0.05 mg/l

Calculate at operating temperature = 110°F or 43°C

VLE: $y_i P_t = x_i \gamma_i P_i$

y_i = mol Fraction Vapor
x_i = mol Fraction liquid
γ_i = activity Coef.

P_i = Vapor Pressure
P_t = total system vapor pressure

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CALCULATION WORKSHEET

Page No. 8 of 12
Job No. 89-5C10-ES Client/Project WHC
Title: 242-A Volatile Organic Removal
Date: Sept 90 by WE Richmond
Checked: 3/8/91 by J Perry

$$\frac{0.05\,\text{mg}}{\ell} \times \frac{1\,\text{g}}{1000\,\text{mg}} \times \frac{1\,\text{mol}}{58\,\text{g}} = 8.62 \times 10^{-7}\,\text{mol}/\ell$$

Since we have assumed essentially pure water

density = 1000g / l ; ∴ 1 l = 55.56 mols H_2O

$\therefore$ M.F Acetone = $8.62E{-7}/55.56 = 1.55E{-8}$

Using methods of App F.

	Acetone	Water
γ_i	= 9.159	$0.999\overline{9}$
P_i	= 476 mmHg	6.4 mmHg
x_i	= 1.55E-8	= 1.0
y_i	= 1.04E-6	= $0.\overline{9}$
mg/l	= 3.35 mg/l	= 1.000×10^6

Using EQ 1

$$R(C_f) - (R-1)C_c = C_s$$

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CALCULATION WORKSHEET

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Job No. 89-5070-ES Client/Project WHC
Title: 242-A Volatile Organic Removal
Date: Sept 90 by WE Richmond
Checked: 3/8/91 by J. Perry

$$R(C_F) - (R-1)3.35\frac{mg}{l} = 0.05\,mg/l$$

$$RC_F = 0.05 + (R-1)3.35$$

$$C_F = \frac{0.05}{R} + \frac{R-1}{R}(3.35)$$

So if feed is ~~say~~ 350 l/min &
slurry is 120 l/min

$$R = 350/120 = 2.92$$

$$C_F = \frac{0.05}{2.92} + \frac{2.92-1}{2.92}(3.35)$$

$$C_F = 1.71E\text{-}2 + 2.20 = 2.22\,mg/l$$

So at $R = 2.92$ $T = 43°C$ Acetone Feed
concentration limit is 2.22 mg/l

Proceed in same fashion to calculate
for other temperatures.

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CALCULATION WORKSHEET

Page No. 10 of 12

Job No. 89-5010-ES Client/Project WHC

Title: 242-A Volatile Organic Removal

Date: Sept 90 by WG Richmond

Checked: 3/8/91 by J. Perry

Temperature (°C)	Y_1 (MF)	CC mg/L	C_F mg/L $\frac{0.05}{R}+\frac{R-1}{R}(C_c)$
5	1.49E-6	4.8	
10	1.41E-6	4.5	
15	1.34E-6	4.3	
20	1.27E-6	4.1	
25	1.21E-6	3.9	
30	1.16E-6	3.7	
35	1.11E-6	3.6	
40	1.06E-6	3.4	
45	1.02E-6	3.3	
50	9.91E-7	3.2	
55	9.6E-7	3.1	
60	9.32E-7	3.0	
65	9.06E-7	2.9	
70	8.83E-7	2.8	
75	8.63E-7	3.7	

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CALCULATION WORKSHEET

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Job No. 89-50.10-ES Client/Project WHC

Title: 242-A Volatile Organic Removal

Date: Sept 90 by WG Richmond

Checked: 3/8/91 by J. Perry

Based on Feed Rate Range and Product Rate Range Find Range For R

$R = \text{Feed}/\text{Product}$

From pp 2 Feed → 337 – 525 l/min

Prod → 120 – 412 l/min

$\max R = 525/120 = 4.375$

$\min R = 337/412 = 0.82$

$R < 1$ Implies Dilution of Feed so minimum $R = 1.0$ corresponding to No concentration

Prepare Graphs of Feed concentration VS R Limits at Various temperatures for operating specifications. For a Range of R corresponding To 1 – 6

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CALCULATION WORKSHEET

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Title: 242-A Volatile Organic Removal
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It Should Be noted That the Calculated Values can be Fitted to a regession line of The Form

$$C_c = aT + b\ln T + c$$

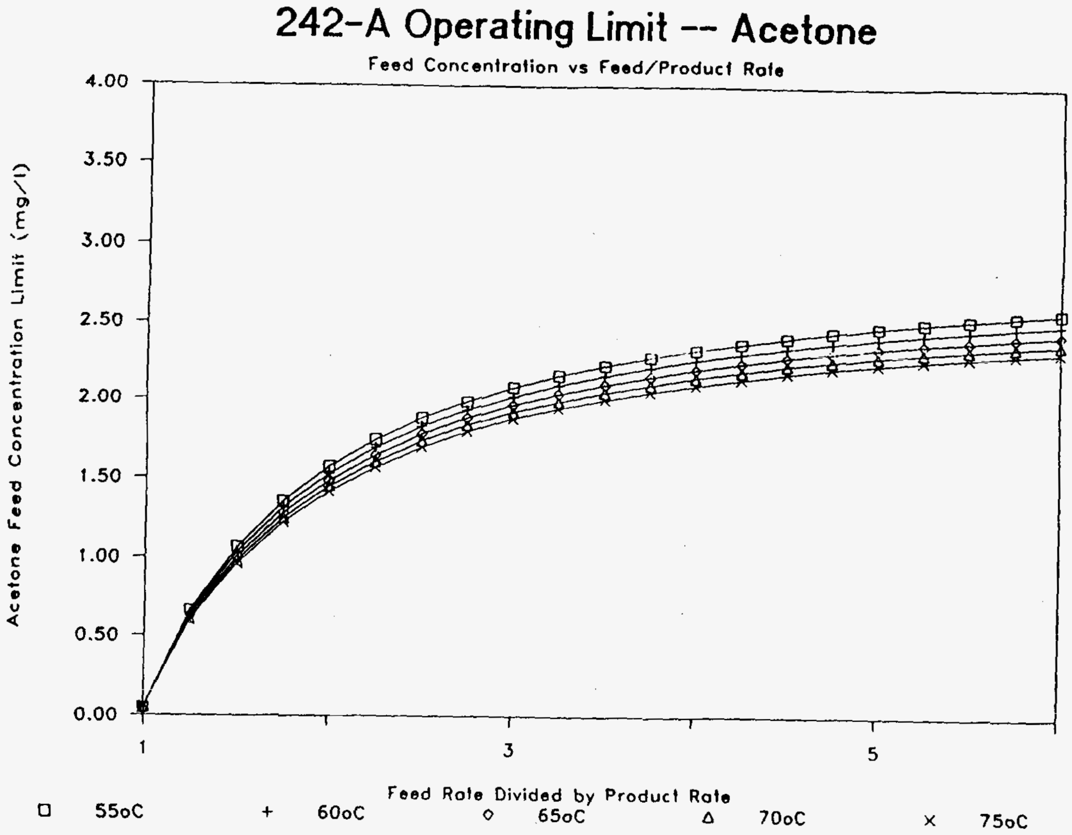
where

C_c is The condensate Concentration in mg/l
T is Temperature Kelvin

Regtission Gives

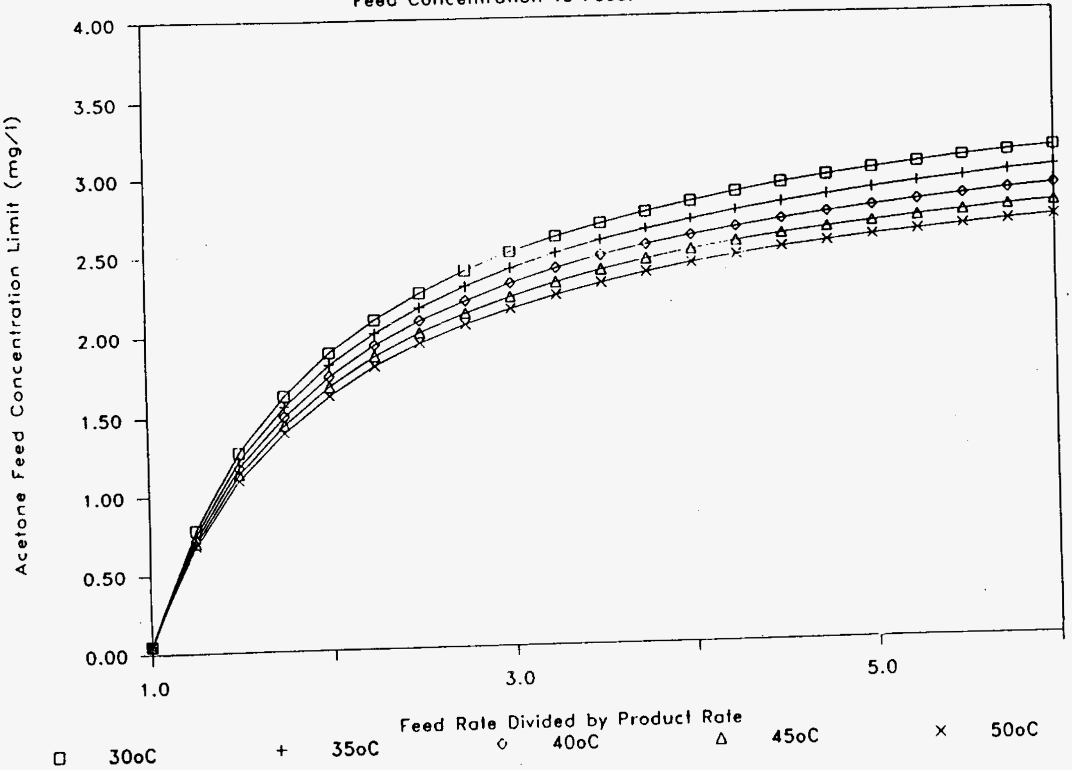
$a = 0.1583$
$b = -58.224$
$c = 288.447$

$R^2 = 0.99995$


242-A Operating Limit -- Acetone
Feed Concentration vs Feed/Product Rate
Acetone Feed Concentration Limit (mg/l)
4.00
3.50
3.00
2.50
2.00
1.50
1.00
0.50
0.00
1
3
5
Feed Rate Divided by Product Rate
□ 55oC
+ 60oC
◇ 65oC
△ 70oC
× 75oC

242-A Operating Limit -- Acetone

Feed Concentration vs Feed/Product Rate



Docket Report on Health-Based Levels and Solubilities Used in the Evaluation of Delisting Petitions, Submitted Under 40 CFR §260.20 and §260.22

November 1989

Prepared by:

Science Applications International Corporation
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Prepared for:

Variances Section, Assistance Branch
Office of Solid Waste
U.S. Environmental Protection Agency
401 M Street, S.W.
Washington, D.C. 20460

EPA Contract No. 68-W9-0091

The Variances Section, in its review of delisting petitions, evaluates levels of carcinogens and systemic toxicants listed in Appendices VII, VIII, and IX of 40 CFR §261. The exposure assumption that is used to assess the hazard of a petitioned waste is ingestion of contaminated ground water, leachate, or wastewater. For both carcinogens and systemic toxicants, the water intake assumption is 2 liters per day for an average 70 kg adult over a 70-year lifetime. The use of a 70-year lifetime considers the effects of carcinogens as a function of cumulative doses, rather than doses received by any small subsection of the population. In addition, in cases where constituents are both carcinogens and systemic toxicants, the more conservative carcinogenic slope factor takes precedence over the toxicant reference dose.

The following equation is used to calculate the delisting health-based levels for carcinogens:

$$D_c = (R \times W \times LT) / (CSF \times I \times A \times ED)$$

where:

D_c = delisting health-based level for carcinogen (mg/l)

R = assumed risk level = 10^{-6}

W = body weight = 70 kg

LT = assumed lifetime = 70 years

CSF = carcinogenic slope factor = experimental potency $(mg/kg/day)^{-1}$

I = intake assumption = 2 L/day

A = absorption factor = 1

ED = exposure duration = 70 years

The following equation is used to calculate the delisting health-based levels for systemic toxicants:

$$D_s = (RfD \times W) / (I \times A)$$

where: D_s = delisting health-based level for systemic toxicant (mg/l)

RfD = reference dose (mg/kg/day)

W = body weight = 70 kg

I = intake assumption = 2 L/day

A = absorption factor = 1

Constituents which have verified health-based levels are listed on the EPA's Integrated Risk Information System (IRIS), which is maintained by the Office of Health and Environmental Assessment in the Office of Research and Development. The information listed on IRIS is designed to be a guide for the evaluation of potential health problems, and is included on IRIS only after an intra-office work group of EPA toxicologists and other scientists have reviewed the facts. IRIS provides verified information for oral and/or inhalation reference doses, risk estimates for carcinogenicity, drinking water health advisories, risk management summaries, and other supplemental data. (IRIS provides the carcinogenic slope factors and the reference doses that are needed in the above equations.) IRIS is currently available to EPA staff through the EPA electronic mail system as well as to the general public, who can access the system through various on-line networks such as DIALCOM, Inc., the Public Health Network (PHN), and the National Library of Medicine's TOXNET. The general public should contact any of the latter networks to obtain an IRIS account. Hard copies of IRIS information for all constituents with verified delisting health-based levels will be provided by the Variances Section upon request.

In addition, IRIS provides Maximum Contaminant Levels (MCLs) for constituents. MCLs are promulgated under the Safe Drinking Water Act (SDWA) of 1974, as amended in 1984, and consider technology and economic feasibility as well as health effects. MCLs are used as the delisting levels for carcinogens and systemic toxicants when available.

Some of the constituents on the delisting docket report entitled "Internal Docket Report on Health-Based Levels and Solubilities Used in the Evaluation of Delisting Petitions, Submitted Under 40 CFR §260.20 and §260.22" are not on IRIS. In these cases, other references, such as health and environmental effects documents (HEEDs), Office of Drinking Water (ODW) health advisories, Carcinogen Assessment Group (CAG) recommendations, and various chemical files are used and will be provided by the Variances Section upon request. The same equations presented above are used for calculating delisting health-based levels.

HEALTH-BASED LEVELS AND SOLUBILITIES
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CAS No.	Compound	HBL (mg/l)	Ref.	Solubility (mg/l) (in H_2O at 25°C)	Ref.
67 64 1	Acetone	4×10^{0}	4	1.0×10^{6}	6
75 05 8	Acetonitrile	2×10^{-1}	4	1.0×10^{6}	6
98 86 2	Acetophenone	4×10^{0}	4	5.5×10^{3}	34
107 02 8	Acrolein	5×10^{-1}	18	2.1×10^{5}	26
79 06 1	Acrylamide	Treatment Technique	48	$>1\times10^{6}$	34
79 10 7	Acrylic acid	3×10^{0}	4	1.0×10^{6}	6
107 13 1	Acrylonitrile	6×10^{-5}	5	7.9×10^{4}	6
116 06 3	Aldicarb	1×10^{-2}	48	6.0×10^{3}	34
309 00 2	Aldrin	2×10^{-6}	5	1.8×10^{-1}	6
107 18 6	Allyl alcohol	2×10^{-1}	4	5.1×10^{5}	6
0859 73 8	Aluminum phosphide	1×10^{-2}	4		
62 53 3	Aniline (Benzeneamine)	6×10^{-3}	5	3.4×10^{4}	34
107 12 7	Anthracene	2×10^{-3}	25,13	4.5×10^{-2}	27
74 [illegible]6 0	Antimony	1×10^{-2}	4		
744[illegible] 38 2	Arsenic	5×10^{-2}	32		
7440 39 3	Barium	1×10^{0}	32		
71 43 2	Benzene	5×10^{-3}	33	1.8×10^{3}	6
92 87 5	Benzidine	2×10^{-7}	5	4.0×10^{2}	6
56 55 3	Benz(a)anthracene	1×10^{-5}	37	5.7×10^{-3}	26
50 32 8	Benzo(a)pyrene	3×10^{-6}	10	1.2×10^{-3}	6
205 99 2	Benzo(b)fluoranthene	2×10^{-5}	25	1.4×10^{-2}	6
207 08 9	Benzo(k)fluoranthene	4×10^{-3}	43	4.3×10^{-3}	6
100 44 7	Benzyl chloride	2×10^{-4}	5	3.3×10^{-3}	29
7440 41 7	Beryllium	7×10^{-6}	5		
111 44 4	Bis(2-chloroethyl)ether	3×10^{-5}	5	1.02×10^{4}	6
108 60 1	Bis(2-chloroisopropyl ether)	1×10^{0}	4	1.7×10^{3}	34
542 88 1	Bis(2-chloro-1-methyl)ether	2×10^{-7}	5	2.2×10^{4}	6
117 81 7	Bis(2-ethylhexyl)phthalate	3×10^{-3}	5	4×10^{-1}	30
75 27 4	Bromodichloromethane	7×10^{-1}	4	4.7×10^{3} (22°C)	51
74 83 9	Bromomethane	5×10^{-2}	4	1.0×10^{3}	28
106 99 0	1,3-Butadiene	3×10^{-4}	14	7.35×10^{2}	6
85 68 7	Butyl benzyl phthalate	9×10^{-1}	7	2.9×10^{0}	27

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CAS No.	Compound	HBL (mg/l)	Ref.	Solubility (mg/l) (in H_2O at 25°C)	Ref.
88 85 7	2-sec-Butyl-4,6-dinitrophenol (Dinoseb)	$4x10^{-2}$	4	$5x10^{1}$	6
40 43 9	Cadmium	$1x10^{-2}$	32		
75 15 0	Carbon disulfide	$4x10^{0}$	4	$2.94x10^{3}$	2
56 23 5	Carbon tetrachloride	$5x10^{-3}$	33	$8.00x10^{2}$	6
75 87 6	Chloral	$7x10^{-2}$	4	Soluble	2
57 74 9	Chlordane	$2x10^{-3}$	48	$5.6x10^{-1}$	6
06 47 8	p-Chloroaniline	$1x10^{-1}$	4	Soluble	2
08 90 7	Chlorobenzene	$1x10^{-1}$	48	$4.7x10^{2}$	6
15 74 7	p-Chloro-m-cresol	$2x10^{-1}$	35	$3.85x10^{3}$(20°C)	2
24 48 1	Chlorodibromomethane	$7x10^{-1}$	4	$4.4x10^{3}$(22°C)	51
67 66 3	Chloroform	$6x10^{-3}$	5	$8.2x10^{3}$	6
07 30 2	Chloromethyl methyl ether	$4x10^{-6}$	8		
95 57 8	2-Chlorophenol	$2x10^{-1}$	4	$2.85x10^{4}$(20°C)	34
40 47 3	Chromium	$5x10^{-2}$	32		
218 01 9	Chrysene	$2x10^{-4}$	25	$1.8x10^{-3}$	6
319 77 3	Cresols	$2x10^{0}$	4	$3.1x10^{4}$	6
57 12 5	Cyanide, (free)	$7x10^{-1}$	4		
460 19 5	Cyanogen	$1x10^{0}$	4	$2.5x10^{5}$	6
506 68 3	Cyanogen bromide	$3x10^{0}$	4		
94 75 7	2,4-Dichlorophenoxyacetic Acid (2,4-D)	$1x10^{-1}$	32	$8.9x10^{2}$	6
72 54 8	DDD	$1x10^{-4}$	5	$1x10^{-1}$	6
72 55 9	DDE	$1x10^{-4}$	5	$4x10^{-2}$	6
50 29 3	DDT	$1x10^{-4}$	5	$5x10^{-3}$	6
	Dibenz(a,h)acridine	$3x10^{-6}$	10	Insoluble	2
53 70 3	Dibenz(a,h)anthracene	$7x10^{-7}$	38	$5.0x10^{-4}$	6
96 12 8	1,2-Dibromo-3-chloropropane	$2x10^{-4}$	48	$1.0x10^{3}$	34
84 74 2	Di-n-butyl phthalate	$4x10^{0}$	4	$1.3x10^{1}$	6
95 50 1	1,2-Dichlorobenzene	$6x10^{-1}$	48	$1.00x10^{2}$	6

HEALTH-BASED LEVELS AND SOLUBILITIES FOR CONSTITUENTS OF CONCERN IN DELISTING PETITIONS

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CAS No.	Compound	HBL (mg/l)	Ref.	Solubility (mg/l) (in H_2O at 25°C)	Ref.
541 73 1	1,3-Dichlorobenzene	3×10^{0}	17	1.23×10^{2}	6
106 46 7	1,4-Dichlorobenzene	7.5×10^{-2}	33	7.9×10^{1}	6
91 94 1	3,3'-Dichlorobenzidine	8×10^{-5}	5	4×10^{0}	6
75 71 8	Dichlorodifluoromethane	7×10^{0}	4	2.80×10^{2}	34
75 34 3	1,1-Dichloroethane	4×10^{-4}	20	5.5×10^{3}(20°C)	6
107 06 2	1,2-Dichloroethane	5×10^{-3}	33	8.520×10^{3}	6
75 35 4	1,1-Dichloroethylene	7×10^{-3}	33	2.250×10^{3}	6
156 59 2	cis-1,2-Dichloroethylene	7×10^{-2}	48	3.500×10^{3}	6
156 60 5	trans-1,2-Dichloroethylene	1×10^{-1}	48	6.30×10^{3}(20°C)	2
75 09 2	Dichloromethane	5×10^{-3}	5	2.0×10^{4}	6
120 83 2	2,4-Dichlorophenol	1×10^{-1}	4	4.6×10^{3}	6
78 87 5	1,2-Dichloropropane	5×10^{-3}	48	2.7×10^{3}	34
542 75 6	1,3-Dichloropropene	2×10^{-4}	5	2.8×10^{3}	6
60 57 1	Dieldrin	2×10^{-6}	5	1.95×10^{-1}	6
66 2	Diethyl phthalate	3×10^{1}	4	8.96×10^{2}	6
60 51 5	Dimethoate	7×10^{-3}	4	2.5×10^{4}	6
57 97 6	7,12-Dimethylbenz(a) anthracene	1×10^{-6}	49	4.4×10^{-3}	6
105 67 9	2,4-Dimethylphenol	2×10^{-2}	13	5.9×10^{2}	26
576 26 1	2,6-Dimethylphenol	2×10^{-3}	4	Slightly Soluble	2
95 65 8	3,4-Dimethylphenol	4×10^{-3}	4	8.17×10^{0}	1
131 11 3	Dimethyl phthalate	4×10^{2}	7	4.32×10^{3}	2
120 61 6	Dimethyl terephthalate	4×10^{0}	4	1.26×10^{1}	1
99 65 0	Dinitrobenzene (meta)	4×10^{-3}	4	4.7×10^{2}	6
534 52 1	4,6-Dinitro-o-cresol	4×10^{-2}	21	2.9×10^{2}	27
51 28 5	2,4-Dinitrophenol	7×10^{-2}	4	5.6×10^{3}	6
121 14 2	Dinitrotoluene	5×10^{-5}	5,50	2.40×10^{2}	6
117 84 0	Di-n-octyl phthalate	6×10^{-1}	7	3×10^{0}	51
123 91 1	1,4-Dioxane	3×10^{-3}	5	4.31×10^{5}	6
122 39 4	Diphenylamine	9×10^{-1}	4	3.57×10^{1}	6
122 66 7	1,2-Diphenylhydrazine	4×10^{-5}	5	1.84×10^{3}	6
298 04 4	Disulfoton	1×10^{-3}	4	Insoluble	2
72 20 8	Endrin	2×10^{-4}	32	2.5×10^{-1}	51
115 29 7	Endosulfan	2×10^{-3}	4	5.3×10^{-1}	51

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CAS No.	Compound	HBL (mg/l)	Ref	Solubility (mg/l) (in H_2O at 25°C)	Ref.
106 89 8	Epichlorohydrin (1-Chloro-2,3-epoxypropane)	Treatment Technique	48	6.0×10^{4}	6
100 41 4	Ethyl benzene	7×10^{-1}	48	1.52×10^{2}	6
60 29 7	Ethyl ether	2×10^{1}	4	6.05×10^{4}	31,2
106 93 4	Ethylene dibromide	5×10^{-5}	48	4.3×10^{3}	6
75 21 8	Ethylene oxide	1×10^{-4}	12	1.0×10^{6}	6
206 44 0	Fluoranthene	2×10^{-1}	28	2.65×10^{-1}	6
86 73 7	Fluorene	2×10^{-3}	25,13	1.7×10^{0}	6
64 18 6	Formic acid	7×10^{1}	4	8.1×10^{5}	6
765 34 4	Glycidylaldehyde	1×10^{-2}	4	$>1\times10^{6}$	6
76 44 8	Heptachlor	4×10^{-4}	48	1.8×10^{-1}	6
024 57 3	Heptachlor epoxide (alpha, beta, gamma isomers)	2×10^{-4}	48	3.5×10^{-1}	6
87 82 1	Hexabromobenzene	7×10^{-2}	4		
118 74 1	Hexachlorobenzene	2×10^{-5}	5	6.0×10^{-3}	6
87 68 3	Hexachlorobutadiene	5×10^{-4}	5	1.5×10^{-1}	6
77 47 4	Hexachlorocyclopentadiene	2×10^{-1}	4	1.8×10^{0}	26
67 72 1	Hexachloroethane	3×10^{-3}	5	5.0×10^{1}	6
70 30 4	Hexachlorophene	1×10^{-2}	4	4×10^{-3}	6
302 01 2	Hydrazine	1×10^{-5}	5	$>1\times10^{6}$	6
74 90 8	Hydrocyanic acid (hydrogen cyanide)	7×10^{-1}	4		
7783 06 4	Hydrogen sulfide	1×10^{-1}	4	4.13×10^{3}	6
193 39 5	Indeno(1,2,3,cd)pyrene	2×10^{-4}	25	5.3×10^{-4}	6
78 83 1	Isobutanol	1×10^{1}	4	7.6×10^{4}	3
78 59 1	Isophorone	9×10^{-3}	52	1.20×10^{4}	34
7439 92 1	Lead	5×10^{-2}	32		
58 89 9	Lindane (gamma-HCH)	2×10^{-4}	33	7.8×10^{0}	51
108 31 6	Maleic anhydride	4×10^{0}	4	Soluble	2
123 33 1	Maleic hydrazide	2×10^{1}	4	Soluble	2
7439 97 6	Mercury	2×10^{-3}	32		
126 98 7	Methacrylonitrile	4×10^{-3}	4	2.5×10^{4}	34
6752 77 5	Methomyl	9×10^{-1}	4	5.8×10^{4}	2

APPENDIX B

ORGANIC EMISSION CALCULATIONS FOR 242-A EVAPORATOR ORGANIC CONSTITUENTS

Appendix B contains vapor-liquid equilibrium and mass balance calculations, performed by Westinghouse Environmental and Geotechnical Services, Inc., used to estimate the quantity of emissions of volatile organic compounds from the 242-A Evaporator vessel vent. Appendix B was included as Appendix 3F of the *242-A Evaporator Dangerous Waste Permit Application*, Revision 0 (DOE-RL 1992). Appendix B contains:

- Calculations of concentrations and emissions from average, maximum and 10 X maximum concentrations of constituents in the process condensate

- Calculations of maximum concentration of the constituent in the feed stream so that 3.0 lb/hr is not exceeded in the vessel vent

- Calculations of maximum concentration of the constituent in the feed stream to ensure the slurry product is acceptable for land disposal.

Calculations were performed for the following constituents:

Acetone
Benzyl Alcohol
Butanal
1-Butanol
2-Butanone
2-Butoxyethanol
3,5-Dimethylpyridine
Ethoxytriethylene glycol
2-Hexanone
Hexone (Methyl Isobutyl Ketone)
2-Pentanone
Phenol
2-Propanol
Pyridine
Tetrahyrofuran
Tetradecane
Tributyl Phosphate
Tridecane

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The organic emissions from C-100 are dependent on the vessel vent flow rate and the exit air concentrations of organics. The vessel vent flow rate is 150 ft^3/min. The exit air concentration (or the vapor phase mole fraction $- y_1$) for the organic constituents must, however, be calculated using the equation for vapor – liquid equilibrium.

$$P_t \, y_i = x_i \, \gamma_i \, p_i$$

P_t = total system vapor pressure
y_i = vapor phase mole fraction of constituent i
x_i = liquid phase mole fraction of constituent i
γ_i = liquid phase activity coefficient for constituent i
p_i = vapor pressure of component i in pure phase at system temperature

If x_i, system pressure, and temperature are known, y_i can be calculated by solving for γ_i and p_i.

γ_i can be solved for in one of three ways:

① γ_i can be solved for using Wilson's Equation for binary solutions

$$\ln \gamma_1 = -\ln(x_1 + \Lambda_{12} x_2) + x_2 \left[\frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{\Lambda_{21} x_1 + x_2} \right]$$

Ref A pp 234 6.11-2

$$\ln \gamma_2 = -\ln(x_2 + \Lambda_{21} x_1) - x_1 \left[\frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{\Lambda_{21} x_1 + x_2} \right]$$

Ref A pp 234 6.11-3

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Λ_{12} and Λ_{21} are calculated using equations 8-10.25 and 8-10.26 pp 291 ref. C.

$\ln \gamma_1^{\infty} = -\ln \Lambda_{12} - \Lambda_{21} + 1$ 8-10.25

$\ln \gamma_2^{\infty} = -\ln \Lambda_{21} - \Lambda_{12} + 1$ 8-10.26

γ_1^{∞} and γ_2^{∞} are infinite dilution activity coeffeceints and must be calculated using the appropriate equations on pp 295 ref. C.

② A second way in which γ_i can be determined is to use the previously described method except instead of using simultaneous equations 8-10.25 and 8-10.26 pp 291 ref. C to solve for Λ_{12} and Λ_{21}, simply set Λ_{21} equal to a range of arbitrary values (in the following calculations, Λ_{21} is assigned typically encountered values ranging from .1 to 1.3) and solve for Λ_{12} using equation 8-10.25 pp 291 ref. C. It should be noted that when the organic constitutents are sufficeintly dilute, equation 6.11-2 ref. A pp 234 reduces to equation 8-10.25 pp 291 ref. C and equation 6.11-3 Ref. A pp 234 reduces to $\gamma_2 = 1$. In addition, so long as γ_1^{∞} is not too large, γ_1 and γ_2 are unaffected by the value assigned to Λ_{21} and $\gamma_1^{\infty} \cong \gamma_1$ and $\gamma_2 \cong 1$.

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③ A third way to solve for γ_i is by using the UNIFAC method.

$$\ln \gamma_i = \ln \gamma_i^c + \ln \gamma_i^R$$ Ref F, pp 314 - 332

γ_i^c and γ_i^R must be calculated.

γ_i^c = γ combinatorial → dependent on differences in molecular size and shape.

$$\ln \gamma_i^c = \ln \frac{\phi_i}{x_i} + \frac{Z}{2} q_i \ln \frac{\theta_i}{\phi_i} + l_i - \frac{\phi_i}{x_i} \sum_j x_j l_j$$

$$\theta_i = \frac{q_i x_i}{\sum_j q_j x_j} \qquad \phi_i = \frac{r_i x_i}{\sum_j r_j x_j}$$

$$r_j = \sum_k \nu_k^i R_k \qquad q_i = \sum_k \nu_k^i Q_k$$

x_i = mol fraction of molecule i in solution

Summations are over all components

R_k, Q_k } Determined from table 8-21 (Ref. F)

ν_k^i = # of groups of type k in molecule i

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γ_i^R is dependent on functional group areas and functional group interactions. $\gamma_i^R = \gamma$ residual.

$$\ln \gamma_i^R = \sum_k \nu_k^i \left(\ln \Gamma_k - \ln \Gamma_k^i \right)$$

ν_k^i = # of groups of type k in molecule i

Γ_k = group residual activity coeffeceint

Γ_k^i = residual activity coeffeciant of group k in a referen solution containing molecules of type i only.

$$\ln \Gamma_k = Q_k \left[1 - \ln \left(\sum_m \theta_m \Psi_{mk} \right) - \sum_m \frac{\theta_m \Psi_{km}}{\sum_n \theta_n \Psi_{nm}} \right]$$

NOTE: SUMMATIONS ARE OVER All GROUPS

$$\ln \Gamma_k^i = Q_k \left[1 - \ln \left(\sum_m \theta_m^i \Psi_{mk} \right) - \sum_m \frac{\theta_m^i \Psi_{km}}{\sum_n \theta_n^i \Psi_{nm}} \right]$$

NOTE: SUMMATIONS ARE OVER All GROUPS IN MOLECULE i only.

$$\theta_m = \frac{Q_m X_m}{\sum_n Q_n X_n}$$

X = Mole fraction of indicated group

Q = Determined from table 8-21 Ref. F

$$\Psi_{mn} = \exp\left(\frac{-a_{mn}}{T} \right)$$

$a_{mn} \Rightarrow$ determined from table 8-22 Ref. F

$T \Rightarrow$ temperature (°K)

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P_i can be solved for in one of two ways:

① One way P_i can be solved for is by one of the three equations on page 657 of Ref. D.

1.) $$\ln\left(\frac{P_i}{P_c}\right) = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^{3} + (VPD)x^{6}\right]$$

$$x = 1 - T/T_c$$

2.) $$\ln(P_i) = (VPA) - \frac{(VPB)}{T} + (VPC)\ln T + \frac{(VPD)(P_c)}{T^2}$$

3.) $$\ln(P_i) = (VPA) - \frac{(VPB)}{(T + (VPC))}$$

Constants for these equations are obtained from the table on pg. 658 – 732 Ref. D

② A second way P_i can be solved for is by using the Clausius - Clapeyron Equation Ref. E pp 209.

$$\ln(P_i) = -\frac{\Delta \hat{H}_v}{RT} + B$$

P_i = vapor pressure of pure substance
R = Gas Constant
B = A constant which varies from one substance to another
$\Delta \hat{H}_v$ = Latent heat of vaporization (or the energy required to vaporiz one mole of liquid)
T = Absolute temperature

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A linear relationship exists between $\ln(P_i)$ and $(1/T)$, therefore, if at least two data points for vapor pressure and temperature are known, an equation which describes P_i at various temperatures can be determined.

$$\frac{\Delta \hat{H}_v}{R} = \text{slope} \quad \frac{\ln\left(P_2/P_1\right)}{\frac{1}{T_2} - \frac{1}{T_1}}$$

$$B = y_{\text{intercept}} = \ln \ln\left(P_i\right) + \frac{\Delta \hat{H}_v}{RT}$$

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Ref. A

Prausnitz, John M., Lichtenthaler, Ruediger N., Azevedo, Edmando Gomes de, "Molecular Thermodydamics of Fluid-Phase Equilibria," Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1986 pp 233-237.

Ref. C

Reid, Robert C., Prausnitz, John M., Poling, Bruce E. "The Properties of Gases and Liquids," 4th Edition, McGraw-Hill, Inc., New York, NY, 1987, pp 290-295.

Ref. D

Reid, Robert C., Prausnitz, John M., Poling, Bruce E. "The Properties of Gasses and Liquids" 4th Edition, McGraw-Hill, Inc., New York, NY, 1987, pp. 656-732.

Ref. E

Felder, R.M., Roussea, R.W., "Elementary Principles of Chemical Processes," John Wiley & Sons, New York, 1978.

Ref. F

Reid, Robert C., Prausnitz, John M., and Poling, Bruce E. "The Properties of Gasses and Liquids," 4th Edition, McGraw-Hill, Inc., New York, NY, 1987, pp. 314 - 332.

Acetone

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Title: Organic Emmissions

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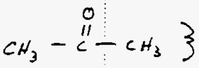
1) Let 1 be Acetone and 2 be H_2O

Acetone

$$\log \gamma_1^{\infty} = \alpha + \epsilon N_1 + \zeta\left(\frac{1}{N_1'} + \frac{1}{N_1''}\right) + \eta (N_1 - N_2)^2$$ Ref C 295 b



$$CH_3-\overset{\overset{O}{\|}}{C}-CH_3$$ } acetone

$N_1 = 3$ $N_1' = N_1'' = 2$ $N_2 = 0$

°K	α	ϵ	ζ	η
298	−1.475	.622	.5	—
333	−1.04	.583	.33	—
373	−.621	.517	.2	—

$$\log \gamma_1^{\infty} = \alpha + 3\epsilon + \zeta$$

note: N_1 and N_2 = total # of carbon atoms in respective molecules

N' and N'' = the # of carbon atoms in respective branches of the indicated molecule

α, ϵ, and ζ can be regressed with respect to temperature to give expressions which can be used to determine ~~α~~, ϵ, and ζ at various temperatures.

$(T) \Rightarrow$ °K

$\alpha = .01137(T) - 4.849$
$\epsilon = -1.406\times10^{-3}(T) + 1.045$
$\zeta = -3.982\times10^{-3}(T) + 1.676$

Acetone

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by	AK [illegible]

$\underline{H_2O}$

$$\log \gamma_2^{\infty} = \alpha + \epsilon N_2 + \zeta\left(\frac{1}{N_2'} + \frac{1}{N_2''} + \frac{1}{N_2'''}\right) + \theta\left(\frac{1}{N_1'} + \frac{1}{N_1''}\right) \quad \text{ref C } 25°C$$

$N_2' = N_2'' = N_2''' = 0 \qquad N_2 = 0 \qquad N_1' = N_1'' = 2$

°K	α	ϵ	ζ	η	θ
298	1.857	0	0	—	−1.019
333	1.493	0	0	—	−.73
373	1.231	0	0	—	−.557

$$\log \gamma_2^{\infty} = \alpha + \theta$$

α and θ can be regressed with respect to temperature to give expressions which can be used to determine α and θ at various temperatures.

$T \Rightarrow °K$

$$\alpha = -8.3 \times 10^{-3}(T) + 4.306$$
$$\theta = 6.117 \times 10^{-3}(T) - 2.816$$

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2.) $\ln \gamma_1^{\infty} = -\ln(\Lambda_{12}) - \Lambda_{21} + 1$ Ref. C 8-10.25

$\ln \gamma_2^{\infty} = -\ln(\Lambda_{21}) - \Lambda_{12} + 1$ Ref. C 8-10.26

T °K	Λ_{12} $\times 10^{-1}$	Λ_{21} $\times 10^{-1}$
288	2.746	2.84
303	2.38	3.176
318	2.05	3.537
333	1.775	3.924
348	1.527	4.338

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3.) $$\ln \gamma_1 = -\ln\left(x_1 + \Lambda_{12} x_2\right) + x_2\left[\frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{\Lambda_{21} x_1 + x_2}\right]$$ Ref. A 6.11-2

$$\ln \gamma_2 = -\ln\left(x_2 + \Lambda_{21} x_1\right) - x_1\left[\frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{\Lambda_{21} x_1 + x_2}\right]$$ Ref A 6.11-3

x_1 & x_2 = mol fraction of respective molecules

Mol Fraction is calculated from ppb concentration in Stream Specific Report App 3A.

ex.) $$1.2575 \times 10^{3}\ \text{ppb} = \frac{1.2575 \times 10^{3}\ \mu g}{1000\ ml} = \frac{1.2575 \times 10^{-3}\ g}{1000\ g} =$$

$$\frac{2.17 \times 10^{-5}\ \text{moles acetone}}{(1.26 \times 10^{-3}\ g\ \text{Acetone}) + (999.999\ g\ H_2O)} = \frac{2.17 \times 10^{-5}\ \text{moles Acetone}}{(2.17 \times 10^{-5}\ \text{moles Acetone}) + (55.5092\ \text{moles}\ H_2O)} = 3.9 \times 10^{-7}\ MF$$

MW Acetone = 58.08 g/mole

MW H_2O = 18.015 g/mol

°K	$x_1 = 3.9 \times 10^{-7}$ MF	$x_1 = 1.582 \times 10^{-6}$ MF	$x_1 = 1.582 \times 10^{-5}$ MF
	γ_1	γ_1	γ_1
288	7.452×10^{0}	7.452×10^{0}	7.452×10^{0}
303	8.313×10^{0}	8.313×10^{0}	8.313×10^{0}
318	9.274×10^{0}	9.274×10^{0}	9.274×10^{0}
333	1.034×10^{1}	1.034×10^{1}	1.034×10^{1}
348	1.154×10^{1}	1.154×10^{1}	1.154×10^{1}

Acetone

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4.)

$$\ln \frac{P_1}{P_c} = (1-X)^{-1}\left[(VPA)X + (VPB)X^{1.5} + (VPC)X^3 + (VPD)X^6\right]$$

Ref. D App A eqn. #1

$X = 1 - T/T_c$

$T_c = 508.1$ °K $P_c = 47$ bars $VPA = -7.45514$

$VPB = 1.202$ $VPC = -2.4396$ $VPD = -3.35590$

Valid From 259 °K to 508.1 °K

$$\ln \frac{P_2}{P_c} = (1-X)^{-1}\left[(VPA)X + (VPB)X^{1.5} + (VPC)X^3 + (VPD)X^6\right]$$

Ref. D App A eqn. #1

$X = 1 - T/T_c$

$T_c = 647.3$ $P_c = 221.2$ $VPA = -7.76451$

$VPB = 1.45838$ $VPC = -2.7758$ $VPD = -1.23303$

Valid From 275 to 647.3

°K	P_1 (bars)	P_2 (bars)
288	1.956×10^{-1}	1.69×10^{-2}
303	3.781×10^{-1}	4.212×10^{-2}
318	6.799×10^{-1}	9.521×10^{-2}
333	1.15×10^{0}	1.98×10^{-1}
348	1.849×10^{0}	3.834×10^{-1}

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5.) $y_i P_t = \gamma_i x_i p_i$

x_i = mole fraction of component i (liquid phase)
y_i = vapor phase mol fraction of component i

P_t = System pressure (vapor phase)

γ_i = activity coeffecient (liquid phase) (component i)

p_i = vapor pressure of pure component at system temp.

$$y_1 = \frac{\gamma_1 x_1 p_1}{P_t}$$

P_t = 750 mm Hg in C-100

$$\Rightarrow (750 \text{ mm Hg})\left(\frac{1.01325 \text{ bars}}{760 \text{ mm Hg}}\right) = .9999 \text{ bars}$$

P_t = .9999 bars

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6.) C-100 stream flow rate = 150 $\frac{ft^3}{min}$

C-100 pressure = 6" WG

$$\text{Emmissions} = \left(150\ \frac{ft^3}{min}\right)\left(28.317\ \frac{l}{ft^3}\right)\left(\frac{60\ min}{hr}\right)\left(\frac{750\ mm\,Hg}{760\ mm\,Hg}\right)\left(\frac{298}{T}\right)\left(\frac{1\ mol}{22.4\ l}\right)$$

$$\underrightarrow{\text{cont'd}}\ \left(\frac{58.08\ g}{mol}\right)\left(\frac{1\ lb}{454\ g}\right)\left(y_i\right) = \frac{\text{lbs of acetone}}{hr}$$

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°K C-100 Acetone Emmissions (x1=ave)

T °K	v1 γ1	p1 bars	x1 mF	y1 mF	Emmissi— lbs/hr
2.88E2	7.452E0	1.956E-1	3.9E-7	5.685E-7	8.45E-4
3.03E2	8.313E0	3.781E-1	3.97E-7	1.226E-6	1.732E-3
3.18E2	9.274E0	6.799E-1	3.97E-7	2.459E-6	3.31E-3
3.33E2	1.034E1	1.15E0	3.97E-7	4.642E-6	5.967E-3
3.48E2	1.154E1	1.849E0	3.97E-7	8.321E-6	1.024E-2

°K C-100 Acetone Emmissions (max)

T °K	v1 γ1	p1 bars	x1 mF	y1 mF	Emmission— lbs/hr.
2.88E2	7.452E0	1.956E-1	1.582E-6	2.306E-6	3.428E-3
3.03E2	8.313E0	3.781E-1	1.582E-6	4.972E-6	7.024E-3
3.18E2	9.273E0	6.799E-1	1.582E-6	9.975E-6	1.343E-2
3.33E2	1.034E1	1.15E0	1.582E-6	1.883E-5	2.42E-2
3.48E2	1.154E1	1.849E0	1.582E-6	3.375E-5	4.152E-2

°K C-100 Acetone Emmissions (max*10)

T °K	v1 γ1	p1 bars	x1 mF	y1 mF	Emmission— lbs/hr.
2.88E2	7.452E0	1.956E-1	1.582E-5	2.306E-5	3.427E-2
3.03E2	8.312E0	3.781E-1	1.582E-5	4.972E-5	7.024E-2
3.18E2	9.272E0	6.799E-1	1.582E-5	9.974E-5	1.342E-1
3.33E2	1.034E1	1.15E0	1.582E-5	1.883E-4	2.42E-1
3.48E2	1.154E1	1.849E0	1.582E-5	3.375E-4	4.151E-1

Acetone

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The process condensate emmission results at 75°C = 348°K, can be used to determine the feed concentration limit. The feed concentration limit is the concentration of volatile constituent in the feed stream, with the assumption that the volatile constituent is completely transferred into the condensate, which will produce 0.71 lbs/hr (.322 Kg/hr) emmissions of acetone from the process condensate. The feed concentration limit is calculated as follows:

obtained from stream specific report

$$\left(\frac{5.10\times10^{4}}{}\ \mu g/\ell\right)\left(\frac{1\ mg}{1000\ \mu g}\right)\left(\frac{1\ hr.}{4.151\times10^{-1}\ lbs}\right)\left(\frac{.71\ lbs}{1\ hr}\right)\left(\frac{R-1}{R}\right)$$

$$= 87.2\left(\frac{R-1}{R}\right) \Rightarrow mg/\ell$$

note: R = feed rate ÷ product rate

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Determination of maximum feed concentration:

$$R \cdot C_f + (1 - R) C_c = C_s$$

R = Ratio of Feed to product Mass Ratio

C_f = Feed Concentration

C_s = Concentration of a given component in Slurry

Note: To determine the maximum feed concentration (C_f) of a given component, (C_s) will be the regulatory limit (HBL or LDR).

C_c = Condensate Concentration of a given component

Note: C_c is calculated from the vapor phase mol fraction for a given component in the slurry.

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C_c is calculated by converting y_i (mol fraction) to y_i (ppm)

$$y_i(MF) = \frac{\text{moles } i}{\text{moles } i + \text{moles } H_2O}$$

In this calculation, the mole contribution of component i is insignificant relative to the mole contribution of H_2O. Therefore,

$$\left(\frac{\text{mol } i}{\cancel{\text{mol } i} + \text{mol } H_2O}\right)\left(\frac{55.5093 \text{ mol } H_2O}{1 \ell}\right)\left(\text{molec. wt}\right)\left(\frac{1000 \text{ mg}}{g}\right)$$

insignificant

$$= \quad \text{mg}/\ell \quad = \quad \text{mg}/\text{Kg} \quad = \text{ppm}$$

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Acetone Slurry Vapor Phase Mol Fraction

T °K	v1 γ_1	p1 bars	x1 mF	Pt bars	y1 mf
2.98E2	8.016E0	3.061E-1	1.83E-7	3.143E-2	1.429E-5
3.03E2	8.313E0	3.781E-1	1.83E-7	4.212E-2	1.365E-5
3.08E2	8.622E0	4.632E-1	1.83E-7	5.584E-2	1.309E-5
3.13E2	8.942E0	5.632E-1	1.83E-7	7.327E-2	1.258E-5
3.18E2	9.274E0	6.799E-1	1.83E-7	9.522E-2	1.212E-5
3.23E2	9.618E0	8.153E-1	1.83E-7	1.226E-1	1.17E-5
3.28E2	9.975E0	9.714E-1	1.83E-7	1.565E-1	1.133E-5
3.33E2	1.034E1	1.15E0	1.83E-7	1.98E-1	1.1E-5
3.38E2	1.073E1	1.355E0	1.83E-7	2.487E-1	1.07E-5
3.43E2	1.113E1	1.587E0	1.83E-7	3.099E-1	1.043E-5
3.48E2	1.154E1	1.849E0	1.83E-7	3.834E-1	1.018E-5

Acetone Slurry Limits (mg/l)

T °K	y1 mF	Cc mg/l	LDR mg/l
2.98E2	1.429E-5	4.606E1	5.9E-1
3.03E2	1.365E-5	4.402E1	5.9E-1
3.08E2	1.309E-5	4.219E1	5.9E-1
3.13E2	1.258E-5	4.055E1	5.9E-1
3.18E2	1.212E-5	3.907E1	5.9E-1
3.23E2	1.17E-5	3.773E1	5.9E-1
3.28E2	1.133E-5	3.654E1	5.9E-1
3.33E2	1.1E-5	3.546E1	5.9E-1
3.38E2	1.07E-5	3.449E1	5.9E-1
3.43E2	1.043E-5	3.362E1	5.9E-1
3.48E2	1.018E-5	3.283E1	5.9E-1

$$C_F = \left(\frac{R+1}{R} + \frac{C_S}{R}\right) C_c$$

Benzyl Alcohol

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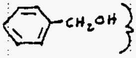
1.) Let 1 be Benzyl Alcohol (BA) and 2 be Water (H_2O).

(BA)

$$\log \gamma_1^\infty = \alpha + \epsilon N_1 + \frac{\zeta}{N_1} + \frac{\theta}{N_2}$$ Ref. C pp. 295 a

$N_1 = 7$ $N_2 = 0$ $\theta = 0$



(BA)

$$\log \gamma_1^\infty = \alpha + 7\epsilon + \zeta/7$$

(H_2O)

$$\log_2^\infty = \alpha + \epsilon N_2 + \frac{\zeta}{N_2} + \frac{\theta}{N_1}$$ Ref. C pp. 295 a

$N_1 = 7$ $N_2 = 0$ $\epsilon = 0$ $\zeta = 0$

$$\log_2^\infty = \alpha + \frac{\theta}{7}$$

Note: N_1, N_2 = total number of carbon atoms in molecules 1 and 2 respectively.

α, ϵ, ζ, and θ are given in table 8-17 Ref. C.

At 25, 60, and 100° C upon plotting α, ϵ, ζ, and θ are found to have a linear relationship with temperature. To facilitate calculations at variable temperatures, the values were regressed to give equations for the adjustable parameters as a function of temperature. The values used and the corresponding regression coefficients are given on the following page:

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(B. A.)

Temp.(K)	α alpha	ϵ epsilon	ζ zeta
298	-9.95E-01	6.22E-01	5.58E-01
333	-7.55E-01	5.83E-01	4.60E-01
373	-4.20E-01	5.17E-01	2.30E-01

α =7.680E-3(T)-3.295E+0
ϵ =-1.410E-3(T)+1.045E+0
ζ =-4.410E-3(T)+1.891E+0

Temp.(K)	α alpha	ϵ epsilon	ζ zeta	$\log \gamma_1^\infty$	γ_1^∞
288	-1.082E+00	6.384E-01	6.204E-01	3.476E+00	2.990E+03
303	-9.668E-01	6.173E-01	5.543E-01	3.433E+00	2.713E+03
318	-8.515E-01	5.961E-01	4.881E-01	3.391E+00	2.461E+03
333	-7.363E-01	5.750E-01	4.220E-01	3.349E+00	2.233E+03
348	-6.210E-01	5.538E-01	3.558E-01	3.307E+00	2.026E+03

(H_2O)

Temp.(K)	Alpha α	theta θ
298	7.60E-01	-6.30E-01
333	6.80E-01	-4.40E-01
373	6.17E-01	-2.80E-01

α =-1.900E-3(T)+1.321E+0
θ =4.651E-3(T)-2.007E+0

Temp.(K)	α alpha	θ theta	$\log \gamma_2^\infty$	γ_2^∞
288	7.739E-01	-6.670E-01	6.786E-01	4.771E+00
303	7.454E-01	-5.972E-01	6.601E-01	4.572E+00
318	7.169E-01	-5.275E-01	6.416E-01	4.381E+00
333	6.884E-01	-4.577E-01	6.230E-01	4.198E+00
348	6.599E-01	-3.880E-01	6.045E-01	4.023E+00

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2.)

$$\ln \gamma_1^\infty = -\ln(\Lambda_{12}) - \Lambda_{21} + 1 \qquad \text{Ref. C } 8\text{-}10.25$$

$$\ln \gamma_2^\infty = -\ln(\Lambda_{21}) - \Lambda_{12} + 1 \qquad \text{Ref. C } 8\text{-}10.26$$

Temp.(K)	γ_1^∞	γ_2^∞	Λ_{12}	Λ_{21}
288	2.990E+03	4.771E+00	5.145E-04	5.694E-01
303	2.713E+03	4.572E+00	5.530E-04	5.945E-01
318	2.461E+03	4.381E+00	5.940E-04	6.202E-01
333	2.233E+03	4.198E+00	6.373E-04	6.472E-01
348	2.026E+03	4.023E+00	6.830E-04	6.752E-01

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3.)

$$\ln \gamma_1 = -\ln(X_1 + \Lambda_{12} X_2) + X_2 \left[\frac{\Lambda_{12}}{X_1 + \Lambda_{12} X_2} - \frac{\Lambda_{21}}{\Lambda_{21} X_1 + X_2} \right]$$ Ref. A 6.11-2

$$\ln \gamma_2 = -\ln(X_2 + \Lambda_{21} X_1) - X_1 \left[\frac{\Lambda_{12}}{X_1 + \Lambda_{12} X_2} - \frac{\Lambda_{21}}{\Lambda_{21} X_1 + X_2} \right]$$ Ref. A 6.11-3

obtained from stream specific report App. 3A

	(ppb) concentration	$X_1 = MF(BA)$	$X_2 = MF(H_2O)$
ave	1.33×10^{1}	2.0×10^{-9}	.999
max	1.80×10^{1}	3.0×10^{-9}	.999
10xmax	1.80×10^{2}	3.0×10^{-8}	.999

ppb to mol fraction (MF) conversion (example):

$$\Rightarrow 1.33 \times 10^{1}\ \text{ppb} = \frac{1.33 \times 10^{1}\ \text{mg}}{\text{litre}} = \frac{1.33 \times 10^{-5}\ g\ (BA)}{1000\ g\ (H_2O + BA)}$$

$$= \frac{1.33\ g\ (BA)}{1.33 \times 10^{-5}\ g (BA) + 999.999\ g (H_2O)} = \frac{1.23 \times 10^{-7}\ \text{moles}\ (BA)}{1.23 \times 10^{-7}\ \text{moles} (BA) + 55.5093\ \text{moles} (H_2O)} =$$

$$= \frac{1.23 \times 10^{-7}\ \text{moles}\ BA}{55.5093\ \text{moles} (H_2O + BA)} = 2 \times 10^{-9}$$

note : Molecular wt. (BA) = 108.140 g/mole
Molecular wt. (H_2O) = 18.015 g/mole

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Temp.(K)	γ_1 (ave)	γ_1 (max)	γ_1 (10x max)	γ_2 (ave)	γ_2 (max)	γ_2 (10x max)
288	2.990E+03	2.990E+03	2.990E+03	1.000E+00	1.000E+00	1.000E+0
303	2.713E+03	2.713E+03	2.712E+03	1.000E+00	1.000E+00	1.000E+0
318	2.461E+03	2.461E+03	2.461E+03	1.000E+00	1.000E+00	1.000E+0
333	2.233E+03	2.233E+03	2.233E+03	1.000E+00	1.000E+00	1.000E+0
348	2.026E+03	2.026E+03	2.026E+03	1.000E+00	1.000E+00	1.000E+0

Benzyl Alcohol

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4.)

$$\ln \frac{P_1}{P_c} = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^{3} + (VPD)x^{6}\right]$$

Ref. D App A equation #1

$$x = 1 - T/T_c$$

T_c = 720.2
VPB = 1.18389

P_c = 44.0
VPC = -9.14255

VPA = -7.09506
VPD = 5.56311

Valid From 303 °K to 720.2 °K

Note: The above equation was used to calculate vapor pressures for temperatures ranging from 288 °K to 348 °K even though these temperatures exceed the range for which the above vapor pressure constants are valid. Upon plotting vapor pressure vs. temperature, vapor pressure appears to approach zero at temperatures below 303 °K.

$$\ln\left(\frac{P_2}{P_c}\right) = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^{3} + (VPD)x^{6}\right]$$

Ref. D App A eqn. #1

$$x = 1 - T/T_c$$

T_c = 647.3
VPB = 1.45838

P_c = 221.2
VPC = -2.7758

VPA = -7.76451
VPD = -1.23303

Valid from 275 °K to 647.3 °K

°K	P_1 (bars)	P_2 (bars)
288	5.667×10^{-5}	1.69×10^{-2}
303	2.099×10^{-4}	4.212×10^{-2}
318	6.792×10^{-4}	9.521×10^{-2}
333	1.953×10^{-3}	1.98×10^{-1}
348	5.061×10^{-3}	3.834×10^{-1}

Benzyl Alcohol

Westinghouse Environmental & Geotechnical Services, Inc.

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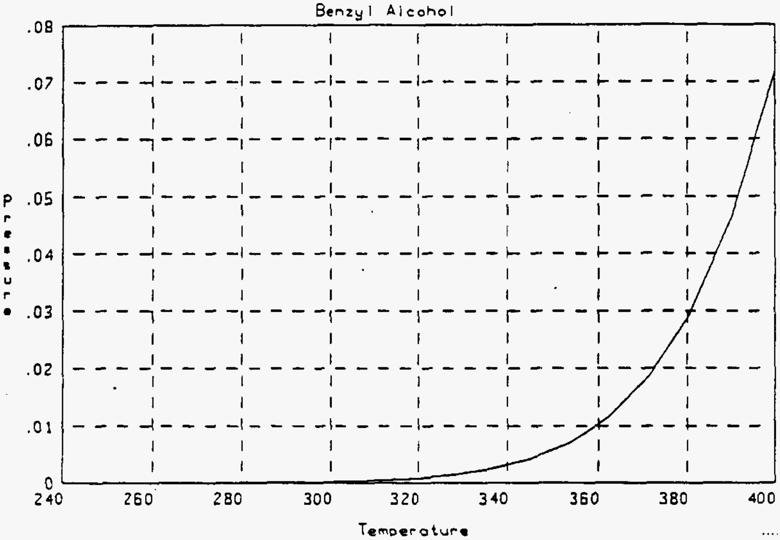
Job No. 89-5010-ES Client/Project WHC /242-A

Title: Organic Emmissions

Date: 1/91 by Tod Perry

Checked: 3/91 by WG Richard



Benzyl Alcohol

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by	Jon Perry
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5.) $Y_i P_t = \gamma_i X_i P_i$

x_i = mol fraction of component i (liquid phase)

Y_i = Vapor Phase Mol Fraction of Component i

P_t = System Vapor Pressure

γ_i = Activity Coeffeceint (Liquid Phase) of Component i

P_i = Vapor Pressur of Component i in Pure Phase At System Temperature

$$Y_1 = \frac{\gamma_1 X_1 P_1}{P_t}$$

P_t = 750 mmHg

$$P_t = 750 \text{ mmHg} \times \frac{1.01325 \text{ bars}}{760 \text{ mmHg}} = .9999 \text{ bars}$$

Temp.(K)	(mF) Y1(ave)	(mF) Y1(max)	(mF) Y1(10max)
288	3.389E-10	5.083E-10	5.083E-09
303	1.139E-09	1.708E-09	1.708E-08
318	3.344E-09	5.015E-09	5.015E-08
333	8.722E-09	1.308E-08	1.308E-07
348	2.051E-08	3.076E-08	3.076E-07

Benzyl Alcohol

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6.)

Given : C-100 Stream flow rate = 150 $\frac{ft^3}{min}$

C-100 pressure = 6" WG

Emissions ($\frac{lbs}{hr}$) can calculated as follows:

$$\left(150\ \frac{ft^3}{min}\right)\left(\frac{28.317\ \ell}{ft^3}\right)\left(\frac{60\ min}{hr}\right)\left(\frac{750\ mm\ Hg}{760\ mm\ Hg}\right)\left(\frac{298}{T}\right)\left(\frac{1\ mol}{22.4\ \ell}\right)$$

$$\rightarrow \text{cont'd} \quad \left(\frac{108.14\ g}{mol}\right)\left(\frac{1\ lb}{454\ g}\right)\left(x_i\right) = \frac{\text{lbs of Benzyl Alcohol}}{hr}$$

ok Benzyl Alcohol C-100 Emissions (xl=ave)

T	xl mf	Emissions lbs/hr
2.88E2	2E-9	9.353E-7
3.03E2	2E-9	2.987E-6
3.18E2	2E-9	8.355E-6
3.33E2	2E-9	2.081E-5
3.48E2	2E-9	4.682E-5

ok Benzyl Alcohol C-100 Emissions (xl=max)

T	xl mf	Emissions lbs/hr
2.88E2	3E-9	1.403E-6
3.03E2	3E-9	4.481E-6
3.18E2	3E-9	1.253E-5
3.33E2	3E-9	3.122E-5
3.48E2	3E-9	7.023E-5

ok Benzyl Alcohol C-100 Emissions (xl=max10)

T	xl mf	Emissions lbs/hr
2.88E2	3E-8	1.403E-5
3.03E2	3E-8	4.48E-5
3.18E2	3E-8	1.253E-4
3.33E2	3E-8	3.121E-4
3.48E2	3E-8	7.022E-4

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Title: Organic Emmissions

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The process condensate emmission results at 75°C = 348°K, can be used to determine the feed concentration limit. The feed concentration limit is the concentration of volatile constituent in the feed stream, with the assumption that the volatile constituent is completely transferred into the condensate, which will produce 0.71 lbs/hr (.322 kg/hr) emmissions of Benzyl Alcohol from the process condensate. The feed concentration limit is calculated as follows:

$$\left(1.80\times10^{2}\ \mu g/\ell\right)\left(\frac{1\ mg}{1000\ \mu g}\right)\left(\frac{1\ hr.}{7.022\times10^{-4}\ lbs}\right)\left(\frac{.71\ lbs}{1\ hr}\right)\left(\frac{R-1}{R}\right)$$

$$= 182\left(\frac{R-1}{R}\right) \Rightarrow mg/\ell$$

note: R = feed rate ÷ product rate

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Determination of maximum feed concentration:

$$R C_f + (1 - R) C_c = C_s$$

R = Ratio of Feed to product Mass Ratio

C_f = Feed Concentration

C_s = Concentration of a given component in Slurry

Note: To determine the maximum Feed concentration (C_f) of a given component, (C_s) will be the regulatory limit (HBL or LDR).

C_c = Condensate Concentration of a given component

Note: C_c is calculated from the vapor phase mol fraction for a given component in the slurry.

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C_c is calculated by conventing y_i (mol fraction) to y_i (ppm)

$$y_i(MF) = \frac{\text{moles } i}{\text{moles } i + \text{moles } H_2O}$$

In this calculation, the mole contribution of component i is insignificant relative to the mole contribution of H_2O. Therefore,

$$\left(\frac{\text{mol } i}{\underbrace{\cancel{\text{mol } i}}_{\text{insignificant}} + \text{mol } H_2O}\right)\left(\frac{55.5093 \text{ mol } H_2O}{1 \ell}\right)\left(\text{molec. wt}\right)\left(\frac{1000 \text{ mg}}{g}\right)$$

$$= \quad \text{mg}/\ell \quad = \quad \text{mg}/\text{Kg} \quad = \text{ppm}$$

Benzyl Alcohol

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Benzyl Alcohol Slurry Vapor Phase Mole Fraction

T °K	vl g/l	pl bars	xl mf	Pt bars	yl mf
2.98E2	2.793E3	1.378E-4	1.67E-7	3.143E-2	2.045E-6
3.03E2	2.703E3	2.099E-4	1.67E-7	4.212E-2	2.25E-6
3.08E2	2.617E3	3.149E-4	1.67E-7	5.584E-2	2.464E-6
3.13E2	2.534E3	4.656E-4	1.67E-7	7.327E-2	2.689E-6
3.18E2	2.453E3	6.792E-4	1.67E-7	9.521E-2	2.922E-6
3.23E2	2.374E3	9.778E-4	1.67E-7	1.226E-1	3.163E-6
3.28E2	2.299E3	1.39E-3	1.67E-7	1.565E-1	3.411E-6
3.33E2	2.225E3	1.953E-3	1.67E-7	1.98E-1	3.664E-6
3.38E2	2.154E3	2.712E-3	1.67E-7	2.487E-1	3.923E-6
3.43E2	2.085E3	3.724E-3	1.67E-7	3.099E-1	4.185E-6
3.48E2	2.019E3	5.061E-3	1.67E-7	3.834E-1	4.45E-6

Benzyl Alcohol Slurry Vapor Phase Condensate Concentration (mg/l)

T °K	yl mf	Cc mg/l	HBL mg/l
2.98E2	2.045E-6	1.228E1	1E0
3.03E2	2.25E-6	1.35E1	1E0
3.08E2	2.464E-6	1.479E1	1E0
3.13E2	2.689E-6	1.614E1	1E0
3.18E2	2.922E-6	1.754E1	1E0
3.23E2	3.163E-6	1.898E1	1E0
3.28E2	3.411E-6	2.047E1	1E0
3.33E2	3.664E-6	2.2E1	1E0
3.38E2	3.923E-6	2.355E1	1E0
3.43E2	4.185E-6	2.512E1	1E0
3.48E2	4.45E-6	2.671E1	1E0

$$C_f = \left(\frac{R-1}{R} + \frac{C_s}{R}\right) C_c$$

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Job No. 89-5010-ES Client/Project WHC/242-A

Title: Organic Emissions

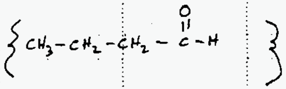
Date: 2/91 by Jon Perry

Checked: 3/91 by

1.) Let 1 be Butanal and 2 be H_2O.

Butanal

$$\log \gamma_1^{\infty} = \alpha + \epsilon N_1 + \frac{\zeta}{N_1} + \frac{\theta}{N_2}$$ Ref C 295 a



$$\left\{ CH_3-CH_2-CH_2-\overset{\overset{O}{\|}}{C}-H \right\} = \text{Butanal} = \text{Butyraldehyde}$$

$N_1 = 4$ $N_2 = 0$

°K	α	ϵ	ζ	η	θ
298	-.780	.622	.320	—	0
333	-.400	.583	.210	—	0
373	-.030	.517	0	—	0

$$\log \gamma_1^{\infty} = \alpha + 4\epsilon + \frac{\zeta}{4}$$

N_1 and N_2 = total # of carbon atoms in respective molecules
N', N'', and N''' = the # of carbon atoms in respective branches of the indicated molecule

α, ϵ, and ζ can be regressed with respect to temperature to give expressions which can be used to determine α, ϵ, and ζ at various temperatures.

$\alpha = 9.982 \times 10^{-3}(T) - 3.744$
$\epsilon = -1.406 \times 10^{-3}(T) + 1.046$
$\zeta = -4.290 \times 10^{-3}(T) + 1.612$

$T \Rightarrow$ °K

Butanal

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Because of the difficulty in locating data which sufficiently describes H_2O at infinite dilation (γ_1^∞) in aldehyde solutions, γ_2^∞ was not calculated. Instead, Λ_{21} was set $=1$, and Λ_{12} was calculated by equation #2. The influence of setting $\Lambda_{21} = 1$ on γ_1 and γ_2 at the variable ranges being used for x_1, x_2, T_1, T_2, Λ_{12}, and Λ_{21} is shown to be insignificant on the following page.

Note: γ_1 and γ_2 were shown to be uneffected by a range of Λ_{21} values ranging from $\Lambda_{21} = .1$ to $\Lambda_{21} = 1.3$ for both the minimum and maximum values of x_1, x_2, T_1, and T_2 incountered in these calculations.

Butanal

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T °K	A21 Λ_{21}	x1	v1 γ_1	v2 γ_2
2.88E2	1E-1	9E-9	6.155E1	1E0
3.03E2	1E-1	9E-9	6.895E1	1E0
3.18E2	1E-1	9E-9	7.723E1	1E0
3.33E2	1E-1	9E-9	8.651E1	1E0
3.48E2	1E-1	9E-9	9.691E1	1E0

T °K	A21 Λ_{21}	x1	v1 γ_1	v2 γ_2
2.88E2	1E-1	1.9E-7	6.155E1	1E0
3.03E2	1E-1	1.9E-7	6.894E1	1E0
3.18E2	1E-1	1.9E-7	7.723E1	1E0
3.33E2	1E-1	1.9E-7	8.651E1	1E0
3.48E2	1E-1	1.9E-7	9.691E1	1E0

T °K	A21 Λ_{21}	x1	v1 γ_1	v2 γ_2
2.88E2	1.3E0	9E-9	6.155E1	1E0
3.03E2	1.3E0	9E-9	6.895E1	1E0
3.18E2	1.3E0	9E-9	7.723E1	1E0
3.33E2	1.3E0	9E-9	8.651E1	1E0
3.48E2	1.3E0	9E-9	9.691E1	1E0

T °K	A21 Λ_{21}	x1	v1 γ_1	v2 γ_2
2.88E2	1.3E0	2.5E-7	6.155E1	1E0
3.03E2	1.3E0	2.5E-7	6.894E1	1E0
3.18E2	1.3E0	2.5E-7	7.723E1	1E0
3.33E2	1.3E0	2.5E-7	8.651E1	1E0
3.48E2	1.3E0	2.5E-7	9.69E1	1E0

Butanal

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2.) $\ln \gamma_1^{\infty} = -\ln(\Lambda_{12}) - \Lambda_{21} + 1$ Ref. C 8-10,25

T °K	Λ_{12} $(\times 10^{-2})$	Λ_{21}
288	1.625	1
303	1.450	1
318	1.295	1
333	1.156	1
348	1.032	1

Butanal

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3.) $$\ln \gamma_1 = -\ln(x_1 + \Lambda_{12} X_2) + X_2 \left[\frac{\Lambda_{12}}{X_1 + \Lambda_{12} X_2} - \frac{\Lambda_{21}}{\Lambda_{21} X_1 + X_2} \right]$$ Ref. A 6.11-2

$$\ln \gamma_2 = -\ln(X_2 + \Lambda_{21} X_1) - X_1 \left[\frac{\Lambda_{21}}{X_1 + \Lambda_{12} X_2} - \frac{\Lambda_{21}}{\Lambda_{21} X_1 + X_2} \right]$$ Ref A 6.11-3

X_1 & X_2 = mol fraction of respective molecules

Mol Fraction is calculated from ppb concentration in Stream Specific Report App 3A.

ex.) $$3.76 \times 10^1 \text{ ppb} = \frac{3.76 \times 10^1 \text{ ug}}{\text{litre}} = \frac{5.21 \times 10^{-7} \text{ moles Butanal}}{1000 \text{ g } (H_2O + \text{Butanal})} =$$

$$\frac{5.21 \times 10^{-7} \text{ moles Butanal}}{3.76 \times 10^{-5} \text{ g Butanal} + 999.999 \text{ g } H_2O} = \frac{5.21 \times 10^{-7} \text{ moles Butanal}}{5.21 \times 10^{-7} \text{ moles Butanal} + 55.5093 \text{ moles } H_2O} = 9 \times 10^{-9} \, MF_{\text{Butanal}}$$

$X_1 = 9 \times 10^{-9}$ MF
$X_1 = 1.9 \times 10^{-8}$ MF
$X_1 = 1.9 \times 10^{-7}$ MF

	$X_1 = 9 \times 10^{-9}$ MF	$X_1 = 1.9 \times 10^{-8}$ MF	$X_1 = 1.90 \times 10^{-7}$ MF	
°K	$\gamma_1 (\times 10^1)$	$\gamma_1 (\times 10^1)$	$\gamma_1 (\times 10^1)$	γ_2
288	6.155	6.155	6.155	1
303	6.895	6.895	6.895	1
318	7.723	7.723	7.723	1
333	8.651	8.651	8.651	1
348	9.691	9.691	9.691	1

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4)
$$\ln \frac{P_1}{P_c} = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^{3} + (VPD)x^{6}\right]$$ Ref. D App. A equation #1

$$x = 1 - T/T_c$$

$T_c = 545.4$
$VPB = .12265$
$P_c = 53.8$
$VPC = -.00073$
$VPA = -7.01403$
$VPD = -8.50911$

Valid From 304 °K to 545.4 °K

Note: The above equation was used to calculate vapor pressures for temperatures ranging from 288 °K to 348 °K even though these temperatures exceed the range for which the above vapor pressure constants are valid. Upon plotting vapor pressure vs. temperature, vapor pressure appears to approach zero at temperatures below 304 °K.

$$\ln\left(\frac{P_2}{P_c}\right) = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^{3} + (VPD)x^{6}\right]$$ Ref. D App A eqn. #1

$$x = 1 - T/T_c$$

$T_c = 647.3$
$VPB = 1.45838$
$P_c = 221.2$
$VPC = -2.7758$
$VPA = -7.76451$
$VPD = -1.23303$

Valid From 275 °K to 647.3 °K

°K	P_1 (bars)	P_2 (bars)
288	9.196×10^{-2}	1.69×10^{-2}
303	1.866×10^{-1}	4.212×10^{-2}
318	3.497×10^{-1}	9.521×10^{-2}
333	6.136×10^{-1}	1.98×10^{-1}
348	1.019×10^{0}	3.834×10^{-1}

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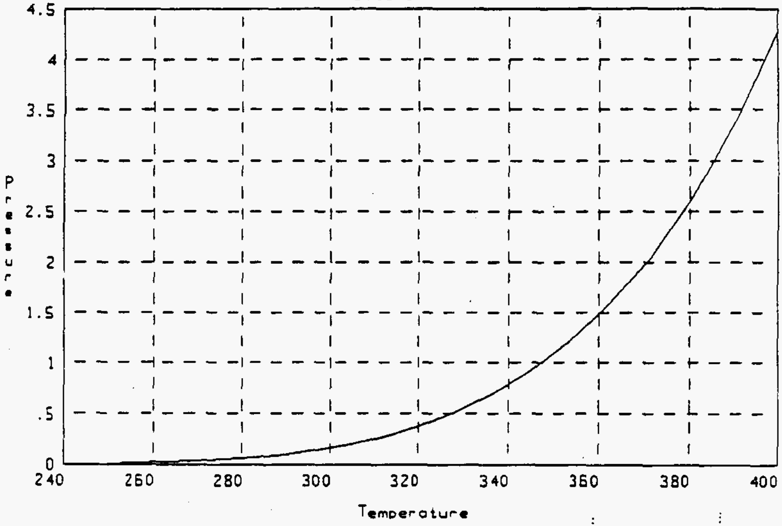

Butanol

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5.) $y_i P_t = \gamma_i x_i p_i$

x_i = mole fraction of component i in liquid phase
y_i = vapor phase mol fraction of component i

P_t = System pressure (vapor phase)

γ_i = activity coeffecient (liquid phase) (component i)

p_i = vapor pressure of pure component at system temp.

$$y_1 = \frac{\gamma_1 x_1 p_1}{P_t}$$

P_t = 750 mm Hg in C-100

$$\Rightarrow \left(750 \text{ mm Hg}\right)\left(\frac{1.01325 \text{ bars}}{760 \text{ mm Hg}}\right) = .9999 \text{ bars}$$

P_t = .9999 bars

Butanal

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6.) C-100 stream flow rate = 150 $\frac{ft^3}{min}$

C-100 pressure = 6" WG

$$\text{Emmissions} = \left(150\ \frac{ft^3}{min}\right)\left(28.317\ \frac{l}{ft^3}\right)\left(\frac{60\ min}{hr}\right)\left(\frac{750\ mm\ Hg}{760\ mm\ Hg}\right)\left(\frac{298}{T}\right)\left(\frac{1\ mol}{22.4\ l}\right)$$

$$\xrightarrow{\text{cont'd}} \left(\frac{72.107\ g}{mol}\right)\left(\frac{1\ lb}{454\ g}\right)\left(y_i\right) = \frac{\text{lbs of Butanal}}{hr}$$

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Butanal Emmissions C-100 (x1=ave)

T °K	v1 γ1	p1 bars	x1 MF	y1 MF	Emmissions lbs/hr.
2.88E2	6.155E1	9.196E-2	9E-9	5.095E-8	9.4E-5
3.03E2	6.895E1	1.866E-1	9E-9	1.158E-7	2.031E-4
3.18E2	7.723E1	3.497E-1	9E-9	2.431E-7	4.063E-4
3.33E2	8.651E1	6.136E-1	9E-9	4.778E-7	7.625E-4
3.48E2	9.691E1	1.019E0	9E-9	8.885E-7	1.357E-3

Butanal Emmissions C-100 (x1=max)

T °K	v1 γ1	p1 bars	x1 MF	y1 MF	Emmissions lbs/hr.
2.88E2	6.155E1	9.196E-2	1.9E-8	1.076E-7	1.984E-4
3.03E2	6.895E1	1.866E-1	1.9E-8	2.445E-7	4.288E-4
3.18E2	7.723E1	3.497E-1	1.9E-8	5.133E-7	8.577E-4
3.33E2	8.651E1	6.136E-1	1.9E-8	1.009E-6	1.61E-3
3.48E2	9.691E1	1.019E0	1.9E-8	1.876E-6	2.864E-3

Butanal Emmissions C-100 (x1=max10)

T °K	v1 γ1	p1 bars	x1 MF	y1 MF	Emmissions lbs/hr.
2.88E2	6.155E1	9.196E-2	1.9E-7	1.075E-6	1.984E-3
3.03E2	6.894E1	1.866E-1	1.9E-7	2.445E-6	4.288E-3
3.18E2	7.723E1	3.497E-1	1.9E-7	5.133E-6	8.577E-3
3.33E2	8.651E1	6.136E-1	1.9E-7	1.009E-5	1.61E-2
3.48E2	9.691E1	1.019E0	1.9E-7	1.876E-5	2.864E-2

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Title: Organic Emissions

Date: 2/91 by Jon Perry

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The process condensate emmission results at 75 °C = 348 °K, can be used to determine the feed concentration limit. The feed concentration limit is the concentration of volatile constituent in the feed stream, with the assumption that the volatile constituent is completely transferred into the condensate, which will produce 0.71 lbs/hr (.322 kg/hr) emmissions of Butanal from the process condensate. The feed concentration limit is calculated as follows:

$$\left(\frac{7.60\times10^{2}\ \mu g/l}{}\right)\left(\frac{1\ mg}{1000\ \mu g}\right)\left(\frac{1\ hr.}{2.864\times10^{-2}\ lbs}\right)\left(\frac{.71\ lbs}{1\ hr}\right)\left(\frac{R-1}{R}\right)$$

$$= 18.84\left(\frac{R-1}{R}\right) \Rightarrow mg/l$$

note: R = feed rate ÷ product rate

Westinghouse Environmental & Geotechnical Services, Inc.

DESIGN ANALYSIS

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Job No. 89-5010-ES Client/Project WHC 642-A

Title: Organic Removal

Date: 2/91 by Jon Perry

Checked: 3/91 by WGRichard

Determination of maximum feed concentration:

$$R \cdot C_f + (1 - R) C_c = C_s$$

R = Ratio of Feed to product Mass Ratio

C_f = Feed Concentration

C_s = Concentration of a given component in Slurry

Note: To determine the maximum Feed concentration (C_f) of a given component, (C_s) will be the regulatory limit (HBL or LDR).

C_c = Condensate Concentration of a given component

Note: C_c is calculated from the vapor phase mol fraction for a given component in the slurry.

Westinghouse Environmental & Geotechnical Services, Inc.

DESIGN ANALYSIS

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Job No. 89-5010-ES Client/Project WHC/242-A
Title: Organic Removal
Date: 2/91 by JD Perry
Checked: 3/91 by WG Richard

C_c is calculated by converting y_i (mol fraction) to y_i (ppm)

$$y_i(MF) = \frac{moles\ i}{moles\ i + moles\ H_2O}$$

In this calculation, the mole contribution of component i is insignificant relative to the mole contribution of H_2O. Therefore,

$$\left(\frac{mol\ i}{\underbrace{\cancel{mol\ i}}_{insignificant} + mol\ H_2O}\right)\left(\frac{55.5093\ mol\ H_2O}{1\ l}\right)(molec.\ wt)\left(\frac{1000\ mg}{g}\right)$$

$$= mg/l = mg/Kg = ppm$$

Butanal

Westinghouse Environmental & Geotechnical Services, Inc.

DESIGN ANALYSIS

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Job No. 89-5010-ES Client/Project WHC/242-A

Title: Organic Removal

Date: 2/91 by Jon Perry

Checked: 3/91 by

Butanal Slurry Vapor Fraction

T °K	v1 l	p1 bars	x1 MF	Pt bars	y1 MF
2.98E2	6.638E1	1.488E-1	2.5E-7	3.143E-2	7.857E-5
3.03E2	6.894E1	1.866E-1	2.5E-7	4.212E-2	7.636E-5
3.08E2	7.16E1	2.32E-1	2.5E-7	5.584E-2	7.435E-5
3.13E2	7.436E1	2.859E-1	2.5E-7	7.328E-2	7.254E-5
3.18E2	7.723E1	3.497E-1	2.5E-7	9.522E-2	7.091E-5
3.23E2	8.021E1	4.247E-1	2.5E-7	1.226E-1	6.946E-5
3.28E2	8.33E1	5.121E-1	2.5E-7	1.565E-1	6.816E-5
3.33E2	8.651E1	6.136E-1	2.5E-7	1.98E-1	6.701E-5
3.38E2	8.984E1	7.307E-1	2.5E-7	2.487E-1	6.6E-5
3.43E2	9.331E1	8.651E-1	2.5E-7	3.099E-1	6.512E-5
3.48E2	9.69E1	1.019E0	2.5E-7	3.834E-1	6.437E-5

Butanal Slurry Limits (mg/l)

T °K	y1 MF	Cc mg/l	HBL mg/l
2.98E2	7.857E-5	3.145E2	1E0
3.03E2	7.636E-5	3.056E2	1E0
3.08E2	7.435E-5	2.976E2	1E0
3.13E2	7.254E-5	2.904E2	1E0
3.18E2	7.092E-5	2.838E2	1E0
3.23E2	6.946E-5	2.78E2	1E0
3.28E2	6.816E-5	2.728E2	1E0
3.33E2	6.701E-5	2.682E2	1E0
3.38E2	6.6E-5	2.642E2	1E0
3.43E2	6.512E-5	2.607E2	1E0
3.48E2	6.437E-5	2.576E2	1E0

$$C_f = \left(\frac{R-1}{R} + \frac{C_s}{R}\right) C_c$$

1- Butanol

Westinghouse Environmental & Geotechnical Services, Inc.

DESIGN ANALYSIS

Page No. 1 of 12
Job No. 89-5010-ES Client/Project 242-A-Part B
Title: Organic Emmissions
Date: 1/91 by Jon Perry
Checked: 3/91 by

1.) Let 1 be 1-Butanol and 2 be H_2O

Butanol :

$$\log \gamma_1^{\infty} = \alpha + \epsilon N_1 + \frac{\zeta}{N_1} + \frac{\theta}{N_2}$$ Ref. C pp 295 a

$N_1 = 4$ N_2 0

$$\left\{ \begin{matrix} N_1 = \text{total \# of carbon atoms in molecule \#1} \\ N_2 = \text{total \# of carbon atoms in molecule \#2} \end{matrix} \right\}$$

$CH_3-CH_2-CH_2-CH_2-OH \Rightarrow$ Butanol

°C	°K	α	ϵ	ζ
25	298	-.995	.622	.558
60	333	-.755	.583	.460
100	373	-.420	.517	.230

$$\log \gamma_1^{\infty} = \alpha + 4\epsilon + \frac{\zeta}{4}$$

α, ϵ, and ζ can be regressed with respect to temperature to give the following expressions which can be used to determine α, ϵ, and ζ at various temperatures. (T) → is in °K

$\alpha = 7.683 \times 10^{-3}(T) - 3.295$
$\epsilon = -1.406 \times 10^{-3}(T) + 1.045$
$\zeta = -4.406 \times 10^{-3}(T) + 1.891$

1- Butanol

Westinghouse Environmental & Geotechnical Services, Inc.

DESIGN ANALYSIS

Page No. 2 of 12

Job No. 89-5010-ES Client/Project 242-A-PartB

Title: Organic Emmissions

Date: 1/91 by Jon Perry

Checked: 3/91 by

H_2O

$$\log \gamma_2^{\infty} = \alpha + \epsilon N_2 + \zeta / N_2 + \frac{\theta}{N_1}$$ Ref C pp 295 a

$N_2 = 0$ $N_1 = 4$

°K	α	ϵ	ζ	θ
298	.760	0	0	−.630
333	.680	0	0	−.440
373	.617	0	0	−.280

$$\log \gamma_2^{\infty} = \alpha + \theta/4$$

α and θ can be regressed with respect to temperature to give expressions which can be used to determine α and θ at various temperatures.

note $T \Rightarrow$ °K

$$\alpha = -1.900 \times 10^{-3} (T) + 1.321 \times 10^{0}$$

$$\theta = 4.651 \times 10^{-3} (T) - 2.007 \times 10^{0}$$

1- Butanol

Westinghouse Environmental & Geotechnical Services, Inc.

DESIGN ANALYSIS

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Job No. 89-5010-ES Client/Project 242-A- Part B

Title: Organic Emmissions

Date 1/91 by Jon Perry

Checked: 3/91 by

2.) $\ln \gamma_1^{\infty} = -\ln(\Lambda_{12}) - \Lambda_{21} + 1$ Ref. C 8-10.25

$\ln \gamma_2^{\infty} = -\ln(\Lambda_{21}) - \Lambda_{12} + 1$ Ref C 8-10.26

T(°K)	Λ_{12} ($\times 10^{-2}$)	Λ_{21} ($\times 10^{-1}$)
288	3.299	6.502
303	3.135	6.681
318	2.978	6.864
333	2.828	7.051
348	2.684	7.244

1- Butanol

Westinghouse Environmental & Geotechnical Services, Inc.

DESIGN ANALYSIS

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Job No. 89-5010-ES

Client/Project 242-A-Part B

Title: Organic Emmissions

Date: 1/91 by Jon Perry

Checked: 3/4/91 by

3) $$\ln \gamma_1 = -\ln(x_1 + \Lambda_{12} x_2) + x_2\left[\frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{\Lambda_{21} x_1 + x_2}\right]$$ Ref. A 6.11-2

$$\ln \gamma_2 = -\ln(x_2 + \Lambda_{21} x_1) - x_1\left[\frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{\Lambda_{21} x_1 + x_2}\right]$$ Ref. A 6.11-3

mol fraction ↓

x_1 = MF of Butanol
x_2 = MF of H_2O

MF is determined from ppb concentration (obtained from stream specific Report App. 3A)

°K	$x_1 = 4.569 \times 10^{-6}$ MF γ_1 $(\times 10^1)$	$x_1 = 2.94 \times 10^{-5}$ γ_1 $(\times 10^1)$	$x_1 = 2.94 \times 10^{-4}$ MF γ_1 $(\times 10^1)$	$x_1 = 4.569 \times 10^{-6}$ MF $x_1 = 2.94 \times 10^{-5}$ $x_1 = 2.94 \times 10^{-4}$ γ_2
288	4.3	4.293	4.227	1
303	4.445	4.437	4.365	1
318	4.594	4.586	4.507	1
333	4.749	4.739	4.654	1
348	4.908	4.898	4.805	1
				1

1- Butanol

Westinghouse Environmental & Geotechnical Services, Inc.

DESIGN ANALYSIS

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Job No. 89-5010-ES Client/Project 242-A-Part B

Title: Organic Emmissions

Date: 1/91 by Jon Perry

Checked: 3/91 by

4.)
$$\ln \frac{P_1}{P_c} = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^3 + (VPD)x^6\right]$$ Ref. D App A eqn. #1

$$x = 1 - T/T_c$$

T_c = 563.1
VPB = .53783

P_c = 44.2
VPC = -9.3424

VPA = -8.00756
VPD = 6.68692

Valid From 275°K to 563.1°K

$$\ln \frac{P_2}{P_c} = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^3 + (VPD)x^6\right]$$ Ref. D App A eqn. #1

$$x = 1 - T/T_c$$

T_c = 647.3°K
VPB = 1.45838

P_c = 221.2 bars
VPC = -2.7758

VPA = -7.76451
VPD = -1.23303

Valid From 275 to 647.3°K

°K	P_1 (bars)	P_2 (bars)
288	4.282×10^{-3}	1.690×10^{-2}
303	1.276×10^{-2}	4.212×10^{-2}
318	3.36×10^{-2}	9.522×10^{-2}
333	7.949×10^{-2}	1.980×10^{-1}
348	1.713×10^{-1}	3.833×10^{-1}

1- Butanol

Westinghouse Environmental & Geotechnical Services, Inc.

DESIGN ANALYSIS

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Job No. 89-5010-ES Client/Project 242-A- Part B
Title: Organic Emmissions
Date: 1/91 by Jon Perry
Checked: 3/91 by

5.) $Y_i \, P_t = \gamma_i \, x_i \, P_i$

x_i = mole Fraction of component i (liquid phase)
Y_i = Vapor Phase Mol Fraction
P_t = System Vapor Pressure
γ_i = Activity Coeffecient (liquid phase) of component i
P_i = Vapor pressure of component i (pure phase) at system Temperature

$$Y_1 = \frac{\gamma_1 \, x_1 \, P1}{P_t}$$

$$P_t = 750 \text{ mmHg} \Rightarrow 750 \text{ mmHg} \times \frac{1.01325 \text{ bars}}{760 \text{ mmHg}}$$

$$P_t = .9999 \text{ bars}$$

1- Butanol

Westinghouse Environmental & Geotechnical Services, Inc.

DESIGN ANALYSIS

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Job No.	89-5010-ES
Client/Project	242-A-Part B
Title:	Organic Emmissions
Date:	1/91 by Jon Perry
Checked:	3/91 by

6.) Given : C-100 stream Flow Rate $= 150\ ft^3/min$

: C-100 Pressure = 6" WG

$$\text{Emmissions} = \left(150\ \frac{ft^3}{min}\right)\left(\frac{28.317\ l}{ft^3}\right)\left(\frac{60\ min}{hr}\right)\left(\frac{750\ mm\ Hg}{760\ mm\ Hg}\right)\left(\frac{298}{T}\right)$$

$$\left(\frac{1\ mole}{22.4\ l}\right)\left(\frac{74.123 g}{mol}\right)\left(\frac{1\ lbs}{454 g}\right)\left(Y_1\right) = \frac{lbs\ \text{Butanol}}{hr.}$$

1-Butano

Westinghouse Environmental & Geotechnical Services, Inc.

DESIGN ANALYSIS

Page No. 8 of 12

Job No. 89-5010-ES Client/Project 242-A-Pan+B

Title: Organic Emmissions

Date: 1/91 by Jon Perry

Checked: 3/91 by WBRichmond

°K Butanol C-100 Emmissions (x1=ave)

T °K	v1 γ1	p1 bars	x1 MF	y1 MF	Emmissions lbs/hr
2.88E2	4.299E1	4.282E-3	4.569E-6	8.413E-7	1.596E-3
3.03E2	4.444E1	1.276E-2	4.569E-6	2.59E-6	4.67E-3
3.18E2	4.593E1	3.36E-2	4.569E-6	7.051E-6	1.211E-2
3.33E2	4.747E1	7.949E-2	4.569E-6	1.724E-5	2.829E-2
3.48E2	4.907E1	1.713E-1	4.569E-6	3.841E-5	6.029E-2

°K Butanol C-100 Emmissions (x1=max)

T °K	v1 γ1	p1 bars	x1 mF	y1 mF	Emmissions lbs/hr
2.88E2	4.293E1	4.282E-3	2.94E-5	5.405E-6	1.025E-2
3.03E2	4.437E1	1.276E-2	2.94E-5	1.664E-5	3E-2
3.18E2	4.586E1	3.36E-2	2.94E-5	4.53E-5	7.781E-2
3.33E2	4.739E1	7.949E-2	2.94E-5	1.108E-4	1.817E-1
3.48E2	4.898E1	1.713E-1	2.94E-5	2.467E-4	3.873E-1

°K Butanol C-100 Emmissions (x1=max10)

T °K	v1 γ1	p1 bars	x1 mF	y1 mF	Emmissions lbs/hr
2.88E2	4.227E1	4.282E-3	2.94E-4	5.322E-5	1.009E-1
3.03E2	4.365E1	1.276E-2	2.94E-4	1.637E-4	2.952E-1
3.18E2	4.507E1	3.36E-2	2.94E-4	4.452E-4	7.648E-1
3.33E2	4.654E1	7.949E-2	2.94E-4	1.088E-3	1.784E0
3.48E2	4.805E1	1.713E-1	2.94E-4	2.42E-3	3.799E0

– Butano

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DESIGN ANALYSIS

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Job No. 89-5010-ES Client/Project 242-A-Part B

Title: Organic Emmissions

Date: 1/91 by Jon Perry

Checked: 3/91 by

The process condensate emmission results at 75°C = 348°K, can be used to determine the feed concentration limit. The feed concentration limit is the concentration of volatile constituent in the feed stream, with the assumption that the volatile constituent is completely transferred into the condensate, which will produce 0.71 lbs/hr (.322 kg/hr) emmissions of Butanol from the process condensate. The feed concentration limit is calculated as follows:

$$\left(\frac{1.21\times10^{6}}{}\ \mu g/l\right)\left(\frac{1\ mg}{1000\ \mu g}\right)\left(\frac{1\ hr.}{3.799\ lbs}\right)\left(\frac{.71\ lbs}{1\ hr}\right)\left(\frac{R-1}{R}\right)$$

$$= 226.14\ \left(\frac{R-1}{R}\right) \Rightarrow mg/l$$

note: R = Feed rate ÷ product rate

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DESIGN ANALYSIS

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Job No. 89-5010-ES		Client/Project WHC/242-A	
Title: 242-A Volatile organic removal			
Date: 1/91		by Jon Perry	
Checked: 3/91		by	

Determination of maximum feed concentration:

$$R C_f + (1 - R) C_c = C_s$$

R = Ratio of Feed to product Mass Ratio

C_f = Feed Concentration

C_s = Concentration of a given component in Slurry

Note: To determine the maximum feed concentration (C_f) of a given component, (C_s) will be the regulatory limit (HBL or LDR).

C_c = Condensate Concentration of a given component

Note: C_c is calculated from the vapor phase mol fraction for a given component in the slurry.

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DESIGN ANALYSIS

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Job No. 89-5010-ES Client/Project WHC/242-A

Title: 242-A- Volatile Organic Removal

Date: 1/91 by Jon Perry

Checked: 3/91 by

C_c is calculated by converting y_i (mol fraction) to y_i (ppm)

$$y_i(MF) = \frac{\text{moles } i}{\text{moles } i + \text{moles } H_2O}$$

In this calculation, the mole contribution of component i is insignificant relative to the mole contribution of H_2O. Therefore,

$$\left(\frac{\text{mol } i}{\underset{\text{insignificant}}{\cancel{\text{mol } i}} + \text{mol } H_2O}\right)\left(\frac{55.5093 \text{ mol } H_2O}{1 \ell}\right)(\text{molec. wt})\left(\frac{1000 \text{ mg}}{g}\right)$$

$$= \text{mg}/\ell = \text{mg}/\text{Kg} = \text{ppm}$$

1- Butano

Westinghouse Environmental & Geotechnical Services, Inc.

DESIGN ANALYSIS

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Job No. 89-5010-ES Client/Project WHC /242-A

Title: 242-A Volatile Organic Removal

Date: 1/91 by Jon Perry

Checked: ______ by ______

Butanol Slurry Vapor Fraction

T °K	v1 Y1	p1 bars	x1 MF	Pt bars	y1 MF
2.98E2	4.396E1	8.996E-3	1.215E-6	3.143E-2	1.529E-5
3.03E2	4.445E1	1.276E-2	1.215E-6	4.212E-2	1.636E-5
3.08E2	4.494E1	1.784E-2	1.215E-6	5.584E-2	1.745E-5
3.13E2	4.544E1	2.464E-2	1.215E-6	7.327E-2	1.856E-5
3.18E2	4.594E1	3.36E-2	1.215E-6	9.522E-2	1.969E-5
3.23E2	4.645E1	4.527E-2	1.215E-6	1.226E-1	2.084E-5
3.28E2	4.696E1	6.031E-2	1.215E-6	1.565E-1	2.2E-5
3.33E2	4.749E1	7.949E-2	1.215E-6	1.98E-1	2.316E-5
3.38E2	4.801E1	1.037E-1	1.215E-6	2.487E-1	2.432E-5
3.43E2	4.854E1	1.339E-1	1.215E-6	3.099E-1	2.549E-5
3.48E2	4.908E1	1.713E-1	1.215E-6	3.834E-1	2.665E-5

Butanol Slurry Limits (mg/l)

T °K	y1 MF	Cc mg/l	LDR mg/l
2.98E2	1.529E-5	6.29E1	5E0
3.03E2	1.636E-5	6.729E1	5E0
3.08E2	1.745E-5	7.179E1	5E0
3.13E2	1.856E-5	7.638E1	5E0
3.18E2	1.969E-5	8.103E1	5E0
3.23E2	2.084E-5	8.575E1	5E0
3.28E2	2.2E-5	9.05E1	5E0
3.33E2	2.316E-5	9.528E1	5E0
3.38E2	2.432E-5	1.001E2	5E0
3.43E2	2.549E-5	1.049E2	5E0
3.48E2	2.665E-5	1.096E2	5E0

$$C_f = \left(\frac{R-1}{R} + \frac{C_s}{R} \right) C_c$$

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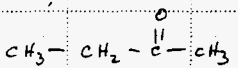
DESIGN ANALYSIS

Page No. 1 of 12
Job No. 89-5010-ES Client/Project WHC/242-A
Title: Organic Emissions
Date: 2/91 by Don Perry
Checked: 3/91 by

1.) Let 1 be 2-Butanone and 2 be H_2O

2-Butanone ;



$$CH_3-CH_2-\overset{O}{\overset{\|}{C}}-CH_3$$

$$\log \gamma_1^{\infty} = \alpha + \epsilon N_1 + \zeta\left(\frac{1}{N_1'} + \frac{1}{N_1''}\right) + \eta\left(N_1 - N_2\right)^2$$ Ref C pp 295 b.

$N_1 = 4$ $N_1' = 2$ $N_1'' = 3$ $N_2 = 0$

°K	α	ϵ	ζ	η
298	−1.475	.622	.500	—
333	−1.040	.583	.330	—
373	,621	.517	,200	—

N_1 = total # of carbon atoms in molecule #1
N_2 = total # of carbon atoms in molecule #2
N_1' & N_1'' = the # of carbon atoms in respective branches of molecule #1 including the functional group carbon atom

$$\log \gamma_1^{\infty} = \alpha + 4\epsilon + \zeta\left(\frac{5}{6}\right)$$

α, E, and ζ can be regressed with respect to temperature to give the following expressions which can be used to determine α, ϵ, and ζ at various temperatures.

$(T) \Rightarrow$ °K

$\alpha = .01137\,(T) - 4.849$
$\epsilon = -1.406\times10^{-3}(T) + 1.045$
$\zeta = -3.982\times10^{-3}(T) + 1.676$

Westinghouse Environmental & Geotechnical Services, Inc.

DESIGN ANALYSIS

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Job No. 89-5010-ES Client/Project WHC/242-A

Title: Organic Emissions

Date: 2/91 by Jon Perry

Checked: 3/91 by WB Richard

H_2O

Ref C pp295C

$$\log \gamma_2^{\infty} = \alpha + \epsilon N_2 + \zeta\left(\frac{1}{N_2'} + \frac{1}{N_2''} + \frac{1}{N_2'''}\right) + \theta\left(\frac{1}{N_1'} + \frac{1}{N_1''}\right)$$

$N_2 = 0$ $N_2' = N_2'' = N_2''' = 0$ $N_1' = 2$ $N_1'' = 3$

°K	α	ϵ	ζ	η	θ
298	1.857	0	0	—	-1.019
333	1.493	0	0	—	-.73
373	1.231	0	0	—	-.557

$$\log \gamma_2^{\infty} = \alpha + \theta\left(5/6\right)$$

α and θ can be regressed w/ respect to temperature to give expressions which can be used to determine α and θ at various temperatures.

$T \Rightarrow$ °K

$$\alpha = -8.3 \times 10^{-3}(T) + 4.306 \times 10^{0}$$
$$\theta = 6.117 \times 10^{-3}(T) - 2.816 \times 10^{0}$$

2-Butanone

Westinghouse Environmental & Geotechnical Services, Inc.

DESIGN ANALYSIS

Page No. 3 of 12

Job No. 89-5010-ES Client/Project WHC/242-A

Title: Organic Emissions

Date: 2/91 by Jon Perry

Checked: 3/91 by

2.) $\ln \gamma_1^{\infty} = -\ln(\Lambda_{12}) - (\Lambda_{21}) + 1$ Ref. C 8-10.25

$\ln \gamma_2^{\infty} = -\ln(\Lambda_{21}) - (\Lambda_{12}) + 1$ Ref. C 8-10.26

T (K)	Λ_{12} $(\times 10^{-2})$	Λ_{21} $(\times 10^{-1})$
288	8.143	2.299
303	7.275	2.59
318	6.476	2.916
333	5.743	3.281
348	5.07	3.69

2-Butanone

Westinghouse Environmental & Geotechnical Services, Inc.

DESIGN ANALYSIS

Page No. 4 of 12
Job No. 89-5010-ES Client/Project WHC/242-A
Title: Organic Emissions
Date: 2/91 by Don Perry
Checked: 3/91 by

3.) $$\ln \gamma_1 = -\ln\left(x_1 + \Lambda_{12} x_2\right) + x_2 \left[\frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{\Lambda_{21} x_1 + x_2}\right]$$ Ref. A 6.11-2

$$\ln \gamma_2 = -\ln\left(x_2 + \Lambda_{21} x_1\right) - x_1 \left[\frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{\Lambda_{21} x_1 + x_2}\right]$$ Ref. A 6.11-3

x_1 = mol fraction of 2-Butanone

x_2 = mol fraction of H_2O

Mol fraction is calculated from the ppb concentration obtained from the stream specific report App 3A

$x_1 = 1.1 \times 10^{-8}$ MF
$x_1 = 3 \times 10^{-8}$ MF
$x_1 = 3 \times 10^{-7}$ MF

	$x_1 = 1.1 \times 10^{-8}$ mF	$x_1 = 3 \times 10^{-8}$ mF	$x_1 = 3 \times 10^{-7}$ mF	
°K	γ_1 $(\times 10^1)$	γ_1 $(\times 10^1)$	γ_1 $(\times 10^1)$	γ_2
288	2.652	2.652	2.652	1
303	2.884	2.884	2.884	1
318	3.136	3.136	3.136	1
333	3.409	3.409	3.409	1
348	3.707	3.707	3.707	1

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4.) $$\ln \frac{P_1}{P_c} = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^3 + (VPD)x^6\right]$$ ref. D App A eqn #1

$x = 1 - T/T_c$

$T_c = 536.8$ $P_c = 42.1$ $VPA = -7.71476$

$VPB = 1.71061$ $VPC = -3.6877$ $VPD = -.75169$

Valid From 255°K to 536.8°K

$$\ln \frac{P_2}{P_c} = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^3 + (VPD)x^6\right]$$ ref. D App A eqn #1

$x = 1 - T/T_c$

$T_c = 647.3$ °K $P_c = 221.2$ $VPA = -7.76451$

$VPB = 1.45838$ $VPC = -2.77580$ $VPD = -1.23303$

Valid From 275 °K to 647.3 °K

°K	P_1 (bars)	P_2 (bars)
288	7.303×10^{-2}	1.690×10^{-2}
303	1.51×10^{-1}	4.212×10^{-2}
318	2.882×10^{-1}	9.522×10^{-2}
333	5.141×10^{-1}	1.980×10^{-1}
348	8.653×10^{-1}	3.833×10^{-1}

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5.) $y_i P_t = \gamma_i x_i p_i$

x_i = mol fraction of component i in liquid phase

y_i = vapor phase mol fraction of component i

P_t = System pressure (vapor phase)

γ_i = activity coeffecient (liquid phase) (component i)

p_i = vapor pressure of pure component at system temp.

$$y_1 = \frac{\gamma_1 x_1 p_1}{P_t}$$

P_t = 750 mm Hg in C-100

$$\Rightarrow (750 \text{ mm Hg})\left(\frac{1.01325 \text{ bars}}{760 \text{ mm Hg}}\right) = .9999 \text{ bars}$$

P_t = .9999 bars

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Checked: 3/91 by WBRichard

6.)

C-100 stream flow rate = 150 $\frac{ft^3}{min}$

C-100 pressure = 6" WG

$$\text{Emmissions} = \left(150\ \frac{ft^3}{min}\right)\left(28.317\ \frac{l}{ft^3}\right)\left(\frac{60\ min}{hr}\right)\left(\frac{750\ mm\ Hg}{760\ mm\ Hg}\right)\left(\frac{298}{T}\right)\left(\frac{1\ mol}{22.4\ l}\right)$$

$$\left(\frac{72.107\ g}{mol}\right)\left(\frac{1}{454}\ \frac{lbs}{g}\right)\left(Y_1\right) = \frac{lbs\ \text{2-Butanone}}{hr}$$

2-Butanone

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Butanone C-100 Emmissions (x1=ave)

T °K	v1 γ1	p1 bars	x1 MF	y1 MF	Emissions lbs/hr
2.88E2	2.652E1	7.303E-2	1.1E-8	2.131E-8	3.932E-5
3.03E2	2.884E1	1.51E-1	1.1E-8	4.79E-8	8.401E-5
3.18E2	3.136E1	2.882E-1	1.1E-8	9.942E-8	1.661E-4
3.33E2	3.409E1	5.141E-1	1.1E-8	1.928E-7	3.077E-4
3.48E2	3.707E1	8.653E-1	1.1E-8	3.528E-7	5.388E-4

Butanone C-100 Emmissions (x1=max)

T °K	v1 γ1	p1 bars	x1 MF	y1 MF	Emissions lbs/hr
2.88E2	2.652E1	7.303E-2	3E-8	5.812E-8	1.072E-4
3.03E2	2.884E1	1.51E-1	3E-8	1.306E-7	2.291E-4
3.18E2	3.136E1	2.882E-1	3E-8	2.712E-7	4.531E-4
3.33E2	3.409E1	5.141E-1	3E-8	5.259E-7	8.392E-4
3.48E2	3.707E1	8.653E-1	3E-8	9.623E-7	1.469E-3

Butanone C-100 Emmissions (x1=max10)

T °K	v1 γ1	p1 bars	x1 MF	y1 MF	Emissions lbs/hr
2.88E2	2.652E1	7.303E-2	3E-7	5.812E-7	1.072E-3
3.03E2	2.884E1	1.51E-1	3E-7	1.306E-6	2.291E-3
3.18E2	3.136E1	2.882E-1	3E-7	2.712E-6	4.531E-3
3.33E2	3.409E1	5.141E-1	3E-7	5.259E-6	8.392E-3
3.48E2	3.707E1	8.653E-1	3E-7	9.623E-6	1.469E-2

2-butanone

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The process condensate emmission results at 75 °C = 348 °K, can be used to determine the feed concentration limit. The feed concentration limit is the concentration of volatile constituent in the feed stream, with the assumption that the volatile constituent is completely transferred into the condensate, which will produce 0.71 lbs/hr (.322 kg/hr) emmissions of 2-Butanone from the process condensate. The feed concentration limit is calculated as follows:

$$\left(\frac{1.20 \times 10^{3}}{} \ \mu g/l\right)\left(\frac{1\ mg}{1000\ \mu g}\right)\left(\frac{1\ \ hr.}{1.469 \times 10^{-2}\ lbs}\right)\left(\frac{.71\ lbs}{1\ hr}\right)\left(\frac{R-1}{R}\right)$$

$$= \quad 58.00 \left(\frac{R-1}{R}\right) \Rightarrow mg/l$$

note: R = Feed rate ÷ product rate

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Determination of maximum feed concentration:

$$R \cdot C_f + (1 - R) C_c = C_s$$

R = Ratio of Feed to product Mass Ratio

C_f = Feed Concentration

C_s = Concentration of a given component in Slurry

Note: To determine the maximum feed concentration (C_f) of a given component, (C_s) will be the regulatory limit (HBL or LDR).

C_c = Condensate Concentration of a given component

Note: C_c is calculated from the vapor phase mol fraction for a given component in the slurry.

2-butanone

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C_c is calculated by converting y_i (mol fraction) to y_i (ppm)

$$y_i(MF) = \frac{\text{moles } i}{\text{moles } i + \text{moles } H_2O}$$

In this calculation, the mole contribution of component i is insignificant relative to the mole contribution of H_2O. Therefore,

$$\left(\frac{\text{mol } i}{\underset{\text{insignificant}}{\cancel{\text{mol } i}} + \text{mol } H_2O}\right)\left(\frac{55.5093 \text{ mol } H_2O}{1 \ell}\right)(\text{molec. wt})\left(\frac{1000 \text{ mg}}{g}\right)$$

$$= \quad \text{mg}/\ell \quad = \quad \text{mg}/\text{Kg} \quad = \quad \text{ppm}$$

2-Butanone

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Butanone Slurry Vapor Fraction

T °K	v1	p1 bars	x1 MF	Pt bars	y1 MF
2.98E2	2.805E1	1.197E-1	1.87E-7	3.143E-2	1.996E-5
3.03E2	2.884E1	1.51E-1	1.87E-7	4.212E-2	1.933E-5
3.08E2	2.965E1	1.888E-1	1.87E-7	5.584E-2	1.875E-5
3.13E2	3.049E1	2.342E-1	1.87E-7	7.327E-2	1.823E-5
3.18E2	3.136E1	2.882E-1	1.87E-7	9.522E-2	1.775E-5
3.23E2	3.224E1	3.52E-1	1.87E-7	1.226E-1	1.731E-5
3.28E2	3.315E1	4.268E-1	1.87E-7	1.565E-1	1.691E-5
3.33E2	3.409E1	5.141E-1	1.87E-7	1.98E-1	1.655E-5
3.38E2	3.506E1	6.152E-1	1.87E-7	2.487E-1	1.622E-5
3.43E2	3.605E1	7.317E-1	1.87E-7	3.099E-1	1.592E-5
3.48E2	3.707E1	8.653E-1	1.87E-7	3.834E-1	1.564E-5

Butanone Slurry Limits(mg/l)

T °K	y1 MF	Cc mg/l	LDR mg/l
2.98E2	1.996E-5	7.991E1	7.5E-1
3.03E2	1.933E-5	7.737E1	7.5E-1
3.08E2	1.875E-5	7.506E1	7.5E-1
3.13E2	1.823E-5	7.296E1	7.5E-1
3.18E2	1.775E-5	7.104E1	7.5E-1
3.23E2	1.731E-5	6.929E1	7.5E-1
3.28E2	1.691E-5	6.77E1	7.5E-1
3.33E2	1.655E-5	6.625E1	7.5E-1
3.38E2	1.622E-5	6.492E1	7.5E-1
3.43E2	1.592E-5	6.372E1	7.5E-1
3.48E2	1.564E-5	6.262E1	7.5E-1

$$C_f = \left(\frac{R-1}{R} + \frac{C_s}{R}\right) C_c$$

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Job No. 84-501D-ES Client/Project WHC/242-A

Title: Organic Emissions

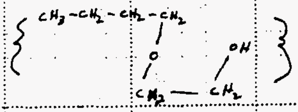
Date: 2/91 by Jon Perry

Checked: 3/91 by WBRichmond

1.) Let 1 be 2-Butoxyethanol and 2 be H_2O.

2-Butoxyethanol

$$\log \gamma_1^{\infty} = \alpha + \epsilon N_1 + \zeta / N_1 + \theta / N_2$$ Ref C 295 a



= 2-Butoxyethanol

$N_1 = 6$ $N_2 = 0$

°K	α	ϵ	ζ	η	θ
298	−.995	.622	.558	—	0
333	−.755	.583	.460	—	0
373	−.420	.517	.230	—	0

$$\log \gamma_1^{\infty} = \alpha + 6 N_1 + \zeta / 6$$

N_1 and N_2 = total # of carbon atoms in respective molecules
N', N^4, and N''' = the # of carbon atoms in respective branches of the indicated molecule

α, ϵ, and ζ can be regressed with respect to temperature to give expressions which can be used to determine α, ϵ, and ζ at various temperatures.

$\alpha = 7.683 \times 10^{-3}(T) - 3.295$
$\epsilon = -1.406 \times 10^{-3}(T) + 1.045$
$\zeta = -4.406 \times 10^{-3}(T) + 1.891$

T => °K

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H_2O

$$\log \gamma_2^{\infty} = \alpha + \epsilon N_2 + \frac{\zeta}{N_2} + \frac{\theta}{N_1}$$

ref 295a

$N_2 = 0 \quad N_1 = 6$

°K	α	ϵ	ζ	η	θ
298	.760	0	0	—	−.630
333	.680	0	0	—	−.440
373	.617	0	0	—	−.280

$$\log \gamma_2^{\infty} = \alpha + \frac{\theta}{6}$$

α and θ can be regressed with respect to temperature to give expressions which can be used to determine α and θ at various temperatures.

$T \Rightarrow$ °K

$\alpha = -1.899 \times 10^{-3} (T) + 1.321$

$\theta = 4.651 \times 10^{-3} (T) - 2.007$

2-Butoxyethanol

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2.) $\ln \gamma_1^\infty = -\ln(\Lambda_{12}) - \Lambda_{21} + 1$ Ref. C 8-10.25 pp 291

$\ln \gamma_2^\infty = -\ln(\Lambda_{21}) - \Lambda_{12} + 1$ Ref. C 8-10.26 pp 291

T °K	Λ_{12} $\times 10^{-3}$	Λ_{21} $\times 10^{-1}$
288	2.072	5.896
303	2.131	6.129
318	2.190	6.371
333	2.248	6.623
348	2.305	6.885

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3.) $$\ln \gamma_1 = -\ln(x_1 + \Lambda_{12} x_2) + x_2 \left[\frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{\Lambda_{21} x_1 + x_2} \right]$$ Ref. A 6.11-2

;

$$\ln \gamma_2 = -\ln(x_2 + \Lambda_{21} x_1) - x_1 \left[\frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{\Lambda_{21} x_1 + x_2} \right]$$ Ref. A 6.11-3

x_1 & x_2 = mol fraction of respective molecules

Mol Fraction is calculated from ppb concentration in Stream Specific Report App 3A.

ex.) $$3.686 \times 10^{2} \text{ ppb} = \frac{3.686 \times 10^{2} \ \mu g}{1 \text{ liter}} = \frac{3.686 \times 10^{-4} \ g}{1000 \ g \ H_2O + \text{2-Butoxyethanol}} =$$

$$= \frac{3.12 \times 10^{-6} \text{ moles 2-Butoxyethanol}}{3.686 \times 10^{-4} \text{ g 2-Butoxyethanol} + 999.999 \text{ g } H_2O} = \frac{3.12 \times 10^{-6} \text{ moles 2-Butoxyethanol}}{3.12 \times 10^{-6} \text{ moles 2-Butoxyethanol} + 55.5093 \text{ moles } H_2O}$$

$= 5.6 \times 10^{-8}$ mF 2-Butoxyethanol

MW of 2-Butoxyethanol = 118.20 g/mole
MW of H_2O = 18.015 g/mole

$x_1 = 5.6 \times 10^{-8}$ MF
$x_1 = 1.4 \times 10^{-7}$ MF
$x_1 = 1.4 \times 10^{-6}$ MF

	$x_1 = 5.6 \times 10^{-8}$ MF	$x_1 = 1.4 \times 10^{-7}$ MF	$x_1 = 1.4 \times 10^{-6}$ MF	
°K	$\gamma_1 (\times 10^{2})$	$\gamma_1 (\times 10^{2})$	$\gamma_1 (\times 10^{-2})$	γ_2
288	7.274	7.274	7.265	1
303	6.910	6.910	6.901	1
318	6.564	6.564	6.556	1
333	6.235	6.235	6.228	1
348	5.923	5.923	5.916	1

2-Butoxyethano

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4) The Clausius - Clapeyron Equation can be used to estimate the vapor pressure.

$$\ln(P_1) = -\frac{\Delta \hat{H}_v}{RT} + B$$ Ref. E pp 209

P_1 = Vapor pressure of pure substance (in this case 2-Butoxyethanol

R = Gas Constant

B = A constant which varies from one substance to another

$\Delta \hat{H}_v$ = Latent heat of vaporization (or the energy required to vaporize one mole of liquid)

T = Absolute temperature

Ref. E = R.M. Felder and R.W. Roussea, "Elementary Principles of Chemical Processes," John Wiley & Sons, New York, 1978.

Note: A linear relationship between ln(P) and 1/T exists, therefore, if at least two data points for P and T are known, an equation which describes P at various temperatures can be determined.

Note: The following data for pressure and temperature was obtained from:

N. Irving Sax, "Dangerous Properties of Industrial Materials" 6th Edition, Van Nostrand Reinhold Company, Inc., New York, New York, 1984, pp 575.

2- Butoxyethanol

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```
Temp.(K)  P(mmHg)      1/T(°K)      ln(P)
-------------------------------------------
4.132E+02 3.000E+02 2.420E-03 5.704E+00
4.442E+02 7.600E+02 2.251E-03 6.633E+00
```

$$\frac{\hat{\Delta H_v}}{R} = \text{slope} = \frac{\ln(P_2/P_1)}{\frac{1}{T_2} - \frac{1}{T_1}} = -5502.27$$

$$B = y_{int} = \ln P + \frac{\hat{\Delta H_v}}{RT}$$

$$B = \ln(300) + \frac{5502.27}{413.15} = 19.022$$

$$\ln P = \frac{-5502.27}{T} + 19.022 \Big\} \text{ The Eqn. Clausius - Clapeyron for 2-Butoxyethanol}$$

Note: Before P can be used in the Vapor Liquid Equilibrium Equation, the units must be converted from mmHg to bars for these calculations

$$1.01325 \text{ bars} = 760 \text{ mm Hg}$$

$$P(\text{mm Hg})\left(\frac{1.01325}{760}\right) = P(\text{bars})$$

°K	P, (bars)
288	1.228×10^{-3}
303	3.162×10^{-3}
318	7.446×10^{-3}
333	1.623×10^{-2}
348	3.309×10^{-2}

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5) $$\ln \frac{P_2}{P_c} = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^{3} + (VPD)x^{6}\right]$$ Ref D App A eqn #1

$$x = 1 - \frac{T_2}{T_c}$$

$T_c = 647.3$
$VPB = 1.45838$
$P_c = 221.2$
$VPC = -2.7758$
$VPA = -7.76451$
$VPD = -1.23303$

Valid From 275 °K to 647.3 °K

°K	P_2 (bars)
288	1.69×10^{-2}
303	4.212×10^{-2}
318	9.521×10^{-2}
333	1.98×10^{-1}
348	3.834×10^{-1}

2-butoxyethanol

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6.) $y_i P_t = \gamma_i x_i p_i$

x_i = mole fraction of component i liquid phase

y_i = vapor phase mol fraction of component i

P_t = System pressure (vapor phase)

γ_i = activity coeffecient (liquid phase) (component i)

p_i = vapor pressure of pure component at system temp.

$$y_1 = \frac{\gamma_1 x_1 p_1}{P_t}$$

P_t = 750 mm Hg in C-100

$$\Rightarrow (750 \text{ mm Hg})\left(\frac{1.01325 \text{ bars}}{760 \text{ mm Hg}}\right) = .9999 \text{ bars}$$

P_t = .9999 bars

2-butoxyethanol

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7.) C-100 stream flow rate = 150 $\frac{ft^3}{min}$

C-100 pressure = 6" WG

$$\text{Emmissions} = \left(150\ \frac{ft^3}{min}\right)\left(28.317\ \frac{l}{ft^3}\right)\left(\frac{60\ min}{hr}\right)\left(\frac{750\ mm\ Hg}{760\ mm\ Hg}\right)\left(\frac{298}{T}\right)\left(\frac{1\ mol}{22.4\ l}\right)$$

$$\underrightarrow{\text{cont'd}}\ \left(\frac{118.20\ g}{mol}\right)\left(\frac{1\ lb}{454\ g}\right)\left(y_i\right) = \frac{\text{lbs of 2-Butoxyethanol}}{hr}$$

2-Butyoxyethanol

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2-Butoxyethanol C-100 Emmissions (xl=ave)

T °K	vl	pl bars	xl MF	yl MF	Emmissions lbs/hr
2.88E2	7.274E2	1.228E-3	5.6E-8	5.003E-8	1.513E-4
3.03E2	6.91E2	3.162E-3	5.6E-8	1.224E-7	3.518E-4
3.18E2	6.564E2	7.446E-3	5.6E-8	2.737E-7	7.499E-4
3.33E2	6.235E2	1.623E-2	5.6E-8	5.669E-7	1.483E-3
3.48E2	5.923E2	3.309E-2	5.6E-8	1.098E-6	2.748E-3

2-Butoxyethanol C-100 Emmissions (xl=max)

T °K	vl	pl bars	xl MF	yl MF	Emmissions lbs/hr
2.88E2	7.274E2	1.228E-3	1.4E-7	1.251E-7	3.783E-4
3.03E2	6.91E2	3.162E-3	1.4E-7	3.059E-7	8.794E-4
3.18E2	6.564E2	7.446E-3	1.4E-7	6.843E-7	1.875E-3
3.33E2	6.235E2	1.623E-2	1.4E-7	1.417E-6	3.707E-3
3.48E2	5.923E2	3.309E-2	1.4E-7	2.744E-6	6.869E-3

2-Butoxyethanol C-100 Emmissions (xl=max10)

T °K	vl	pl bars	xl MF	yl MF	Emmissions lbs/hr
2.88E2	7.265E2	1.228E-3	1.4E-6	1.249E-6	3.778E-3
3.03E2	6.901E2	3.162E-3	1.4E-6	3.055E-6	8.784E-3
3.18E2	6.556E2	7.446E-3	1.4E-6	6.835E-6	1.872E-2
3.33E2	6.228E2	1.623E-2	1.4E-6	1.416E-5	3.703E-2
3.48E2	5.916E2	3.309E-2	1.4E-6	2.741E-5	6.861E-2

2-Butoxyethanol

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The process condensate emmission results at 75 °C = 348 °K, can be used to determine the feed concentration limit. The feed concentration limit is the concentration of volatile constituent in the feed stream, with the assumption that the volatile constituent is completely transferred into the condensate, which will produce 0.71 lbs/hr (.322 kg/hr) emissions of 2-Butoxyethanol from the process condensate. The feed concentration limit is calculated as follows:

$$\left(\frac{9.20 \times 10^{3}}{} \mu g/l\right)\left(\frac{1 \text{ mg}}{1000 \mu g}\right)\left(\frac{1 \text{ hr.}}{6.861 \times 10^{-2} \text{ lbs}}\right)\left(\frac{.71 \text{ lbs}}{1 \text{ hr}}\right)\left(\frac{R-1}{R}\right)$$

$$= 95.20 \left(\frac{R-1}{R}\right) \Rightarrow \text{mg}/l$$

note: R = feed rate ÷ product rate

2- Butoxyethanol

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Determination of maximum feed concentration:

$$R\,C_f + (1-R)\,C_c = C_s$$

R = Ratio of Feed to product Mass Ratio

C_f = Feed Concentration

C_s = Concentration of a given component in Slurry

Note: To determine the maximum feed concentration (C_f) of a given component, (C_s) will be the regulatory limit (HBL or LDR).

C_c = Condensate Concentration of a given component

Note: C_c is calculated from the vapor phase mol fraction for a given component in the slurry.

2-Butoxyethanol

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C_c is calculated by converting y_i (mol fraction) to y_i (ppm)

$$y_i(MF) = \frac{\text{moles } i}{\text{moles } i + \text{moles } H_2O}$$

In this calculation, the mole contribution of component i is insignificant relative to the mole contribution of H_2O. Therefore,

$$\left(\frac{\text{mol } i}{\cancel{\text{mol } i} + \text{mol } H_2O}\right)\left(\frac{55.5093 \text{ mol } H_2O}{1 \ell}\right)(\text{molec. wt})\left(\frac{1000 \text{ mg}}{g}\right)$$

insignificant

$$= \text{mg}/\ell = \text{mg}/\text{Kg} = \text{ppm}$$

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2-Butoxyethanol Slurry Vapor Phase Mol Fraction

T	v1	p1	x1	Pt	y1
2.98E2	7.029E2	2.332E-3	1.52E-7	3.143E-2	7.925E-6
3.03E2	6.909E2	3.162E-3	1.52E-7	4.212E-2	7.884E-6
3.08E2	6.792E2	4.246E-3	1.52E-7	5.584E-2	7.85E-6
3.13E2	6.677E2	5.648E-3	1.52E-7	7.327E-2	7.823E-6
3.18E2	6.563E2	7.446E-3	1.52E-7	9.522E-2	7.802E-6
3.23E2	6.452E2	9.733E-3	1.52E-7	1.226E-1	7.786E-6
3.28E2	6.343E2	1.262E-2	1.52E-7	1.565E-1	7.775E-6
3.33E2	6.235E2	1.623E-2	1.52E-7	1.98E-1	7.769E-6
3.38E2	6.129E2	2.073E-2	1.52E-7	2.487E-1	7.766E-6
3.43E2	6.025E2	2.628E-2	1.52E-7	3.099E-1	7.767E-6
3.48E2	5.923E2	3.309E-2	1.52E-7	3.834E-1	7.771E-6

2-Butoxyethanol Slurry Limits (mg/l)

T	y1	Cc	HBL
2.98E2	7.925E-6	5.2E1	1E0
3.03E2	7.884E-6	5.173E1	1E0
3.08E2	7.85E-6	5.151E1	1E0
3.13E2	7.823E-6	5.133E1	1E0
3.18E2	7.802E-6	5.119E1	1E0
3.23E2	7.786E-6	5.109E1	1E0
3.28E2	7.775E-6	5.102E1	1E0
3.33E2	7.769E-6	5.097E1	1E0
3.38E2	7.766E-6	5.095E1	1E0
3.43E2	7.767E-6	5.096E1	1E0
3.48E2	7.771E-6	5.098E1	1E0

$$C_f = \left(\left(\frac{R-1}{R} \right) + \frac{C_s}{R} \right) C_c$$

3,5 Dimethylpyridine

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The UNIFAC method can be used to determine activity coefficients (γ_i).

Ref. F
Robert C. Reid, John M. Prausnitz, Bruce E. Poling, "The Properties of Gases and Liquids," 4th Edition, McGraw-Hill, Inc., New York, NY, 1987, pp. 314 - 332.

$$\ln \gamma_i = \underset{(\text{combinatorial})}{\ln \gamma_i^C} + \underset{(\text{residual})}{\ln {}_i^R}$$

note: The combinatorial part of this equation deals with pure component properties only and is dependent on diffences in molecular size and shape

$$\ln \gamma_i^C = \ln \frac{\phi_i}{x_i} + \frac{z}{2} q_i \ln \frac{\theta_i}{\phi_i} + l_i - \frac{\phi_i}{x_i} \sum_j x_j l_j$$

$$\theta_i = \frac{q_i x_i}{\sum_j q_j x_j} \qquad \phi_i \; \frac{r_i x_i}{\sum_j r_j x_j}$$

$$r_i = \sum_k \nu_k^i R_k \qquad q_i = \sum_k \nu_k^i Q_k$$

x_i = mol fraction of molecule i in solution
Summations are over all components
$\left.\begin{matrix} R_k \\ Q_k \end{matrix}\right\}$ Determined from table B-21 (Ref. F)
ν_k^i = # of groups of type k in molecule i

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$$\ln \gamma_i^R = \sum_k \nu_k^i \left(\ln \Gamma_k - \ln \Gamma_k^i \right)$$

ν_k^i = # of groups of type k in molecule i
Γ_k = group residual activity coefficient
Γ_k^i = residual activity coeffecient of group k in a reference solution containing molecules of type i only.

$$\ln \Gamma_k = Q_k \left[1 - \ln \left(\sum_m \theta_m \Psi_{mk} \right) - \sum_m \frac{\theta_m \Psi_{km}}{\sum_n \theta_n \Psi_{nm}} \right]$$

Note: Summations are over all groups

$$\ln \Gamma_k^i = Q_k \left[1 - \ln \left(\sum_m \theta_m^i \Psi_{mk} \right) - \sum_m \frac{\theta_m^i \Psi_{km}}{\sum_n \theta_n^i \Psi_{nm}} \right]$$

Note: Summations are over all groups in molecule i only.

$$\theta_m = \frac{Q_m X_m}{\sum_n Q_n X_n}$$

X_m = mole fraction of group in
Q ⇒ determined from table 8-21 Ref. F

$$\Psi_{mn} = \exp\left(\frac{-a_{mn}}{T} \right)$$

a_{mn} ⇒ determined from table 8-22 Ref. F
T = temperature (°K)

3,5 Dimethylpyridine

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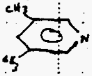

The following information is available in Ref. E

molecule		group name	group main #	ν_j^i	R_j	Q_j
3,5 Dimethyl pyridine	(1)	CH_3	1	$\nu_1^1 = 2$	.9011	.848
	(1)	C_5H_3N	18	$\nu_{18}^1 = 1$	2.667	1.553
H_2O	(2)	H_2O	7	$\nu_7^2 = 1$	.9200	1.400

$$r_i = \sum_k \nu_k^i R_k$$

$$r_1 = (2)(.9011) + (1)(2.667) = 4.469$$

$$r_2 = (1)(.9200) = 9.2 \times 10^{-1}$$

$$q_i = \sum_k \nu_k^i Q_k$$

$$q_1 = (2)(.848) + (1)(1.553) = 3.249$$

$$q_2 = (1)(1.400) = 1.400$$

$$\phi_i = \frac{r_i x_i}{\sum_j r_j x_j}$$

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x_i = mol fraction which is calculated from ppb concentration (obtained from Stream Specific Report – App. 3A).

ex.) 2.07×10^{1} ppb $= \dfrac{2.07\times10^{1}\ \text{mg}}{1\ \text{litre}} = \dfrac{1.93\times10^{-7}\ \text{moles } 3,5\text{DMP}}{1000\ \text{g}} = \dfrac{1.93\times10^{-7}\ \text{moles } \overset{3,5}{\text{DMP}}}{2.07\times10^{-5}\ \text{g } \overset{3,5}{\text{DMP}} + 999.999\ \text{g } H_2O} =$

$= \dfrac{1.93\times10^{-7}\ \text{moles } \overset{3,5}{\text{DMP}}}{1.93\times10^{-7}\ \text{moles } \overset{3,5}{\text{DMP}} + 55.5093\ \text{moles } H_2O} = 3\times10^{-9}$ MF 3,5 Dimethylpyridine

$$\phi_1 = \frac{(4.469)(3\times10^{-9})}{(4.469)(3\times10^{-9}) + (9.2\times10^{-1})(1)} = 1.457\times10^{-8} \quad \text{at } x_i = 3\times10^{-9}$$

$$\phi_2 = \frac{(.92)(1)}{(4.469)(3\times10^{-9}) + (.92)(1)} = 1 \quad \text{at } x_i = 3\times10^{-9}$$

$$\theta_i = \frac{q_i\, x_i}{\sum_j q_j\, x_j}$$

$$\theta_1 = \frac{(3.249)(3\times10^{-9})}{(3.249)(3\times10^{-9}) + (1.4)(1)} = 6.962\times10^{-9} \quad \text{at } x_1 = 3\times10^{-9}$$

$$\theta_2 = \frac{(1.4)(1)}{(3.249)(3\times10^{-9}) + (1.4)(1)} = 1 \quad \text{at } x_1 = 3\times10^{-9}$$

$$l_i = \frac{z}{2}(r_i - q_i) - (r_i - 1) \qquad z = 10$$

$$l_1 = 5(4.469 - 3.249) - (4.469 - 1) = 2.632$$

$$l_2 = 5(.92 - 1.4) - (.92 - 1) = -2.32$$

3,5 Dimethylpyridine

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$$\ln \gamma_1^c = \ln \frac{\phi_i}{x_i} + \overset{z=10}{\frac{z}{2}}\, q_i \ln \frac{\theta_i}{\phi_i} + l_i - \frac{\phi_i}{x_i} \sum_j x_j l_j$$

$$\ln \gamma_1^c = \ln\left(\frac{1.457\times10^{-8}}{3\times10^{-9}}\right) + 5(3.249)\ln\left(\frac{6.962\times10^{-9}}{1.457\times10^{-8}}\right) + 2.632 - \left(\frac{1.457\times10^{-8}}{3\times10^{-9}}\right)\left[(3\times10^{-9})(2.632) + (1)(-2.32)\right]$$

$\gamma_1^c = 32.53$ at $x_1 = 3\times10^{-9}$ mf

$\gamma_2^c = 1$ at $x_1 = 3\times10^{-9}$ mf

3,5 Dimethylpyridine

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$$\ln \Gamma_k^i = Q_k \left[1 - \ln\left(\sum_m \Theta_m^i \Psi_{mk} \right) - \sum_m \frac{\Theta_m^i \Psi_{km}}{\sum_n \Theta_n^i \Psi_{nm}} \right]$$

$$X_m = \frac{\nu_m^i}{\sum_n \nu_n^i} \qquad \Theta_m^i = \frac{Q_m X_m^i}{\sum_n Q_n X_n} \qquad \Psi_{mn} = \exp\left(\frac{-a_{mn}}{T} \right)$$

note : let 1 designate $\rightarrow CH_3$, $18 \rightarrow C_5H_3N$, $7 \rightarrow H_2O$

note : small $x_i \rightarrow$ designates mol fraction of molecule in solution (as on previous pages)

Capital $X_i \rightarrow$ to be used below, designates mol fraction of a functional group in solution

Capital $X_{(i)}^{(i)} \rightarrow$ to be used below, designates mol fraction of a functional group with respect to the indicated molecule

$$X_1^{(1)} = \frac{2}{2+1} = .667 = 2/3$$

$$X_{18}^{(1)} = \frac{1}{2+1} = .333 = 1/3$$

$$X_7^{(2)} = \frac{1}{1} = 1$$

$$\Psi_{1 \rightarrow 18} = \Psi_{118} = \exp \frac{-287.7}{T} = 3.683 \times 10^{-1} \qquad \text{at } T = 288°K$$

$$\Psi_{18 \rightarrow 1} = \Psi_{181} = \exp \frac{101.6}{T} = 1.423 \qquad \text{at } T = 288°K$$

$$\Psi_{11} = 1$$

$$\Psi_{1818} = 1$$

$$\Psi_{77} = 1$$

3,5 Dimethylpyr.dine

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$$\theta_1^{(1)} = \frac{(.848)(2/3)}{(.848)(2/3) + (1.553)(1/3)} = 5.22 \times 10^{-1}$$

$$\theta_{18}^{(1)} = \frac{(1.553)(1/3)}{.848\,(2/3) + 1.553\,(1/3)} = 4.78 \times 10^{-1}$$

$$\theta_7^{(2)} = \frac{(1.4)(1)}{(1.4)(1)} = 1$$

$$\ln \Gamma_1^{1} = .848 \left\{ 1 - \ln \left[(\theta^{1})(\psi_{11}) + (\theta_{18}^{1})(\psi_{181}) \right] - \left[\frac{(\theta_1^{1})(\psi_{11})}{(\theta_1^{1})(\psi_{11}) + (\theta_{18}^{1})(\psi_{181})} + \frac{(\theta_{18}^{1})(\psi_{118})}{(\theta_1^{1})(\psi_{118}) + (\theta_{18}^{1})(\psi_{1818})} \right] \right\}$$

$\Gamma_1^{1} = 1.106$ at $T = 288\,°K$

$\Gamma_{18}^{1} = 1.113$ at $T = 288\,°K$

$\Gamma_7^{2} = 1$ at $T = 288\,°K$

3,5 Dimethylpyridine

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$$\ln \Gamma_k = Q_k \left[1 - \ln\left(\sum_m \theta_m \Psi_{mk} \right) - \sum_m \frac{\theta_m \Psi_{km}}{\sum_n \theta_n \Psi_{nm}} \right]$$

$$X_1 = \frac{(3\times10^{-9})(2)}{(3\times10^{-9})(2+1)+(1)(1)} = 6\times10^{-9} \quad \text{at } x_1 = 3\times10^{-9}$$

$$X_{18} = \frac{(3\times10^{-9})(1)}{(3\times10^{-9})(2+1)+(1)(1)} = 3\times10^{-9} \quad \text{at } x_1 = 3\times10^{-9}$$

$$X_7 = \frac{(1)(1)}{3\times10^{-9}(2+1)+(1)(1)} = 1 \quad \text{at } x_1 = 3\times10^{-9}$$

$$\left.\begin{aligned}
\Psi_{118} &= 3.683\times10^{-1} \\
\Psi_{181} &= 1.423 \\
\Psi_{17} &= \exp\left(\frac{-1318}{T}\right) = 1.029\times10^{-2} \\
\Psi_{71} &= \exp\left(\frac{-300}{T}\right) = 3.529\times10^{-1} \\
\Psi_{718} &= \exp\left(\frac{-459}{T}\right) = 2.032\times10^{-1} \\
\Psi_{187} &= \exp\left(\frac{332.9}{T}\right) = 3.177
\end{aligned}\right\} \text{at } T = 288\,^\circ\text{K}$$

note: $\Psi_{11} = \Psi_{1818} = \Psi_{77} = 1$

3,5 Dimethylpyridine

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$$\theta_1 = \frac{(.848)(6\times10^{-9})}{(.848)(6\times10^{-9}) + (1.553)(3\times10^{-9}) + (1)(1.4)} = 3.634\times10^{-9} \quad (\text{at } x_1 = 3\times10^{-9})$$

$$\theta_{18} = \frac{(1.553)(3\times10^{-9})}{(.848)(6\times10^{-9}) + (1.553)(3\times10^{-9}) + (1)(1.4)} = 3.328\times10^{-9} \quad (\text{at } x_1 = 3\times10^{-9})$$

$$\theta_7 = \frac{(1.4)(1)}{(.848)(6\times10^{-9}) + (1.553)(3\times10^{-9}) + (1)(1.4)} = 1 \quad (\text{at } x_1 = 3\times10^{-9})$$

$$\ln \Gamma_1 = .848 \left\{ 1 - \ln\left[\theta_1(\psi_{11}) + \theta_{18}(\psi_{181}) + \theta_7(\psi_{71})\right] - \left[\frac{\theta_1 \psi_{11}}{\theta_1(\psi_{11}) + \theta_{18}(\psi_{181}) + \theta_7(\psi_{71})} + \frac{\theta_{18} \psi_{118}}{\theta_1(\psi_{118}) + \theta_{18}(\psi_{1818}) + \theta_7(\psi_{718})} + \frac{\theta_7 \psi_{17}}{\theta_1(\psi_{17}) + \theta_{18}(\psi_{187}) + \theta_7(\psi_{77})} \right] \right\}$$

$\Gamma_1 = 5.599$

$\Gamma_{18} = 4.043\times10^{-1}$

$\Gamma_7 = 1$

3,5 Dimethylpyridine

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$$\ln \gamma_i^R = \sum_k \nu_k^{i} \left(\ln \Gamma_k - \ln \Gamma_k^{i} \right)$$

$$\ln \gamma_1^R = 2\left[\ln(5.599) - \ln(1.106)\right] + 1\left[\ln(4.043\times10^{-1}) - \ln(1.113)\right]$$

$\gamma_1^R = 9.305$ at 288 °K $x_1 = 3\times10^{-9}$ mf

$$\ln \gamma_2^R = 1\left[\ln(1) - \ln(1)\right]$$

$\gamma_2^R = 1$ at 288 °K $x_1 = 3\times10^{-9}$

$$\ln \gamma_1 = \ln \gamma_1^C + \ln \gamma_1^R$$

$$\ln \gamma_1 = \ln(32.53) + \ln(9.305)$$

$\gamma_1 = 302.7$ at 288 °K $x_1 = 3\times10^{-9}$ mf

$$\ln \gamma_2 = \ln(1) + \ln(1)$$

$\gamma_2 = 1$ at 288 °K $x_1 = 3\times10^{-9}$ mf

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combinatorial

3,5-Dimethylpyridine Activity Coeffeceint Information

T K	x1 mf	phi1 ϕ_1	theta1 θ_1	l1 l_1	V1C γ_1^c
2.88E2	3E-9	1.457E-8	6.962E-9	2.632E0	3.253E1
3.03E2	3E-9	1.457E-8	6.962E-9	2.632E0	3.253E1
3.18E2	3E-9	1.457E-8	6.962E-9	2.632E0	3.253E1
3.33E2	3E-9	1.457E-8	6.962E-9	2.632E0	3.253E1
3.48E2	3E-9	1.457E-8	6.962E-9	2.632E0	3.253E1

residual

3,5-Dimethylpyridine Activity Coeffeceint Information

O18 θ_{18}	U187 Ψ_{187}	U718 Ψ_{718}	F18 Γ_{18}	V1R γ_1^R	V1 γ_1
3.328E-9	3.177E0	2.032E-1	4.043E-1	9.305E0	3.027E2
3.328E-9	3E0	2.198E-1	4.706E-1	9.936E0	3.232E2
3.328E-9	2.849E0	2.361E-1	5.329E-1	1.041E1	3.385E2
3.328E-9	2.717E0	2.52E-1	5.906E-1	1.074E1	3.492E2
3.328E-9	2.603E0	2.674E-1	6.435E-1	1.095E1	3.563E2

3,5 Dimethylpyridine

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$$\ln(P_i) = VPA - \frac{VPB}{(T+VPC)}$$

Ref. D, App A eq. 3

VPA = 10.2648 VPB = 4106.95 VPC = -44.45

Valid from 400 °K to 460 °K.

Note: Because the temperatures of interest in our calculations (288 - 348 °K) exceed the range in which the above equation is valid, data points for temperature and pressure shall be generated between 400 °K and 460 °K (using the above equation). The data points will then be used to develop an equation (Clausius Clapeyron Equation) which can be used to calculate vapor pressures for 3,5 Dimethylpyridine at the temperatures of interest.

T(K)	P(bars)
4.000E+02	2.763E-01
4.150E+02	4.411E-01
4.300E+02	6.788E-01
4.450E+02	1.012E+00
4.600E+02	1.465E+00

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The Clausius - Clapeyron Equation can be used to estimate the vapor pressure.

$$\ln(P_1) = -\frac{\Delta \hat{H}_v}{RT} + B$$

Ref. E pp 209

P_1 = Vapor pressure of pure substance (in this case 3,5 Dimethylpyridine)

R = Gas Constant

B = A constant which varies from one substance to another

$\Delta \hat{H}_v$ = Latent heat of vaporization (or the energy required to vaporize one mole of liquid)

T = Absolute temperature

Ref. E = R.M. Felder and R.W. Rousseau, "Elementary Principles of Chemical Processes," John Wiley & Sons, New York, 1978.

Note: A linear relationship between ln(P) and 1/T exists, therefore, if at least two data points for P and T are known, an equation which describes P at various temperatures can be determined.

3,5 Dimethypyridine

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Checked:	3/91	by	

T ⇒ °K

(bars)

1/T	ln(P)
2.500E-03	-1.286E+00
2.410E-03	-8.186E-01
2.326E-03	-3.874E-01
2.247E-03	1.152E-02
2.174E-03	3.816E-01

$$\frac{\Delta \hat{H}_v}{R} = \text{slope} = \frac{\ln\left(P_2/P_1\right)}{\frac{1}{T_2} - \frac{1}{T_1}} = -5115$$

$$B = y_{\text{intercept}} = \ln P + \frac{\Delta \hat{H}_v}{RT} = 11.5$$

The Clausius Clapeyron Equation for 3,5 Dimethylpyridine is:

$$\ln(P') = \frac{-5115}{T} + 11.5$$

T (°K)	P' (bars)
288	1.91×10^{-3}
303	4.602×10^{-3}
318	1.02×10^{-2}
333	2.106×10^{-2}
348	4.083×10^{-2}

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Job No. 89-5010-ES Client/Project WHC/242-A

Title: Organic Emmissions

Date: 3/91 by Jon Perry

Checked: 3/91 by AWRichard

$$\ln \frac{P_2}{P_c} = (1-x)^{-1}\left[(VPA)(x) + (VPB)(x)^{1.5} + (VPC)(x)^3 + (VPD)(x)^6\right]$$

Ref. D
App A
eqn. #1

$$x = 1 - T/T_c$$

$T_c = 647.3$
$P_c = 221.2$
$VPA = -7.76451$
$VPB = 1.45838$
$VPC = -2.7758$
$VPD = -1.23303$

Valid from 275 °K to 647.3 °K

T °K	P_2 (bars)
288	1.69×10^{-2}
303	4.212×10^{-2}
318	9.521×10^{-2}
333	1.98×10^{-1}
348	3.834×10^{-1}

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$$y_i P_t = \gamma_i x_i p_i$$

x_i = mol fraction of component i (liquid phase)
y_i = vapor phase mol fraction of component i
P_t = System pressure (vapor phase)
γ_i = activity coeffecient (liquid phase) (component i)
p_i = vapor pressure of pure component at system temp.

$$y_1 = \frac{\gamma_1 x_1 p_1}{P_t}$$

P_t = 750 mm Hg in C-100

$$\Rightarrow (750 \text{ mm Hg})\left(\frac{1.01325 \text{ bars}}{760 \text{ mm Hg}}\right) = .9999 \text{ bars}$$

P_t = .9999 bars

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Job No. 89-5010-ES Client/Project WHC/242-A

Title: Organic Emmissions

Date: 3/91 by Jon Perry

Checked: 3/91 by WC

C-100 stream flow rate = 150 $\frac{ft^3}{min}$

C-100 pressure = 6" WG

$$\text{Emmissions} = \left(150\ \frac{ft^3}{min}\right)\left(28.317\ \frac{l}{ft^3}\right)\left(\frac{60\ min}{hr}\right)\left(\frac{750\ mm\ Hg}{760\ mm\ Hg}\right)\left(\frac{298}{T}\right)\left(\frac{1\ mol}{22.4\ l}\right)$$

$$\xrightarrow{\text{cont'd}} \left(\frac{107.156\ g}{mol}\right)\left(\frac{1\ lb}{454\ g}\right)\left(y_i\right) = \frac{\text{lbs of 3,5-Dimethylpyridine}}{hr}$$

3,5-Dimethylpy---

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Title: Organic Emmissions
Date: 3/91 by Jon Perry
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°K 3,5-Dimethylpyridine C-100 Emmissions (xl=ave) f

T °K	Vl gl	pl bars	xl mf	yl mf	Emmissions lbs/hr
2.88E2	3.027E2	1.91E-3	3E-9	1.735E-9	4.757E-6
3.03E2	3.232E2	4.602E-3	3E-9	4.463E-9	1.163E-5
3.18E2	3.385E2	1.02E-2	3E-9	1.036E-8	2.574E-5
3.33E2	3.492E2	2.106E-2	3E-9	2.207E-8	5.233E-5
3.48E2	3.563E2	4.083E-2	3E-9	4.365E-8	9.905E-5

°K 3,5-Dimethylpyridine C-100 Emmissions (xl=max) f

T °K	Vl gl	pl bars	xl mf	yl mf	Emmissions lbs/hr
2.88E2	3.027E2	1.91E-3	4E-9	2.313E-9	6.343E-6
3.03E2	3.232E2	4.602E-3	4E-9	5.951E-9	1.551E-5
3.18E2	3.385E2	1.02E-2	4E-9	1.382E-8	3.431E-5
3.33E2	3.492E2	2.106E-2	4E-9	2.942E-8	6.978E-5
3.48E2	3.563E2	4.083E-2	4E-9	5.82E-8	1.321E-4

°K 3,5-Dimethylpyridine C-100 Emmissions (xl=max10) f

T °K	Vl gl	pl bars	xl mf	yl mf	Emmissions lbs/hr
2.88E2	3.027E2	1.91E-3	4E-8	2.313E-8	6.343E-5
3.03E2	3.232E2	4.602E-3	4E-8	5.951E-8	1.551E-4
3.18E2	3.385E2	1.02E-2	4E-8	1.382E-7	3.431E-4
3.33E2	3.492E2	2.106E-2	4E-8	2.942E-7	6.978E-4
3.48E2	3.563E2	4.083E-2	4E-8	5.82E-7	1.321E-3

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Title: Organic Emmissions

Date: 3/91 by Joe Perry

Checked: 3/91 by

The process condensate emmission results at 75 °C = 348 °K, can be used to determine the feed concentration limit. The feed concentration limit is the concentration of volatile constituent in the feed stream, with the assumption that the volatile constituent is completely transferred into the condensate, which will produce 0.71 lbs/hr (.322 kg/hr) emmissions of 3,5 Dimethylpyridine from the process condensate. The feed concentration limit is calculated as follows:

$$\left(2.4 \times 10^{2} \ \mu g/l\right)\left(\frac{1 \ mg}{1000 \ \mu g}\right)\left(\frac{1 \ hr.}{1.321 \times 10^{-3} \ lbs}\right)\left(\frac{.71 \ lbs}{1 hr}\right)\left(\frac{R-1}{R}\right)$$

$$= 129 \left(\frac{R-1}{R}\right) mg/l$$

note: R = feed rate ÷ product rate

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Determination of maximum feed concentration:

$$R\,C_f + (1 - R)\,C_c = C_s$$

R = Ratio of feed to product Mass Ratio

C_f = Feed Concentration

C_s = Concentration of a given component in Slurry

Note: To determine the maximum feed concentration (C_f) of a given component, (C_s) will be the regulatory limit (HBL or LDR).

C_c = Condensate Concentration of a given component

Note: C_c is calculated from the vapor phase mol fraction for a given component in the slurry.

2,5 Dimethylpy

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Checked: 3/91 by W. Gehling

C_c is calculated by converting y_i (mol fraction) to y_i (ppm)

$$y_i(MF) = \frac{\text{moles } i}{\text{moles } i + \text{moles } H_2O}$$

In this calculation, the mole contribution of component i is insignificant relative to the mole contribution of H_2O. Therefore,

$$\left(\frac{\text{mol. } i}{\cancel{\text{mol } i} + \text{mol } H_2O}\right)\left(\frac{55.5093 \text{ mol } H_2O}{1 \ell}\right)(\text{molec. wt})\left(\frac{1000 \text{ mg}}{g}\right)$$

insignificant

$$= \text{mg}/\ell = \text{mg}/\text{Kg} = \text{ppm}$$

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Title: Organic Removal

Date: 3/91 by Jon Perry

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3,5-Dimethylpyridine Slurry Vapor Phase Mole Fraction

T °K	Vl cc	pl bars	xl mf	Pt bars	yl mf
2.98E2	3.17E2	3.467E-3	1.68E-7	3.143E-2	5.874E-6
3.03E2	3.232E2	4.602E-3	1.68E-7	4.212E-2	5.933E-6
3.08E2	3.288E2	6.053E-3	1.68E-7	5.584E-2	5.989E-6
3.13E2	3.339E2	7.892E-3	1.68E-7	7.327E-2	6.043E-6
3.18E2	3.385E2	1.02E-2	1.68E-7	9.522E-2	6.094E-6
3.23E2	3.425E2	1.309E-2	1.68E-7	1.226E-1	6.144E-6
3.28E2	3.461E2	1.666E-2	1.68E-7	1.565E-1	6.193E-6
3.33E2	3.492E2	2.106E-2	1.68E-7	1.98E-1	6.24E-6
3.38E2	3.52E2	2.643E-2	1.68E-7	2.487E-1	6.286E-6
3.43E2	3.543E2	3.296E-2	1.68E-7	3.099E-1	6.331E-6
3.48E2	3.563E2	4.083E-2	1.68E-7	3.834E-1	6.375E-6

3,5-Dimethylpyridine Slurry Limits (mg/l)

T °K	yl mf	Cc mg/l	HBL mg/l
2.98E2	5.874E-6	3.494E1	1E0
3.03E2	5.933E-6	3.529E1	1E0
3.08E2	5.989E-6	3.562E1	1E0
3.13E2	6.043E-6	3.594E1	1E0
3.18E2	6.094E-6	3.625E1	1E0
3.23E2	6.144E-6	3.655E1	1E0
3.28E2	6.193E-6	3.683E1	1E0
3.33E2	6.24E-6	3.711E1	1E0
3.38E2	6.286E-6	3.739E1	1E0
3.43E2	6.331E-6	3.766E1	1E0
3.48E2	6.375E-6	3.792E1	1E0

$$C_f = \left(\frac{R-1}{R} + \frac{C_s}{R}\right) C_c$$

Ethoxytriethyleneglyco

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Job No. 89-5010-ES

Client/Project WHC/242-A

Title: Organic Emissions

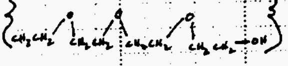
Date: 2/91 by Jon Perry

Checked: 3/91 by AW Richardson

1.) Let 1 be Ethoxytriethyleneglycol (ETEG) and 2 be H_2O.

(ETEG)

$$\log \gamma_1^\infty = \alpha + \epsilon N_1 + \frac{\zeta}{N_1} + \frac{\theta}{N_2}$$ Ref C 295 a



= (ETEG)

$N_1 = 8$ $N_2 = 0$

°K	α	ϵ	ζ	η	θ
298	−.995	.622	.558	—	0
333	−.755	.583	.460	—	0
373	−.420	.517	.230	—	0

$$\log \gamma_1^\infty = \alpha + 8\epsilon + \frac{\zeta}{8}$$

N_1 and N_2 = total # of carbon atoms in respective molecules
N', N'', and N''' = the # of carbon atoms in respective branches of the indicated molecule

α, ϵ, and ζ can be regressed with respect to temperature to give expressions which can be used to determine α, ϵ, and ζ at various temperatures.

$\alpha = 7.683 \times 10^{-3}(T) - 3.295$
$\epsilon = -1.406 \times 10^{-3}(T) + 1.045$
$\zeta = -4.406 \times 10^{-3}(T) + 1.891$

T → °K

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Title: Organic Emissions

Date: 2/91 by Jon Perry

Checked: 3/91 by W.G. Richmond

H_2O

$$\log \gamma_2^{\infty} = \alpha + \epsilon N_2 + \frac{\zeta}{N_2} + \frac{\theta}{N_1}$$

ref 295a

$N_2 = 0 \quad N_1 = 8$

°K	α	ϵ	ζ	η	θ
298	.760	0	0	—	−.630
333	.680	0	0	—	−.440
373	.617	0	0	—	−.280

$$\log \gamma_2^{\infty} = \alpha + \frac{\theta}{8}$$

α and θ can be regressed with respect to temperature to give expressions which can be used to determine α and θ at various temperatures.

$T \Rightarrow$ °K

$$\alpha = -1.900 \times 10^{-3}(T) + 1.321$$
$$\theta = 4.657 \times 10^{-3}(T) - 2.007$$

ethoxytriethyleneglycol

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Title: Organic Emissions

Date: 2/91 by Dn Ray

Checked: 3/91 by WB Richmond

2.) $\ln \gamma_1^{\infty} = -\ln(\Lambda_{12}) - \Lambda_{21} + 1$ Ref. C 8-10.25

$\ln \gamma_2^{\infty} = -\ln(\Lambda_{21}) - \Lambda_{12} + 1$ Ref. C 8-10.26

T °K	Λ_{12} $(\times 10^{-4})$	Λ_{21} $(\times 10^{-1})$
288	1.196	5.541
303	1.343	5.799
318	1.507	6.069
333	1.689	6.351
348	1.890	6.647

ethoxytriethyleneglycol

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3.) $$\ln \gamma_1 = -\ln\left(X_1 + \Lambda_{12} X_2\right) + X_2 \left[\frac{\Lambda_{12}}{X_1 + \Lambda_{12} X_2} - \frac{\Lambda_{21}}{\Lambda_{21} X_1 + X_2}\right]$$ Ref. A 6.11-2

;

$$\ln \gamma_2 = -\ln\left(X_2 + \Lambda_{21} X_1\right) - X_1 \left[\frac{\Lambda_{12}}{X_1 + \Lambda_{12} X_2} - \frac{\Lambda_{21}}{\Lambda_{21} X_1 + X_2}\right]$$ Ref A 6.11-3

X_1 & X_2 = mol fraction of respective molecules

Mol Fraction is calculated from ppb concentration in Stream Specific Report App 3A.

ex.) $$8.20 \times 10^{1}\ \text{ppb} = \frac{8.20 \times 10^{-5}\ \text{g}}{\text{litre} = 1000\ \text{g}} = \frac{4.6 \times 10^{-7}\ \text{moles (ETEG)}}{8.2 \times 10^{-5}\ \text{g ETEG} + 999.999\ \text{g}\ H_2O} =$$

$$= \frac{4.6 \times 10^{-7}\ \text{moles ETEG}}{4.6 \times 10^{-7}\ \text{moles ETEG} + 55.5093\ \text{moles}\ H_2O} = 8 \times 10^{-9}\ \text{MF ETEG}$$

Molec. Wt ETEG = 178.26
Molec. Wt. H_2O = 18.05

$X_1 = 8 \times 10^{-9}$ MF
$X_1 = 1.2 \times 10^{-8}$ MF
$X_1 = 1.21 \times 10^{-7}$ MF

	$X_1 = 8 \times 10^{-9}$ MF	$X_1 = 1.2 \times 10^{-8}$ MF	$X_1 = 1.21 \times 10^{-7}$ MF	
°K	γ_1	γ_1	γ_1	γ_2
288	1.306×10^{4}	1.306×10^{4}	1.304×10^{4}	1
303	1.133×10^{4}	1.133×10^{4}	1.131×10^{4}	1
318	9.829×10^{3}	9.829×10^{3}	9.815×10^{3}	1
333	8.527×10^{3}	8.526×10^{3}	8.515×10^{3}	1
348	7.397×10^{3}	7.397×10^{3}	7.388×10^{3}	1

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4) The Clausius - Clapeyron Equation can be used to estimate the vapor pressure.

$$\ln(P_1) = -\frac{\Delta\hat{H}_v}{RT} + B$$ Ref. E pp. 209

P_1 = Vapor pressure of pure substance (in this case Ethoxytriethylene-glycol)

R = Gas Constant

B = A constant which varies from one substance to another

$\Delta\hat{H}_x$ = Latent heat of vaporization (or the energy required to vaporize one mole of liquid)

T = Absolute temperature

Ref. E = R.M. Felder and R.W. Rousseau, "Elementary Principles of Chemical Processes," John Wiley & Sons, New York, 1978.

Note: A linear relationship between ln(P) and 1/T exists, therefore, if at least two data points for P and T are known, an equation which describes P at various temperatures can be determined.

Note: The following data for pressure and temperature was obtained from:

N. Irving, Sax, "Dangerous Properties of Industrial Materials 6th Edition, Van Nostrand Reinhold Company, Inc., New York, New York, 1984, pp. 1313.

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Temp.(C)	Temp.(K)	P(mmHg)	1/T(K)	ln(P)
2.000E+01	2.932E+02	1.000E-02	3.411E-03	-4.605E+00
2.554E+02	5.286E+02	7.600E+02	1.892E-03	6.633E+00

$$\frac{\Delta \hat{H}}{R} = \text{slope} = \frac{\ln (P_2/P_1)}{\frac{1}{T_2} - \frac{1}{T_1}} = -7393.74$$

$$B = y_{int} = \ln P + \frac{\Delta \hat{H}_v}{RT}$$

$$= \ln (.01) + \frac{7393.74}{293.2}$$

$$= 20.62$$

The Clausius - Clapeyron Eqn. for (ETEG) can be written as;

$$\ln P = -\frac{7393.74}{T} + 20.62$$

Note: Before P can be used in the Vapor Liquid Equilibrium Equation, the units must be converted from mmHg to bars (for these calculations)

$$P_{(mm\,Hg)}\left(\frac{1.01325}{760}\right) = P_{(bars)}$$

°K	P_i bars
288	8.514×10^{-6}
303	3.035×10^{-5}
318	9.595×10^{-5}
333	2.735×10^{-4}
348	7.121×10^{-4}

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$$\ln \frac{P_2}{P_c} = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^3 + (VPD)x^6\right]$$ Ref D App A eqn #1

$$x = 1 - \frac{T_2}{T_c}$$

$T_c = 647.3$
$VPB = 1.45838$
$P_c = 221.2$
$VPC = -2.7758$
$VPA = -7.76451$
$VPD = -1.23303$

Valid From 275 °K to 647.3 °K

°K	P_2 (bars)
288	1.69×10^{-2}
303	4.212×10^{-2}
318	9.521×10^{-2}
333	1.98×10^{-1}
348	3.834×10^{-1}

Ethoxytriethyleneglycol

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5.) $y_i P_t = \gamma_i x_i p_i$

x_i = mole fraction of component i (liquid phase)
y_i = vapor phase mol fraction of component i
P_t = System pressure (vapor phase)
γ_i = activity coeffecient (liquid phase) (component i)
p_i = vapor pressure of pure component at system temp.

$$y_1 = \frac{\gamma_1 x_1 p_1}{P_t}$$

P_t = 750 mm Hg in C-100

$$\Rightarrow (750 \text{ mm Hg})\left(\frac{1.01325 \text{ bars}}{760 \text{ mm Hg}}\right) = .9999 \text{ bars}$$

P_t = .9999 bars

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6.) C-100 stream flow rate = 150 $\frac{ft^3}{min}$

C-100 pressure = 6" WG

$$\text{Emmissions} = \left(150\ \frac{ft^3}{min}\right)\left(28.317\ l/ft^3\right)\left(\frac{60\ min}{hr}\right)\left(\frac{750\ mm\ Hg}{760\ mm\ Hg}\right)\left(\frac{298}{T}\right)\left(\frac{1\ mol}{22.4\ l}\right)$$

$$\xrightarrow{\text{cont'd}} \left(\frac{178.26\ g}{mol}\right)\left(\frac{1\ lb}{454\ g}\right)\left(y_i\right) = \frac{\text{lbs of Ethoxytriethyleneglycol}}{hr}$$

Ethoxytriethyleneglycol

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Date:	2/91	by	Jon Perry
Checked:	3/91	by	WB Richard

Ethoxytriethyleneglycol C-100 Emmissions (xl=ave)

T °K	vl	pl bars	xl MF	yl MF	Emmissions lbs/hr
2.88E2	1.306E4	8.514E-6	8E-9	8.897E-10	4.059E-6
3.03E2	1.133E4	3.035E-5	8E-9	2.751E-9	1.193E-5
3.18E2	9.829E3	9.595E-5	8E-9	7.545E-9	3.117E-5
3.33E2	8.527E3	2.735E-4	8E-9	1.866E-8	7.36E-5
3.48E2	7.397E3	7.121E-4	8E-9	4.214E-8	1.591E-4

Ethoxytriethyleneglycol C-100 Emmissions (xl=max)

T °K	vl	pl bars	xl MF	yl MF	Emmissions lbs/hr
2.88E2	1.306E4	8.514E-6	1.2E-8	1.335E-9	6.087E-6
3.03E2	1.133E4	3.035E-5	1.2E-8	4.126E-9	1.789E-5
3.18E2	9.829E3	9.595E-5	1.2E-8	1.132E-8	4.675E-5
3.33E2	8.526E3	2.735E-4	1.2E-8	2.798E-8	1.104E-4
3.48E2	7.397E3	7.121E-4	1.2E-8	6.321E-8	2.386E-4

Ethoxytriethyleneglycol C-100 Emmissions (xl=max10)

T °K	vl	pl bars	xl MF	yl MF	Emmissions lbs/hr
2.88E2	1.304E4	8.514E-6	1.21E-7	1.343E-8	6.127E-5
3.03E2	1.131E4	3.035E-5	1.21E-7	4.154E-8	1.801E-4
3.18E2	9.815E3	9.595E-5	1.21E-7	1.14E-7	4.708E-4
3.33E2	8.515E3	2.735E-4	1.21E-7	2.818E-7	1.112E-3
3.48E2	7.388E3	7.121E-4	1.21E-7	6.367E-7	2.403E-3

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The process condensate emmission results at 75°C = 348°K, can be used to determine the feed concentration limit. The feed concentration limit is the concentration of volatile constituent in the feed stream, with the assumption that the volatile consitituent is completely transferred into the condensate, which will produce 0.71 lbs/hr (.322 kg/hr) emmissions of Ethoxytriethylene glycol from the process condensate. The feed concentration limit is calculated as follows:

$$\left(\frac{1.20\times10^{3}}{} \ \mu g/l\right)\left(\frac{1\ mg}{1000\ \mu g}\right)\left(\frac{1\ \ hr.}{2.403\times10^{-3}\ \ lbs}\right)\left(\frac{.71\ lbs}{1\ hr}\right)\left(\frac{R-1}{R}\right)$$

$$= \quad 355 \left(\frac{R-1}{R}\right) \Longrightarrow mg/l$$

note: R = feed rate ÷ product rate

— Ethoxytriethyleneglycol

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Determination of maximum feed concentration:

$$R\,C_f + (1 - R)\,C_c = C_s$$

R = Ratio of Feed to product Mass Ratio

C_f = Feed Concentration

C_s = Concentration of a given component in Slurry

Note: To determine the maximum feed concentration (C_f) of a given component, (C_s) will be the regulatory limit (HBL or LDR).

C_c = Condensate Concentration of a given component

Note: C_c is calculated from the vapor phase mol fraction for a given component in the slurry.

Ethoxytriethyleneglycol

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C_c is calculated by converting y_i (mol fraction) to y_i (ppm)

$$y_i(MF) = \frac{\text{moles } i}{\text{moles } i + \text{moles } H_2O}$$

In this calculation, the mole contribution of component i is insignificant relative to the mole contribution of H_2O. Therefore,

$$\left(\frac{\text{mol } i}{\underset{\text{insignificant}}{\cancel{\text{mol } i}} + \text{mol } H_2O}\right)\left(\frac{55.5093 \text{ mol } H_2O}{1 \ell}\right)(\text{molec. wt})\left(\frac{1000 \text{ mg}}{g}\right)$$

$$= \quad mg/\ell \quad = \quad mg/Kg \quad = \text{ppm}$$

Ethoxytriethyleneglycol

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Ethoxytriethyleneglycol Slurry Vapor Phase Mole Fraction

T °K	v1	p1 bars	x1 MF	Pt bars	y1 MF
2.98E2	1.186E4	2.015E-5	1.01E-7	3.143E-2	7.682E-7
3.03E2	1.131E4	3.035E-5	1.01E-7	4.212E-2	8.234E-7
3.08E2	1.079E4	4.51E-5	1.01E-7	5.584E-2	8.803E-7
3.13E2	1.029E4	6.618E-5	1.01E-7	7.327E-2	9.39E-7
3.18E2	9.817E3	9.595E-5	1.01E-7	9.521E-2	9.991E-7
3.23E2	9.363E3	1.375E-4	1.01E-7	1.226E-1	1.061E-6
3.28E2	8.93E3	1.949E-4	1.01E-7	1.565E-1	1.124E-6
3.33E2	8.517E3	2.735E-4	1.01E-7	1.98E-1	1.188E-6
3.38E2	8.124E3	3.798E-4	1.01E-7	2.487E-1	1.253E-6
3.43E2	7.748E3	5.224E-4	1.01E-7	3.099E-1	1.319E-6
3.48E2	7.39E3	7.121E-4	1.01E-7	3.834E-1	1.386E-6

Ethoxytriethyleneglycol Slurry Limits (mg/l)

T °K	yl MF	Cc mg/l	HBL mg/l
2.98E2	7.682E-7	7.601E0	1E0
3.03E2	8.234E-7	8.147E0	1E0
3.08E2	8.803E-7	8.711E0	1E0
3.13E2	9.39E-7	9.291E0	1E0
3.18E2	9.991E-7	9.887E0	1E0
3.23E2	1.061E-6	1.05E1	1E0
3.28E2	1.124E-6	1.112E1	1E0
3.33E2	1.188E-6	1.175E1	1E0
3.38E2	1.253E-6	1.24E1	1E0
3.43E2	1.319E-6	1.306E1	1E0
3.48E2	1.386E-6	1.372E1	1E0

$$C_f = \left(\frac{R-1}{R} + \frac{C_s}{R}\right) C_c$$

α- Hexanone

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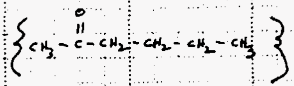
1.) Let 1 be 2-Hexanone and 2 be H_2O.

2-Hexanone

$$\log \gamma_1^{\infty} = \alpha + \epsilon N_1 + \zeta\left(\frac{1}{N_1'} + \frac{1}{N_1''}\right) + \eta(N_1 - N_2)^2$$

Ref C295b

 = 2-Hexanone

$$\left\{CH_3-\overset{\overset{O}{\|}}{C}-CH_2-CH_2-CH_2-CH_3\right\} = \text{2-Hexanone}$$

$N_1 = 6$ $N_2 = 0$ $N_1' = 2$ $N_1'' = 5$

°K	α	ϵ	ζ	η
298	−1.475	.622	.500	0
333	−1.040	.583	.330	0
373	−.621	.517	.200	0

$$\log \gamma_1^{\infty} = \alpha + 6\epsilon + \zeta\left(\tfrac{7}{10}\right)$$

N_1 and N_2 = total # of carbon atoms in respective molecules
N', N'', and N''' = the # of carbon atoms in respective branches of the indicated molecule

α, ϵ, and ζ can be regressed with respect to temperature to give expressions which can be used to determine α, ϵ, and ζ at various temperatures.

$\alpha = 1.137\times10^{-2}(T) - 4.849$
$\epsilon = -1.406\times10^{-3}(T) + 1.045$
$\zeta = -3.982\times10^{-3}(T) + 1.676$

T → °K

2-Hexanone

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H_2O

$$\log \gamma_2^{\infty} = \alpha + \epsilon N_2 + \zeta\left(\frac{1}{N_2'} + \frac{1}{N_2''} + \frac{1}{N_2'''}\right) + \theta\left(\frac{1}{N_1'} + \frac{1}{N_1''}\right)$$

ref
295 C

$N_2 = 0$ $N_1 = 6$ $N_1' = 2$ $N_1'' = 5$

°K	α	ϵ	ζ	η	θ
298	1.857	0	0	—	−1.019
333	1.493	0	0	—	−.730
373	1.231	0	0	—	−.557

$$\log \gamma_2^{\infty} = \alpha + \theta\left(7/10\right)$$

α and θ can be regressed with respect to temperature to give expressions which can be used to determine α and θ at various temperatures.

$T \Rightarrow$ °K

$\alpha = -8.3 \times 10^{-3}(T) + 4.306$

$\theta = 6.117 \times 10^{-3}(T) - 2.816$

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2.) $\ln \gamma_1^{\infty} = -\ln(\Lambda_{12}) - \Lambda_{21} + 1$ Ref. C 8-10.25

$\ln \gamma_2^{\infty} = -\ln(\Lambda_{21}) - \Lambda_{12} + 1$ Ref. C 8-10.26

T °K	Λ_{12} $(\times 10^{-3})$	Λ_{21} $(\times 10^{-1})$
288	5.298	1.795
303	5.133	2,063
318	4.954	2.37
333	4,758	2.723
348	4.547	3.129

2-Hexanone

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3.) $$\ln \gamma_1 = -\ln (X_1 + \Lambda_{12} X_2) + X_2 \left[\frac{\Lambda_{12}}{X_1 + \Lambda_{12} X_2} - \frac{\Lambda_{21}}{\Lambda_{21} X_1 + X_2} \right]$$ Ref. A 6.11-2

$$\ln \gamma_2 = -\ln (X_2 + \Lambda_{21} X_1) - X_1 \left[\frac{\Lambda_{12}}{X_1 + \Lambda_{12} X_2} - \frac{\Lambda_{21}}{\Lambda_{21} X_1 + X_2} \right]$$ Ref A 6.11-3

X_1 & X_2 = mol fraction of respective molecules

Mol Fraction is calculated from ppb concentration in Stream Specific Report App 3A.

ex.) 7.75×10^{0} ppb $= \frac{7.75 \times 10^{0} \text{ mg}}{l} = \frac{7.75 \times 10^{-6} \text{ g 2-Hexanone}}{1000 \text{ g } H_2O + \text{2-Hexanone}} =$

$= \frac{7.7 \times 10^{-8} \text{ moles 2-Hexanone}}{7.75 \times 10^{-6} \text{ g 2-Hexanone} + 999.999 \text{ g } H_2O} = \frac{7.7 \times 10^{-8} \text{ moles 2-Hexanone}}{7.7 \times 10^{-8} \text{ moles 2-Hexanone} + 55.5093 \text{ moles } H_2O} =$

$= 1 \times 10^{-9}$ MF 2-Hexanone

$X_1 = 1 \times 10^{-9}$ MF
$X_1 = 2 \times 10^{-9}$ MF
$X_1 = 2 \times 10^{-8}$ MF

°K	$X_1 = 1 \times 10^{-9}$ MF $\gamma_1 (\times 10^2)$	$X_1 = 2 \times 10^{-9}$ MF $\gamma_1 (\times 10^2)$	$X_1 = 2 \times 10^{-8}$ MF $\gamma_1 (\times 10^2)$	γ_2
288	4.287	4.287	4.287	1
303	4.309	4.309	4.309	1
318	4.33	4.33	4.33	1
333	4.351	4.351	4.351	1
348	4.372	4.372	4.372	1

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4) The Clausius - Clapeyron Equation can be used to estimate the vapor pressure.

$$\ln(P_1) = -\frac{\Delta \hat{H}_v}{RT} + B$$ Ref. E pp 209

P_1 = Vapor pressure of pure substance (in this case 2-Hexanone)

R = Gas Constant

B = A constant which varies from one substance to another

$\Delta \hat{H}_v$ = Latent heat of vaporization (or the energy required to vaporize one mole of liquid)

T = Absolute temperature

Ref. E = R.M. Felder and R.W. Roussea, "Elementary Principles of Chemical Processes," John Wiley & Sons, New York, 1978.

Note: $1/T$ can be regressed with respect to $\ln(P_1)$ to give an expression which can be used to determine P_1 at various temperatures.

Note: The following data for pressure and temperature was obtained from:

"CRC Handbook of Chemistry and Physics, 60th Edition, 2nd Printing, CRC Press, Inc., Boca, Florida, 1980, pp D208.

2-Hexanone

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C	Temp.(K)	P(mmHg)	ln(P)	1/T
7.7	2.809E+02	1.000E+00	0.000E+00	3.561E-03
38.8	3.120E+02	1.000E+01	2.303E+00	3.205E-03
62	3.352E+02	4.000E+01	3.689E+00	2.984E-03
79.8	3.530E+02	1.000E+02	4.605E+00	2.833E-03
111	3.842E+02	4.000E+02	5.991E+00	2.603E-03
127.5	4.007E+02	7.600E+02	6.633E+00	2.496E-03

$$\text{Slope} = \frac{\Delta \hat{H}_i}{R} = -6.219 \times 10^{3}$$

$$y_{int} = B = 2.220 \times 10^{1}$$

Using the Clausius – Clapeyron Equation for 2-Hexanone

$$\ln(P_1) = \frac{-6.219 \times 10^{3}}{T} + 2.22 \times 10^{1}$$

Note: Befor P_1 can be used in the Vapor Liquid Equilibrium Equation the units must be converted from mmHg to bars for these calculations

1.01325 bars = 760 mmHg

$$P_1(\text{mmHg})\left(\frac{1.01325}{760}\right) = P(\text{bars})$$

°K	P_1 (bars)
288	2.445×10^{-3}
303	7.12×10^{-3}
318	1.875×10^{-2}
333	4.524×10^{-2}
348	1.012×10^{-1}

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5.) $y_i P_t = \gamma_i x_i p_i$

x_i = mole fraction of component i (liquid phase)
y_i = vapor phase mol fraction of component i
P_t = System pressure (vapor phase)
γ_i = activity coeffecient (liquid phase) (component i)
p_i = vapor pressure of pure component at system temp.

$$y_1 = \frac{\gamma_1 x_1 p_1}{P_t}$$

P_t = 750 mm Hg in C-100

$$\Rightarrow \left(750 \text{ mm Hg}\right)\left(\frac{1.01325 \text{ bars}}{760 \text{ mm Hg}}\right) = .9999 \text{ bars}$$

P_t = .9999 bars

2-Hexanone

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$$\ln \frac{P_2}{P_c} = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^{3} + (VPD)x^{6}\right]$$

Ref. D App A eqn #1

$$x = 1 - \frac{T_1}{T_c}$$

$T_c = 647.3$

$VPB = 1.45838$

$P_c = 221.2$

$VPC = -2.7758$

$VPA = -7.76451$

$VPD = -1.23303$

Valid From 275 °K to 647.3 °K

°K	P_2 (bars)
288	1.69×10^{-2}
303	4.212×10^{-2}
318	9.521×10^{-2}
333	1.98×10^{-1}
348	3.834×10^{-1}

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6.) C-100 stream flow rate = 150 $\frac{ft^3}{min}$

C-100 pressure = 6" WG

$$\text{Emmissions} = \left(150\ \frac{ft^3}{min}\right)\left(28.317\ \frac{l}{ft^3}\right)\left(\frac{60\ min}{hr}\right)\left(\frac{750\ mm\ Hg}{760\ mm\ Hg}\right)\left(\frac{298}{T}\right)\left(\frac{1\ mol}{22.4\ l}\right)$$

$$\xrightarrow{\text{int'd}} \left(\frac{100.16\ g}{mol}\right)\left(\frac{1\ lb}{454\ g}\right)\left(y_i\right) = \frac{\text{lbs of 2-Hexanone}}{hr}$$

2-Hexanone

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°K 2-Hexanone C-100 Emmissions (xl=ave)

T °K	vl ρl	pl bars	xl MF	yl MF	Emissions lbs/hr
2.88E2	4.287E2	2.445E-3	1E-9	1.048E-9	2.687E-6
3.03E2	4.309E2	7.12E-3	1E-9	3.068E-9	7.474E-6
3.18E2	4.33E2	1.875E-2	1E-9	8.117E-9	1.884E-5
3.33E2	4.351E2	4.524E-2	1E-9	1.968E-8	4.363E-5
3.48E2	4.372E2	1.012E-1	1E-9	4.424E-8	9.384E-5

°K 2-Hexanone C-100 Emmissions (xl=max)

T °K	vl ρl	pl bars	xl MF	yl MF	Emissions lbs/hr
2.88E2	4.287E2	2.445E-3	2E-9	2.096E-9	5.373E-6
3.03E2	4.309E2	7.12E-3	2E-9	6.136E-9	1.495E-5
3.18E2	4.33E2	1.875E-2	2E-9	1.623E-8	3.768E-5
3.33E2	4.351E2	4.524E-2	2E-9	3.937E-8	8.727E-5
3.48E2	4.372E2	1.012E-1	2E-9	8.849E-8	1.877E-4

°K 2-Hexanone C-100 Emmissions (xl=max10)

T °K	vl ρl	pl bars	xl MF	yl MF	Emissions lbs/hr
2.88E2	4.287E2	2.445E-3	2E-8	2.096E-8	5.373E-5
3.03E2	4.308E2	7.12E-3	2E-8	6.136E-8	1.495E-4
3.18E2	4.33E2	1.875E-2	2E-8	1.623E-7	3.768E-4
3.33E2	4.351E2	4.524E-2	2E-8	3.937E-7	8.727E-4
3.48E2	4.372E2	1.012E-1	2E-8	8.849E-7	1.877E-3

2-Hexanone

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The process condensate emmission results at 75°C = 348°K, can be used to determine the feed concentration limit. The feed concentration limit is the concentration of volatile constituent in the feed stream, with the assumption that the volatile consitituent is completely transferred into the condensate, which will produce 0.71 lbs/hr (.322 kg/hr) emissions of 2-Hexanone from the process condensate. The feed concentration limit is calculated as follows:

$$\left(1.10\times10^{2}\ \mathrm{Mg}/l\right)\left(\frac{1\ \mathrm{mg}}{1000\ \mathrm{Mg}}\right)\left(\frac{1\ \mathrm{hr.}}{1.877\times10^{-3}\ \mathrm{lbs}}\right)\left(\frac{.71\ \mathrm{lbs}}{1\ \mathrm{hr}}\right)\left(\frac{R-1}{R}\right)$$

$$= 41.61\left(\frac{R-1}{R}\right) \Rightarrow \mathrm{mg}/l$$

note: R = feed rate ÷ product rate

2- Hexanone

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Determination of maximum feed concentration:

$$R\,C_f + (1-R)\,C_c = C_s$$

R = Ratio of Feed to product Mass Ratio

C_f = Feed Concentration

C_s = Concentration of a given component in Slurry

Note: To determine the maximum feed concentration (C_f) of a given component, (C_s) will be the regulatory limit (HBL or LDR).

C_c = Condensate Concentration of a given component

Note: C_c is calculated from the vapor phase mol fraction for a given component in the slurry.

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C_c is calculated by converting y_i (mol fraction) to y_i (ppm)

$$y_i(MF) = \frac{\text{moles } i}{\text{moles } i + \text{moles } H_2O}$$

In this calculation, the mole contribution of component i is insignificant relative to the mole contribution of H_2O. Therefore,

$$\left(\frac{\text{mol } i}{\underbrace{\cancel{\text{mol } i}}_{\text{insignificant}} + \text{mol } H_2O}\right)\left(\frac{55.5093 \text{ mol } H_2O}{1\,l}\right)(\text{molec. wt})\left(\frac{1000 \text{ mg}}{g}\right)$$

$$= \frac{mg}{l} = \frac{mg}{Kg} = ppm$$

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2-Hexanone Slurry Vapor Phase Mol Fraction

T °K	vl [illegible]	pl bars	xl MF	Pt bars	yl MF
2.98E2	4.301E2	5.045E-3	1.8E-7	3.143E-2	1.243E-5
3.03E2	4.308E2	7.12E-3	1.8E-7	4.212E-2	1.311E-5
3.08E2	4.315E2	9.935E-3	1.8E-7	5.584E-2	1.382E-5
3.13E2	4.322E2	1.372E-2	1.8E-7	7.327E-2	1.456E-5
3.18E2	4.329E2	1.875E-2	1.8E-7	9.522E-2	1.534E-5
3.23E2	4.336E2	2.537E-2	1.8E-7	1.226E-1	1.616E-5
3.28E2	4.343E2	3.403E-2	1.8E-7	1.565E-1	1.7E-5
3.33E2	4.351E2	4.524E-2	1.8E-7	1.98E-1	1.789E-5
3.38E2	4.358E2	5.963E-2	1.8E-7	2.487E-1	1.881E-5
3.43E2	4.365E2	7.798E-2	1.8E-7	3.099E-1	1.977E-5
3.48E2	4.372E2	1.012E-1	1.8E-7	3.834E-1	2.077E-5

2-Hexanone Slurry Limits (mg/l)

T °K	yl MF	Cc mg/l	HBL mg/l
2.98E2	1.243E-5	6.909E1	1E0
3.03E2	1.311E-5	7.287E1	1E0
3.08E2	1.382E-5	7.683E1	1E0
3.13E2	1.456E-5	8.097E1	1E0
3.18E2	1.534E-5	8.53E1	1E0
3.23E2	1.616E-5	8.982E1	1E0
3.28E2	1.7E-5	9.454E1	1E0
3.33E2	1.789E-5	9.946E1	1E0
3.38E2	1.881E-5	1.046E2	1E0
3.43E2	1.977E-5	1.099E2	1E0
3.48E2	2.077E-5	1.155E2	1E0

$$C_f = \left(\frac{R-1}{R} + \frac{C_s}{R} \right) C_c$$

Hexone (MIBK)

Westinghouse Environmental & Geotechnical Services, Inc.

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Job No. 89-5010-ES Client/Project WHC/242-A

Title: Organic Emissions

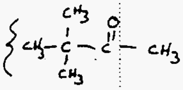
Date: 2/91 by Dn Perry

Checked: 3/91 by

1.) Let 1 be Hexone (MIBK) and 2 be H_2O.

Hexone

$$\log \gamma_1^{\infty} = \alpha + \epsilon N_1 + \zeta\left(\frac{1}{N_1'} + \frac{1}{N_1''}\right) + \eta(N_1 - N_2)^2$$ Ref C 295 b



$$\left\{ CH_3-C(CH_3)_2-C(=O)-CH_3 \right\}$$ = (MIBK) Hexone

$N_1 = 6$ $N_2 = 0$ $N_1' = 5$ $N_1'' = 2$

°K	α	ϵ	ζ	η
298	-1.475	.622	.500	0
333	-1.040	.583	.330	0
373	-.621	.517	.200	0

$$\log \gamma_1^{\infty} = \alpha + 6\epsilon + \zeta\left(\frac{7}{10}\right)$$

N_1 and N_2 = total # of carbon atoms in respective molecules
N', N'', and N''' = the # of carbon atoms in respective branches of the indicated molecule

α, ϵ, and ζ can be regressed with respect to temperature to give expressions which can be used to determine α, ϵ, and ζ at various temperatures.

$\alpha = 1.137 \times 10^{-2} (T) - 4.849$
$\epsilon = -1.406 \times 10^{-3} (T) + 1.045$
$\zeta = -3.982 (T) + 1.676$

T => °K

Hexone (MIBK)

Westinghouse Environmental & Geotechnical Services, Inc.

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H_2O

$$\log \gamma_2^{\infty} = \alpha + \epsilon N_2 + \zeta\left(\frac{1}{N_2'} + \frac{1}{N_2''} + \frac{1}{N_2'''}\right) + \theta\left(\frac{1}{N_1'} + \frac{1}{N_1''}\right)$$ ref 295 C

$N_2 = 0$ $N_1 = 6$ $N_1' = 5$ $N_1'' = 2$

°K	α	ϵ	ζ	η	θ
298	1.857	0	0	—	−1.019
333	1.493	0	0	—	−.73
373	1.231	0	0	—	−.557

$$\log \gamma_2^{\infty} = \alpha + \theta\left(\frac{7}{10}\right)$$

α and θ can be regressed with respect to temperature to give expressions which can be used to determine α and θ at various temperatures.

$T \Rightarrow$ °K

$\alpha = -8.3 \times 10^{-3}(T) + 4.306$
$\theta = 6.117 \times 10^{-3}(T) - 2.816$

Hexone (mibk)

Westinghouse Environmental & Geotechnical Services, Inc.

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Title: Organic Emissions

Date: 2/91 by Jon Perry

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2.) $\ln \gamma_1^\infty = -\ln(\Lambda_{12}) - \Lambda_{21} + 1$ Ref. C 8-10.25

$\ln \gamma_2^\infty = -\ln(\Lambda_{21}) - \Lambda_{12} + 1$ Ref. C 8-10.26

T °K	Λ_{12} $(\times 10^{-3})$	Λ_{21} $(\times 10^{-1})$
288	5.298	1.795
303	5.133	2.063
318	4.954	2.37
333	4.758	2.723
348	4.547	3.129

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3.)
$$\ln \gamma_1 = -\ln(x_1 + \Lambda_{12} x_2) + x_2 \left[\frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{\Lambda_{21} x_1 + x_2} \right]$$
Ref. A 6.11-2

$$\ln \gamma_2 = -\ln(x_2 + \Lambda_{21} x_1) - x_1 \left[\frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{\Lambda_{21} x_1 + x_2} \right]$$
Ref A 6.11-3

x_1 & x_2 = mol fraction of respective molecules

Mol Fraction is calculated from ppb concentration in Stream Specific Report App 3A.

ex.)
$$9.247 \times 10^{0}\ \text{ppb} = \frac{9.47\ \mu g}{l} = \frac{9.47 \times 10^{-6}\ g}{1000\ g} = \frac{9.5 \times 10^{-8}\ \text{moles MIBK}}{999.999\ g\ H_2O + 9.5 \times 10^{-8}\ g\ \text{MIBK}} =$$

$$\frac{9.5 \times 10^{-8}\ \text{moles MIBK}}{(55.5093\ \text{moles}\ H_2O) + (9.5 \times 10^{-8}\ \text{moles MIBK})} = 2 \times 10^{-9}\ \text{MF MIBK}$$

mw MIBK = 100.16 g/mole
mw H_2O = 18.015 g/mole

	$x_1 = 2 \times 10^{-9}$	$x_1 = 1.2 \times 10^{-8}$	1.22×10^{-7}	$x_1 = 2 \times 10^{-9}$ $x_1 = 1.2 \times 10^{-8}$ $x_1 = 1.22 \times 10^{-7}$
°K	γ_1 ($\times 10^2$)	γ_1 ($\times 10^2$)	γ_1 ($\times 10^2$)	γ_2
288	4.287	4.287	4.287	1
303	4.308	4.308	4.308	1
318	4.33	4.33	4.33	1
333	4.351	4.351	4.351	1
348	4.372	4.372	4.372	1

Hexone (MIBK)

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4.) $$\ln \frac{P_1}{P_c} = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^3 + (VPD)x^6\right]$$ Ref. D App A equation #1

$$x = 1 - T/T_c$$

T_c = 571
VPB = 2.92801

P_c = 32.7
VPC = −5.27311

VPA = −8.54349
VPD = −2.54507

Valid From 295 °K to 571 °K

Note: The above equation was used to calculate vapor pressures for temperatures ranging from 288 °K to 348 °K even though these temperatures exceed the range for which the above vapor pressure constants are valid. Upon plotting vapor pressure vs. temperature, vapor pressure appears to approach zero at temperatures below 295 °K.

$$\ln\left(\frac{P_2}{P_c}\right) = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^3 + (VPD)x^6\right]$$ Ref. D App A eqn. #1

$$x = 1 - T/T_c$$

T_c = 647.3
VPB = 1.45838
Valid From 275 °K

P_c = 221.2
VPC = −2.7758
to 647.3 °K

VPA = −7.76451
VPD = −1.23303

°K	P_1 (bars)	P_2 (bars)
288	1.455×10^{-2}	1.69×10^{-2}
303	3.426×10^{-2}	4.212×10^{-2}
318	7.299×10^{-2}	9.521×10^{-2}
333	1.429×10^{-1}	1.98×10^{-1}
348	2.605×10^{-1}	3.834×10^{-1}

[illegible]

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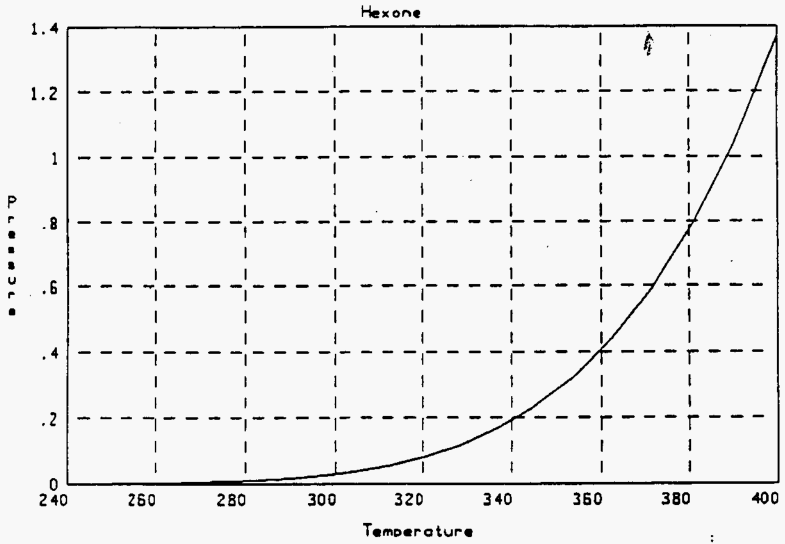

Hexone (MIBK)

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5.) $y_i P_t = \gamma_i x_i p_i$

x_i = mole fraction of component i in liquid phase
y_i = vapor phase mol fraction of component i
P_t = System pressure (vapor phase)
γ_i = activity coefficient (liquid phase) (component i)
p_i = vapor pressure of pure component at system temp.

$$y_1 = \frac{\gamma_1 x_1 p_1}{P_t}$$

P_t = 750 mm Hg in C-100

$$\Rightarrow \left(750 \text{ mm Hg}\right)\left(\frac{1.01325 \text{ bars}}{760 \text{ mm Hg}}\right) = .9999 \text{ bars}$$

P_t = .9999 bars

Hexone (MIBK)

Westinghouse Environmental & Geotechnical Services, Inc.

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Title: Organic Emissions

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6.) C-100 stream flow rate = 150 $\frac{ft^3}{min}$

C-100 pressure = 6" WG

$$\text{Emmissions} = \left(150\ \frac{ft^3}{min}\right)\left(28.317\ \frac{l}{ft^3}\right)\left(\frac{60\ min}{hr}\right)\left(\frac{750\ mm\ Hg}{760\ mm\ Hg}\right)\left(\frac{298}{T}\right)\left(\frac{1\ mol}{22.4\ l}\right)$$

$$\xrightarrow{\text{cont'd}} \left(\frac{100.16\ g}{mol}\right)\left(\frac{1\ lb}{454\ g}\right)\left(Y_i\right) = \frac{\text{lbs of (MIBK)}}{hr}$$

Hexone (MIBK)

Westinghouse Environmental & Geotechnical Services, Inc.

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MIBK C-100 Emmissions (x1=ave)

T °K	v1 δ	p1 bars	x1 MF	y1 MF	lbs/hr. Emmissions
2.88E2	4.287E2	1.455E-2	9E-9	5.617E-8	1.44E-4
3.03E2	4.308E2	3.426E-2	9E-9	1.329E-7	3.237E-4
3.18E2	4.33E2	7.299E-2	9E-9	2.845E-7	6.603E-4
3.33E2	4.351E2	1.429E-1	9E-9	5.598E-7	1.241E-3
3.48E2	4.372E2	2.605E-1	9E-9	1.025E-6	2.175E-3

MIBK C-100 Emmissions (x1=max)

T °K	v1 δ	p1 bars	x1 MF	y1 MF	lbs/hr. Emmissions
2.88E2	4.287E2	1.455E-2	1.2E-8	7.489E-8	1.919E-4
3.03E2	4.308E2	3.426E-2	1.2E-8	1.772E-7	4.316E-4
3.18E2	4.33E2	7.299E-2	1.2E-8	3.793E-7	8.804E-4
3.33E2	4.351E2	1.429E-1	1.2E-8	7.463E-7	1.654E-3
3.48E2	4.372E2	2.605E-1	1.2E-8	1.367E-6	2.9E-3

MIBK C-100 Emmissions (x1=max10)

T °K	v1 δ	p1 bars	x1 mF	y1 molFraction	lbs/hr. Emmissions
2.88E2	4.287E2	1.455E-2	1.22E-7	7.614E-7	1.951E-3
3.03E2	4.308E2	3.426E-2	1.22E-7	1.801E-6	4.388E-3
3.18E2	4.329E2	7.299E-2	1.22E-7	3.856E-6	8.95E-3
3.33E2	4.351E2	1.429E-1	1.22E-7	7.588E-6	1.682E-2
3.48E2	4.372E2	2.605E-1	1.22E-7	1.39E-5	2.948E-2

Hexone (MIBK)

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Title: Organic Emissions
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The process condensate emmission results at 75 °C = 348 °K, can be used to determine the feed concentration limit. The feed concentration limit is the concentration of volatile constituent in the feed stream, with the assumption that the volatile constituent is completely transferred into the condensate, which will produce 0.71 lbs/hr (.322 kg/hr) emmissions of <u>Hexone (MIBK)</u> from the process condensate. The feed concentration limit is calculated as follows:

$$\left(\frac{6.80\times10^{2}}{} \ \mu g/l\right)\left(\frac{1\ mg}{1000\ \mu g}\right)\left(\frac{1\quad hr.}{2.948\times10^{-2}\quad lbs}\right)\left(\frac{.71\ lbs}{1\ hr}\right)\left(\frac{R-1}{R}\right)$$

$$= \quad 16.38\left(\frac{R-1}{R}\right) \Rightarrow mg/l$$

note: R = Feed rate ÷ product rate

Hexone (MIBK)

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Determination of maximum feed concentration:

$$R\,C_f + (1-R)\,C_c = C_s$$

R = Ratio of Feed to product Mass Ratio

C_f = Feed Concentration

C_s = Concentration of a given component in Slurry

Note: To determine the maximum feed concentration (C_f) of a given component, (C_s) will be the regulatory limit (HBL or LDR).

C_c = Condensate Concentration of a given component

Note: C_c is calculated from the vapor phase mol fraction for a given component in the slurry.

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Checked: 3/91 by W.R. Lehland

C_c is calculated by converting y_i (mol fraction) to y_i (ppm)

$$y_i(MF) = \frac{\text{moles } i}{\text{moles } i + \text{moles } H_2O}$$

In this calculation, the mole contribution of component i is insignificant relative to the mole contribution of H_2O. Therefore,

$$\left(\frac{\text{mol } i}{\underbrace{\cancel{\text{mol } i}}_{\text{insignificant}} + \text{mol } H_2O}\right)\left(\frac{55.5093 \text{ mol } H_2O}{1 \ell}\right)(\text{molec. wt})\left(\frac{1000 \text{ mg}}{g}\right)$$

$$= \text{mg}/\ell = \text{mg}/\text{Kg} = \text{ppm}$$

[illegible] ketone (MIBK)

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Title: Organic Removal
Date: 2/91 by Jon Kerry
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MIBK Slurry Vapor Phase Mol Fraction

T °K	v1 l	p1 bars	x1 MF	Pt bars	y1 MF
2.98E2	4.301E2	2.607E-2	5.9E-8	3.143E-2	2.104E-5
3.03E2	4.308E2	3.426E-2	5.9E-8	4.212E-2	2.068E-5
3.08E2	4.315E2	4.454E-2	5.9E-8	5.584E-2	2.031E-5
3.13E2	4.322E2	5.73E-2	5.9E-8	7.327E-2	1.994E-5
3.18E2	4.33E2	7.299E-2	5.9E-8	9.522E-2	1.958E-5
3.23E2	4.337E2	9.212E-2	5.9E-8	1.226E-1	1.923E-5
3.28E2	4.344E2	1.152E-1	5.9E-8	1.565E-1	1.887E-5
3.33E2	4.351E2	1.429E-1	5.9E-8	1.98E-1	1.853E-5
3.38E2	4.358E2	1.759E-1	5.9E-8	2.487E-1	1.819E-5
3.43E2	4.365E2	2.148E-1	5.9E-8	3.099E-1	1.786E-5
3.48E2	4.372E2	2.605E-1	5.9E-8	3.834E-1	1.753E-5

MIBK Slurry Limits (mg/l)

T °K	y1 MF	Cc mg/l	LDR mg/l
2.98E2	2.104E-5	1.17E2	3.3E-1
3.03E2	2.068E-5	1.15E2	3.3E-1
3.08E2	2.031E-5	1.129E2	3.3E-1
3.13E2	1.994E-5	1.109E2	3.3E-1
3.18E2	1.958E-5	1.089E2	3.3E-1
3.23E2	1.923E-5	1.069E2	3.3E-1
3.28E2	1.887E-5	1.049E2	3.3E-1
3.33E2	1.853E-5	1.03E2	3.3E-1
3.38E2	1.819E-5	1.011E2	3.3E-1
3.43E2	1.786E-5	9.928E1	3.3E-1
3.48E2	1.753E-5	9.747E1	3.3E-1

$$C_f = \left(\frac{R-1}{R} + \frac{C_s}{R}\right) C_c$$

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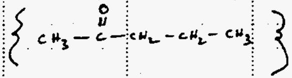
Title: Organic Emmissions
Date: 2/91 by Jon Perry
Checked: 3/91 by WRichard

1.) Let 1 be 2- Pentanone and 2 be H_2O.

2- Pentanone

$$\log \gamma_1^{\infty} = \alpha + \epsilon N_1 + \zeta\left(\frac{1}{N_1'} + \frac{1}{N_1''}\right) + \eta(N_1 - N_2)^2$$ Ref C 295 b



$$\left\{ CH_3-\overset{\overset{O}{\parallel}}{C}-CH_2-CH_2-CH_3 \right\} = \text{2-Pentanone} = \text{methyl propyl ketone}$$

$N_1 = 5$ $N_2 = 0$ $N_1' = 2$ $N_1'' = 4$

°K	α	ϵ	ζ	η
298	−1.475	.622	.500	0
333	−1.040	.583	.330	0
373	−.621	.517	.200	0

$$\log \gamma_1^{\infty} = \alpha + 5\epsilon + \zeta(3/4)$$

N_1 and N_2 = total # of carbon atoms in respective molecules
N', N'', and N''' = the # of carbon atoms in respective branches of the indicated molecule

α, ϵ, and ζ can be regressed with respect to temperature to give expressions which can be used to determine α, ϵ, and ζ at various temperatures.

$\alpha = 1.137\times10^{-2}(T) - 4.849$
$\epsilon = -1.406\times10^{-3}(T) + 1.045$
$\zeta = -3.982\times10^{-3}(T) + 1.676$

T => °K

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H_2O

$$\log \gamma_2^{\infty} = \alpha + \varepsilon N_2 + \zeta\left(\frac{1}{N_2'} + \frac{1}{N_2''} + \frac{1}{N_2'''}\right) + \theta\left(\frac{1}{N_1'} + \frac{1}{N_1''}\right)$$

ref
295 C

$N_2 = 0$ $N_1 = 5$ $N_1' = 2$ $N_1'' = 4$

°K	α	ε	ζ	η	θ
298	1.857	0	0	—	−1.019
333	1.493	0	0	—	−.73
373	1.231	0	0	—	−.557

$$\log \gamma_2^{\infty} = \alpha + \theta\left(3/4\right)$$

α and θ can be regressed with respect to temperature to give expressions which can be used to determine α and θ at various temperatures.

$T \Rightarrow$ °K

$\alpha = -8.3 \times 10^{-3}(T) + 4.306$

$\theta = 6.117 \times 10^{-3}(T) - 2.816$

2- Pentanone

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2.) $\ln \gamma_1^{\infty} = -\ln(\Lambda_{12}) - \Lambda_{21} + 1$ Ref. C 8-10.25

$\ln \gamma_2^{\infty} = -\ln(\Lambda_{21}) - \Lambda_{12} + 1$ Ref. C 8-10.26

T °K	Λ_{12} $(\times 10^{-2})$	Λ_{21} $(\times 10^{-1})$
288	2.131	1.994
303	1.979	2.271
318	1.83	2.585
333	1.685	2.943
348	1.544	3.35

2-Pentanone

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3.) $$\ln \gamma_1 = -\ln(X_1 + \Lambda_{12} X_2) + X_2 \left[\frac{\Lambda_{12}}{X_1 + \Lambda_{12} X_2} - \frac{\Lambda_{21}}{\Lambda_{21} X_1 + X_2} \right]$$ Ref. A 6.11-2

$$\ln \gamma_2 = -\ln(X_2 + \Lambda_{21} X_1) - X_1 \left[\frac{\Lambda_{12}}{X_1 + \Lambda_{12} X_2} - \frac{\Lambda_{21}}{\Lambda_{21} X_1 + X_2} \right]$$ Ref A 6.11-3

X_1 & X_2 = mol fraction of respective molecules

Mol Fraction is calculated from ppb concentration in Stream Specific Report App 3A.

ex.) 8.75×10^0 ppb $= \frac{8.75 \times 10^0 \ \mu g}{l} = \frac{8.75 \times 10^{-6} g}{1000 g} =$

$$\frac{1.02 \times 10^{-7} \text{ moles 2-pentanone}}{8.75 \times 10^{-6} g \text{ 2-pentanone} + 999.999 g H_2O} = \frac{1.02 \times 10^{-7} \text{ moles 2-pentanone}}{1.02 \times 10^{-7} \text{ moles 2-pentanone} + 55.5093 \text{ moles } H_2O} = 2 \times 10^{-9} \text{ MF 2-Pentanone}$$

$X_1 = 2 \times 10^{-9}$ MF
$X_1 = 3 \times 10^{-9}$ MF
$X_1 = 2.5 \times 10^{-8}$ MF

	$X_1 = 2 \times 10^{-9}$ MF	$X_1 = 3 \times 10^{-9}$ MF	$X_1 = 2.5 \times 10^{-8}$ MF	
°K	$\gamma_1 (\times 10^2)$	$\gamma_1 (\times 10^2)$	$\gamma_1 (\times 10^2)$	γ_2
288	1.045	1.045	1.045	1
303	1.095	1.095	1.095	1
318	1.147	1.147	1.147	1
333	1.202	1.202	1.202	1
348	1.259	1.259	1.259	1

α-Pentanone

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4) $\ln P_1 = (VPA) - \dfrac{VPB}{(T + VPC)}$ Ref. D App. A eqn. #3

VPA = 9.3829 VPB = 2934.87 VPC = −62.25

Valid From 275 °K to 410 °K

$$\ln \frac{P_2}{P_c} = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^{3} + (VPD)x^{6}\right]$$ Ref. D App A eqn #1

$x = 1 - T/T_c$

T_c = 647.3 P_c = 221.2 VPA = −7.76451

VPB = 1.45838 VPC = −2.7758 VPD = +1.23303

Valid From 275 °K to 647.3 °K

°K	P_1 (bars)	P_2 (bars)
288	2.685×10^{-2}	1.69×10^{-2}
303	6.035×10^{-2}	4.212×10^{-2}
318	1.234×10^{-1}	9.521×10^{-2}
333	2.33×10^{-1}	1.98×10^{-1}
348	4.115×10^{-1}	3.834×10^{-1}

2-Pentanone

Westinghouse Environmental & Geotechnical Services, Inc.

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5.) $Y_i P_t = \gamma_i X_i P_i$

x_i = mole fraction of component i liquid phase

y_i = vapor phase mol fraction of component i

P_t = System pressure (vapor phase)

γ_i = activity coeffecient (liquid phase) (component i)

p_i = vapor pressure of pure component at system temp.

$$Y_1 = \frac{\gamma_1 X_1 P_1}{P_t}$$

P_t = 750 mm Hg in C-100

$$\Rightarrow (750 \text{ mm Hg})\left(\frac{1.01325 \text{ bars}}{760 \text{ mm Hg}}\right) = .9999 \text{ bars}$$

P_t = .9999 bars

2-Pentanone

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6.) C-100 stream flow rate = 150 $\frac{ft^3}{min}$

C-100 pressure = 6" WG

$$\text{Emmissions} = \left(150\ \frac{ft^3}{min}\right)\left(28.317\ \frac{l}{ft^3}\right)\left(\frac{60\ min}{hr}\right)\left(\frac{750\ mm\ Hg}{760\ mm\ Hg}\right)\left(\frac{298}{T}\right)\left(\frac{1\ mol}{22.4\ l}\right)$$

$$\xrightarrow{\text{cont'd}} \left(\frac{86.134\ g}{mol}\right)\left(\frac{1\ lb}{454\ g}\right)\left(y_i\right) = \frac{\text{lbs of 2-Pentanone}}{hr}$$

2-Pentanone

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2-Pentanone C-100 Emmissions (xl=ave)

T °K	vl γl	pl bars	xl mF	yl mF	Emmissions lbs/hr
2.88E2	1.045E2	2.685E-2	2E-9	5.611E-9	1.237E-5
3.03E2	1.095E2	6.035E-2	2E-9	1.321E-8	2.768E-5
3.18E2	1.147E2	1.234E-1	2E-9	2.83E-8	5.649E-5
3.33E2	1.202E2	2.33E-1	2E-9	5.599E-8	1.067E-4
3.48E2	1.259E2	4.115E-1	2E-9	1.036E-7	1.89E-4

2-Pentanone C-100 Emmissions (xl=max)

T °K	vl γl	pl bars	xl mF	yl mF	Emmissions lbs/hr
2.88E2	1.045E2	2.685E-2	3E-9	8.417E-9	1.855E-5
3.03E2	1.095E2	6.035E-2	3E-9	1.982E-8	4.153E-5
3.18E2	1.147E2	1.234E-1	3E-9	4.245E-8	8.474E-5
3.33E2	1.202E2	2.33E-1	3E-9	8.399E-8	1.601E-4
3.48E2	1.259E2	4.115E-1	3E-9	1.554E-7	2.835E-4

2-Pentanone C-100 Emmissions (xl=max10)

T °K	vl γl	pl bars	xl mF	yl mF	Emmissions lbs/hr
2.88E2	1.045E2	2.685E-2	2.5E-8	7.014E-8	1.546E-4
3.03E2	1.095E2	6.035E-2	2.5E-8	1.652E-7	3.461E-4
3.18E2	1.147E2	1.234E-1	2.5E-8	3.538E-7	7.062E-4
3.33E2	1.202E2	2.33E-1	2.5E-8	6.999E-7	1.334E-3
3.48E2	1.259E2	4.115E-1	2.5E-8	1.295E-6	2.363E-3

2-Pentanone

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Title: Organic Emmissions

Date: 2/91 by Jon Perry

Checked: 3/91 by WG Richmond

The process condensate emmission results at 75 °C = 348 °K, can be used to determine the feed concentration limit. The feed concentration limit is the concentration of volatile constituent in the feed stream, with the assumption that the volatile constituent is completely transferred into the condensate, which will produce 0.71 lbs/hr (.322 Kg/hr) emissions of 2-Pentanone from the process condensate. The feed concentration limit is calculated as follows:

$$\left(\frac{1.20 \times 10^{2}}{} \ \mu g/l\right)\left(\frac{1 \ mg}{1000 \ \mu g}\right)\left(\frac{1 \ hr.}{2.363 \times 10^{-3} \ lbs}\right)\left(\frac{.71 \ lbs}{1 \ hr}\right)\left(\frac{R-1}{R}\right)$$

$$= \quad 36.06 \left(\frac{R-1}{R}\right) \Rightarrow mg/l$$

note: R = Feed rate ÷ product rate

2- Pentanone

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Determination of maximum feed concentration:

$$R\,C_f + (1-R)\,C_c = C_s$$

R = Ratio of feed to product Mass Ratio

C_f = Feed Concentration

C_s = Concentration of a given component in Slurry

Note: To determine the maximum feed concentration (C_f) of a given component, (C_s) will be the regulatory limit (HBL or LDR).

C_c = Condensate Concentration of a given component

Note: C_c is calculated from the vapor phase mol fraction for a given component in the slurry.

2-Pentanone

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C_c is calculated by converting y_i (mol fraction) to y_i (ppm)

$$y_i(MF) = \frac{\text{moles } i}{\text{moles } i + \text{moles } H_2O}$$

In this calculation, the mole contribution of component i is insignificant relative to the mole contribution of H_2O. Therefore,

$$\left(\frac{\text{mol } i}{\underbrace{\cancel{\text{mol } i}}_{\text{insignificant}} + \text{mol } H_2O}\right)\left(\frac{55.5093 \text{ mol } H_2O}{1\,l}\right)(\text{molec. wt})\left(\frac{1000 \text{ mg}}{g}\right)$$

$$= \text{mg}/l = \text{mg}/\text{Kg} = \text{ppm}$$

2-Pentanone

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2-Pentanone Slurry Vapor Phase Mol Fraction

T °K	vl Li	pl bars	xl MF	Pt bars	yl MF
2.98E2	1.078E2	4.66E-2	2.09E-7	3.143E-2	1.05E-6
3.03E2	1.095E2	6.035E-2	2.09E-7	4.212E-2	1.381E-6
3.08E2	1.112E2	7.734E-2	2.09E-7	5.584E-2	1.797E-6
3.13E2	1.129E2	9.813E-2	2.09E-7	7.327E-2	2.316E-6
3.18E2	1.147E2	1.234E-1	2.09E-7	9.522E-2	2.957E-6
3.23E2	1.165E2	1.537E-1	2.09E-7	1.226E-1	3.743E-6
3.28E2	1.183E2	1.9E-1	2.09E-7	1.565E-1	4.698E-6
3.33E2	1.202E2	2.33E-1	2.09E-7	1.98E-1	5.851E-6
3.38E2	1.22E2	2.836E-1	2.09E-7	2.487E-1	7.233E-6
3.43E2	1.24E2	3.427E-1	2.09E-7	3.099E-1	8.88E-6
3.48E2	1.259E2	4.115E-1	2.09E-7	3.834E-1	1.083E-5

2-Pentanone Slurry LImits (mg/l)

T °K	yl MF	Cc mg/l	HBL mg/l
2.98E2	1.05E-6	5.02E0	1E0
3.03E2	1.381E-6	6.602E0	1E0
3.08E2	1.797E-6	8.593E0	1E0
3.13E2	2.316E-6	1.107E1	1E0
3.18E2	2.957E-6	1.414E1	1E0
3.23E2	3.743E-6	1.79E1	1E0
3.28E2	4.698E-6	2.246E1	1E0
3.33E2	5.851E-6	2.798E1	1E0
3.38E2	7.233E-6	3.458E1	1E0
3.43E2	8.88E-6	4.246E1	1E0
3.48E2	1.083E-5	5.178E1	1E0

$$C_f = \left(\frac{R-1}{R} + \frac{C_s}{R}\right) C_c$$

Phenol

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Title: Organic Emmissions

Date: 2/91 by Jon Perry

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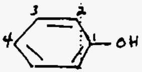
1.) Let 1 be Phenol and 2 be H_2O.

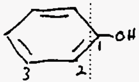
Phenol

$$\log \gamma_1^{\infty} = \alpha + \epsilon N_1 + \zeta\left(\frac{1}{N_1'} + \frac{1}{N_1''}\right) + \eta\left(N_1 - N_2\right)^2$$ Ref. C 295 b

$N_1 = 6$ $N_2 = 0$



$N_1' = 4$



$N_1'' = 3$

Note: with the exception of the functional group carbon atom, each carbon atom is accounted for.

°K	α	ϵ	ζ	η
298	−1.22	.622	.17	0
333	−1.023	.583	.252	0
373	−.87	.517	.4	0

N_1 and N_2 = total # of carbon atoms in respective molecules

N', N'' = the # of carbon atoms in respective branches of the indicated molecule

α, ϵ, and ζ can be regressed with respect to temperature to give expressions which can be used to determine α, ϵ, and ζ at various temperatures.

$\alpha = 4.647 \times 10^{-3}(T) - 2.593$

$\epsilon = -1.41 \times 10^{-3}(T) + 1.045$

$\zeta = 3.082 \times 10^{-3}(T) - .757$

$T \Rightarrow$ °K

Phencl

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H_2O

$$\log \gamma_2^{\infty} = \alpha + \epsilon N_2 + \zeta\left(\frac{1}{N_2'} + \frac{1}{N_2''} + \frac{1}{N_2'''}\right) + \theta\left(\frac{1}{N_1'} + \frac{1}{N_1''}\right)$$ ref. c 295 c

$N_2 = 0$ $N_1' = 4$ $N_1'' = 3$

°K	α	ϵ	ζ	η	θ
353	1.208	0	0	—	−.690

$$\log \gamma_2^{\infty} = \alpha + \theta\left(\tfrac{7}{12}\right)$$

Note: Since values for α and θ are given at one temperature only, the values for α and θ at 353°K will be used to calculate γ_2^{∞} at other temperatures.

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2.) $\ln \gamma_1^{\infty} = -\ln(\Lambda_{12}) - \Lambda_{21} + 1$ Ref. C 8-10.25

$\ln \gamma_2^{\infty} = -\ln(\Lambda_{21}) - \Lambda_{12} + 1$ Ref. C 8-10.26

T °K	Λ_{12} $(\times 10^{-3})$	Λ_{21} $\times 10^{-1}$
288	3.96	4.237
303	4.251	4.236
318	4.558	4.235
333	4.887	4233
348	5.24	4.232

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3.) $$\ln \gamma_1 = -\ln\left(X_1 + \Lambda_{12} X_2\right) + X_2\left[\frac{\Lambda_{12}}{X_1 + \Lambda_{12} X_2} - \frac{\Lambda_{21}}{\Lambda_{21} X_1 + X_2}\right]$$ Ref. A 6.11-2

$$\ln \gamma_2 = -\ln\left(X_2 + \Lambda_{21} X_1\right) - X_1\left[\frac{\Lambda_{12}}{X_1 + \Lambda_{12} X_2} - \frac{\Lambda_{21}}{\Lambda_{21} X_1 + X_2}\right]$$ Ref A 6.11-3

X_1 & X_2 = mol fraction of respective molecules

Mol Fraction is calculated from ppb concentration in Stream Specific Report App 3A.

ex.) $$1.19 \times 10^{1}\ \text{ppb} = \frac{1.19 \times 10^{1}\ \text{mg}}{\text{litre}} = \frac{1.19 \times 10^{-5}\ \text{g}}{1000\ \text{g}} = \frac{1.26 \times 10^{-7}\ \text{moles phenol}}{1.19 \times 10^{-5}\ \text{g phenol} + 999.999\ \text{g } H_2O}$$

$$= \frac{1.26 \times 10^{-7}\ \text{moles phenol}}{1.26 \times 10^{-7}\ \text{moles phenol} + 55.5093\ \text{moles } H_2O} = 2 \times 10^{-9}\ \text{mF Phenol}$$

$x_1 = 2 \times 10^{-9}$ MF
$x_1 = 6 \times 10^{-9}$ MF
$x_1 = 6.3 \times 10^{-9}$ MF

	$x_1 = 2 \times 10^{-9}$ mF	$X_1 = 6 \times 10^{-9}$ mF	$x_1 = 6.3 \times 10^{-9}$ MF	
°K	γ_1 ($\times 10^2$)	γ_1 ($\times 10^2$)	γ_1 ($\times 10^2$)	γ_2
288	4.488	4.488	4.488	1
303	4.186	4.186	4.186	1
318	3.905	3.905	3.905	1
333	3.642	3.642	3.642	1
348	3.398	3.398	3.398	1

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4.)

$$\ln \frac{P_1}{P_c} = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^3 + (VPD)x^6\right]$$

Ref. D App A eqn #1

$x = 1 - T/T_c$

$T_c = 694.4$ $P_c = 61.3$ $VPA = -8.7555$

$VPB = 2.92651$ $VPC = -6.31601$ $VPD = -1.36889$

Valid From 380 °K to 694.4 °K

$$\ln \frac{P_2}{P_c} = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^3 + (VPD)x^6\right]$$

Ref. D App A eqn. #1

$x = 1 - T/T_c$

$T_c = 647.3$ $P_c = 221.2$ $VPA = -7.76451$

$VPB = 1.45838$ $VPC = -2.7758$ $VPD = -1.23303$

Valid From 275 °K to 647.3 °K

°K	P_1 (bars)	P_2 (bars)
288	2.573×10^{-4}	1.69×10^{-2}
303	8.686×10^{-4}	4.242×10^{-2}
318	2.555×10^{-3}	9.521×10^{-2}
333	6.68×10^{-3}	1.98×10^{-1}
348	1.579×10^{-2}	3.834×10^{-1}

Phenol

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5.) $y_i P_t = \gamma_i x_i p_i$

x_i = mole fraction of component i (liquid phase)
y_i = vapor phase mol fraction of component i
P_t = System pressure (vapor phase)
γ_i = activity coeffecient (liquid phase) (component i)
p_i = vapor pressure of pure component at system temp.

$$y_1 = \frac{\gamma_1 x_1 p_1}{P_t}$$

P_t = 750 mm Hg in C-100

$$\Rightarrow (750\ \text{mm Hg})\left(\frac{1.01325\ \text{bars}}{760\ \text{mm Hg}}\right) = .9999\ \text{bars}$$

P_t = .9999 bars

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6.) C-100 stream flow rate = 150 $\frac{ft^3}{min}$

C-100 pressure = 6" WG

$$\text{Emmissions} = \left(150\ \frac{ft^3}{min}\right)\left(28.317\ \frac{l}{ft^3}\right)\left(\frac{60\ min}{hr}\right)\left(\frac{750\ mm\ Hg}{760\ mm\ Hg}\right)\left(\frac{298}{T}\right)\left(\frac{1\ mol}{22.4\ l}\right)$$

$$\underset{\longrightarrow}{\text{cnt'd}}\ \left(\frac{94.113\ g}{mol}\right)\left(\frac{1\ lb}{454\ g}\right)\left(y_i\right) = \frac{\text{lbs of Phenol}}{hr}$$

Phenol

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Title: Organic Emmissions

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Phenol C-100 Emmissions (xl=ave)

T °K	vl δl	pl bars	xl MF	yl MF	Emmissions lbs/hr
2.88E2	4.488E2	2.573E-4	2E-9	2.31E-10	5.562E-7
3.03E2	4.186E2	8.686E-4	2E-9	7.273E-10	1.665E-6
3.18E2	3.905E2	2.555E-3	2E-9	1.996E-9	4.353E-6
3.33E2	3.642E2	6.68E-3	2E-9	4.867E-9	1.014E-5
3.48E2	3.398E2	1.579E-2	2E-9	1.073E-8	2.138E-5

Phenol C-100 Emmissions (xl=max)

T °K	vl δl	pl bars	xl MF	yl MF	Emmissions lbs/hr
2.88E2	4.488E2	2.573E-4	6E-9	6.929E-10	1.669E-6
3.03E2	4.186E2	8.686E-4	6E-9	2.182E-9	4.995E-6
3.18E2	3.905E2	2.555E-3	6E-9	5.987E-9	1.306E-5
3.33E2	3.642E2	6.68E-3	6E-9	1.46E-8	3.041E-5
3.48E2	3.398E2	1.579E-2	6E-9	3.218E-8	6.415E-5

Phenol C-100 Emmissions (xl=max10)

T °K	vl δl	pl bars	xl MF	yl MF	Emmissions lbs/hr
2.88E2	4.648E2	2.573E-4	6.3E-8	7.534E-9	1.815E-5
3.03E2	4.39E2	8.686E-4	6.3E-8	2.402E-8	5.499E-5
3.18E2	4.146E2	2.555E-3	6.3E-8	6.674E-8	1.456E-4
3.33E2	3.915E2	6.68E-3	6.3E-8	1.648E-7	3.432E-4
3.48E2	3.698E2	1.579E-2	6.3E-8	3.678E-7	7.33E-4

Phenol

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The process condensate emmission results at 75°C = 348 °K, can be used to determine the feed concentration limit. The feed concentration limit is the concentration of volatile constituent in the feed stream, with the assumption that the volatile constituent is completely transferred into the condensate, which will produce 0.71 lbs/hr (.322 kg/hr) emmissions of Phenol from the process condensate. The feed concentration limit is calcalated as follows:

$$\left(3.30\times10^{2}\ \mu g/l\right)\left(\frac{1\ mg}{1000\ \mu g}\right)\left(\frac{1\ hr.}{7.33\times10^{-4}\ lbs}\right)\left(\frac{.71\ lbs}{1\ hr}\right)\left(\frac{R-1}{R}\right)$$

$$= 320\left(\frac{R-1}{R}\right) \Rightarrow mg/l$$

note: R = feed rate ÷ product rate

Phenol

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Determination of maximum feed concentration:

$$R \cdot C_f + (1-R) C_c = C_s$$

R = Ratio of feed to product Mass Ratio

C_f = Feed Concentration

C_s = Concentration of a given component in Slurry

Note: To determine the maximum feed concentration (C_f) of a given component, (C_s) will be the regulatory limit (HBL or LDR).

C_c = Condensate Concentration of a given component

Note: C_c is calculated from the vapor phase mol fraction for a given component in the slurry.

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Checked: 3/91 by

C_c is calculated by converting y_i (mol fraction) to y_i (ppm)

$$y_i(MF) = \frac{\text{moles } i}{\text{moles } i + \text{moles } H_2O}$$

In this calculation, the mole contribution of component i is insignificant relative to the mole contribution of H_2O. Therefore,

$$\left(\frac{\text{mol } i}{\underset{\text{insignificant}}{\cancel{\text{mol } i}} + \text{mol } H_2O}\right)\left(\frac{55.5093 \text{ mol } H_2O}{1 \ell}\right)\left(\text{molec. wt}\right)\left(\frac{1000 \text{ mg}}{g}\right)$$

$$= \quad mg/\ell \quad = \quad mg/Kg \quad = \quad ppm$$

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Phenol Slurry Vapor Phase Mol Fraction

T °K	v1 γ1	p1 bars	x1 MF	Pt bars	y1 MF
2.98E2	4.282E2	5.886E-4	1.187E-6	3.143E-2	9.518E-6
3.03E2	4.184E2	8.686E-4	1.187E-6	4.212E-2	1.024E-5
3.08E2	4.088E2	1.262E-3	1.187E-6	5.584E-2	1.097E-5
3.13E2	3.995E2	1.808E-3	1.187E-6	7.327E-2	1.17E-5
3.18E2	3.903E2	2.555E-3	1.187E-6	9.522E-2	1.243E-5
3.23E2	3.814E2	3.563E-3	1.187E-6	1.226E-1	1.316E-5
3.28E2	3.726E2	4.908E-3	1.187E-6	1.565E-1	1.387E-5
3.33E2	3.641E2	6.68E-3	1.187E-6	1.98E-1	1.458E-5
3.38E2	3.557E2	8.992E-3	1.187E-6	2.487E-1	1.527E-5
3.43E2	3.476E2	1.198E-2	1.187E-6	3.099E-1	1.594E-5
3.48E2	3.396E2	1.579E-2	1.187E-6	3.834E-1	1.66E-5

Phenol Slurry Limits (mg/kg)

T °K	y1 MF	Cc mg/kg	LDR mg/kg
2.98E2	9.518E-6	4.973E1	6.2E0
3.03E2	1.024E-5	5.35E1	6.2E0
3.08E2	1.097E-5	5.731E1	6.2E0
3.13E2	1.17E-5	6.113E1	6.2E0
3.18E2	1.243E-5	6.494E1	6.2E0
3.23E2	1.316E-5	6.873E1	6.2E0
3.28E2	1.387E-5	7.247E1	6.2E0
3.33E2	1.458E-5	7.616E1	6.2E0
3.38E2	1.527E-5	7.977E1	6.2E0
3.43E2	1.594E-5	8.33E1	6.2E0
3.48E2	1.66E-5	8.672E1	6.2E0

$$C_f = \left(\frac{R-1}{R} + \frac{C_s}{R} \right) C_c$$

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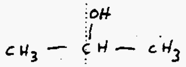
1.) Let 1 be <u>2- Propanol</u> and 2 be <u>H_2O</u>.

<u>2- Propanol</u>:

$$\log \gamma_1^{\infty} = \alpha + 3\epsilon + \zeta\left(\frac{1}{N_1'} + \frac{1}{N_1''}\right) + \eta\left(N_1 - N_2\right)^2$$ Ref C 295 b



$$\left\{ CH_3 - \overset{OH}{\overset{|}{C}H} - CH_3 \right\} = \text{2- propanol} = \text{isopropyl alcohol}$$

$N_1 = 3$ $N_2 = 0$ $N_1' = 2$ $N_1'' = 2$

°K	α	ϵ	ζ	η
298	−1.22	.622	.17	0
333	−1.023	.583	.252	0
373	−.87	.517	.4	0

$$\log \gamma_1^{\infty} = \alpha + 3\epsilon + \zeta$$

N_1 and N_2 = total # of carbon atoms in respective molecules
N', N'', and N''' = the # of carbon atoms in respective branches of the indicated molecule

α, ϵ, and ζ can be regressed with respect to temperature to give expressions which can be used to determine α, ϵ, and ζ at various temperatures.

$\alpha = 4.647 \times 10^{-3} (T) - 2.593$
$\epsilon = -1.41 \times 10^{-3} (T) + 1.045$
$\zeta = 3.082 \times 10^{-3} (T) - .757$

T => °K

2-Propanol

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H_2O

$$\log \gamma_2^{\infty} = \alpha + \epsilon N_2 + \zeta\left(\frac{1}{N_2'} + \frac{1}{N_2''} + \frac{1}{N_2'''}\right) + \theta\left(\frac{1}{N_1'} + \frac{1}{N_1''}\right) \quad \begin{matrix}\text{ref C} \\ 295\ \text{C}\end{matrix}$$

$N_2 = 0 \qquad N_1' = 2 = N_1''$

°K	α	ϵ	ζ	η	θ
353	1.208	0	0	—	−.690

$$\log \gamma_2^{\infty} = \alpha + \theta$$

Notes: Values for α and θ are given at one temperature only (80 °C = 353 °K). Values for α and θ at 80 °C will be used at other temperatures to calculate γ_2^{∞}.

2-Propanol

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2.) $\ln \gamma_1^{\infty} = -\ln(\Lambda_{12}) - \Lambda_{21} + 1$ Ref. C 8-10.25

$\ln \gamma_2^{\infty} = -\ln(\Lambda_{21}) - \Lambda_{12} + 1$ Ref. C 8-10.26

T °K	Λ_{12} $(\times 10^{-1})$	Λ_{21} $(\times 10^{-1})$
288	2.281	6.565
303	1.981	6.765
318	1.725	6.94
333	1.505	7.094
348	1.316	7.23

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3.) $\ln \gamma_1 = -\ln(X_1 + \Lambda_{12} X_2) + X_2 \left[\frac{\Lambda_{12}}{X_1 + \Lambda_{12} X_2} - \frac{\Lambda_{21}}{\Lambda_{21} X_1 + X_2} \right]$ Ref. A 6.11-2

$\ln \gamma_2 = -\ln(X_2 + \Lambda_{21} X_1) - X_1 \left[\frac{\Lambda_{12}}{X_1 + \Lambda_{12} X_2} - \frac{\Lambda_{21}}{\Lambda_{21} X_1 + X_2} \right]$ Ref A 6.11-3

X_1 & X_2 = mol fraction of respective molecules

Mol Fraction is calculated from ppb concentration in Stream Specific Report App 3A.

ex.) 2.35×10^{1} ppb $= \frac{2.35 \times 10^{1}\text{ mg}}{\text{litre}} = \frac{2.35 \times 10^{-5}\text{ g}}{1000\text{ g}} = \frac{3.91 \times 10^{-7}\text{ moles (6-propanol)}}{2.35 \times 10^{-5}\text{ g 2-propanol} + 999.99\text{g } H_2O}$

$= \frac{3.91 \times 10^{-7}\text{ moles 2-propanol}}{3.91 \times 10^{-7}\text{ moles 2-propanol} + 55.5093\text{ moles } H_2O} = 7 \times 10^{-9}$ MF 2-propanol

$X_1 = 7 \times 10^{-9}$ mF
$X_1 = 1 \times 10^{-8}$ mF
$X_1 = 1.02 \times 10^{-7}$ mF

°K	$X_1 = 7 \times 10^{-9}$ mF $\gamma_1 (\times 10^{0})$	$X_1 = 1 \times 10^{-8}$ mF $\gamma_1 (\times 10^{0})$	$X_1 = 1.02 \times 10^{-7}$ mF $\gamma_1 (\times 10^{0})$	γ_2
288	6.182	6.182	6.182	1
303	6.976	6.976	6.976	1
318	7.872	7.872	7.872	1
333	8.883	8.883	8.883	1
348	10.02	10.02	10.02	1

2-Propanol

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4.)

$$\ln \frac{P_1}{P_c} = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^{3} + (VPD)x^{6}\right]$$

Ref. D App A eqn #1

$x = 1 - T/T_c$

$T_c = 508.3$
$P_c = 47.6$
$VPA = -8.16927$
$VPB = -9.43213 \times 10^{-2}$
$VPC = -8.1004$
$VPD = 7.85000$

Valid From 250 °K to 508.3 °K

$$\ln \frac{P_2}{P_c} = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^{3} + (VPD)x^{6}\right]$$

Ref. D App A eqn. #1

$x = 1 - T/T_c$

$T_c = 647.3$
$P_c = 221.2$
$VPA = -7.76451$
$VPB = 1.45838$
$VPC = -2.7758$
$VPD = -1.23303$

Valid From 275 °K to 647.3 °K

°K	P_1 (bars)	P_2 (bars)
288	3.003×10^{-2}	1.69×10^{-2}
303	7.799×10^{-2}	4.242×10^{-2}
318	1.817×10^{-1}	9.521×10^{-2}
333	3.852×10^{-1}	1.98×10^{-1}
348	7.525×10^{-1}	3.834×10^{-1}

2-Propanol

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5.) $y_i P_t = \gamma_i x_i p_i$

x_i = mole fraction component i (liquid phase)
y_i = vapor phase mol fraction of component i

P_t = System pressure (vapor phase)

γ_i = activity coeffecient (liquid phase) (component i)

p_i = vapor pressure of pure component at system temp.

$$y_1 = \frac{\gamma_1 x_1 p_1}{P_t}$$

P_t = 750 mm Hg in C-100

$$\Rightarrow (750 \text{ mm Hg})\left(\frac{1.01325 \text{ bars}}{760 \text{ mm Hg}}\right) = .9999 \text{ bars}$$

P_t = .9999 bars

2-Propanol

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6.) C-100 stream flow rate = 150 $\frac{ft^3}{min}$

C-100 pressure = 6" WG

$$\text{Emmissions} = \left(150\ \frac{ft^3}{min}\right)\left(28.317\ \frac{l}{ft^3}\right)\left(\frac{60\ min}{hr}\right)\left(\frac{750\ mm\ Hg}{760\ mm\ Hg}\right)\left(\frac{298}{T}\right)\left(\frac{1\ mol}{22.4\ l}\right)$$

$$\underrightarrow{\text{cont'd}}\ \left(\frac{60.096\,g}{mol}\right)\left(\frac{1\ lb}{454\ g}\right)\left(y_i\right) = \frac{\text{lbs of 2-propanol}}{hr}$$

2-Propanol

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2-Propanol C-100 Emmissions (x1=ave)

T °K	v1 γl	p1 bars	x1 MF	y1 MF	Emmissions lbs/hr.
2.88E2	6.182E0	3.003E-2	7E-9	1.299E-9	1.998E-6
3.03E2	6.976E0	7.799E-2	7E-9	3.809E-9	5.567E-6
3.18E2	7.872E0	1.817E-1	7E-9	1.001E-8	1.395E-5
3.33E2	8.883E0	3.852E-1	7E-9	2.396E-8	3.186E-5
3.48E2	1.002E1	7.525E-1	7E-9	5.28E-8	6.72E-5

2-Propanol C-100 Emmissions (x1=max)

T °K	v1 γl	p1 bars	x1 MF	y1 MF	Emmissions lbs/hr.
2.88E2	6.182E0	3.003E-2	1E-8	1.856E-9	2.855E-6
3.03E2	6.976E0	7.799E-2	1E-8	5.441E-9	7.953E-6
3.18E2	7.872E0	1.817E-1	1E-8	1.431E-8	1.992E-5
3.33E2	8.883E0	3.852E-1	1E-8	3.422E-8	4.552E-5
3.48E2	1.002E1	7.525E-1	1E-8	7.543E-8	9.6E-5

2-Propanol C-100 Emmissions (x1=max10)

T °K	v1 γl	p1 bars	x1 MF	y1 MF	Emmissions lbs/hr.
2.88E2	6.182E0	3.003E-2	1.02E-7	1.893E-8	2.912E-5
3.03E2	6.976E0	7.799E-2	1.02E-7	5.55E-8	8.112E-5
3.18E2	7.872E0	1.817E-1	1.02E-7	1.459E-7	2.032E-4
3.33E2	8.883E0	3.852E-1	1.02E-7	3.491E-7	4.643E-4
3.48E2	1.002E1	7.525E-1	1.02E-7	7.694E-7	9.792E-4

2-Propanol

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The process condensate emmission results at 75 °C = 348 °K, can be used to determine the feed concentration limit. The feed concentration limit is the concentration of volatile constituent in the feed stream, with the assumption that the volatile constituent is completely transferred into the condensate, which will produce 0.71 lbs/hr (.322 Kg/hr) emmissions of 2- propanol from the process condensate. The feed concentration limit is calculated as follows:

$$\left(\frac{3.40 \times 10^{2}}{}\ \mu g/l\right)\left(\frac{1\ mg}{1000\ \mu g}\right)\left(\frac{1\ \ hr.}{9,792 \times 10^{-4}\ lbs}\right)\left(\frac{.71\ lbs}{1\ hr}\right)\left(\frac{R-1}{R}\right)$$

$$= \quad 247 \left(\frac{R-1}{R}\right) \Longrightarrow mg/l$$

note: R = feed rate ÷ product rate

2- Propanol

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Determination of maximum feed concentration:

$$R C_f + (1-R) C_c = C_s$$

R= Ratio of Feed to product Mass Ratio

C_f = Feed Concentration

C_s = Concentration of a given component in Slurry

Note: To determine the maximum feed concentration (C_f) of a given component, (C_s) will be the regulatory limit (HBL or LDR).

C_c = Condensate Concentration of a given component

Note: C_c is calculated from the vapor phase mol fraction for a given component in the slurry.

2-Propanol

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C_c is calculated by converting y_i (mol fraction) to y_i (ppm)

$$y_i(MF) = \frac{\text{moles } i}{\text{moles } i + \text{moles } H_2O}$$

In this calculation, the mole contribution of component i is insignificant relative to the mole contribution of H_2O. Therefore,

$$\left(\frac{\text{mol } i}{\cancel{\text{mol } i} + \text{mol } H_2O}\right)\left(\frac{55.5093 \text{ mol } H_2O}{1 \ell}\right)(\text{molec. wt})\left(\frac{1000 \text{ mg}}{g}\right)$$

insignificant

$$= \text{mg}/\ell = \text{mg}/\text{Kg} = \text{ppm}$$

2-propanol

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°K 2-Propanol Slurry Vapor Phase Mol Fraction

T °K	v1 γ1	p1 bars	x1 MF	Pt bars	y1 MF
2.98E2	6.7E0	5.747E-2	3E-7	3.143E-2	3.675E-6
3.03E2	6.976E0	7.799E-2	3E-7	4.212E-2	3.875E-6
3.08E2	7.262E0	1.046E-1	3E-7	5.584E-2	4.08E-6
3.13E2	7.561E0	1.386E-1	3E-7	7.327E-2	4.291E-6
3.18E2	7.872E0	1.817E-1	3E-7	9.522E-2	4.507E-6
3.23E2	8.195E0	2.357E-1	3E-7	1.226E-1	4.728E-6
3.28E2	8.532E0	3.028E-1	3E-7	1.565E-1	4.954E-6
3.33E2	8.883E0	3.852E-1	3E-7	1.98E-1	5.184E-6
3.38E2	9.248E0	4.857E-1	3E-7	2.487E-1	5.419E-6
3.43E2	9.628E0	6.07E-1	3E-7	3.099E-1	5.659E-6
3.48E2	1.002E1	7.525E-1	3E-7	3.834E-1	5.902E-6

°K 2-Propanol Slurry Limits (mg/l)

T °K	y1 MF	Cc mg/l	HBL mg/l
2.98E2	3.675E-6	1.226E1	1E0
3.03E2	3.875E-6	1.293E1	1E0
3.08E2	4.08E-6	1.361E1	1E0
3.13E2	4.291E-6	1.431E1	1E0
3.18E2	4.507E-6	1.503E1	1E0
3.23E2	4.728E-6	1.577E1	1E0
3.28E2	4.954E-6	1.653E1	1E0
3.33E2	5.184E-6	1.729E1	1E0
3.38E2	5.419E-6	1.808E1	1E0
3.43E2	5.659E-6	1.888E1	1E0
3.48E2	5.902E-6	1.969E1	1E0

$$C_f = \left(\frac{R-1}{R} + \frac{C_s}{R} \right) C_c$$

Pyridine

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The UNIFAC method is used to determine activity coefficients (γ_i).

Ref. F

Robert C. Reid, John M. Prausnitz, Bruce E. Poling, "The Properties of Gases and Liquids," 4th Edition, McGraw-Hill, Inc., New York, NY, 1987, pp. 314-332.

$$\ln \gamma_i = \underset{\text{(combinatorial)}}{\ln \gamma_i^{C}} + \underset{\text{(residual)}}{\ln {}_i^{R}}$$

note: The combinatorial part of this equation deals with pure component properties only and is dependent on diffences in molecular size and shape.

$$\ln \gamma_i^{c} = \ln \frac{\phi_i}{x_i} + \frac{z}{2} q_i \ln \frac{\theta_i}{\phi_i} + l_i - \frac{\phi_i}{x_i} \sum_j x_j l_j$$

$$\theta_i = \frac{q_i x_i}{\sum_j q_j x_j} \qquad \phi_i \ \frac{r_i x_i}{\sum_j r_j x_j}$$

$$r_i = \sum_k \nu_k^{i} R_k \qquad q_i = \sum_k \nu_k^{i} Q_k$$

x_i = mol Fraction of molecule i in solution
Summations are over all components
R_k, Q_k } Determined from table 8-21 (Ref. F)
ν_k^{i} = # of groups of type k in molecule i

Pyridine

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$$\ln \gamma_i^R = \sum_k \nu_k^i \left(\ln \Gamma_k - \ln \Gamma_k^i \right)$$

ν_k^i = # of groups of type k in molecule i

Γ_k = group residual activity coefficient

Γ_k^i = residual activity coeffecient of group k in a reference solution containing molecules of type i only.

$$\ln \Gamma_k = Q_k \left[1 - \ln \left(\sum_m \theta_m \Psi_{mk} \right) - \sum_m \frac{\theta_m \Psi_{km}}{\sum_n \theta_n \Psi_{nm}} \right]$$

Note : Summations are over all groups

$$\ln \Gamma_k^i = Q_k \left[1 - \ln \left(\sum_m \theta_m \Psi_{mk} \right) - \sum_m \frac{\theta_m \Psi_{km}}{\sum_n \theta_n \Psi_{nm}} \right]$$

Note : Summations are over all groups in molecule i only.

$$\theta_m = \frac{Q_m X_m}{\sum_n Q_n X_n}$$

X_m = mole fraction of group m

Q ⇒ determined from table 8-21 Ref. F

$$\Psi_{mn} = \exp\left(\frac{-a_{mn}}{T} \right)$$

a_{mn} ⇒ determined from table 8-22 Ref. F

T = temperature (°K)

Pyridine

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 => pyridine

The following information is available in Ref. E

molecule		group name	group main #	ν_j^i	R_j^i	Q_j
Pyridine	(1)	C_5H_5N	18	1	2.9993	2.113
H_2O	(2)	H_2O	7	1	.9200	1.400

$$r_i = \sum_k \nu_k^i R_k$$

$$r_1 = (1)(2.9993) = 2.9993$$

$$r_2 = (1)(.9200) = .9200$$

$$q_i = \sum_k \nu_k^i Q_k$$

$$q_1 = (1)(2.113) = 2.1113$$

$$q_2 = (1)(1.400) = 1.400$$

$$\phi_i = \frac{r_i \quad x_i}{\sum_j r_j \; x_j}$$

Pyridine

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x_i = mol fraction which is calculated from ppb concentration (obtained from Stream Specific Report – App. 3A).

ex. 5.04×10^2 ppb $= 5.04 \times 10^2 \, \text{mg/litre} = \dfrac{6.37 \times 10^{-6} \text{ moles pyridine}}{1000\,g} =$

$$= \frac{6.37 \times 10^{-6} \text{ moles pyridine}}{5.04 \times 10^{-4} g \text{ pyridine} + 999.999 g\, H_2O} = \frac{6.37 \times 10^{-6} \text{ moles pyridine}}{6.37 \times 10^{-6} \text{ moles pyridine} + 55.5093 \text{ moles } H_2O} = 1.15 \times 10^{-7} \text{ MF Pyridine}$$

$$\phi_1 = \frac{(2.9993)(1.15 \times 10^{-7})}{(2.9993)(1.15 \times 10^{-7}) + (.9200)(1)} = 3.749 \times 10^{-7} \quad \text{at } x_1 = 1.15 \times 10^{-7}$$

$$\phi_2 = \frac{(9200)(1)}{(2.9993)(1.15 \times 10^{-7}) + (.9200)(1)} = 1 \quad \text{at } x_1 = 1.15 \times 10^{-7}$$

$$\theta_i = \frac{q_i x_i}{\sum_j q_j x_j}$$

$$\theta_1 = \frac{(2.1113)(1.15 \times 10^{-7})}{(2.1113)(1.15 \times 10^{-7}) + (1.400)(1)} = 1.736 \times 10^{-7} \quad \text{at } x_1 = 1.15 \times 10^{-7}$$

$$\theta_2 = \frac{(1.400)(1)}{(2.1113)(1.15 \times 10^{-7}) + (1.400)(1)} = 1 \quad \text{at } x_1 = 1.15 \times 10^{-7}$$

$$l_i = \frac{z}{2}(r_i - q_i) - (r_i - 1) \qquad z = 10$$

$$l_1 = \frac{10}{2}(2.9993 - 2.1113) - (2.9993 - 1) = 2.432$$

$$l_2 = \frac{10}{2}(.9200 - 1.400) - (.9200 - 1) = -2.32$$

Pyridine

Westinghouse Environmental & Geotechnical Services, Inc.

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Job No. 89-5010-ES Client/Project WHC/242-A

Title: Organic ~~Rem~~ Emissions

Date: 3/91 by Jon Kerry

Checked: 3/91 by WG Richard

$$\ln \gamma_1^c = \ln \frac{\phi_i}{x_i} + \frac{z}{2} q_i \ln \frac{\theta_i}{\phi_i} + l_i - \frac{\phi_i}{x_i} \sum_j x_j l_j$$

$z = 10$

$$\ln \gamma_1^c = \ln\left(\frac{3.749\times10^{-7}}{1.15\times10^{-7}}\right) + (5)(2.1113)\ln\left(\frac{1.736\times10^{-7}}{3.749\times10^{-7}}\right) + 2.432 - \left(\frac{3.749\times10^{-7}}{1.15\times10^{-7}}\right)\overset{l_i}{\Big[}(1.15\times10^{-7})(2.432) + (1)(-2.32)\Big]$$

$\gamma_1^c = 2.093\times10^{1}$ at $x_1 = 1.15\times10^{-7}$

$\gamma_2^c = 1$ at $x_1 = 1.15\times10^{-7}$

Pyridine

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Title: Organic Emissions
Date: 3/91 by Jon Perry
Checked: 3/21 by WBRichard

$$\ln \Gamma_k^i = Q_k \left[1 - \ln\left(\sum_m \Theta_m^i \Psi_{mk}\right) - \sum_m \frac{\Theta_m^i \Psi_{km}}{\sum_n \Theta_n^i \Psi_{nm}} \right]$$

$$X_m = \frac{\nu_m^i}{\sum_n \nu_n^i} \qquad \Theta_m^i = \frac{Q_m X_m^i}{\sum_n Q_n X_n} \qquad \Psi_{mn}^{ii} = \exp\left(\frac{-a_{mn}}{T}\right)$$

note; small x_i → mol fraction of molecule in solution
Capital X_i → mol fraction of functional group in solution
Capital X_i^i → mol fraction of functional group with respect to the indicated molecule

$$X_{18}^{(1)} = \frac{1}{1} = 1$$
$$X_7^{2} = \frac{1}{1} = 1$$

note 18 designates → C_5H_5N, 7 → H_2O

$$\Psi_{18\to18} = \Psi_{1818} = \exp\frac{-0}{T} = 1$$

$$\Psi_{7\to7} = \Psi_{77} = \exp\frac{-0}{T} = 1$$

$$\Theta_{18}^{(1)} = \frac{(2.113)(1)}{(2.113)(1)} = 1$$

$$\Theta_7^{(2)} = \frac{(1.400)(1)}{(1.400)(1)} = 1$$

$$\ln \Gamma_{18}^{(1)} = (2.113)\left\{1 - \ln\left[(\Theta_{18}^{(1)})(\Psi_{1818})\right] - \left[\frac{(\Theta_{18}^{(1)})(\Psi_{1818})}{(\Theta_{18}^{(1)})(\Psi_{1818})}\right]\right\}$$

$$\Gamma_{18}^{(1)} = 1$$

$$\Gamma_7^{(2)} = 1$$

Pyridine

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Job No. 89-500-ES Client/Project WHC/242-A
Title: Organic Emissions
Date: 3/91 by Jon Perry
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$$\ln \Gamma_k = Q_k \left[1 - \ln\left(\sum_m \theta_m \psi_{mk} \right) - \sum_m \frac{\theta_m \psi_{km}}{\sum_n \theta_n \psi_{nm}} \right]$$

$$X_{18} = \frac{(1.15\times10^{-7})(1)}{(1.15\times10^{-7})(1) + (1)(1)} = 1.15\times10^{-7}$$

$$X_7 = \frac{(1)(1)}{(1.15\times10^{-7})(1) + (1)(1)} = 1$$

$$\psi_{18\to7} = \psi_{187} = \exp\left(\frac{-332.9}{T}\right) = 3.177 \quad \text{at } T = 288\,°K$$

$$\psi_{7\to18} = \psi_{718} = \exp\left(\frac{-459}{T}\right) = 2.032\times10^{-1} \quad \text{at } T = 288\,°K$$

note: $\psi_{77} = 1$, $\psi_{1818} = 1$

$$\theta_{18} = \frac{(2.113)(1.15\times10^{-7})}{(2.113)(1.15\times10^{-7}) + (1.400)(1)} = 1.736\times10^{-7}$$

$$\theta_7 = \frac{(1.400)(1)}{(2.113)(1.15\times10^{-7}) + (1.400)(1)} = 1$$

Pyridine

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$$\ln \Gamma_{18} = 2.113 \left\{ 1 - \ln\left[(\theta_{18})(\psi_{1818}) + (\theta_7)(\psi_{718}) \right] - \left[\frac{(\theta_{18})(\psi_{1818})}{(\theta_{18})(\psi_{1818}) + (\theta_7)(\psi_{718})} + \frac{(\theta_7)(\psi_{187})}{(\theta_{18})(\psi_{187}) + (\theta_7)(\psi_{77})} \right] \right\}$$

$\Gamma_{18} = 2.917 \times 10^{-1}$ at $T = 288\,°K$ and $x_1 = 1.15 \times 10^{-7}$ mf.

$$\ln \Gamma_7 = 1.400 \left\{ 1 - \ln\left[(\theta_{18})(\psi_{187}) + (\theta_7)(\psi_{77}) \right] - \left[\frac{(\theta_{18})(\psi_{718})}{(\theta_{18})(\psi_{1818}) + (\theta_7)(\psi_{718})} + \frac{(\theta_7)(\psi_{77})}{(\theta_{18})(\psi_{187}) + (\theta_7)(\psi_{77})} \right] \right\}$$

$\Gamma_7 = 1$

Pyridine

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Title: Organic Emissions

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$$\ln \gamma_i^R = \sum_k \nu_k^i \left(\ln \Gamma_k - \ln \Gamma_k^i\right)$$

$$\ln \gamma_1^R = 1\left(\ln(2.917\times10^{-1}) - \ln(1)\right)$$

$\gamma_1^R = 2.917\times10^{-1}$ at 288 °k $x_1 = 1.15\times10^{-7}$ mf.

$$\ln \gamma_2^R = 1\left(\ln(1) - \ln(1)\right)$$

$\gamma_2^R = 1$ at 288 °k $x_1 = 1.15\times10^{-7}$ mf

$$\ln \gamma_1 = \ln \gamma_1^C + \ln \gamma_1^R$$

$$\ln \gamma_1 = \ln(1) + \ln(2.917\times10^{-1})$$

$\gamma_1 = 6.104$ at 288 °k $x_1 = 1.15\times10^{-7}$ mf.

$$\ln \gamma_2 = \ln \gamma_2^C + \ln{}_2^R$$

$$\gamma_2 = \ln(1) + \ln(1)$$

$$\gamma_2 = 1$$

Pyridine

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Title: Organic Emissions
Date: 3/91 by Jon Perry
Checked: 3/91 by W6Richard

combinatorial

Title: Pyridine Activity Coeffegeint Calculations

Element	T °K	x1 x_1	phi1 Φ	theta1 θ	l1 ℓ_1	V1C γ_1^c
1	2.88E2	1.15E-7	3.749E-7	1.736E-7	2.432E0	2.093E1
2	3.03E2	1.15E-7	3.749E-7	1.736E-7	2.432E0	2.093E1
3	3.18E2	1.15E-7	3.749E-7	1.736E-7	2.432E0	2.093E1
4	3.33E2	1.15E-7	3.749E-7	1.736E-7	2.432E0	2.093E1
5	3.48E2	1.15E-7	3.749E-7	1.736E-7	2.432E0	2.093E1

Residual group

Title: Pyridine Activity Coeffeceint Calculations

Element	O18 Θ	U187 Ψ_{187}	U718 Ψ_{718}	~~F18~~ ln	V1R γ_1^R	V1 γ_1
1	1.736E-7	3.177E0	2.032E-1	2.917E-1	2.917E-1	6.104E0
2	1.736E-7	3E0	2.198E-1	3.586E-1	3.586E-1	7.505E0
3	1.736E-7	2.849E0	2.361E-1	4.247E-1	4.247E-1	8.888E0
4	1.736E-7	2.717E0	2.52E-1	4.885E-1	4.885E-1	1.022E1
5	1.736E-7	2.603E0	2.674E-1	5.489E-1	5.489E-1	1.149E1

Pyridine

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Title: Organic Emissions
Date: 2/91 by Jon Perry
Checked: 3/91 by WGKirkwood

$$\ln \frac{P_1}{P_c} = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^{3} + (VPD)x^{6}\right]$$ Ref. D App A eqn. #1

$x = 1 - T/T_c$

$T_c = 620$ $P_c = 56.3$ $VPA = -7.07689$

$VPB = 1.21511$ $VPC = -2.76681$ $VPD = -2.87472$

Valid From 340°K to 620°K

$$\ln \frac{P_2}{P_c} = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^{3} + (VPD)x^{6}\right]$$ Ref. D App A eqn. #1

$x = 1 - T/T_c$

$T_c = 647.3$ $P_c = 221.2$ $VPA = -7.76451$

$VPB = 1.45838$ $VPC = -2.77758$ $VPD = -1.23303$

Valid From 275°K to 647.3°K

°K	P_1 (bars)	P_2 (bars)
288	1.556×10^{-2}	1.69×10^{-2}
303	3.594×10^{-2}	4.212×10^{-2}
318	7.554×10^{-2}	9.521×10^{-2}
333	1.466×10^{-1}	1.98×10^{-1}
348	2.66×10^{-1}	3.834×10^{-1}

Pyridine

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Date: 3/91 by Jon Perry
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Note: The temperature range in which the vapor pressures (for Pyridine) were calculated (see previous page), exceed the limits in which the equation used to calculate the vapor pressures is valid. Upon plotting vapor pressure versus temperature over the temperature range of interest (288 °K – 348 °K), vapor pressure appears to approach zero at temperatures below 340 °K. See plot on following page.

Pyridine

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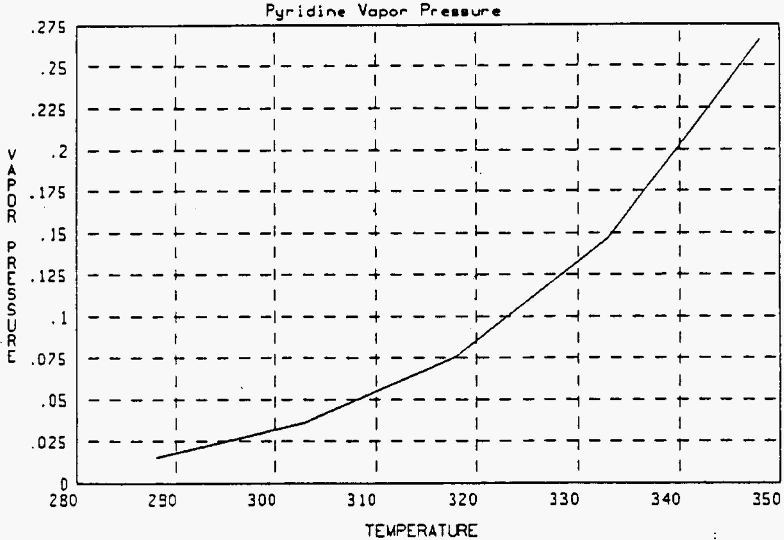
Title: Organic Emissions

Date: 3/91 by Jon Perry

Checked: 3/91 by WGRichwine



Pyridine

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$$y_i P_t = \gamma_i x_i p_i$$

x_i = mole fraction of component i (liquid phase)

y_i = vapor phase mol fraction of component i

P_t = System pressure (vapor phase)

γ_i = activity coeffecient (liquid phase) (component i)

p_i = vapor pressure of pure component at system temp.

$$y_1 = \frac{\gamma_1 x_1 p_1}{P_t}$$

P_t = 750 mm Hg in C-100

$$\Rightarrow \left(750 \text{ mm Hg}\right)\left(\frac{1.01325 \text{ bars}}{760 \text{ mm Hg}}\right) = .9999 \text{ bars}$$

P_t = .9999 bars

Pyridine

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C-100 stream flow rate = 150 $\frac{ft^3}{min}$

C-100 pressure = 6" WG

$$\text{Emmissions} = \left(150\ \frac{ft^3}{min}\right)\left(28.317\ l/ft^3\right)\left(\frac{60\ min}{hr}\right)\left(\frac{750\ mm\ Hg}{760\ mm\ Hg}\right)\left(\frac{298}{T}\right)\left(\frac{1\ mol}{22.4\ l}\right)$$

$$\xrightarrow{\text{cont'd}}\left(\frac{79.102\ g}{mol}\right)\left(\frac{1\ lb}{454\ g}\right)\left(y_i\right) = \frac{\text{lbs of pyridine}}{hr}$$

Pyridine

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Title: Organic Emissions
Date: 3/91 by Jon Perry
Checked: 3/91 by WG Richard

Pyridine C-100 Emmissions (xl=ave)

T °K	Vl L	pl bars	xl mF	yl mF	Emmissions lbs/hr
2.88E2	6.104E0	1.556E-2	1.15E-7	1.093E-8	2.211E-5
3.03E2	7.505E0	3.594E-2	1.15E-7	3.102E-8	5.968E-5
3.18E2	8.888E0	7.554E-2	1.15E-7	7.722E-8	1.416E-4
3.33E2	1.022E1	1.466E-1	1.15E-7	1.724E-7	3.018E-4
3.48E2	1.149E1	2.66E-1	1.15E-7	3.514E-7	5.886E-4

Pyridine C-100 Emmissions (xl=max)

T °K	Vl L	pl bars	xl mF	yl mF	Emmissions lbs/hr
2.88E2	6.104E0	1.556E-2	1.25E-7	1.188E-8	2.404E-5
3.03E2	7.505E0	3.594E-2	1.25E-7	3.371E-8	6.487E-5
3.18E2	8.888E0	7.554E-2	1.25E-7	8.394E-8	1.539E-4
3.33E2	1.022E1	1.466E-1	1.25E-7	1.874E-7	3.281E-4
3.48E2	1.149E1	2.66E-1	1.25E-7	3.819E-7	6.398E-4

Pyridine C-100 Emmissions (xl=max10)

T °K	Vl L	pl bars	xl mF	yl mF	Emmissions lbs/hr
2.88E2	6.104E0	1.556E-2	1.253E-6	1.19E-7	2.41E-4
3.03E2	7.505E0	3.594E-2	1.253E-6	3.38E-7	6.502E-4
3.18E2	8.888E0	7.554E-2	1.253E-6	8.414E-7	1.542E-3
3.33E2	1.022E1	1.466E-1	1.253E-6	1.879E-6	3.289E-3
3.48E2	1.149E1	2.66E-1	1.253E-6	3.829E-6	6.413E-3

Pyridine

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Title: Organic Emissions

Date: 3/91 by Dn Perry

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The process condensate emmission results at 75 °C = 348 °K, can be used to determine the feed concentration limit. The feed concentration limit is the concentration of volatile constituent in the feed stream, with the assumption that the volatile constituent is completely transferred into the condensate, which will produce 0.71 lbs/hr (.322 kg/hr) emissions of Pyridine from the process condensate. The feed concentration limit is calculated as follows:

$$\left(\frac{5.50\times10^{3}}{}\ \mu g/l\right)\left(\frac{1\ mg}{1000\ \mu g}\right)\left(\frac{1\ hr.}{6.413\times10^{-3}\ lbs}\right)\left(\frac{.71\ lbs}{1\ hr}\right)\left(\frac{R-1}{R}\right)$$

$$= 609\ \left(\frac{R-1}{R}\right)\ mg/l$$

note: R = Feed rate ÷ product rate

-- Pyridine

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Title: Organic Removal

Date: 3/91 by D. Perry

Checked: 3/91 by W. Richard

Determination of maximum feed concentration:

$$R \cdot C_f + (1-R)\,C_c = C_s$$

R = Ratio of Feed to product Mass Ratio

C_f = Feed Concentration

C_s = Concentration of a given component in Slurry

Note: To determine the maximum Feed concentration (C_f) of a given component, (C_s) will be the regulatory limit (HBL or LDR).

C_c = Condensate Concentration of a given component

Note: C_c is calculated from the vapor phase mol fraction for a given component in the slurry.

Pyridine

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C_c is calculated by converting y_i (mol fraction) to y_i (ppm)

$$y_i(MF) = \frac{\text{moles } i}{\text{moles } i + \text{moles } H_2O}$$

In this calculation, the mole contribution of component i is insignificant relative to the mole contribution of H_2O. Therefore,

$$\left(\frac{\text{mol. } i}{\underset{\text{insignificant}}{\cancel{\text{mol } i}} + \text{mol } H_2O}\right)\left(\frac{55.5093 \text{ mol } H_2O}{1\,\ell}\right)(\text{molec. wt})\left(\frac{1000 \text{ mg}}{g}\right)$$

$$= \text{mg}/\ell = \text{mg}/\text{Kg} = \text{ppm}$$

Pyridine

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ok Pyridine Slurry Vapor Phase Mole Fraction

T °K	V1 l	p1 bars	x1 mf	Pt bars	y1 mf
2.98E2	7.038E0	2.75E-2	7.5E-8	3.143E-2	4.617E-7
3.03E2	7.505E0	3.594E-2	7.5E-8	4.212E-2	4.802E-7
3.08E2	7.969E0	4.648E-2	7.5E-8	5.584E-2	4.976E-7
3.13E2	8.431E0	5.954E-2	7.5E-8	7.327E-2	5.138E-7
3.18E2	8.888E0	7.554E-2	7.5E-8	9.521E-2	5.289E-7
3.23E2	9.339E0	9.502E-2	7.5E-8	1.226E-1	5.429E-7
3.28E2	9.784E0	1.185E-1	7.5E-8	1.565E-1	5.558E-7
3.33E2	1.022E1	1.466E-1	7.5E-8	1.98E-1	5.678E-7
3.38E2	1.065E1	1.801E-1	7.5E-8	2.487E-1	5.787E-7
3.43E2	1.107E1	2.196E-1	7.5E-8	3.099E-1	5.886E-7
3.48E2	1.149E1	2.66E-1	7.5E-8	3.834E-1	5.977E-7

ok Pyridine Slurry Limits (mg/l)

T	y1 mf	Cc mg/l	LDR mg/l
2.98E2	4.617E-7	2.027E0	3.3E-1
3.03E2	4.802E-7	2.109E0	3.3E-1
3.08E2	4.976E-7	2.185E0	3.3E-1
3.13E2	5.138E-7	2.256E0	3.3E-1
3.18E2	5.289E-7	2.322E0	3.3E-1
3.23E2	5.429E-7	2.384E0	3.3E-1
3.28E2	5.558E-7	2.441E0	3.3E-1
3.33E2	5.678E-7	2.493E0	3.3E-1
3.38E2	5.787E-7	2.541E0	3.3E-1
3.43E2	5.886E-7	2.585E0	3.3E-1
3.48E2	5.977E-7	2.625E0	3.3E-1

$$C_f = \left(\frac{R-1}{R} + \frac{C_s}{R} \right) C_c$$

Tetrahydrofuran

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Job No. 89-5010-ES Client/Project WHC/242-A

Title: Organic Emmissions

Date: 2/91 by Jon Perry

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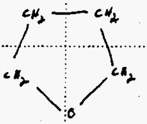
1.) Let 1 be Tetrahydrofuran (THF) and 2 be H_2O.

THF

$$\log \gamma_1^{\infty} = \alpha + \epsilon N_1 + \zeta\left(\frac{1}{N_1'} + \frac{1}{N_1''}\right) + \eta\left(N_1 - N_2\right)^2$$ Ref. C 295 b



= THF

$N_1 = 4$
$N_2 = 0$
$N_1' = 2$
$N_1'' = 2$

°K	α	ϵ	ζ	η	θ
293	-.770	.640	.195	0	—

$$\log \gamma_1^{\infty} = \alpha + 4\epsilon + \zeta$$

N_1 and N_2 = Total # of carbon atoms in respective molecules.

N', N'', N''' = The # of carbon atoms in respective branches of the indicated molecule

Note: Values for α, ϵ, and ζ are given at one temperature only (293° K). The values for α, ϵ, and ζ at 293 °K will be used at other temperatures to calculate γ_1^{∞}.

Tetrahydrofuran

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Title: Organic Emmissions
Date: 2/91 by Jon Perry
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Because of difficulty in locating data which sufficiently describes H_2O at infinite dilution (γ_2^∞) in an Ether solution, (γ_2^∞) was not calculated. Instead, Λ_{21} was set $= 1$ and Λ_{12} was calculated by equation #2. The influence of setting $\Lambda_{21} = 1$ on γ_1 and γ_2 at the variable ranges being used for x_1, x_2, T_1, T_2, Λ_{12}, and Λ_{21} were shown (see below) to be insignificant.

Note: γ_1 and γ_2 are essentially uneffected by a range of Λ_{21} values ranging from $\Lambda_{21} = .1$ to $\Lambda_{21} = 1.3$ for both the minimum and maximum values of x_1, x_2, T_1, and T_2 incountered in these calculations.

✓ Tetrahydrofuran Test (A21=1.3) (x1=1.1E-8)

T	A21 Λ_{21}	x1	v1 γ_1	v2 γ_2
2.88E2	1.3E0	1.1E-8	9.66E1	1E0
3.03E2	1.3E0	1.1E-8	9.66E1	1E0
3.18E2	1.3E0	1.1E-8	9.66E1	1E0
3.33E2	1.3E0	1.1E-8	9.66E1	1E0
3.48E2	1.3E0	1.1E-8	9.66E1	1E0

✓ Tetrahydrofuran Test (A21=.1) (x1=1.1E-8)

T	A21 Λ_{21}	x1	v1 γ_1	v2 γ_2
2.88E2	1E-1	1.1E-8	9.661E1	1E0
3.03E2	1E-1	1.1E-8	9.661E1	1E0
3.18E2	1E-1	1.1E-8	9.661E1	1E0
3.33E2	1E-1	1.1E-8	9.661E1	1E0
3.48E2	1E-1	1.1E-8	9.661E1	1E0

Tetrahydrofuran

Westinghouse Environmental & Geotechnical Services, Inc.

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Title: Organic Emmissions

Date: 2/91 by Jon Perry

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$A_{21} = 1.3$ $x_1 = 4.25 \times 10^{-7}$

T °K	A21 A_{21}	x1	v1 γ_1	v2 γ_2
2.88E2	1.3E0	4.25E-7	9.659E1	1E0
3.03E2	1.3E0	4.25E-7	9.659E1	1E0
3.18E2	1.3E0	4.25E-7	9.659E1	1E0
3.33E2	1.3E0	4.25E-7	9.659E1	1E0
3.48E2	1.3E0	4.25E-7	9.659E1	1E0

Tetrahydrofuran Test (A21=.1) (x1=4.25E-7)

T °K	A21 A_{21}	x1	v1 γ_1	v2 γ_2
2.88E2	1E-1	4.25E-7	9.66E1	1E0
3.03E2	1E-1	4.25E-7	9.66E1	1E0
3.18E2	1E-1	4.25E-7	9.66E1	1E0
3.33E2	1E-1	4.25E-7	9.66E1	1E0
3.48E2	1E-1	4.25E-7	9.66E1	1E0

Tetrahydrofuran

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2.)

$$\ln \gamma_1^\infty = -\ln(\Lambda_{12}) - \Lambda_{21} + 1$$ Ref. C 8-10.25

T (°K)	Λ_{12} ($\times 10^{-2}$)	Λ_{21}
288	1.035	1
303	1.035	1
318	1.035	1
333	1.035	1
348	1.035	1

Tetrahydrofuran

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$$\ln(P_1) = (VPA) - \frac{(VPB)}{T + (VPC)}$$

Ref. D App A eqn #3

$VPA = 9.4867$ $VPB = 2768.38$ $VPC = -46.9$

Valid from 270 °K to 370 °K

$$\ln\left(\frac{P_2}{P_c}\right) = (1-X)^{-1}\left[(VPA)X + (VPB)X^{1.5} + (VPC)X^3 + (VPD)X^6\right]$$

Ref. D App A eqn. #1

$$X = 1 - T/T_c$$

$T_c = 647.3$ $P_c = 221.2$ $VPA = -7.76451$

$VPB = 1.45838$ $VPC = -2.7758$ $VPD = -1.23303$

Valid from 275 °K to 647.3 °K

°K	P_1 (bars)	P_2 (bars)
288	1.359×10^{-1}	1.69×10^{-2}
303	2.663×10^{-1}	4.212×10^{-2}
318	4.843×10^{-1}	9.521×10^{-2}
333	8.273×10^{-1}	1.98×10^{-1}
348	1.34×10^{0}	3.834×10^{-1}

Tetrahydrofuran

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$y_i P_t = \gamma_i x_i p_i$

x_i = mole fraction of component i liquid phase
y_i = vapor phase mol fraction of component i
P_t = System pressure (vapor phase)
γ_i = activity coeffecient (liquid phase) (component i)
p_i = vapor pressure of pure component at system temp.

$$y_1 = \frac{\gamma_1 x_1 p_1}{P_t}$$

P_t = 750 mm Hg in C-100

$$\Rightarrow \left(750 \text{ mm Hg}\right)\left(\frac{1.01325 \text{ bars}}{760 \text{ mm Hg}}\right) = .9999 \text{ bars}$$

P_t = .9999 bars

Tetrahydrofuran

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C-100 stream flow rate = 150 $\frac{ft^3}{min}$

C-100 pressure = 6" WG

$$\text{Emmissions} = \left(150\ \frac{ft^3}{min}\right)\left(28.317\ \frac{\ell}{ft^3}\right)\left(\frac{60\ min}{hr}\right)\left(\frac{750\ mm\,Hg}{760\ mm\,Hg}\right)\left(\frac{298}{T}\right)\left(\frac{1\ mol}{22.4\ \ell}\right)$$

$$\xrightarrow{\text{cont'd}} \left(\frac{72.107\ g}{mol}\right)\left(\frac{1\ lb}{454\ g}\right)\left(y_i\right) = \frac{\text{lbs of (THF)}}{hr}$$

Tetrahydrofuran

Westinghouse Environmental & Geotechnical Services, Inc.

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Title: Organic Emmissions

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Tetrahydrofuran C-100 Emmissions (x1=ave)

T °K	v1 g/l	p1 bars	x1 mf	y1 mf	Emmissions lbs/hr
2.88E2	9.66E1	1.359E-1	1.1E-8	1.445E-7	2.666E-4
3.03E2	9.66E1	2.663E-1	1.1E-8	2.83E-7	4.964E-4
3.18E2	9.66E1	4.843E-1	1.1E-8	5.147E-7	8.602E-4
3.33E2	9.66E1	8.273E-1	1.1E-8	8.792E-7	1.403E-3
3.48E2	9.66E1	1.34E0	1.1E-8	1.424E-6	2.174E-3

Tetrahydrofuran C-100 Emmissions (x1=max)

T °K	v1 g/l	p1 bars	x1 mf	y1 mf	Emmissions lbs/hr
2.88E2	9.66E1	1.359E-1	4.2E-8	5.516E-7	1.018E-3
3.03E2	9.66E1	2.663E-1	4.2E-8	1.081E-6	1.895E-3
3.18E2	9.66E1	4.843E-1	4.2E-8	1.965E-6	3.284E-3
3.33E2	9.66E1	8.273E-1	4.2E-8	3.357E-6	5.357E-3
3.48E2	9.66E1	1.34E0	4.2E-8	5.436E-6	8.302E-3

Tetrahydrofuran C-100 Emmissions (x1=max10)

T °K	v1 g/l	p1 bars	x1 mf	y1 mf	Emmissions lbs/hr
2.88E2	9.66E1	1.359E-1	4.25E-7	5.581E-6	1.03E-2
3.03E2	9.66E1	2.663E-1	4.25E-7	1.093E-5	1.918E-2
3.18E2	9.66E1	4.843E-1	4.25E-7	1.989E-5	3.323E-2
3.33E2	9.66E1	8.273E-1	4.25E-7	3.397E-5	5.421E-2
3.48E2	9.66E1	1.34E0	4.25E-7	5.501E-5	8.4E-2

Tetrahydrofuran

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The process condensate emmission results at 75 °C = 348 °K, can be used to determine the feed concentration limit. The feed concentration limit is the concentration of volatile constituent in the feed stream, with the assumption that the volatile constituent is completely transferred into the condensate, which will produce 0.71 lbs/hr (.322 kg/hr) emmissions of tetrahydrofuran from the process condensate. The feed concentration limit is calculated as follows:

$$\left(\frac{1.70\times10^{3}}{}\ \mu g/l\right)\left(\frac{1\ mg}{1000\ \mu g}\right)\left(\frac{1\ \ hr.}{8.4\times10^{-2}\ \ lbs}\right)\left(\frac{.71\ lbs}{1\ hr}\right)\left(\frac{R-1}{R}\right)$$

$$= 14.37\left(\frac{R-1}{R}\right) \Longrightarrow mg/l$$

note: R = Feed rate ÷ product rate

Tetrahydrofuran

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Determination of maximum feed concentration:

$$R\,C_f + (1-R)\,C_c = C_s$$

R = Ratio of Feed to product Mass Ratio

C_f = Feed Concentration

C_s = Concentration of a given component in Slurry

Note: To determine the maximum feed concentration (C_f) of a given component, (C_s) will be the regulatory limit (HBL or LDR).

C_c = Condensate Concentration of a given component

Note: C_c is calculated from the vapor phase mol fraction for a given component in the slurry.

Tetrahydrofuran

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C_c is calculated by converting y_i (mol fraction) to y_i (ppm)

$$y_i(MF) = \frac{\text{moles } i}{\text{moles } i + \text{moles } H_2O}$$

In this calculation, the mole contribution of component i is insignificant relative to the mole contribution of H_2O. Therefore,

$$\left(\frac{\text{mol } i}{\cancel{\text{mol } i} + \text{mol } H_2O}\right)\left(\frac{55.5093 \text{ mol } H_2O}{1 \ell}\right)\left(\text{molec. wt}\right)\left(\frac{1000 \text{ mg}}{g}\right)$$

insignificant

$$= \text{mg}/\ell = \text{mg}/\text{Kg} = \text{ppm}$$

Tetrahydrofuran

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Job No. 89-5010-ES Client/Project WHC/242-A

Title: Organic Removal

Date: 2/91 by Jon Perry

Checked: 3/91 by WEPritchard

°K Tetrahydrofuran Slurry Vapor phase Mole Fraction

T °K	vl γ_1	pl bars	xl mf	Pt bars	yl mf
2.98E2	9.66E1	2.147E-1	2.5E-7	3.144E-2	1.65E-4
3.03E2	9.66E1	2.663E-1	2.5E-7	4.213E-2	1.527E-4
3.08E2	9.66E1	3.276E-1	2.5E-7	5.585E-2	1.417E-4
3.13E2	9.66E1	3.998E-1	2.5E-7	7.328E-2	1.318E-4
3.18E2	9.66E1	4.843E-1	2.5E-7	9.523E-2	1.228E-4
3.23E2	9.66E1	5.827E-1	2.5E-7	1.226E-1	1.148E-4
3.28E2	9.66E1	6.965E-1	2.5E-7	1.565E-1	1.075E-4
3.33E2	9.66E1	8.273E-1	2.5E-7	1.98E-1	1.009E-4
3.38E2	9.66E1	9.769E-1	2.5E-7	2.487E-1	9.487E-5
3.43E2	9.66E1	1.147E0	2.5E-7	3.099E-1	8.939E-5
3.48E2	9.66E1	1.34E0	2.5E-7	3.834E-1	8.439E-5

°K Tetrahydrofuran Slurry Limits (mg/l)

T °K	yl mf	Cc g/l	HBL mg/l
2.98E2	1.65E-4	6.603E2	1E0
3.03E2	1.527E-4	6.111E2	1E0
3.08E2	1.417E-4	5.67E2	1E0
3.13E2	1.318E-4	5.273E2	1E0
3.18E2	1.228E-4	4.917E2	1E0
3.23E2	1.148E-4	4.594E2	1E0
3.28E2	1.075E-4	4.303E2	1E0
3.33E2	1.009E-4	4.038E2	1E0
3.38E2	9.487E-5	3.797E2	1E0
3.43E2	8.939E-5	3.578E2	1E0
3.48E2	8.439E-5	3.378E2	1E0

$$C_f = \left(\frac{R-1}{R} + \frac{C_s}{R}\right) C_c$$

Tetradecane

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Job No. 89-5010-ES Client/Project WHC/242-A

Title: Organic Emissions

Date: 3/91 by Jon Perry

Checked: 3/91 by

Because tetradecane is essentially insoluble in water, the organic emissions for tetradecane can be most accurately calculated by treating water and tetradecane as a non-interacting mixture. This is accomplished by setting the activity coefficients of both water and tetradecane equal to one.

$\gamma_1 = 1$

$\gamma_2 = 1$

1 → tetradecane

2 → H_2O

Tetradecane

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Job No. 89-5010-ES Client/Project WHC/242-A

Title: Organic Emmissions

Date: 3/91 by Jon Perry

Checked: 3/91 by

Y_1 and Y_2 = mole fractions of respective molecules.

mole Fraction is calculated from the ppb concentration (obtained from stream specific report App. 3A)

ex) 9.11×10^1 ppb $= \dfrac{9.11 \times 10^1 \text{ mg}}{1 \text{ litre}} = \dfrac{9.11 \times 10^{-5} \text{ g}}{1000 \text{ g}} = \dfrac{4.59 \times 10^{-7} \text{ moles tetradecane}}{9.11 \times 10^{-5} \text{ g}_{\text{tetradecane}} + 999.999 \text{ g}_{H_2O}}$

$= \dfrac{4.59 \times 10^{-7} \text{ moles tetradecane}}{4.59 \times 10^{-7} \text{ moles}_{\text{tetradecane}} + 55.5093 \text{ moles } H_2O} = 8 \times 10^{-9}$ MF tetradecane

Tetradecane

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Title: Organic Emissions
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Checked: 3/91 by W. Rushmid

The Clausius - Clapeyron Equation can be used to estimate the vapor pressure.

$$\ln(P_1) = -\frac{\Delta\hat{H}_v}{RT} + B$$ Ref. E pp. 209

P_1 = Vapor pressure of pure substance

R = Gas Constant

B = A constant which varies from one substance to another

$\Delta\hat{H}_v$ = Latent heat of vaporization (or the energy required to vaporize one mole of liquid)

T = Absolute temperature

Ref. E = R.M. Felder and R.W. Roussea, "Elementary Principles of Chemical Processes," John Wiley & Sons, New York, 1978.

Note: A linear relationship between $\ln(P)$ and $\frac{1}{T}$ exists, therefore, if at least two data points for P and T are known, an equation which describes P at various temperatures can be determined.

The following data points for pressure and temperature were taken from:

"CRC Handbook of Chemistry and Physics, 60th Edition, 2nd Printing, CRC Press, Inc., Boca, Florida, 1980, pp D208.

Tetradecane

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Title: Organic Emissions

Date: 3/91 by J. Perry

Checked: 3/91 by W. Richard

Temp.(C)	T(K)	P(mmHg)	1/T	LN(P)
76.4	349.55	1	2.861E-03	0.000E+00
120.7	393.85	10	2.539E-03	2.303E+00
152.7	425.85	40	2.348E-03	3.689E+00
178.5	451.65	100	2.214E-03	4.605E+00
226.8	499.95	400	2.000E-03	5.991E+00
252.5	525.65	760	1.902E-03	6.633E+00

y intercept = 19.87

slope = −6922.47

Clausius Clapeyron Eqn:

$$\ln(P_1) = \frac{-6922.47}{T} + 19.87$$

T(°K)	P_1 (bars)
288	2.061×10^{-5}
303	6.776×10^{-5}
318	1.991×10^{-4}
333	5.307×10^{-4}
348	1.3×10^{-3}

Tetradecane

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Title: Organic Emissions

Date: 3/91 by J. Perry

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$$\ln\left(\frac{P_2}{P_c}\right) = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^{3} + (VPD)x^{6}\right]$$

Ref. D

eqn. #1

$$x = 1 - T/T_c$$

$T_c = 647.3$ $P_c = 221.2$ $VPA = -7.76451$

$VPB = 1.45838$ $VPC = -2.7758$ $VPD = -1.23303$

Valid from 275 °K to 647.3 °K

T (K)	P_2 (bars)
288	1.69×10^{-2}
303	4.212×10^{-2}
318	9.521×10^{-2}
333	1.98×10^{-1}
348	3.834×10^{-1}

Tetradecane

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$$y_i P_t = \gamma_i x_i p_i$$

x_i = mol fraction of component i in liquid phase
y_i = vapor phase mol fraction of component i
P_t = System pressure (vapor phase)
γ_i = activity coeffecient (liquid phase) (component i)
p_i = vapor pressure of pure component at system temp.

$$y_1 = \frac{\gamma_1 x_1 p_1}{P_t}$$

P_t = 750 mm Hg in C-100

$$\Rightarrow (750 \text{ mm Hg})\left(\frac{1.01325 \text{ bars}}{760 \text{ mm Hg}}\right) = .9999 \text{ bars}$$

P_t = .9999 bars

Tetradecane

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Checked:	3/91 by WBHildebrand

C-100 stream flow rate = 150 $\frac{ft^3}{min}$

C-100 pressure = 6" WG

$$\text{Emmissions} = \left(150\ \frac{ft^3}{min}\right)\left(28.317\ \frac{l}{ft^3}\right)\left(\frac{60\ min}{hr}\right)\left(\frac{750\ mm\ Hg}{760\ mm\ Hg}\right)\left(\frac{298}{T}\right)\left(\frac{1\ mol}{22.4\ l}\right)$$

$$\underset{\longrightarrow}{\text{cont'd}}\ \left(\frac{198.394\ g}{mol}\right)\left(\frac{1\ lb}{454\ g}\right)\left(y_i\right) = \frac{\text{lbs of tetradecane}}{hr}$$

Tetradecane

Westinghouse Environmental & Geotechnical Services, Inc.

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Job No. 89-5010-ES Client/Project WHC 1242-A

Title: Organic Emissions

Date: 3/91 by Jim Perry

Checked: 3/91 by

Tetradecane C-100 Emmissions (xl=ave)

T °K	vl	pl bars	xl mf	yl mf	Emmissions lb/hr
2.88E2	1E0	2.061E-5	8E-9	1.649E-13	8.373E-10
3.03E2	1E0	6.776E-5	8E-9	5.421E-13	2.616E-9
3.18E2	1E0	1.991E-4	8E-9	1.593E-12	7.322E-9
3.33E2	1E0	5.307E-4	8E-9	4.246E-12	1.864E-8
3.48E2	1E0	1.3E-3	8E-9	1.04E-11	4.37E-8

Tetradecane C-100 Emmissions (xl=max)

T °K	vl	pl bars	xl mf	yl mf	Emmissions lbs/hr
2.88E2	1E0	2.061E-5	4E-8	8.247E-13	4.187E-9
3.03E2	1E0	6.776E-5	4E-8	2.711E-12	1.308E-8
3.18E2	1E0	1.991E-4	4E-8	7.963E-12	3.661E-8
3.33E2	1E0	5.307E-4	4E-8	2.123E-11	9.321E-8
3.48E2	1E0	1.3E-3	4E-8	5.201E-11	2.185E-7

Tetradecane C-100 Emmissions (xl=max10)

T °K	vl	pl bars	xl mf	yl mf	Emmissions lbs/hr
2.88E2	1E0	2.061E-5	4E-7	8.247E-12	4.187E-8
3.03E2	1E0	6.776E-5	4E-7	2.711E-11	1.308E-7
3.18E2	1E0	1.991E-4	4E-7	7.963E-11	3.661E-7
3.33E2	1E0	5.307E-4	4E-7	2.123E-10	9.321E-7
3.48E2	1E0	1.3E-3	4E-7	5.201E-10	2.185E-6

Tetradecane

Westinghouse Environmental & Geotechnical Services, Inc.

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Job No. 89-5010-ES Client/Project WHC /242-A
Title: Organic Emissions
Date: 3/91 by Jon Perry
Checked: 3/91 by

The process condensate emmission results at 75°C = 348°K, can be used to determine the feed concentration limit. The feed concentration limit is the concentration of volatile constituent in the feed stream, with the assumption that the volatile constituent is completely transferred into the condensate, which will produce 0.71 lbs/hr (.322 kg/hr) emmissions of Tetradecane from the process condensate. The feed concentration limit is calculated as follows:

$$\left(\frac{4.40\times10^{3}}{} \mu g/l\right)\left(\frac{1 \text{ mg}}{1000\ \mu g}\right)\left(\frac{1 \text{ hr.}}{2.185\times10^{-6} \text{ lbs}}\right)\left(\frac{.71 \text{ lbs}}{1 \text{ hr}}\right)\left(\frac{R-1}{R}\right)$$

$$= 1.430\times10^{6}\left(\frac{R-1}{R}\right) \text{ mg/l}$$

note: R = feed rate ÷ product rate

Tetradecane

Westinghouse Environmental & Geotechnical Services, Inc.

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Job No. 89-5010-ES Client/Project WHC/242-A

Title: Organic Removal

Date: 3/91 by Jon Perry

Checked: 3/91 by

Determination of maximum feed concentration:

$$R\,C_f + (1-R)\,C_c = C_s$$

R = Ratio of feed to product Mass Ratio

C_f = Feed Concentration

C_s = Concentration of a given component in Slurry

Note: To determine the maximum feed concentration (C_f) of a given component, (C_s) will be the regulatory limit (HBL or LDR).

C_c = Condensate Concentration of a given component

Note: C_c is calculated from the vapor phase mol fraction for a given component in the slurry.

Tetradecane

Westinghouse Environmental & Geotechnical Services, Inc.

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Job No. 89-5010-ES Client/Project WHC/242-A

Title: Organic Removal

Date: 3/91 by J. Perry

Checked: 3/91 by WB Richard

C_c is calculated by converting y_i (mol fraction) to y_i (ppm)

$$y_i(MF) = \frac{\text{moles } i}{\text{moles } i + \text{moles } H_2O}$$

In this calculation, the mole contribution of component i is insignificant relative to the mole contribution of H_2O. Therefore,

$$\left(\frac{\text{mol } i}{\cancel{\text{mol } i} + \text{mol } H_2O}\right)\left(\frac{55.5093 \text{ mol } H_2O}{1\,l}\right)(\text{molec. wt})\left(\frac{1000 \text{ mg}}{g}\right)$$

insignificant

$$= \text{mg}/l = \text{mg}/\text{Kg} = \text{ppm}$$

Tetradecane

Westinghouse Environmental & Geotechnical Services, Inc.

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Job No. 89-5010-ES Client/Project WHC/242-A

Title: Organic Removal

Date: 3/91 by J. Perry

Checked: 3/91 by WG Richmond

Tetradecane Slurry Vapor Phase mole fraction

T °K	vl	pl bars	xl MF	Pt bars	yl MF
2.98E2	1E0	4.618E-5	9.1E-8	3.143E-2	1.337E-10
3.03E2	1E0	6.776E-5	9.1E-8	4.212E-2	1.464E-10
3.08E2	1E0	9.818E-5	9.1E-8	5.584E-2	1.6E-10
3.13E2	1E0	1.406E-4	9.1E-8	7.327E-2	1.746E-10
3.18E2	1E0	1.991E-4	9.1E-8	9.521E-2	1.902E-10
3.23E2	1E0	2.788E-4	9.1E-8	1.226E-1	2.07E-10
3.28E2	1E0	3.866E-4	9.1E-8	1.565E-1	2.248E-10
3.33E2	1E0	5.307E-4	9.1E-8	1.98E-1	2.439E-10
3.38E2	1E0	7.217E-4	9.1E-8	2.487E-1	2.641E-10
3.43E2	1E0	9.728E-4	9.1E-8	3.099E-1	2.857E-10
3.48E2	1E0	1.3E-3	9.1E-8	3.834E-1	3.086E-10

Tetradecane Slurry Limits (mg/l)

T °K	yl MF	Cc mg/l	HBL mg/l
2.98E2	1.337E-10	1.472E-3	1E0
3.03E2	1.464E-10	1.612E-3	1E0
3.08E2	1.6E-10	1.762E-3	1E0
3.13E2	1.746E-10	1.923E-3	1E0
3.18E2	1.902E-10	2.095E-3	1E0
3.23E2	2.07E-10	2.279E-3	1E0
3.28E2	2.248E-10	2.476E-3	1E0
3.33E2	2.439E-10	2.686E-3	1E0
3.38E2	2.641E-10	2.909E-3	1E0
3.43E2	2.857E-10	3.146E-3	1E0
3.48E2	3.086E-10	3.399E-3	1E0

$$C_f = \left(\frac{R-1}{R} + \frac{C_s}{R}\right) C_c$$

Tributyl Phosphate

Westinghouse Environmental & Geotechnical Services, Inc.

DESIGN ANALYSIS

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Job No. 89-5010-ES Client/Project WHC/242-A
Title: Organic Emissions
Date: 3/91 by Jon Perry
Checked: 3/91 by

Because tributyl phosphate is essentially insoluble in water, the organic emissions for tributyl phosphate can be most accurately calculated by treating water and tributyl phosphate as a non-interacting mixture. This is accomplished by setting the activity coefficients of both water and ~~tribtyl~~ tributyl phosphate equal to one.

$$\gamma_1 = 1$$

$$\gamma_2 = 1$$

1 → tributyl phosphate (TBP)

2 → H_2O

Tributyl Phosphate

Westinghouse Environmental & Geotechnical Services, Inc.

DESIGN ANALYSIS

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Job No. 89-5010-ES Client/Project WHC/242-A

Title: Organic Emission

Date: 3/91 by Jon Petty

Checked: 3/9 by WGKirchand

X_1 and X_2 = mole fractions of respective molecules

Mole Fraction is calculated from the ppb concentration (obtained from the stream specific report App 3A).

ex.) 3.620×10^{3} ppb $= \dfrac{3.62 \times 10^{-3} \text{ g TBP}}{1 \ell} = \dfrac{1.359 \times 10^{-5} \text{ moles TBP}}{1000 \text{ g TBP} + H_2O} =$

$$= \frac{1.359 \times 10^{-5} \text{ moles TBP}}{3.62 \times 10^{-3} \text{ g TBP} + 999.996 \text{ g } H_2O} = \frac{1.359 \times 10^{-5} \text{ moles TBP}}{1.359 \times 10^{-5} \frac{\text{moles}}{\text{TBP}} + 55.5091 \frac{\text{moles}}{H_2O}} = 2.45 \times 10^{-7} \frac{\text{mf}}{\text{TBP}}$$

TBP MW = 266.36

H_2O MW = 18.015

Tributyl Phosphate

Westinghouse Environmental & Geotechnical Services, Inc.

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An equation describing the vapor pressure of TBP at various temperatures is given in reference G equation (3).

$$\ln(P_1) = -\frac{7735}{T} + 20.53$$

P_1 => bars

T => °K

T °K	P_1 (bars)
288	1.786×10^{-3}
303	6.751×10^{-3}
318	2.251×10^{-2}
333	6.732×10^{-2}
348	1.832×10^{-1}

Tributyl Phosphate

Westinghouse Environmental & Geotechnical Services, Inc.

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$$\ln\left(\frac{P_2}{P_c}\right) = (1-x)^{-1}\left[(VPA)x + (VPB)x^{1.5} + (VPC)x^{3} + (VPD)x^{6}\right]$$ Ref D eqn. #1

$T_c = 647.3$
$VPB = 1.45838$

$P_c = 221,2$
$VPC = -2,7758$

$VPA = -7.76451$
$VPD = -1.23303$

$$x = 1 - T/T_c$$

Valid from 275°K to 647.3°K

T (°K)	P_2 (bars)
288	1.69×10^{-2}
303	4.212×10^{-2}
318	$9,521 \times 10^{-2}$
333	$1,98 \times 10^{-1}$
348	$3,834 \times 10^{-1}$

Tributyl Phosphate

Westinghouse Environmental & Geotechnical Services, Inc.

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Title: Organic Emissions

Date: 3/91 by J. Perry

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$$y_i P_t = \gamma_i x_i p_i$$

x_i = mol fraction of component i in liquid phase

y_i = vapor phase mol fraction of component i

P_t = system pressure (vapor phase)

γ_i = activity coeffecient (liquid phase) (component i)

p_i = vapor pressure of pure component at system temp.

$$y_1 = \frac{\gamma_1 x_1 p_1}{P_t}$$

P_t = 750 mm Hg in C-100

$$\Rightarrow (750 \text{ mm Hg})\left(\frac{1.01325 \text{ bars}}{760 \text{ mm Hg}}\right) = .9999 \text{ bars}$$

P_t = .9999 bars

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Title: Organic Emissions

Date: 3/91 by J. Perry

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C-100 stream flow rate = 150 $\frac{ft^3}{min}$

C-100 pressure = 6" WG

$$\text{Emmissions} = \left(150\ \frac{ft^3}{min}\right)\left(28.317\ \frac{l}{ft^3}\right)\left(\frac{60\ min}{hr}\right)\left(\frac{750\ mm\ Hg}{760\ mm\ Hg}\right)\left(\frac{298}{T}\right)\left(\frac{1\ mol}{22.4\ l}\right)$$

$$\xrightarrow{\text{cont'd}} \left(\frac{266.36\ g}{mol}\right)\left(\frac{1\ lb}{454\ g}\right)\left(y_i\right) = \frac{\text{lbs of Tributyl Phosphate}}{hr}$$

Tributyl Phosphate

Westinghouse Environmental & Geotechnical Services, Inc.

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°K Tributyl Phosphate C-100 Emissions (xl=ave)

T °K	vl	pl bars	xl mF	yl mF	Emissions lbs/hr
2.88E2	1E0	1.786E-3	2.45E-7	4.377E-10	2.983E-6
3.03E2	1E0	6.751E-3	2.45E-7	1.654E-9	1.072E-5
3.18E2	1E0	2.251E-2	2.45E-7	5.515E-9	3.404E-5
3.33E2	1E0	6.732E-2	2.45E-7	1.65E-8	9.724E-5
3.48E2	1E0	1.832E-1	2.45E-7	4.49E-8	2.532E-4

°K Tributyl Phosphate C-100 Emissions (xl=max)

T °K	vl	pl bars	xl mF	yl mF	Emissions lbs/hr
2.88E2	1E0	1.786E-3	1.393E-6	2.488E-9	1.696E-5
3.03E2	1E0	6.751E-3	1.393E-6	9.405E-9	6.093E-5
3.18E2	1E0	2.251E-2	1.393E-6	3.136E-8	1.936E-4
3.33E2	1E0	6.732E-2	1.393E-6	9.379E-8	5.529E-4
3.48E2	1E0	1.832E-1	1.393E-6	2.553E-7	1.44E-3

°K Tributyl Phosphate C-100 Emissions (xl=max10)

T °K	vl	pl bars	xl mf	yl mf	Emissions lbs/hr
2.88E2	1E0	1.786E-3	1.394E-5	2.49E-8	1.697E-4
3.03E2	1E0	6.751E-3	1.394E-5	9.412E-8	6.098E-4
3.18E2	1E0	2.251E-2	1.394E-5	3.138E-7	1.937E-3
3.33E2	1E0	6.732E-2	1.394E-5	9.386E-7	5.533E-3
3.48E2	1E0	1.832E-1	1.394E-5	2.554E-6	1.441E-2

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The process condensate emmission results at 75°C = 348°K, can be used to determine the feed concentration limit. The feed concentration limit is the concentration of volatile constituent in the feed stream, with the assumption that the volatile constituent is completely transferred into the condensate, which will produce 0.71 lbs/hr (.322 kg/hr) emmissions of Tributyl Phosphate from the process condensate. The feed concentration limit is calculated as follows:

$$\left(\frac{2.06 \times 10^{5}}{} \ \mu g/l\right)\left(\frac{1\ mg}{1000\ \mu g}\right)\left(\frac{1\ hr.}{1.441 \times 10^{-2}\ lbs}\right)\left(\frac{.71\ lbs}{1\ hr}\right)\left(\frac{R-1}{R}\right)$$

$$= 1.01 \times 10^{4} \left(\frac{R-1}{R}\right) \ mg/l$$

note: R = feed rate ÷ product rate

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Title: Organic Removal

Date: 3/91 by J. Perry

Checked: 3/91 by

Determination of maximum feed concentration:

$$R C_f + (1 - R) C_c = C_s$$

R= Ratio of Feed to product Mass Ratio

C_f = Feed Concentration

C_s = Concentration of a given component in Slurry

Note: To determine the maximum Feed concentration (C_f) of a given component, (C_s) will be the regulatory limit (HBL or LDR).

C_c = Condensate Concentration of a given component

Note: C_c is calculated from the vapor phase mol fraction for a given component in the slurry.

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C_c is calculated by converting y_i (mol fraction) to y_i (ppm)

$$y_i(MF) = \frac{\text{moles } i}{\text{moles } i + \text{moles } H_2O}$$

In this calculation, the mole contribution of component i is insignificant relative to the mole contribution of H_2O. Therefore,

$$\left(\frac{\text{mol } i}{\underset{\text{insignificant}}{\cancel{\text{mol } i}} + \text{mol } H_2O}\right)\left(\frac{55.5093 \text{ mol } H_2O}{1 \ell}\right)(\text{molec. wt})\left(\frac{1000 \text{ mg}}{g}\right)$$

$$= \text{mg}/\ell = \text{mg}/\text{Kg} = \text{ppm}$$

Tributyl Phosphate

Westinghouse Environmental & Geotechnical Services, Inc.

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Job No. 89-5010-ES Client/Project WHC/242-A

Title: Organic Removal

Date: 3/91 by J. Perry

Checked: 3/91 by WHRichard

Tributyl Phosphate Slurry Vapor Phase Mole Fraction

T °K	vl	pl bars	xl mf	Pt bars	yl mf
2.98E2	1E0	4.399E-3	6.8E-8	3.143E-2	2.992E-10
3.03E2	1E0	6.751E-3	6.8E-8	4.212E-2	4.591E-10
3.08E2	1E0	1.022E-2	6.8E-8	5.584E-2	6.949E-10
3.13E2	1E0	1.526E-2	6.8E-8	7.327E-2	1.038E-9
3.18E2	1E0	2.251E-2	6.8E-8	9.521E-2	1.531E-9
3.23E2	1E0	3.28E-2	6.8E-8	1.226E-1	2.231E-9
3.28E2	1E0	4.725E-2	6.8E-8	1.565E-1	3.213E-9
3.33E2	1E0	6.732E-2	6.8E-8	1.98E-1	4.579E-9
3.38E2	1E0	9.493E-2	6.8E-8	2.487E-1	6.456E-9
3.43E2	1E0	1.325E-1	6.8E-8	3.099E-1	9.012E-9
3.48E2	1E0	1.832E-1	6.8E-8	3.834E-1	1.246E-8

Tributyl Phosphate Cf Based on Cc from slurry (mg/l)

T °K	yl mf	Cc g/l	HBL g/l
2.98E2	2.992E-10	4.423E-3	1E0
3.03E2	4.591E-10	6.788E-3	1E0
3.08E2	6.949E-10	1.027E-2	1E0
3.13E2	1.038E-9	1.535E-2	1E0
3.18E2	1.531E-9	2.263E-2	1E0
3.23E2	2.231E-9	3.298E-2	1E0
3.28E2	3.213E-9	4.751E-2	1E0
3.33E2	4.579E-9	6.77E-2	1E0
3.38E2	6.456E-9	9.545E-2	1E0
3.43E2	9.012E-9	1.333E-1	1E0
3.48E2	1.246E-8	1.842E-1	1E0

$$C_f = \left(\frac{R-1}{R} + \frac{C_s}{R} \right) C_c$$

Tridecane

Westinghouse Environmental & Geotechnical Services, Inc.

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Job No. 89-5010-ES Client/Project WHC/242-A

Title: Organic Emissions

Date: 3/91 by Jon Perry

Checked: 3/91 by WG Rich

Because tridecane is essentially insoluble in water, the organic emissions for tridecane can be most accurately calculated by treating water and tridecane as a non-interacting mixture. This is accomplished by setting the activity coefficients of both water and tridecane equal to one.

$$\gamma_1 = 1$$

$$\gamma_2 = 1$$

$1 \longrightarrow$ tridecane

$2 \longrightarrow H_2O$

Tridecane

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X_1 and X_2 = mole fractions of respective molecules.

Mole fraction is calculated from the ppb concentration (obtained from stream specific report App. 3A)

ex

$$8.62 \times 10^{1}\ ppb = \frac{8.62 \times 10^{1}\ \mu g}{litre} = \frac{4.68 \times 10^{-7}\ \text{moles of tridecane}}{1000 g}$$

$$= \frac{4.68 \times 10^{-7}\ \text{moles tridecane}}{8.62 \times 10^{-5}\ g\ \text{tridecane} + 999.999\ g\ H_2O} = \frac{4.68 \times 10^{-7}\ \text{moles tridecane}}{4.68 \times 10^{-7}\ \text{moles tridecane} + 55.5093\ \text{moles}\ H_2O} = 8 \times 10^{-9}\ \text{mf tridecane}$$

Tridecane

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The Claussius – Clapeyron Equation can be used to estimate the vapor pressure.

$$\ln(P_1) = \frac{-\Delta \hat{H}_v}{RT} + B \qquad \text{Ref. E pp 209}$$

P_1 = Vapor pressure of pure substance

R = Gas constant

B = A constant which varies from one substance to another

$\Delta \hat{H}_v$ = Latent heat of vaporization (or energy required to vaporize one mole of liquid)

T = Absolute temperature

Ref. E = R.M. Felder and R.W. Roussea, "Elementary Principles of Chemical Processes," John Wiley & Sons, New York, 1978.

Note: A linear relationship between $\ln(P)$ and $\frac{1}{T}$ exists, therefore, if at least two data points for P and T are known, an equation which describes P at various temperatures can be determined.

The following data points for pressure and temperature were taken from:

"CRC Handbook of Chemistry and Physics, 60th Edition, 2nd Printing, CRC Press, Inc., Boca, Florida, 1980, pp D 208.

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```
   T(C)       P(mmHg)       T(K)         1/T        LN(Pmm)
--------------------------------------------------------------
 5.940E+01   1.000E+00   3.326E+02   3.007E-03   0.000E+00
 1.040E+02   1.000E+01   3.772E+02   2.651E-03   2.303E+00
 1.377E+02   4.000E+01   4.109E+02   2.434E-03   3.689E+00
 1.625E+02   1.000E+02   4.357E+02   2.295E-03   4.605E+00
 2.094E+02   4.000E+02   4.826E+02   2.072E-03   5.991E+00
 2.340E+02   7.600E+02   5.072E+02   1.972E-03   6.633E+00

              Regression Output:
Constant                                  1.928E+01
Std Err of Y Est                          2.014E-02
R Squared                                 9.999E-01
No. of Observations                       6.000E+00
Degrees of Freedom                        4.000E+00

X Coefficient(s)        -6.406E+03
Std Err of Coef.         2.350E+01
```

$y_{int} = 19.28$

$\text{Slope} = -6406$

Claussius Clapeyron Eqn.

$$\ln(P_1) = -\frac{6406}{T} + 19.28$$

°K	P_1 bar
288	6.888×10^{-5}
303	2.071×10^{-4}
318	5.616×10^{-4}
333	1.391×10^{-3}
348	3.189×10^{-3}

Tridecane

Westinghouse Environmental & Geotechnical Services, Inc.

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$$\ln\left(\frac{P_2}{P_c}\right) = (1-X)^{-1}\left[(VPA)X + (VPB)X^{1.5} + (VPC)X^{3} + (VPD)X^{6}\right]$$ Ref D AH A eqn. #1

$X = 1 - T/T_c$

$T_c = 647.3$ $P_c = 221.2$ VPA = -7.76451

VPB = 1.45838 VPC = -2.7758 VPD = -1.23303

Valid From 275 °K to 647.3 °K

T (°K)	P_2 bars
288	1.69×10^{-2}
303	4.212×10^{-2}
318	9.521×10^{-2}
333	1.98×10^{-1}
348	3.834×10^{-1}

Tridecane

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$$y_i P_t = \gamma_i x_i p_i$$

x_i = mol fraction of component i (liquid phase)
y_i = vapor phase mol fraction of component i
P_t = System pressure (vapor phase)
γ_i = activity coeffecient (liquid phase) (component i)
p_i = vapor pressure of pure component at system temp.

$$y_1 = \frac{\gamma_1 x_1 p_1}{P_t}$$

P_t = 750 mm Hg in C-100

$$\Rightarrow (750 \text{ mm Hg})\left(\frac{1.01325 \text{ bars}}{760 \text{ mm Hg}}\right) = .9999 \text{ bars}$$

P_t = .9999 bars

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C-100 stream flow rate = 150 $\frac{ft^3}{min}$

C-100 pressure = 6" WG

$$\text{Emmissions} = \left(150\ \frac{ft^3}{min}\right)\left(28.317\ \frac{l}{ft^3}\right)\left(\frac{60\ min}{hr}\right)\left(\frac{750\ mm\ Hg}{760\ mm\ Hg}\right)\left(\frac{298}{T}\right)\left(\frac{1\ mol}{22.4\ l}\right)$$

$$\underset{\longrightarrow}{\text{cont'd}}\ \left(\frac{184.367\ g}{mol}\right)\left(\frac{1\ lb}{454\ g}\right)\left(y_i\right) = \frac{\text{lbs of tridecane}}{hr}$$

Tridecane

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Title: organic emissions
Date: 3/91 by J. Perry
Checked: 3/91 by W6 Richmond

°K Tridecane C-100 Emmissions (xl=ave)

T °K	vl	pl bars	xl MF	yl MF	Emmissions lbs/hr
2.88E2	1E0	6.888E-5	8E-9	5.511E-13	2.6E-9
3.03E2	1E0	2.071E-4	8E-9	1.657E-12	7.432E-9
3.18E2	1E0	5.616E-4	8E-9	4.493E-12	1.92E-8
3.33E2	1E0	1.391E-3	8E-9	1.113E-11	4.543E-8
3.48E2	1E0	3.189E-3	8E-9	2.551E-11	9.96E-8

°K Tridecane C-100 Emmissions (xl=max)

T °K	vl	pl bars	xl MF	yl MF	Emmissions lbs/hr
2.88E2	1E0	6.888E-5	3.4E-8	2.342E-12	1.105E-8
3.03E2	1E0	2.071E-4	3.4E-8	7.044E-12	3.159E-8
3.18E2	1E0	5.616E-4	3.4E-8	1.909E-11	8.159E-8
3.33E2	1E0	1.391E-3	3.4E-8	4.731E-11	1.931E-7
3.48E2	1E0	3.189E-3	3.4E-8	1.084E-10	4.233E-7

°K Tridecane C-100 Emmissions (xl=max10)

T °K	vl	pl bars	xl MF	yl MF	Emmissions lbs/hr
2.88E2	1E0	6.888E-5	3.42E-7	2.356E-11	1.111E-7
3.03E2	1E0	2.071E-4	3.42E-7	7.085E-11	3.177E-7
3.18E2	1E0	5.616E-4	3.42E-7	1.921E-10	8.207E-7
3.33E2	1E0	1.391E-3	3.42E-7	4.759E-10	1.942E-6
3.48E2	1E0	3.189E-3	3.42E-7	1.091E-9	4.258E-6

Tridecane

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Title: organic emission

Date: 3/91 by J. Perry

Checked: 3/91 by WGHistand

The process condensate emmission results at 75°C = 348°K, can be used to determine the feed concentration limit. The feed concentration limit is the concentration of volatile constituent in the feed stream, with the assumption that the volatile constituent is completely transferred into the condensate, which will produce 0.71 lbs/hr (.322 kg/hr) emmissions of tridecane from the process condensate. The feed concentration limit is calculated as follows:

$$\left(\frac{3.5\times10^{3}}{} \ \mu g/l\right)\left(\frac{1 \ mg}{1000 \ \mu g}\right)\left(\frac{1 \ hr.}{4.258\times10^{-6} \ lbs}\right)\left(\frac{.71 \ lbs}{1 \ hr}\right)\left(\frac{R-1}{R}\right)$$

$$= 5.836\times10^{5} \left(\frac{R-1}{R}\right) \ mg/l$$

note: R = feed rate ÷ product rate

Tridecane

Westinghouse Environmental & Geotechnical Services, Inc.

DESIGN ANALYSIS

Page No. 10 of 12

Job No. 89-5010-ES Client/Project WHC/242-A

Title: Organic Removal

Date: 3/91 by Jon Perry

Checked: 3/91 by WG Richmond

Determination of maximum feed concentration:

$$R\,C_f + (1-R)\,C_c = C_s$$

R = Ratio of Feed to product Mass Ratio

C_f = Feed Concentration

C_s = Concentration of a given component in Slurry

Note: To determine the maximum feed concentration (C_f) of a given component, (C_s) will be the regulatory limit (HBL or LDR).

C_c = Condensate Concentration of a given component

Note: C_c is calculated from the vapor phase mol fraction for a given component in the slurry.

Westinghouse Environmental & Geotechnical Services, Inc.

DESIGN ANALYSIS

Page No. 11 of 12

Job No. 89-5010 - ES Client/Project WHC/242-A

Title: Organic Removal

Date: 3/91 by Jim Perry

Checked: 3/91 by WG Pritchard

C_c is calculated by converting y_i (mol fraction) to y_i (ppm)

$$y_i(MF) = \frac{\text{moles } i}{\text{moles } i + \text{moles } H_2O}$$

In this calculation, the mole contribution of component i is insignificant relative to the mole contribution of H_2O. Therefore,

$$\left(\frac{\text{mol } i}{\underset{\text{insignificant}}{\cancel{\text{mol } i}} + \text{mol } H_2O}\right)\left(\frac{55.5093 \text{ mol } H_2O}{1 \ell}\right)(\text{molec. wt})\left(\frac{1000 \text{ mg}}{g}\right)$$

$$= \text{mg}/\ell = \text{mg}/\text{Kg} = \text{ppm}$$

Tridecane

Westinghouse Environmental & Geotechnical Services, Inc.

DESIGN ANALYSIS

Page No. 12 of 12

Job No. 89-5010-ES Client/Project WHC/242-A

Title: Organic Removal

Date: 3/91 by J. Perry

Checked: 3/91 by

Tridecane Slurry Vapor Phase Mole Fraction

T °K	vl	pl bars	xl MF	Pt bars	yl MF
2.98E2	1E0	1.453E-4	9.8E-8	3.143E-2	4.53E-10
3.03E2	1E0	2.071E-4	9.8E-8	4.212E-2	4.82E-10
3.08E2	1E0	2.92E-4	9.8E-8	5.584E-2	5.124E-10
3.13E2	1E0	4.07E-4	9.8E-8	7.327E-2	5.444E-10
3.18E2	1E0	5.616E-4	9.8E-8	9.521E-2	5.78E-10
3.23E2	1E0	7.67E-4	9.8E-8	1.226E-1	6.132E-10
3.28E2	1E0	1.038E-3	9.8E-8	1.565E-1	6.5E-10
3.33E2	1E0	1.391E-3	9.8E-8	1.98E-1	6.886E-10
3.38E2	1E0	1.85E-3	9.8E-8	2.487E-1	7.29E-10
3.43E2	1E0	2.438E-3	9.8E-8	3.099E-1	7.711E-10
3.48E2	1E0	3.189E-3	9.8E-8	3.834E-1	8.151E-10

Tridecane Slurry Limits (mg/l)

T °K	yl MF	Cc mg/l	HBL mg/l
2.98E2	4.53E-10	4.636E-3	1E0
3.03E2	4.82E-10	4.932E-3	1E0
3.08E2	5.124E-10	5.244E-3	1E0
3.13E2	5.444E-10	5.572E-3	1E0
3.18E2	5.78E-10	5.915E-3	1E0
3.23E2	6.132E-10	6.275E-3	1E0
3.28E2	6.5E-10	6.653E-3	1E0
3.33E2	6.886E-10	7.047E-3	1E0
3.38E2	7.29E-10	7.46E-3	1E0
3.43E2	7.711E-10	7.891E-3	1E0
3.48E2	8.151E-10	8.342E-3	1E0

$$C_f = \left(\frac{R-1}{R} + \frac{C_s}{R}\right) C_c$$

APPENDIX C

CALCULATED ORGANIC EMISSIONS FROM 242-A EVAPORATOR VESSEL VENT FOR CAMPAIGNS 94-1 AND 94-2

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• Stacks

006608

Westinghouse
Hanford Company

Internal
Memo

From: TWRS Environmental Compliance 77510-95-021
Phone: 373-9379 R2-06
Date: May 10, 1995
Subject: CALCULATED ORGANIC EMISSIONS FROM 242-A EVAPORATOR VESSEL VENT FOR CAMPAIGNS 94-1 AND 94-2

To: R. D. Gustavson

cc:			
DD Bachand	R1-51	RJ Nicklas	R1-43
LE Borneman	R2-06	WE Ross	S5-07
JG Coenenberg	H6-24	BH Von Bargen	R1-43
PR Gunter	R1-52		

References: "242-A Evaporator Dangerous Waste Permit Application", DOE/RL-90-42, Rev 0, Jun 28, 1991.

The calculated emissions of organic constituents from the 242-A Evaporator vessel vent during campaigns 94-1 and 94-2 are:

	Operating Period	Maximum Emission Rate	Limit from 40 CFR 265	Total Emissions
Campaign 94-1	43 days	9.36×10^{-2} kg/hr (0.206 lb/hr)	1.4 kg/hr (3 lb/hr)	18.4 kgs (40.5 lbs)
Campaign 94-2	43 days	5.77×10^{-2} kg/hr (0.120 lb/hr)	1.4 kg/hr (3 lb/hr)	45.0 kgs (99.1 lbs)

Documentation of organic emissions is required per 40 CFR 265.1035(b)(2). Engineering calculations can be used to determine the emission rates as allowed in 40 CFR 265.1032(c). These values were determined using Evaporator candidate feed tank sample results and the attached equilibrium calculations, which are similar to those given in the Evaporator Dangerous Waste Permit Application, Appendices 3E and 3F.

The maximum emission rate is the rate from the feed tank which had the highest concentration of volatile organics. For Campaign 94-1, feed tank 106-AW had the highest organic concentrations, primarily acetone. For Campaign 94-2, feed tank 107-AP had the highest organic concentrations, primarily butanol. A weighted average emission rate was used to determine the total emissions. For Campaign 94-1, tank 106-AW was only 13% of the volume. This explains why Campaign 94-1 has a greater maximum emission rate, but a smaller total emission.

The total quantity for the annual period from April 15, 1994 (startup of Campaign 94-1) to April 15, 1995 is 63.4 kgs (139.8 lbs). The limit given in 40 CFR 265, Subpart AA is 2800 kgs (3.1 tons). The organic emissions given here are about 2% of the allowed emissions.

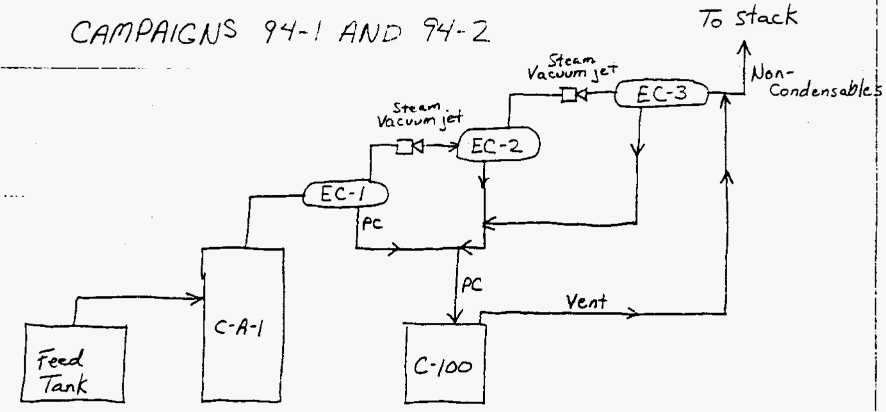
Mark Bowman

Mark Bowman
TWRS Environmental Compliance

Calculations
By M.W. Bowman

Checked by

CALCULATE VESSEL VENT ORGANIC EMISSIONS FOR 242-A CAMPAIGNS 94-1 AND 94-2



Flowrate: Total Vent: ~600 ft^3/min
C-100 Vent: ~150 ft^3/min

Per calculations in Appendix 3E of the "242-A Evaporator Dangerous Waste Permit Application" (DOE/RL-90-42), pg 3E-29, the primary source of emission is C-100 tank. Calculations there show the emissions from condenser vent is ~1000 times smaller than C-100 emissions because the three condensers serve as stages of scrubbing for organic removal.

* Assumption: all organic emissions are from C-100 vent.

* Assumption: there is no flow measurement on C-100. The flow is assumed to be 150 ft^3/min (Part B), although it may actually be less.

$Q_{100} \equiv$ C-100 tank volumetric air flow = 150 ft^3/min

1

Calculations
by MW Bowman

Checked by

Define:

$\dot{m}_T \equiv$ total mass flow of organics out of C-100, kg/hr

$\dot{m}_i \equiv$ mass flow of organic component i, kg/hr

$\dot{n}_{100} \equiv$ mole flow from C-100, mol/hr

$P_T \equiv$ pressure total in C-100, atm

$T \equiv$ temperature, C-100, °K

$y_i \equiv$ mole fraction of component i in vapor phase, unitless

$x_i \equiv$ " " " " in liquid phase, unitless

$P_i \equiv$ vapor pressure of component i, atm

$\gamma_i \equiv$ activity coefficient of component i, unitless

$R =$ gas constant $= .08206$ l-atm/mol·°K

$X_{100_i} \equiv$ conc. of component i in C-100, gm/l

$X_{F_i} \equiv$ conc. of component i in the feed, gm/l

$MW_i \equiv$ molecular wt of component i, gm/mol

$R_G =$ gas constant $= .08206 \frac{\text{l-atm}}{\text{mol-°K}}$

$R \equiv$ ratio of feed flowrate divided by slurry flowrate, unitless

Calculations by MNBowman
Checked by JA Campbell

1. Calculate $\dot{n}_{100}$. molar flowrate from C-100

$$P_T Q_{100} = \dot{n}_{100} RT$$

$$\dot{n}_{100} = \frac{P_T Q_{100}}{RT}$$

* Assumption: pressure in C-100 is 750 mmHg, from Part B, pg 3E-23

$$P_T = \frac{750 \text{ mHg}}{760 \text{ mHg/atm}} = .987 \text{ atm}$$

* Assumption: temperature of the off-gas is 75°C, from Part B, pg 3E-27.
NOTE - This is the maximum T used in the Part B calculations (worst case). The temp in C-100 is normally limited to < 62°C (145°F)

$$T = 75°C + 273 = 348°K$$

$$Q_{100} = 150 \text{ ft}^3/\text{min} \left(28.317 \, \ell/\text{ft}^3\right)\left(60 \text{ min}/\text{hr}\right)$$

$$= 2.55 \times 10^5 \, \ell/\text{hr}$$

$$\dot{n}_{100} = \frac{P_T Q_{100}}{R_G T} = \frac{.987 \text{ atm} \left(2.55 \times 10^5 \, \ell/\text{hr}\right)}{.08206 \frac{\ell\text{-atm}}{\text{mol}\cdot°\text{K}} \left(348°K\right)}$$

$$\dot{n}_{100} = 8.81 \times 10^3 \text{ mol/hr}$$

Calculations by MWBowman
Checked by JA Cy

2. Determine the equation for relating mass flowrate to mol flowrate

$\dot{m}_i \equiv$ mass flow of component i from C-100

$$\dot{m}_i = y_i \, \dot{n}_{100} (MW_i)$$

where y_i = gas phase mol fraction of component i (unitless)
MW_i = molecular wt of component i (gm/mol)

$$\dot{m}_i = y_i \, (8.81 \times 10^3 \text{ mol/hr}) \frac{(MW_i)}{1000 \text{ gm/kg}}$$

NOTE - $\frac{1}{1000}$ converts gms to kgs.

3. Determine the relationship between y_i, mole fraction in gas phase, and x_i, mol fraction in liquid phase.

$$y_i P_T = \gamma_i x_i P_i$$

This is the standard equation for vapor-liquid equilibrium, given in 3E-3 of the Part B. It relates the mol fraction in the gas phase to the mol fraction in the liquid phase using the vapor pressure of pure component, P_i, and activity coefficient, γ_i. P_i can be obtained from reference books, but γ_i must be calculated based on various parameters. Fortunately, the Part B provides P_i and γ_i for all compounds in Appendix 3F.

Calculations by MW Bowman
Checked by VA Campbell

4. Relate x_i, the mol fraction in C-100 liquid phase, to X_{F_i}, the mass concentration (gm/L) in the feed tank.

x_i = mol fraction (C-100) of component i (unitless)

X_{F_i} = mass conc. (feed tank) of component i (gm/ℓ)

a. First, relate x_i to X_{100i}, the concentration of component i in C-100 (gm/ℓ).

$$x_i = \frac{\text{mols of } i}{\text{mols total}} = \frac{\text{mols of } i}{(\text{mols of } i) + (\text{mols of } H_2O)}$$

* Assumption: the mols of all components are trivial compared to the mols of water. Example: if Acetone is 1300 μg/L, this is

$$\frac{1300\ \mu g/L}{10^6\ (58.1\ gm/mol)} = 2.24 \times 10^{-5}\ mol/\ell$$

$$H_2O \text{ is } \frac{1000\ gm/L}{18\ gm/mol} = 55.6\ mol/\ell$$

The mols of H_2O is 10^6 X the moles of Acetone

$$x_i = \frac{\text{mols of } i}{(\text{mols of } i) + (\text{mols of } H_2O)} \approx \frac{\text{mols of } i}{\text{mols of } H_2O}$$

$$\text{mols of } i = \frac{X_{100i}}{(MW_i)}$$

X_{100i} units: gm/ℓ
MW_i units: gm/mol

$$x_i = \frac{\dfrac{X_{100i}}{(MW_i)}}{\dfrac{X_{H_2O}}{(MW_{H_2O})}}$$

NOTE: x_i is unitless

for H_2O, $X_{H_2O} = 1000$ gm/ℓ $MW_{H_2O} = 18$ gm/mol

Calculations by MW Bowman
Checked by JA Campbell

$$x_i = \frac{\frac{X_{100i}}{(mw_i)}}{\frac{X_{H_2O}}{(mw_{H_2O})}} = \frac{\frac{X_{100i}}{(mw_i)}}{\frac{1000\ gm/l}{18\ gm/mol}}$$

$$x_i = (1.8 \times 10^{-2}\ l/mol) \frac{X_{100i}}{(mw_i)}$$

b. Now relate X_{100i}, concentration of component i in C-100, to X_{Fi}, concentration of component i in the feed.

The standard equations for relating PC concentration (X_{100i}) to feed concentration (X_{Fi}) are:

$$\cancel{X_F} \quad X_{Fi} = X_{100i}\left(\frac{R-1}{R}\right); \text{ and } \quad X_{100i} = X_{Fi}\left(\frac{R}{R-1}\right)$$

Where $R \equiv$ ratio of feed flow rate divided by slurry flowrate.

* Assumption: these equations assume that all the constituent in the feed goes into the process condensate.

$$x_i = (1.8 \times 10^{-2}\ l/mol) \frac{X_{100i}}{(mw_i)}$$

$$= (1.8 \times 10^{-2}\ l/mol) \frac{X_{Fi}}{(mw_i)} \left(\frac{R}{(R-1)}\right)$$

Calculations by MWBowman
Checked by

5. Combining equations:

- from #2:

$$\dot{m}_i = y_i \dot{n}_{100} (mw_i)$$

$$= y_i (8.81 \times 10^3 \text{ mol/hr}) \frac{(mw_i)}{1000 \text{ gm/kg}}$$

- from #3:

$$y_i P_T = \gamma_i \chi_i P_i \qquad P_T = .987 \text{ atm}$$

$$y_i = \gamma_i \chi_i \frac{P_i}{P_T} = \gamma_i \chi_i \frac{P_i}{.987 \text{ atm}}$$

- from #4b

$$\chi_i = (1.8 \times 10^{-2} \text{ l/mol}) \frac{X_{F_i}}{(mw_i)} \left(\frac{R}{R-1}\right)$$

Combing #3 and #4b

$$y_i = \gamma_i \left(\frac{P_i}{.987 \text{ atm}}\right) \chi_i$$

$$= \gamma_i \left(\frac{P_i}{.987 \text{ atm}}\right) \underbrace{(1.8 \times 10^{-2} \text{ l/mol}) \frac{X_{F_i}}{(mw_i)} \left(\frac{R}{R-1}\right)}_{\chi_i}$$

combining this with #2:

Calculations by

Checked by

$$\dot{m}_i = y_i \left(8.81\times10^{3}\ \text{mol/hr}\right)\frac{(mw_i)}{1000\ \text{gm/kg}}$$

$$\dot{m}_i = \underbrace{\gamma_i\left(\frac{P_i}{.987\,\text{atm}}\right)\left(1.8\times10^{-2}\ \ell/\text{mol}\right)\frac{X_{F_i}}{(mw_i)}\left(\frac{R}{R-1}\right)}_{y_i}\left(8.81\times10^{3}\ \text{mol/hr}\right)\frac{(mw_i)}{1000\ \text{gm/kg}}$$

Simplify: combine constants and cancel mw_i from the equation:

$$\dot{m}_i = \left(0.161\ \frac{\ell\text{-kg}}{\text{hr-gm-atm}}\right)\gamma_i P_i X_{F_i}\left(\frac{R}{R-1}\right)$$

Check units: γ_i is unitless

P_i is atm

X_{F_i} is gm/ℓ

R is unitless

$$\frac{\cancel{\ell}\text{-kg}}{\text{hr-}\cancel{\text{gm}}\text{-}\cancel{\text{atm}}} \times \cancel{\text{atm}} \times \frac{\cancel{\text{gm}}}{\cancel{\ell}} = \text{kg/hr} \qquad \text{OK}$$

Calculation by MW Bowman
Checked by TA Campbell

6. Determine equation for individual components

$$\dot{m}_i = \left(0.161 \frac{\ell\text{-kg}}{\text{hr-gm-atm}}\right) \gamma_i P_i X_{Fi} \left(\frac{R}{R-1}\right)$$

Normally $R=2$ and the equation becomes $\left(\frac{R}{R-1}\right)=2$

$$\dot{m}_i = \left(0.322 \frac{\ell\text{-kg}}{\text{hr-gm-atm}}\right) \gamma_i P_i X_{Fi}$$

The values for γ_i, P_i are given in the Part B.
See attached table.

Constituent	MW_i (gm/mol)	γ_i	P_i (atm)	Part B Ref. Page No.	$\dot{m}_i$ (kg/hr)
Acetone	58.1	11.5	1.82	3F-15	6.74 X_{Fi}
1-Butanol	74.12	49.1	0.169	3F-54	2.67 X_{Fi}
2-Butanone (MEK)	72.1	37.1	0.854	3F-66	10.2 X_{Fi}
2-Butoxyethanol	118.2	592	0.0327	3F-80	6.23 X_{Fi}
2-Proponol	60.09	10.0	0.743	3F-179	2.39 X_{Fi}
Tri-butyl Phosphate	266.3	1.0	0.181	3F-234	5.83E-2 X_{Fi}
Tetrahydrofuran	72.11	96.6	1.32	3F-211	41.1 X_{Fi}
Benzyl Alcohol	108.13	2019	0.00506	3F-32	3.29 X_{Fi}
Butanal	72.1	96.9	1.01	3F-42	31.5 X_{Fi}
Methyl Isobutyl Ketone	100.16	437	0.257	3F-143	36.2 X_{Fi}

Calculations by WW Bowman

Checked by

10/19

Constituent	MW_i (gm/mol)	γ_i	P_i (atm)	Part B Ref. Page No.	$\dot{m}_i$ (kg/hr)
2-Pentanone	86.13	126	0.406	3F-155	16.5 X_{Fi}
2-Hexanone	100.16	437	0.100	3F-130	14.1 X_{Fi}
Tridecane	184.41	1.0	0.00315	3F-246	1.01E-3 X_{Fi}
Tetradecane	198.4	1.0	0.00128	3F-223	4.12E-4 X_{Fi}

Notes: Molecular weights are from the TOMES database. The values for P_i given in the Part B were converted from bars to atm. The values for $\dot{m}_i$ assume R = 2.

Calculations by MWBowman

Checked by

/1

Calculation by MWBowman
Checked by TA

Campaign 94-1 (Data from Process Control Plan (WHC-SD-WM-PCP-008 Rev1)

Tank 102-AW   Ref: PCP, WHC-SD-WM-PCP-008 Rev 1

Acetone = 595 µg/L
Butanal = 6 µg/L
1-Butanol = 145 µg/L

NOTE-
These are 90% confidence intervals (where the analyte was seen in more than one samp.

Acetone: $\dot{m}_{Acetone} = 6.74 \frac{\ell\text{-kg}}{\text{hr gm}} (595\ \mu\text{gm}/\ell)\left(\frac{1\text{gm}}{10^6\mu\text{gm}}\right)$

$= 4.01 \times 10^{-3}$ kg/hr

Butanal: $\dot{m}_{Butanal} = 31.5 \frac{\ell\text{-kg}}{\text{hr-gm}} (6\ \mu\text{gm}/\ell)\left(\frac{1\text{gm}}{10^6\mu\text{gm}}\right)$

$= 1.89 \times 10^{-4}$ kg/hr

1-Butanol $\dot{m}_{Butanol} =$ ~~145 µgm/l~~
$2.67 \frac{\ell\text{-kg}}{\text{hr-gm}} (145\ \mu\text{gm}/\ell)\left(\frac{1\text{gm}}{10^6\mu\text{gm}}\right)$

$= 3.87 \times 10^{-4}$ kg/hr

Sum: $(4.01 \times 10^{-3}) + (1.89 \times 10^{-4}) + (3.87 \times 10^{-4})$

$= 4.59 \times 10^{-3}$ kg/hr

Tank 106-AW   Ref: PCP, WHC-SD-WM-PCP-008

Acetone = 13,700 µgm/l
Butanal = 9 µgm/l
1-Butanol = 67 µgm/l
2-Hexanone = 57 µgm/l (~~Also called MIBK~~) MWB
Tetradecane = 4400 µgm/l
Tridecane = 5300 µgm/l

90% confidence intervals (where the analyte was seen in more than one sample).

4

Calculations by NW Bowman
Checked by

Acetone: $\dot{m}_{ACETONE} = 6.74 \frac{\ell\text{-kg}}{\text{hr-gm}} (13,700\ \mu g/\ell)\left(\frac{1\ gm}{10^6\ \mu gm}\right)$

$= 9.23 \times 10^{-2}$ kg/hr

Butanal: $\dot{m}_{BUTANAL} = 31.5 \frac{\ell\text{-kg}}{\text{hr-gm}} (9\ \mu g/\ell)(1\ gm/10^6\ \mu gm)$

$= 2.84 \times 10^{-4}$ kg/hr

1-Butanol: $\dot{m}_{BUTANOL} = 2.67 \frac{\ell\text{-kg}}{\text{hr-gm}} (67\ \mu gm/\ell)(1\ gm/10^6\ \mu gm)$

$= 1.79 \times 10^{-4}$ kg/hr

2-Hexanone $\dot{m}_{HEXANONE} = \overset{mwB}{\cancel{16.5}}$
$14.1 \frac{\ell\text{-kg}}{\text{hr-gm}} (57\ \mu gm/\ell)(1\ gm/10^6\ \mu gm)$

$= 8.04 \times 10^{-4}$ kg/hr

Tetradecane $\dot{m}_{Tetrad} = 4.12 \times 10^{-4} \frac{\text{kg-}\ell}{\text{hr-gm}} (4400\ \mu gm/\ell)(1\ gm/10^6\ \mu gm)$

$= 1.81 \times 10^{-6}$ kg/hr

Tridecane $\dot{m}_{Trid} = 1.01 \times 10^{-3} \frac{\text{kg-}\ell}{\text{hr-gm}} (5300\ \mu gm/\ell)(1\ gm/10^6\ \mu gm)$

$= 5.35 \times 10^{-6}$ kg/hr

Sum: $(9.23 \times 10^{-2}) + (2.84 \times 10^{-4}) + (1.79 \times 10^{-4}) +$
$(8.04 \times 10^{-4}) + (1.81 \times 10^{-6}) + (5.35 \times 10^{-6})$

$= 9.36 \times 10^{-2}$ kg/hr

Calculations by MW Bowman
Checked by GA Campbell

Tank 103-AP

Acetone = 808 μg/l
1-Butanol = 6.5 μg/l
2-Butoxyethanol = 400 μg/l
2-Hexanone = 8.2 μg/l

90% Confidence intervals (for analytes detected in more than one sample).

Acetone: $\dot{m}_{ACE} = 6.74 \frac{l\text{-}kg}{hr\text{-}gm} (808\ \mu g/l)(1\ gm/10^6\ \mu g)$
$= 5.45 \times 10^{-3}\ kg/hr$

1-Butanol: $\dot{m}_{Butanol} = 2.67 \frac{l\text{-}kg}{hr\text{-}gm} (6.5\ \mu g/l)(1g/10^6\ \mu g)$
$= 1.74 \times 10^{-5}\ kg/hr$

Butoxyethanol $\dot{m}_{BUTX} = 6.23 \frac{l\text{-}kg}{hr\text{-}gm} (400\ \mu g/l)(1g/10^6\ \mu g)$
$= 2.49 \times 10^{-3}\ kg/hr$

2-Hexanone $\dot{m}_{HEX} = 14.1 \frac{l\text{-}kg}{hr\text{-}gm} (8.2\ \mu g/l)(1g/10^6\ \mu g)$
$= 1.16 \times 10^{-4}\ kg/hr$

Sum: $(5.45 \times 10^{-3}) + (1.74 \times 10^{-5}) + (2.49 \times 10^{-3}) + (1.16 \times 10^{-4})$
$= 8.07 \times 10^{-3}\ kg/hr$

Based on the individual results from each tank, the maximum emission seen was 9.36×10^{-2} kg/hr (0.206 lb/hr). The prime contributor was acetone from tank 106-AW.

Calculations by MW Bowman
Checked by

To determine an average emission, a composite (weighted average) must be determined. The Process Control Plan (WHC-SD-WM-PCP-008, Rev 1), Appendix G states the composite analysis for radionuclides used the following:

41%	102-AW
13%	106-AW
46%	103-AP

A weighted average is then:

$$.41\,(4.59 \times 10^{-3}\ \mathrm{kg/hr}) + .13\,(9.36 \times 10^{-2}\ \mathrm{kg/hr}) +$$
$$.46\,(8.07 \times 10^{-3}\ \mathrm{kg/hr})$$
$$= 1.78 \times 10^{-2}\ \mathrm{kg/hr} \qquad (3.92 \times 10^{-2}\ \mathrm{lb/hr})$$

Total Emissions:
From the Post Run Document, WHC-SD-WM-PE-053, Rev 0, the 242-A Evaporator operated for 43 days (Pg 3).

mwB ~~RA~~ $m_{TOT} = 1.78 \times 10^{-2}\ \mathrm{kg/hr}\,(43\ \mathrm{days})(24\ \mathrm{hr/day})$
$$= 18.4\ \mathrm{kg} \qquad (40.5\ \mathrm{lbs})$$

Maximum Rate:	9.36×10^{-2} kg/hr	0.206 lb/hr
Average Rate:	1.78×10^{-2} kg/hr	3.92×10^{-2} lb/hr
Total Emitted:	18.4 ~~lbs~~ mwB kg	40.5 lbs
Operating Days:	43 days	

Calculations by M W Bowman

Checked by

Campaign 94-2

Data from Process Control Plan, WHC-SD-WM-PCP-009 Rev 0

Data ~~from~~ mwB for 108-AP from E.Q. Le, Internal Memo #71730-94-001

Tank 101-AP

2-Butanone = $\leq 500\ \mu g/l$

Tetrahydrofuran: $\leq 500\ \mu g/l$

Benzyl Alcohol: $\leq 2000\ \mu g/l$

1-Butanol: $\leq 2000\ \mu g/l$

Butoxyethanol: $\leq 2000\ \mu g/l$

Although these numbers are all "less than", will use maximum in calculations.

2-Butanone: $\dot{m}_{BUTN} = 10.2\ \frac{l\text{-}kg}{hr\text{-}gm}\ (500\ \mu g/l)\left(\frac{1\ g}{10^6\ \mu g}\right)$

$= 5.10 \times 10^{-3}$ kg/hr

Tetrahydrofuran:

$\dot{m}_{Tetfrn} = 41.1\ \frac{l\text{-}kg}{hr\text{-}gm}\ (500\ \mu g/l)\left(\frac{1\ g}{10^6\ \mu g}\right)$

$= 2.06 \times 10^{-2}$ kg/hr

Benzyl Alcohol:

$\dot{m}_{BNZL} = 3.29\ \frac{l\text{-}kg}{hr\text{-}gm}\ (2000\ \mu g/l)\left(\frac{1\ g}{10^6\ \mu g}\right)$

$= 6.58 \times 10^{-3}$ kg/hr

1-Butanol $\dot{m}_{BUTANOL} = 2.67\ \frac{l\text{-}kg}{hr\text{-}gm}\ (2000\ \mu g/l)\left(\frac{1\ g}{10^6\ \mu g}\right)$

$= 5.34 \times 10^{-3}$ kg/hr

2-Butoxyethanol

$\dot{m}_{BUTXY} = 6.23\ \frac{l\text{-}kg}{hr\text{-}gm}\ (2000\ \mu g/l)\left(\frac{1\ g}{10^6\ \mu g}\right)$

$= 1.25 \times 10^{-2}$ kg/hr

Sum $(5.10 \times 10^{-3}) + (2.06 \times 10^{-2}) + (6.58 \times 10^{-3}) + (5.34 \times 10^{-3})$

$+ (1.25 \times 10^{-2}) = 5.01 \times 10^{-2}$ kg/hr

Calculations by MW Bowman

Checked by

Tank 107-AP

TBP = 3755 µg/l
Benzyl Alcohol = <2000 µg/l
1-Butanol = 14,392 µg/l
2-Butoxyethanol = <2000 µg/l

Results are 90% confidence intervals for all values which are above detection limits.

TBP: $\dot{m}_{TBP} = 5.83 \times 10^{-2} (3755\ \mu g/l)\left(\frac{1g}{10^6 \mu g}\right)$
$= 2.19 \times 10^{-4}$ kg/hr

Benzyl Alcohol:
$\dot{m}_{Benz} = 3.29 \frac{l\text{-}kg}{hr\text{-}gm} (2000\ \mu g/l)\left(\frac{1g}{10^6 \mu g}\right)$
$= 6.58 \times 10^{-3}$ kg/hr

1-Butanol: $\dot{m}_{BUTNOL} = 2.67 \frac{l\text{-}kg}{hr\text{-}gm} (14,392\ \mu g/l)\left(\frac{1g}{10^6 \mu g}\right)$
$= 3.84 \times 10^{-2}$ kg/hr

2-Butoxy ethanol: $\dot{m}_{BUTX} = 6.23 \frac{l\text{-}kg}{hr\text{-}gm} (2000\ \mu g/l)\left(\frac{1g}{10^6 \mu g}\right)$
$= 1.25 \times 10^{-2}$ kg/hr

sum: $(2.19 \times 10^{-4}) + (6.58 \times 10^{-3}) + (3.84 \times 10^{-2}) + (1.25 \times 10^{-2})$
$= 5.77 \times 10^{-2}$ kg/hr

Tank 108-AP

Acetone = 376 µg/l
Benzyl Alcohol = <1000 µg/l
1-Butanol = 1820 µg/l
2-Butanone = 56 µg/l
2-Butoxyethanol = 1,240 µg/l
2-Hexanone = 50 µg/l
2-Propanol = 78 µg/l
Tetradecane = <1000 µg/l
Tetrahydrofuran = 54 µg/l

All values are 90% confidence intervals if above the detection limits.

TBP = 3280 µg/l
Tridecane = <1000 µg/l

Calculations by MW Bowman
Checked by

Acetone: $\dot{m}_{ACE} = 6.74 \frac{\ell\text{-kg}}{\text{hr-gm}} (376\ \mu g/\ell)\left(\frac{1g}{10^6 \mu g}\right)$

$= 2.53 \times 10^{-3}$ kg/hr

Benzyl Alcohol: $\dot{m}_{Benz} = 3.29 \frac{\ell\text{-kg}}{\text{hr-gm}} (1000\ \mu g/\ell)\left(\frac{1g}{10^6 \mu g}\right)$

$= 3.29 \times 10^{-3}$ kg/hr

1-Butanol: $\dot{m}_{BUTNOL} = 2.67 \frac{\ell\text{-kg}}{\text{hr-gm}} (1820\ \mu g/\ell)\left(\frac{1g}{10^6 \mu g}\right)$

$= 4.86 \times 10^{-3}$ kg/hr

2-Butanone: $\dot{m}_{BUTNONE} = 10.2 \frac{\ell\text{-kg}}{\text{hr-gm}} (56\ \mu g/\ell)\left(\frac{1g}{10^6 \mu g}\right)$

$= 5.71 \times 10^{-4}$ kg/hr

2-Butoxyethanol: $\dot{m}_{BUTXY} = 6.23 \frac{\ell\text{-kg}}{\text{hr-gm}} (1240)\left(\frac{1g}{10^6 \mu g}\right)$

$= 7.73 \times 10^{-3}$ kg/hr

2-Hexanone: $\dot{m}_{HEX} = 14.1 \frac{\ell\text{-kg}}{\text{hr-gm}} (50\ \mu g/\ell)\left(\frac{1g}{10^6 \mu g}\right)$

$= 7.05 \times 10^{-4}$ kg/hr

2-Propanol: $\dot{m}_{prop} = 2.39 \frac{\ell\text{-kg}}{\text{hr-gm}} (78\ \mu g/\ell)\left(\frac{1g}{10^6 \mu g}\right)$

$= 1.86 \times 10^{-4}$ kg/hr

Tetradecane $\dot{m}_{TET} = 4.12 \times 10^{-4} \frac{\ell\text{-kg}}{\text{hr-gm}} (1000\ \mu g/\ell)\left(\frac{1g}{10^6 \mu g}\right)$

$= 4.12 \times 10^{-7}$ kg/hr

Tetrahydrofuran $\dot{m}_{FUR} = 41.1 \frac{\ell\text{-kg}}{\text{hr-gm}} (54\ \mu g/\ell)\left(\frac{1g}{10^6 \mu g}\right)$

$= 2.22 \times 10^{-3}$ kg/hr

TBP $\dot{m}_{TBP} = 5.83 \times 10^{-2} \frac{\ell\text{-kg}}{\text{hr-gm}} (3280\ \mu g/\ell)\left(\frac{1g}{10^6 \mu g}\right)$

$= 1.91 \times 10^{-4}$ kg/hr

Tridecane $\dot{m}_{Tri} = 1.01 \times 10^{-3} \frac{\ell\text{-kg}}{\text{hr-gm}} (1000\ \mu g/\ell)\left(\frac{1g}{10^6 \mu g}\right)$

$= 1.01 \times 10^{-6}$ kg/hr

Summation $= 2.23 \times 10^{-2}$ kg/hr

Calculations by MWBowman
Checked by TA

To determine an average emission rate, a composite (weighted average) must be determined. The PCP (WHC-SD-WM-PCP-009, Rev 0) states the following composite was used:

32%	101-AP
34%	107-AP
34%	108-AP

The weighted average is

$$.32\,(5.01\times10^{-2}\,\text{kg/hr}) + .34\,(5.77\times10^{-2}\,\text{kg/hr}) + .34\,(2.23\times10^{-2}\,\text{kg/hr})$$

$$= 4.32\times10^{-2}\,\text{kg/hr}$$

Total Emissions:

From the draft Post Run Document (WHC-SD-WM-PE-054) the Evaporator operated 1040 hrs (43 days). This is total time (1416 hrs), minus planned outages (308.5 hrs), minus unplanned outages (68 hrs)

$$m_{TOT} = 4.32\times10^{-2}\,\text{kg/hr}\,(1040\,\text{hrs})$$

$$= 45.0\,\text{kg} \qquad (99.1\,\text{lbs})$$

Maximum rate :	5.77×10^{-2} kg/hr	0.120 lbs/hr
Average rate :	4.32×10^{-2} kg/hr	9.53×10^{-2} lbs/hr
Total Emitted :	45.0 kg	99.1 lbs
Operating Days :	43 days	

DISTRIBUTION SHEET

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		Date June 20, 1996
Project Title/Work Order Organic Emission Calculations for the 242-A Evaporator Vessel Vent System, WHC-SD-WM-ES-380, Rev. 0		EDT No. 615281
		ECN No. N/A

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