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ESTIMATING RELEASES AND  
WASTE-TREATMENT EFFICIENCIES FOR THE  
TOXIC CHEMICAL RELEASE  
INVENTORY FORM

Section 313 of the  
Emergency Planning and Community  
Right-to-Know Act of 1986

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where

$F_{\text{vap}}$  = fraction of fluid vaporized, dimensionless

$C_{p1}$  = heat capacity of liquid at a constant pressure at temperature of system, Btu/lb-°F

$T_1$  = temperature of liquid in system, °F

$T_b$  = boiling point of liquid at atmospheric pressure, °F

$H_{\text{vap}}$  = heat of vaporization, Btu/lb

This fraction can be multiplied by the generation rate obtained with equations in Subsection 6.2.1 (liquid discharge) or Subsection 6.2.4 (two-phase discharge) to obtain the quantity of chemical emitted to air as it is being discharged.

For a chemical in a mixture, use the boiling point and heat capacity of the chemical as before. The system temperature will be the same for all the chemicals in the mixture. Multiply the fraction flashed by the release rate calculated according to instructions for mixtures in Section 6.2.1.

### 6.2.3 Vaporization Model

A liquid chemical that is spilled onto the ground may spread out over an area, vaporize, and thus result in an air emission. A vaporization model developed by Clements can be used to estimate the rate of evaporation if the size (area) of the spill is known or can be estimated. This is a simple vaporization model, but other available spill models (TRC 1986) are more complex and may require more input data.

$$W = \frac{MKAP^\circ}{RT_1}$$

where

$W$  = vapor generation rate, lb/second

$M$  = molecular weight of chemical

$A$  = area of spill, ft<sup>2</sup>

$P^\circ$  = vapor pressure of chemical, psia, at temperature  $T_1$  [can assume 25°C (77°F) if not known]

$R$  = universal gas constant, 10.73 psia-ft<sup>3</sup>/°R-lb mole

$T_l$  = temperature of liquid spilled, °R = °F + 460

K = gas-phase mass transfer coefficient, ft/second

$$K = 0.00438 (U)^{0.78} \left[ \frac{D}{3.1 \times 10^{-4}} \right]^{2/3}$$

where D = diffusion coefficient for chemical in air, ft<sup>2</sup>/second  
U = Windspeed, miles/h

Diffusion coefficients can be found in chemical handbooks, usually in cm<sup>2</sup>/second (converted to ft<sup>2</sup>/second by multiplying cm<sup>2</sup>/second by 1.08 x 10<sup>-3</sup>).

If D is not available, use the following equation instead to calculate K.

$$K = 0.00438 (U)^{0.78} \left( \frac{18}{M} \right)^{1/3}, \text{ ft/second}$$

For a chemical in a spilled mixture, use the partial pressure,  $P_A$ , for the chemical instead of the chemical's vapor pressure. See Section 3.1.1 to calculate  $P_A$ ; M and K remain chemical specific parameters.

#### 6.2.4 Two-Phase Discharge

This method, which is based on the Fauske/Cude method, involves calculating the rate of discharge from two-phase (liquid-gas) critical flows. It is applicable to releases of saturated liquids stored under pressure at a temperature above the normal boiling point, and it is valid only if the calculated fraction of liquid flashing (see Section 6.2.2) is less than 1. This method assumes that the two phases (as discharged) are homogeneous and in mutual equilibrium. A simple empirical method, it yields approximate solutions. Alternative methods are required for more complex situations. The accuracy of this method is questionable for discharges involving long lengths of pipe where two-phase flow may develop within the line.

Two-phase critical flows can occur in failures of connections to the vapor space of vessels containing superheated liquids under pressure. They can also occur in failures of pipework containing superheated liquids remote from the vessel, where a fully developed critical flow would be established. Critical flow exists when velocity of the fluid attains sonic velocity, which can be determined by calculating the critical pressure ratio and using the