GEN 55 (REV.6/74)

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PLAINTIFF'S
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Calculations to Determine Need for Air Monitoring

The attached appendices show equations for estimating air contamination in typical CCCTC Laboratories. These equations should be used by the chemists in individual labs to determine if, as a result of current experiments, there is a potential danger of exceeding the Permissible Exposure Level (PEL) of a specific chemical. Judgement on the part of individual chemists is required to make this determination.

Equation 1 in the attachment will allow the estimation of the volume of liquid necessary to produce an ambient air concentration equal to the PEL. This equation should be used in the event of spills to estimate the potential exposure.

Equation 2 estimates the volume of a liquid chemical a given laboratory can handle and remain at or below the PEL in a given 8 hour period. This assumes the chemical is evaporated evenly during the 8 hour period. It should be useful in experiments where units are operated continuously during the shift. This calculation uses data from the recent survey of air flows at various CCCTC locations (1). Data provided in this survey for individual laboratories are volume, air turnover rate at standard conditions and air turnover rates when exhaust fans are operating. When using chemicals with extremely low PEL's it may be desirable to use the exhaust fans constantly. In this event the exhaust fan turnover rate should be used in the calculations.

These calculations should serve as the preliminary evaluation to determine if ambient air monitoring is required. They should insure proper prioritization of air monitoring.

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1. Air Measurement Reading Report, Callins Haggard and Associates.

APPENDIX I

EQUATION FOR ESTIMATING AIR CONTAMINATION
IN TYPICAL CCCTC LABORATORIES

$PV = nRT$ - Ideal Gas Law equation

Let: $Pi = PPM \times 10^{-6}$ = pressure of gas in room = PEL

V = Volume of Lab in Liters = 188, 724

$$n = \frac{\text{density (g/ml)} - \text{ml(liquid)}}{MW}$$

$$R = 0.083 \frac{\text{l atm}}{\text{mole °K}}$$

T = Absolute Temp - assume 300°K average

Then $N = \frac{PV}{RT}$

$$ml = \frac{PV\ MW}{RT\ \text{density}}$$

$$= \frac{PPM \cdot 10^{-6} \cdot 1.9 \times 10^{5} \cdot MW}{0.083 \cdot 300 \cdot \text{density}}$$

$$= \frac{PPM \cdot 0.19 \cdot MW}{24.9 \cdot \text{density}}$$

$$\text{ml(liquid)} = \frac{PPM \cdot MW \cdot 7.6 \times 10^{-3}}{\text{density}} \qquad \text{Equation 1}$$

Example: A chemist wishes to calculate the volume of n-butyl acetate that will give a concentration near the PEL in his laboratory.

PEL	=	200 ppm
Density	=	0.883 g/ml
MW	=	116 g/mole

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$$\text{ml} = \frac{200 \cdot 116 \cdot 7.6 \times 10^{-3}}{0.883} = 199.7 \text{ ml}$$

He may want to apply a safety factor and say that a spill of greater than 150 ml would call for evacuation of the lab for a few minutes.

Example: How much benzene is required to contaminate the air to the PEL

PEL	=	1 ppm
Density	=	0.88
MW	=	.79

$$\text{ml} = \frac{1 \cdot 76 \cdot 7.6 \times 10^{-3}}{0.88} = 0.65 \text{ ml}$$

APPENDIX II

EQUATION FOR ESTIMATING THE VOLUME OF A LIQUID CHEMICAL A GIVEN LABORATORY CAN HANDLE AND REMAIN AT OR BELOW THE PEL IN AN EIGHT HOUR SHIFT

Equation 1 (Appendix I) gives an air contaminate concentration assuming no removal of the contaminant by air turnover in the laboratory. Current air turnover rates for each laboratory were reported in a recent study (1). These data are available in the library.

Based on the exponential dilution theory it takes about 7 to 9 complete turnovers to reduce a contaminant to the zero level. However, most of the contaminant is removed in 2 or 3 turnovers.

Using equation 1, and 8 hour shift and the air turnover rate we develop equation 2.

$$\text{ml (liquid)} = \frac{\text{PPM} \cdot \text{MW} \cdot 7.6 \times 10^{-3}}{\text{density}} \cdot \frac{480 \text{ minutes}}{\text{Turnover rate in min.} \times 3}$$

where ml (liquid) is the volume of liquid that can be vaporized over an 8 hour shift and not exceed the PEL. Condensing this equation:

$$\text{ml (liquid)} = \frac{\text{PPM} \cdot \text{MW} \cdot 1.2}{\text{density} \cdot \text{Turnover rate}} \qquad \text{Equation 2}$$

A typical calculation for benzene in lab No. 66 which has an air turnover rate of 5.6 minutes is:

$$\text{ml (liquid)} = \frac{1 \cdot 78 \cdot 1.2}{0.88 \cdot 5.6} = 19$$

thus 19 ml of benzene could be evaporated over an 8 hour period in lab No. 66 and keep the contamination level to 1 ppm.