

TOXIC VAPOR CONCENTRATIONS IN THE CONTROL ROOM FOLLOWING A POSTULATED ACCIDENTAL RELEASE



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**TOXIC VAPOR CONCENTRATIONS IN THE
CONTROL ROOM FOLLOWING A
POSTULATED ACCIDENTAL RELEASE**

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1. Introduction

An accidental release of a toxic gas can harm or even kill the individuals who are exposed to the gas beyond its toxicity limits. Under most circumstances, the consideration of such an event would fall in the category of industrial safety.

There are, however, situations that can be postulated in which a toxic gas release could interfere with the safe operation of a nuclear plant. (See General Design Criterion 19, Appendix A, Part 50, Title 10, Code of Federal Regulations). For instance, a catastrophic release of chlorine from a rail car, in which the entire load of chlorine is spilled, could lead to the incapacitation or even death of the control room operators. This is a consequence of low probability (Hornyik; Murphy et al.; Simmons et al.). A number of events may have to occur in a sequential fashion to produce dangerous levels of chlorine within the control room. The chlorine tank must rupture, the wind direction must be toward the control room fresh air inlets, and the flow conditions must be such as to allow the chlorine to reach the inlets with concentrations sufficiently high to overcome the operators. The staff at U.S. Nuclear Regulatory Commission (NRC) has concluded that, notwithstanding the low probabilities, this type of an accident scenario should be considered in its safety evaluation of nuclear reactor plants.

The NRC staff has developed a number of guidelines and criteria to assure that the requirements of General Design Criterion 19 are met. These can be found in Standard Review Plans 2.2 and 6.4 and in Regulatory Guides 1.78 and 1.95. One aspect of the safety evaluation of nuclear

reactor plants is the assessment of the toxic vapor concentrations that may result from a liquid spill. The present report summarizes an acceptable method for such an assessment, and lists some typical toxic substances and their pertinent physical properties.

Many of the assumptions underlying the mathematical formulation in this report may seem rather simplistic and arbitrary. However, it is believed that they are reasonably conservative. As soon as more realistic models or direct experimental data become available, the present treatment will be modified.

It should also be pointed out that the probabilistic nature of the catastrophic spill of toxic chemicals, during transportation and in storage, is not considered here. That is, the frequency of shipment and cargo size of each toxic chemical past the nuclear plant site, the accident rates of on-site release and of each shipment type (trucks, rails, barges, etc.), the distribution of wind speeds and directions, and the uncertainty of the weather conditions will not be included in the assessment of vapor concentrations. The accident probabilities of trucks, rails, and barges, per vehicle mile, have been estimated by Directorate of Regulatory Standards. An analysis of the risks in the water transportation of hazardous materials has been made by the Committee on Hazardous Materials. The statistical nature of the hazards to nuclear power plants from surface traffic accidents and from off-site release of toxic vapors has been extensively studied by Hornyik. The risk of catastrophic spill of chlorine during transportation has been investigated by Murphy et al. and Simmons et al.

2. Calculation of Vapor Concentrations in Air

In a postulated accident, it is assumed that the entire container of the toxic substance ruptures. This is the worst case compared with partial ruptures where the content leaks out in a steady flow. Part of the substance will vaporize and diffuse into the atmosphere. The vapor is assumed to form a cloud or a plume, which will disperse into the atmosphere and, simultaneously, move toward the control room air intake. The vapor concentration is further reduced by dilution with the air in the control room ventilation system.

Any interaction that can take place rapidly between the spilled substance and the environment (air, earth, water) must be identified and evaluated. For example, fast chemical reactions may generate toxic gaseous products, or may reduce the hazard of the spilled substances.

2.1 Mass Transfer

The volatility of a substance is a direct function of its vapor pressure. Most solid substances have relatively low vapor pressures at a high ambient temperature of 40°C. Compressed gases, liquefied gases, and many liquids have sufficiently high vapor pressures, so that, when released to the atmosphere, they will either vaporize or evaporate. For compressed and liquefied gases and those liquids whose normal boiling points are far below the ambient temperature, instantaneous flashing (rapid formation of a cloud) will first take place. The remaining liquid will vaporize by drawing heat from the surroundings. On the other hand, if the normal boiling point is above the ambient temperature, the liquid will evaporate into the atmosphere.

2.1.1 Surface Area of a Spill

The rate of mass transfer, i.e., vaporization or evaporation, of a liquid into the atmosphere is, among other things, directly proportional to the surface area of the spill. Let us approximate the initial shape of the liquid body by a cylinder, with the height equal to the radius of the base. The liquid spreads quickly by gravity to a thin pancake on ground. Its surface area, A , may be estimated by the following equation (Van Ulden):

$$A(t) = \pi \left\{ r_0^2 + 2t \left[\frac{gV_0(\rho_l - \rho)}{\pi \rho_l} \right]^{1/2} \right\} \quad (2.1-1)$$

$$\text{and } V_0 = \pi r_0^3 \quad (2.1-2)$$

where

r_0	=	initial radius of the spill	(cm)
g	=	gravitational constant	= 981 (cm/sec ²)
V_0	=	volume of the spill	(cm ³)
ρ_l	=	density of the liquid or gas	(g/cm ³)
ρ	=	density of air	(g/cm ³)
t	=	time	(sec)

To be sure, the rate of area spread depends on the surface tension, viscosity, and density of the liquid. A more sophisticated formula should be developed to include these physical properties. At present, eq. (2.1-1) is adopted as a first approximation for the spill area. Equation (2.1-1) also neglects the mass loss, atmospheric turbulence, and temperature and wind effects. Note that V_0 is the volume of the liquid spill remaining after instantaneous flashing to puff has taken place.

The surface area, however, does not in reality expand indefinitely as eq. (2.1-1) indicates. During vaporization and evaporation, the liquid continuously loses mass, and hence the total volume reduces with time. Thus, the liquid will attain a maximum surface area at some time depending upon the mass transfer rate. If the spill occurs on a surface that will restrict the spread of the spill under all postulated accident conditions, e.g., inside a building or within a domed area, then the maximum area of the spill can be calculated. In most cases, the condition of the ground cannot be described accurately, and therefore, the maximum area of the spill cannot be easily computed. In these cases, the maximum area of spill is estimated from the initial volume by assuming a spill thickness of 1 cm. It is believed that this minimum thickness is realistic and still conservative.

2.1.2 Vaporization of Low-Boiling-Point Liquids and Compressed Gases

For the liquids and compressed gases whose normal boiling points are lower than the ambient temperature, the heat balance in the instantaneous puff formation is given by the following equation:

$$m_T C_p (T_o - T_b) = m_{vo} H_v \quad (2.1-3)$$

where

- m_T = total initial mass of the liquid (g)
- C_p = heat capacity of the liquid (cal/g°C)
- T_o = ambient temperature (°C)
- T_b = normal boiling point of the liquid (°C) < T_o
- m_{vo} = mass of the instantaneously vaporized liquid (g)
- H_v = heat of vaporization of the liquid (cal/g)

For compressed gases such as liquid nitrogen and helium, T_0 should be the actual storage temperature of the liquid. For other gases and liquids, it is assumed that they have attained the ambient temperature before the instantaneous flashing takes place. The ratio m_{V0}/m_T is the maximum fraction of the liquid which forms the instantaneous puff.

2.1.2.1 Atmospheric and Solar Radiation

The remaining liquid, $(m_T - m_{V0})$, will vaporize by absorption of heat from atmospheric (long-wave) radiation and solar (short-wave) radiation, convection of air, and ground conduction. Reflection of radiation by the liquid surface and re-emission of radiation by the liquid body are ignored here, as quantitative treatment on these two subjects is lacking for various liquids except water (Koberg; Patterson et al.). If the liquid is spilled inside a building, the direct solar radiation may be disregarded.

The atmospheric and solar radiation fluxes may be computed using the existing formulas (Koberg; Patterson et al.). However, there is more confidence in employing the observed or empirical data available in the literature. The maximum expected solar and atmospheric radiation fluxes at various north latitudes (30° to 45°) for each month of the year have been tabulated (Langhaar; Perry and Chilton, 12-21). These clear-day values include direct and scattered radiation on a horizontal surface, and are based on analyses of Weather Bureau records for a number of states throughout the United States. Both the daily average and noon values are presented. The highest value is $275 \text{ cal/m}^2\text{-sec}$ at noon on June 1 and July 1 at 30°N . On cloudy days, the clear-day fluxes are

reduced by $(0.61S + 0.35)$, where S = number of hours of sunshine divided by the total number of possible sunshine (Fritz and MacDonald).

The atmospheric and solar radiation fluxes have also been experimentally measured at various locations in the southwestern region, i.e., latitude 27°N to 40°N (Fritz and MacDonald; Koberg). These values are daily averages for everyday of each month. The maximum values are (at Roosevelt Reservoir, AR) $115 \text{ cal/m}^2 - \text{sec}$ and $97 \text{ cal/m}^2 - \text{sec}$ for atmospheric and solar radiation, respectively.

It may be interesting to compare the experimental data of the atmospheric radiation flux with a calculated value using the following modified Brunt's formula (Koberg):

$$q_{LW} = \sigma_{SB} (C_1 + 0.0263 \sqrt{p_{H_2O}}) (T_a + 273)^4 \quad (2.1-4)$$

where q_{LW} = atmospheric radiation flux ($\text{cal/m}^2 \text{ sec}$)

σ_{SB} = Stefan - Boltzmann constant = 1.355×10^{-8}
 $\text{cal/m}^2 \text{ sec } ^{\circ}\text{K}^4$

T_a = ambient temperature ($^{\circ}\text{C}$)

C_1 = 0.735 for $T_a > 34^{\circ}\text{C}$

p_{H_2O} = vapor pressure of water (mbar)

For $T_a = 40^{\circ}\text{C}$ and assuming 50% relative humidity in air, $p_{H_2O} = 38.3$ mbar (List p. 347). q_{LW} is computed to be $117 \text{ cal/m}^2 \text{ sec}$, which is comparable to the experimental value cited above.

2.1.2.2 Forced Convection of Air

The heat flux, q_c , due to forced convection of air over the spill is:

$$q_c = hc (T_a - T_b) \quad (2.1-5)$$

where hc is the heat transfer coefficient ($\text{cal/m}^2 \cdot \text{sec} \cdot ^\circ\text{C}$).

The heat transfer coefficient of air blowing over a flat surface has been computed (Bolz and Tuve, p. 538) for a mean air temperature of 21°C . The computation was based on the following heat transfer equation:

$$h_c = (\text{constant}) \frac{k}{L} \left(\frac{L u \rho}{\mu} \right)^{0.6} \left(\frac{C_a \mu}{k} \right)^{0.3} \quad (2.1-6)$$

where k = thermal conductivity of air at T_a ($\text{cal/cm sec } ^\circ\text{C}$)

L = characteristic length (m)

u = wind velocity (m/sec)

μ = viscosity of air (g/cm sec)

C_a = heat capacity of air ($\text{cal/g } ^\circ\text{C}$)

ρ = density of air (g/cm^3)

The computed values of hc are tabulated for several assumed wind velocities (Bolz and Tuve). The value extrapolated for the wind velocity of 1 m/sec is $1.6 \text{ cal/m}^2 \text{ sec } ^\circ\text{C}$.

2.1.2.3 Earth Conduction

The heat transfer by earth conduction, q_d , is given by the following equation (Bird et al., p. 354),

$$q_d = k_E (T_E - T_b) [\pi k_E t / \rho_E C_{PE}]^{-1/2}$$

where k_E = thermal conductivity of earth's crust ($\text{cal/cm sec } ^\circ\text{C}$)

ρ_E = density of earth's crust (g/cm^3)

C_{PE} = heat capacity of earth's crust ($\text{cal/g } ^\circ\text{C}$)

t = time (sec)

T_E = ground temperature ($^{\circ}\text{C}$)

The average thermal conductivity of earth's crust is 4×10^{-3} cal/cm sec $^{\circ}\text{C}$ (Lange, p. 1503). This may be compared with the thermal conductivities of limestone, sandstone, and granite, which range from 1.36×10^{-3} cal/cm sec $^{\circ}\text{C}$ to 9.5×10^{-3} cal/cm sec $^{\circ}\text{C}$ (Weast, E-3). The overall average density of earth's crust of various consistencies (dry, moist, mud, loose, and packed) is 1.52 g/cm^3 (Perry and Chilton, 3-90). The heat capacities of several substances resembling earth's crust (clay, granite, limestone, sand, stones, and bricks) vary from 0.191 to 0.224 cal/g $^{\circ}\text{C}$ (Perry and Chilton 3-136).

Using $k_E = 4 \times 10^{-3}$ cal/cm sec $^{\circ}\text{C}$, $\rho_E = 1.52 \text{ g/cm}^3$, and $C_{pE} = 0.2$ cal/g $^{\circ}\text{C}$, eq. (2.1-7) becomes

$$q_d = 197 (T_E - T_b)/t^{1/2} \quad (\text{cal/m}^2\text{-sec}) \quad (2.1-8)$$

2.1.2.4 Vaporization Rate

The rate of total heat transfer, in cal/sec, of the remaining liquid after instantaneous flashing is given by the following equation

$$\frac{dQ}{dt} = A (t) (q_r + q_c + q_d) \quad (2.1-9)$$

$$= A (t) \{ q_r + h_c (T_a - T_b) + 197 (T_E - T_b)/t^{1/2} \} \quad (2.1-10)$$

where q_r = solar and atmospheric radiation fluxes.

The vaporization rate, (dm_v/dt) , in g/sec, is then

$$(dm_v/dt) = \frac{1}{H_v} \left(\frac{dQ}{dt} \right) \quad (2.1-11)$$

$$= \frac{A(t)}{H_v} \{ q_r + h_c (T_a - T_b) + 197 (T_E - T_b)/t^{1/2} \} \quad (2.1-12)$$

where m_v = mass of the vapor.

2.1.3 Evaporation of Normal-Boiling-Point Liquids

When exposed to the atmosphere, the liquids with normal boiling points above the ambient temperature will evaporate by diffusion into the air. The main driving force here is the vapor pressure difference, i.e., concentration gradient, between the liquid phase and the air. As the liquids may be spilled in either a confined area with or without ventilation, or in an open area with wind blowing over the liquid surface, the appropriate formula for the mass transfer in each case will be presented.

2.1.3.1 Gaseous Diffusion in Still Air

The rate of a vapor diffusing into still air may be computed from the Fickian diffusion equation (Bird et al., p. 596) :

$$(dm_v/dt) = \frac{A(t) p_{pv} 10^4}{P} \left(\frac{D}{\pi t}\right)^{1/2} \frac{g}{\text{sec}} \quad (2.1-13)$$

where $A(t)$ = surface area of the spill at time, t , (m^2)

p = vapor pressure of the liquid (mm Hg)

P = ambient atmospheric pressure (mm Hg)

p_v = vapor density of the liquid (g/cm^3)

D = diffusion coefficient of the liquid into air (cm^2/sec). The experimental values of D for a number of compounds diffusing into air have been tabulated (Bolz and Tuve, p. 546; Perry and Chilton, 3-222). They vary from 0.03 to 0.2 cm^2/sec . The diffusion coefficient, D_{AB} , of a gas A diffusing into a gas B may also be estimated by the following formula (Bird et al., p. 511; Reid & Sherwood, p. 523; Perry and Chilton, 3-230) (see also Sissom and Pitts, p. 189):

$$D_{AB} = 0.0018583 \frac{(T_a + 273)^{3/2} \left(\frac{1}{M_A} + \frac{1}{M_B}\right)^{1/2}}{P \sigma_{AB}^2 \Omega_{AB}} \quad (2.1-14)$$

where M_A = molecular weight of gas A (g/mole)

M_B = molecular weight of gas B (g/mole)

P = atmospheric pressure (atm)

σ = Lennard - Jones parameter

Ω_{AB} = dimensionless function of temperature and intermolecular potential field E_{AB}

The Lennard-Jones parameter is empirically estimated to be an arithmetic mean of the two gases:

$$\sigma_{AB} = (\sigma_A + \sigma_B) / 2 \quad (2.1-15)$$

The intermolecular potential field is empirically estimated to be a geometric mean of the two gases:

$$E_{AB} = (E_A E_B)^{1/2} \quad (2.1-16)$$

The values of σ , E , and Ω for a few compounds are available in the literature (Bird et al, p. 744; Reid and Sherwood, p. 524, p. 632).

Eventually, the air space in the confined building will be saturated with the toxic vapor of the spill, and the vapor concentration will approach the following value (assuming ideal-gas behavior of the vapor):

$$C_s = \frac{P_s M}{R_g (T_a + 273)} \quad (2.1-17)$$

where C_s = saturation concentration (g/cm³)

R_g = universal gas constant

M = molecular weight of the liquid (g/mole)

T_a = ambient temperature (°C)

P_s = saturation vapor pressure of the liquid (mm Hg)

This would be the maximum vapor concentration of a liquid that is spilled in a confined space, such as a basement.

2.1.3.2 Mass Transfer by Forced Convection

The evaporation of a liquid in an open space with wind or in a confined area with good ventilation can be described as a mass transfer process by forced convection.

The evaporation rate may be calculated by the following formulas (Eckert and Drake, pp. 470-476):

$$(dm_v/dt) = h_d M A(t) (P_s - P_a)/R_g (T_a + 273) \quad (2.1-18)$$

where, for a laminar flow (Eckert and Drake, pp. 176, 177, 475):

$$h_d = 0.664 \frac{D}{L} (Re)^{1/2} (Sc)^{1/3} \quad (2.1-19)$$

and for a turbulent flow (Eckert and Drake p. 215):

$$h_d = 0.037 \frac{D}{L} (Re)^{0.8} (Sc)^{1/3} \quad (2.1-20)$$

Re = Reynold number = L u ρ/μ

Sc = Schmidt number = μ/Dρ

h_d = mass transfer coefficient (cm/sec)

R_g = universal gas constant

D = diffusion coefficient (cm²/sec)

u = wind speed (cm/sec)

ρ = density of air (g/cm³)

L = characteristic length (cm)

μ = viscosity of air (g/cm sec)

M = molecular weight of the liquid (g/mole)

P_s = saturation vapor pressure of the liquid at temperature
 T_a (mm Hg)

P_a = actual vapor pressure of the liquid in air (mm Hg)

For water, P_a may be computed from the relative humidity (List, p. 347). For other liquids, P_a would normally be zero.

The diameter of the spill area may be taken as the characteristic length, L . The spill area and thus the characteristic length vary with time (eq. (2.1-1)).

2.1.4 Comparison of Calculations With Empirical Data

A few calculations of evaporation rates are compared with the available empirical data. However, the empirical observations were made on evaporation of water from confined sources, such as pools and ponds, where the surface areas are already fixed. Therefore, it is not possible to check the dynamic process of simultaneous spreading and evaporation of the liquid.

2.1.4.1 Annual Evaporation of Water

The annual evaporation of water from a standard evaporation pan of the Weather Bureau has been measured at many stations throughout the United States. The data for the period of 1946-1955 have been collected (Kohler et al.).

The annual mean temperatures, wind speeds, and relative humidities of several geographic regions of the United States have been compiled (Lerner, pp. 182-193). Using this information, it is possible to calculate the annual evaporation of water by eqs. (2.1-18) and (2.1-19). A comparison of the calculated annual evaporation using eq. (2.1-19) (laminar flow) with the experimental data for ten widely separated locations is presented in Table 1. In the calculations, the arithmetic mean of the relative humidities was used for each location, and the characteristic length was 1.2 m (diameter of the standard evaporation pan of the National Weather Service). The agreement is good, with the maximum variation being within a factor of 2.

2.1.4.2 Empirical Formulas for Evaporation of Water

Several formulas for the prediction of evaporation of water from pools have been developed empirically (Chow, 11-4; Merritt; Patterson, et al.; Davis and Sorensen). These are summarized in Table 2 together with the calculated evaporation rates for water at 38°C with a relative humidity of 10% and wind speed of 1 m/sec. The experimental datum obtained under this condition for evaporation on drying trays (Bolz and Tuve) is also shown. Using $L = 1.2$ m, the evaporation rates computed from eqs. (2.1-18) and (2.1-19) (laminar flow) are also presented in Table 2.

The empirical formulas predict evaporation rates ranging from 0.070 to 0.44 $\text{g/m}^2 \text{ sec}$, with an average of 0.26 $\text{g/m}^2 \text{ sec}$. The agreement between the empirical formulas and the experimental value, and hence eqs. (2.1-18) and (2.1-19), is within a factor of 2 in most cases. The empirical

Table 1 Comparison of Calculated Evaporation Rates
of Water With Experimental Data*

Location	Annual Average Temperature (°C)	Annual Average Wind Speed (cm/sec)	Average Relative Humidity (%) High-Low	Annual Evaporation (cm)	
				Experimental	Eq. (2.1-19)
Phoenix, AR	21.3	268	53-32	183	179
Los Angeles, CA	16.5	277	75-53	117	85
Denver, CO	11.1	402	69-41	81	91
Louisville, KY	13.1	371	81-59	91	66
New Orleans, LA	20.2	375	88-63	124	84
Portland, ME	7.2	393	80-60	61	46
Albuquerque, NM	13.8	398	57-37	137	126
Bismark, ND	5.2	478	78-56	86	49
El Paso, TX	17.4	434	52-35	183	177
Seattle, WA	10.6	420	83-74	61	43

*Data for annual average temperatures, wind speeds, and relative humidity obtained from Lerner, pp. 182-193. Data for annual evaporation from Kohler et al.

Table 2 Comparison of Calculated Evaporation Rates
of Water by Several Formulas

Ambient Temperature = 38°C

Relative Humidity = 10%

Wind Speed = 1 m/sec

<u>Formula</u>	<u>Equation</u>	<u>Evaporation Rate</u> <u>(g/m² sec)</u>
FitzGerald	$E = (0.4 + 0.199 w) (ps - pa)$	0.44
Meyer, small pool:	$E = 0.5 (1 + 0.1 w) (ps - pa)$	0.32
large reservoir:	$E = 0.37 (1 + 0.1 w) (ps - pa)$	0.23
Horton	$E = 0.4 \{ps [2 - \exp(-0.2w)] - pa\}$	0.29
Rohwer	$E = 0.771 (0.44 + 0.118w) (1.465 - 0.0186P)$ $(ps - pa)$	0.26
Harbeck	$E = 0.0599 w (ps - pa)$	0.070
Patterson	$E = 0.345 (1 + 0.1w) (ps - pa)$	0.22
Kohler, Davis	$E = (0.37 + 0.1 w) (ps - pa)^{0.88}$	0.29
<u>Experimental</u>		
Bolz and Tuve	Drying trays	0.15
Eq. (2.1-19)		0.14

E = evaporation rate (inches/day)

w = wind speed (miles/hr)

P, ps, pa in inches Hg.

expressions do not account for the ambient temperature, except through its influence on vapor pressures, or for the reservoir size. Both of these factors are accounted for in eqs. (2.1-18) and (2.1-19). Under these circumstances, it is not expected that the agreement between the empirical expressions and eqs. (2.1-18) and (2.1-19) to be better than a factor of 2.

2.2 Vapor Dispersion

The vapor from instantaneous flashing (puff) and from continuous vaporization or evaporation (plume) moves in the direction of the wind and disperses by diffusion into the atmosphere. The dispersion is assumed to follow a Gaussian distribution for short travel times (a few minutes to one hour). That is, an individual puff may or may not be well-described by a Gaussian formulation, but an ensemble of puffs is assumed to disperse in a Gaussian function. This diffusion model is applicable only to the vapors whose densities do not differ greatly from that of air (Slade). The wind is assumed to be in the direction from the source of spill to the control room air intake. It should be noted that topological variations of the terrain between the source and receptor are ignored in this treatment.

2.2.1 Instantaneous Puff Release

The diffusion equation for an instantaneous puff with a finite initial volume and a receptor at the air intake is given by the following equation (Yanskey, et al., 3-2; Slade, p. 115):

$$\chi(x, y, z, h) = \frac{Q}{(2\pi)^{3/4} \sigma_{XI} \sigma_{YI} \sigma_{ZI}} \cdot \exp \left\{ -\frac{1}{2} \left[\frac{x^2}{\sigma_{XI}^2} + \frac{y^2}{\sigma_{YI}^2} \right] \right\} \\ \cdot \left\{ \exp \left[-\frac{1}{2} \frac{(z-h)^2}{\sigma_{ZI}^2} \right] + \exp \left[-\frac{1}{2} \frac{(z+h)^2}{\sigma_{ZI}^2} \right] \right\} \quad (2.2-1)$$

Where χ = concentration (g/m^3)

Q = source strength (g) = m_{V0}

σ_{XI} , σ_{YI} , σ_{ZI} = adjusted standard deviations of the puff concentration in the horizontal along-wind (X), horizontal cross-wind (Y), and vertical cross-wind directions (Z), respectively (m).

x , y , z = distances from the puff center in the X, Y, and Z directions, respectively (m). z is also the effective above-ground elevation of the receptor, e.g., the fresh-air intake of a control room.

h = effective above-ground elevation of the source.

To account for the initial volume of the puff, it is assumed that

$$\sigma_{XI}^2 = \sigma_{XI}^2 + \sigma_0^2 \quad (2.2-2)$$

$$\sigma_{YI}^2 = \sigma_{YI}^2 + \sigma_0^2 \quad (2.2-3)$$

$$\sigma_{ZI}^2 = \sigma_{ZI}^2 + \sigma_0^2 \quad (2.2-4)$$

$$\sigma_{XI}^2 = \sigma_{YI}^2 \quad (2.2-5)$$

and letting $x = x_0 - ut$ (2.2-6)

$$\sigma_0 = \left[m_{V0} / (2^{1/2} \pi^{3/2} \rho_V) \right]^{1/3} \quad (2.2-7)$$

where

σ_0 = initial standard deviation of the puff (m)

σ'_{XI} , σ'_{YI} , σ'_{ZI} = standard deviation of puff concentration in the

X, Y and Z directions, respectively (m)

m_{v0} = mass of the instantaneously released puff (g)

ρ_v = density of the puff (g/m^3)

x_0 = ground distance between the source of spill and receptor (m)

u = wind speed (m/sec)

t = time after release (sec)

Then, eq. (2.2-1) may be used for the calculation of the center-line concentration where $y = 0$.

The fresh air intakes in nuclear power plants are usually situated on the top or sides of a building. To account conservatively for building effects on the puff dispersion, eq. (2.2-1) is modified as follows.

For the vapors much heavier than air,

$$z = h = 0 \quad (2.2-8)$$

and for the vapors lighter than air, h is replaced by z in eq. (2.2-1).

2.2.2 Continuous Plume Diffusion

The diffusion equation for the continuous release of a plume with a finite initial volume and a receptor at z above the ground level is given by the following equation (Yanskey et al., 3-39; Slade, p. 99):

$$\chi(x,y,z,h) = \frac{Q'}{2\pi u \sigma_Y \sigma_Z} \exp \left\{ -\frac{y^2}{2\sigma_Y^2} \right\} \left\{ \exp \left[-\frac{(z-h)^2}{2\sigma_Z^2} \right] + \exp \left[-\frac{(z+h)^2}{2\sigma_Z^2} \right] \right\} \quad (2.2-9)$$

where

σ_Y, σ_Z = standard deviations of the plume concentration in the Y and Z directions, respectively (m)

Q' = continuous source strength (g/sec)

To give credit for the finite initial size of the spill, σ_Y here is replaced by $(\sigma_Y^2 + \sigma_{Y_0}^2)^{1/2}$, where σ_{Y_0} is the effective width of the spill. Although the distribution of a circular spill of a liquid in the cross-wind direction is not a normal function (it is of the form $p = (1 - F^2)^{1/2}$, where $-1.0 \leq F \leq 1.0$), σ_{Y_0} may be approximated by the following method (Turner):

$$\sigma_{Y_0} \cong r \pi^{1/2} / 4.3 \quad (2.2-10)$$

where r = radius of the spill. Similarly, σ_Z may be replaced by $(\sigma_Z^2 + \sigma_{Z_0}^2)^{1/2}$. However, σ_{Z_0} may be assumed to be zero since it is usually very small.

If r and Q' change significantly with time, they should be replaced by their mean values over suitably short time intervals. Then the concentration calculations can be carried out with constant r and Q' over each time interval.

Again, to account conservatively for building wake and plume bypass around the receptor, it is assumed that, for the vapors much heavier than air, $z=h=0$, and for the vapors lighter than air, h is replaced by z in eq. (2.2-9).

2.2.3 Standard Deviations and Stability Conditions

The average curves of σ_Y and σ_Z as a function of down-wind distance have been constructed for various weather stability categories (Hilsmeier and Gifford). The stability categories, i.e., the Pasquill's types of weather condition, are defined as:

Pasquill's Stability Category

Weather Condition

A	extremely unstable
B	moderately unstable
C	slightly unstable
D	neutral
E	slightly stable
F	moderately stable
G	extremely stable

The curves for types E and F for release from a few minutes to 10 minutes are available in the reference (Hilsmeier and Gifford). These conditions encompass the worst expected situation for nearly all the nuclear power plant sites. The type G curve has been constructed by extrapolation (Yansky et al., 3-6). Calculations that are based on the type G curve are likely to be extremely conservative.

Although the Pasquill-Gifford curves are appropriate only for plumes, they may be assumed to be applicable for estimating the puff dispersion coefficients. Alternatively, the power function approximations of Islitzer and Slade (Slade, p. 175) may be used for the distance from 100 m to 4 km. The power function approximations, shown below, give much smaller dispersion coefficients than the Pasquill-Gifford curves. Note that all these standard deviation curves and functions may not be applicable to distances shorter than 100 meters.

Weather Condition	σ_{YI}	σ_{ZI}
Unstable	0.14 (x) ^{0.92}	0.53 (x) ^{0.73}
Neutral	0.06 (x) ^{0.92}	0.15 (x) ^{0.70}
Very stable	0.02 (x) ^{0.89}	0.05 (x) ^{0.61}

2.3 Control Room Air Exchange

The ventilation layout of the reactor control building varies from plant to plant. Conservatively, it is assumed that the outside air enters directly into the control room through an air intake. The dilution factor, F, is given by:

$$F = 1 - \exp(-W\tau/V_r) \quad (2.3-1)$$

where

W = air flow rate in control room (m³/sec)

V_r = control room air space (m³)

τ = time duration (sec)

2.4 Summary of Vapor Concentrations Calculations

2.4.1 Calculation of Concentration

The concentration of the toxic chemical, C_o, in g/m³, at the air intake just outside the control room is the sum of the puff and plume concentrations at any instant. The concentration, C_o, at the outside air intake at time t_i is

$$C_o(t_i) = m_{v, \text{puff}}(x/Q)_{t_i} + (dm_v/dt)_{t_i, \text{plume}}(x/Q) \quad (2.4-1)$$

The concentration build-up inside control room C_r, in g/m³, at time t_i is

$$C_r(t_i) = C_r(t_{i-1}) + [C_o(t_i) - C_r(t_{i-1})] [1 - \exp(-W\tau/V_r)]$$

where $\tau = t_i - t_{i-1}$

(2.4-2)

2.4.2 Summary of Conservatism

In summary, the present method of estimating the vapor concentration of a toxic chemical in the control room following a postulated accidental release, contains several conservative assumptions. Among them are the following:

1. The entire inventory or cargo in one container is released;
2. The area of the spill is predicted by eq. (2.1-1), with a minimum thickness of 1 cm;
3. The vapor, in the form of a puff or plume, moves directly toward the air intakes of the control room;
4. The center-line concentration of the vapor is calculated using the formulas in section 2.2.

The following values may be assumed in the calculation of vapor concentration using the formulas in this report:

Diffusion coefficient (if not available), D	0.2 cm ² /sec
Solar and atmospheric radiation fluxes	275 cal/m ² -sec
Air exchange rate in control room (if not known),	
W/V _r	1/hr

The site meteorological parameters, based on the available data, should be used. It is recommended that a few combinations of the ambient temperatures, Pasquill types, and wind speeds be assumed to give the most conservative assessment of the toxic vapor concentrations. A plot of the

vapor concentration inside the control room as a function of time after the postulated chemical spill should be helpful.

3. Toxic Substances

3.1 General Considerations

There are six broad classes of chemical substances that are hazardous to human beings, namely, toxic, asphyxiate, explosive, corrosive, flammable, and radioactive substances. When an explosive or flammable material is accidentally released, it is highly likely to explode or burn before its vapor reaches the control room. For this reason, only those substances whose toxicity limits are less than their lower limits of explosion and flammability will be considered for control room habitability here.

A list of these chemicals is presented in the Appendix. An earlier list was published by the Committee on the Safety of Nuclear Installations. The present list is by no means inclusive, but is representative of the substances that may be encountered. Some of these substances have been reported to be stored or transported at or near nuclear power plants. This information was obtained from applications of construction permits of nuclear power plants, as received by U. S. Nuclear Regulatory Commission, and from British Chemical Industry, Jones Bardelmeier and Company, Ltd., National Academy of Sciences, Navaz, and Simmons et al. Following the suggestion of the Danish Ministry of the Environment (Steering Committee), a number of the chemical agents reported to be potentially usable for warfare are also included in the list (Department of Defense, Hersh, Prentiss, Rothschild). Radioactive materials, however, are excluded.

It should be noted that any chemical which can generate airborne toxic products by chemical reactions or otherwise, should also be classified as a potential toxic substance. Metallic sodium and potassium are good examples. The so-called binary gas system of chemical warfare is another case in point. However, the probability of coincidental release and reacting of two such chemicals in the same vicinity has, in the review to date, been so low that the event need not be considered here.

It may be desirable to compile and tabulate the inventory and application purpose(s) of each chemical substance that is stored and transported regularly at and/or near all the nuclear reactor installations. This is not attempted here, as each nuclear power plant will be reviewed on a case-to-case basis.

3.2 Sources of Physical Data

Included in Appendix are the physical properties that are necessary for the calculations of vapor concentration in the control room after a postulated accidental release, as discussed in Section 2. These physical data were taken mainly from handbooks and references (Braker and Mossman, Dean, Dreisbach, Henderson and Haggard, Lange, Perry, Timmermans, Weast). A few were obtained from chemical manufacturers and the Thermodynamic Research Center (Zwolinski).

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Appendix
Physical Properties of Toxic Chemicals

	MW	BP	VD	SG	CP	HV	VP	D	% F.
Acetaldehyde	44.1	20.2	1.52	.783	.51	136.2			4-57
Acetic anhydride	102.1	140.0	3.52	1.057	.398	92.2	10.		2.7-10
Acetone	58.1	56.2	2.00	.791	.528	128.1	400.	.134	2.5-13
Acetone cyanohydrin	85.1	82.0	2.95	.932			.8		
Acrolein	56.1	52.5	1.94	.841	.511	126.1	475.		2.8-31
Acrylonitrile	53.1	77.3	1.83	.806	.500		225.		3.1-17
Allyl chloride	76.5	45.0	2.64	.938	.313	90.5	650.		
Ammonia	17.0	- 33.4	.597	.674	1.1	327.4			15.5-2
Aniline	93.1	184.4	3.22	1.022	.521	103.7	1.5	.079	1.3-25
Arsine	77.9	- 62.5	2.69	1.604		51.2			
Benzene	78.1	80.1	2.77	0.88	0.419	103.6	190.	0.077	1.2-9.1
Bromine	159.8	58.7	5.5	3.12	.107	44.9	380.	.109	
Bromobenzylcyanide	196.0	242.	6.7	1.47		55.7	0.07		2.0-11.5
Butadiene	54.1	- 4.4	1.92	.621	.545	99.8			
Butanol	74.1	117.5	2.55	.81	.563	141.3	18.	.092	1.4-11.2
Carbon dioxide	44.0	- 78.5	1.53	.468	.184	83.2			
Carbon disulfide	76.1	46.5	2.64	1.293	.241	84.1	625.	.109	1-75
Carbon monoxide	28.0	-191.5	.968	.789	.515	51.6			
Carbon tetrachloride	153.8	76.8	5.3	1.597	.201	47.3	211.	.081	
Chlorine	70.9	- 34.1	2.49	1.570	.226	68.8			
CNB	119.7	75.	4.1	1.14					
CNC	129.6	60.	4.5	1.40			127.		
CNS	144.5	60.	5.0	1.47					
Cresol	108.1	198.	3.72	1.01	.55	102.9	1.		
Cyanogen chloride	61.5	13.1	1.98	1.218		103.		.136	
Diethylamine	73.1	55.5	2.53	.685	.564	96.4	425.	.109	1.8-10.
Dimethylformamide	73.1	153.	2.51	.953		155.4	3.7		
Diphenylchloroarsine	264.5	307.	9.15	1.387		56.6	.0016		
Diphenylcyanoarsine	255.0	290.	8.75	1.32		79.3	.00005		
Diphosgene	197.9	127.	6.9	1.66			10.3		
Epichlorohydrin	92.5	116.1	3.21	1.181			40.		
Ethyl acetate	88.1	77.2	3.04	.895	.459	102.	186.	.0935	2.5-9
Ethyl benzene	106.2	136.2	3.66	.867	.409	95.1	20.	.081	
Ethyl chloride	64.5	12.3	2.22	.924	.368	90.6			3.8-15.4
Ethylchloroarsine	174.9	156.	6.0	1.69		52.5	9.5		
Ethylene dichloride	99.0	83.5	3.35	1.253	.301	77.3	165.		

Appendix
Physical Properties of Toxic Chemicals (continued)

	MW	BP	VD	SG	CP	HV	VP	D
Ethylene oxide	44.1	10.7	1.49	.897	.476	138.5		<i>3.0-100</i>
Ethyl ether	74.1	34.6	2.56	.708	.547	83.9		.0955 <i>1.4-4</i>
Fluorine	38.0	-188.3	1.70	1.503	.367	39.8		
Formaldehyde (37% solution)	30.0	97.0	1.07	1.10			198.	<i>7.0-73</i>
Helium	4.0	-268.9	.137	.125	.86	4.84		
Hexylene glycol	118.2	197.1	4.0	.923	.537	151.	.3	
Hydrazine	32.0	113.5	1.1	1.008	.74	305.	30.	<i>4.7-100</i>
Hydrochloric acid	36.5	- 85.0	1.268	1.194	.90	103.1		
Hydrogen cyanide	27.0	25.7	.947	.687	.627	247.0		.212 <i>6.0-40</i>
Hydrogen fluoride	20.0	19.5	1.27	1.003	.61	80.5		<i>4.3-45</i>
Hydrogen sulfide	34.1	- 60.8	1.19	.993	.478	131.		
Isopropyl alcohol	60.1	80.3	2.07	.785	.78	159.4	106.	.106 <i>2.0-11</i>
Isopropylamine	59.1	32.4	2.03	.694	.385	110.		
Lewisite	207.4	190.	7.2	1.89		58.	1.	
Methanol	32.0	64.7	1.11	.792	.600	262.8	260.	.162 <i>6.5-5</i>
Methyldichloroarsine	160.9	133.	5.5	1.83		49.	10.	
Mustard gas	159.1	227.8	5.4	1.27		94.	.4	
Mustard-lewisite mixture	178.5	190.	6.0	1.66		58.	1.0	
Nitric acid, conc. (70% solution)	63.0	120.5	2.29	1.41	.615	114.9	10.	
Nitrogen	28.0	-195.8	.97	.806	.474	47.5		
Nitrogen mustard (HN-1)	170.1	85.	5.9	1.09		77.	.5	
Nitrogen mustard (HN-2)	156.1	75.	5.4	1.15		78.8	1.16	
Nitrogen mustard (HN-3)	204.5	137.	6.9	1.24		72.	.038	
Pentaborane -9	63.2	58.4	2.2	.61	.571	121.8	400.	
Perchloryl fluoride	102.5	- 46.7	3.73	2.003	.265	45.1		
Phenol	94.1	181.9	3.24	1.058	.561	174.4	1.0	
Phenyldichloroarsine	222.9	252.	7.75	1.65		67.	.113	
Phosgene	98.9	8.2	3.4	1.419	.243	59.0		.117
Phosgene oxime	113.9	53.	4.0					
Propionaldehyde	58.1	48.8	2.0	.806	.522	122.8	560.	
Propylene oxide	58.1	34.3	2.0	.831				
Sarin	140.1	147.	4.86	1.089		84.9	5.5	

Appendix
Physical Properties of Toxic Chemicals (continued)

	MW	BP	VD	SG	CP	HV	VP	D
Soman	182.2	167.	6.33	1.022		78.5	.75	
Styrene	104.1	145.2	3.6	.906	.416	101.7	20.	1.6-6.1
Sulfur dioxide	64.1	- 10.0	2.26	1.46	.361	92.8		
Sulfuric acid	98.1	330.	3.4	1.83	.339	122.1		
Tabun	162.3	246.	5.63	1.073		79.6	.1	
Tetraethyl lead	323.5	200.	11.2	1.659			1.	
Tetramethyl lead	267.3	110.	9.2	1.995			60.	
Toluene	92.1	110.	3.14	.866	.421	98.6	55.	.0924 1.27-7 7
Trichloroethylene	131.4	87.2	4.53	1.466	.223	62.3	140.	2.6-13.4
Vinyl acetate	86.1	72.	3.0	.932	.433	95.2	230.	4-22
Vinyl chloride	62.5	- 13.9	2.15	.920	.38	79.8		
Xylene	106.2	140.0	3.66	.870	.400	96.0	20.	1.1-7.0

60 TOTAL

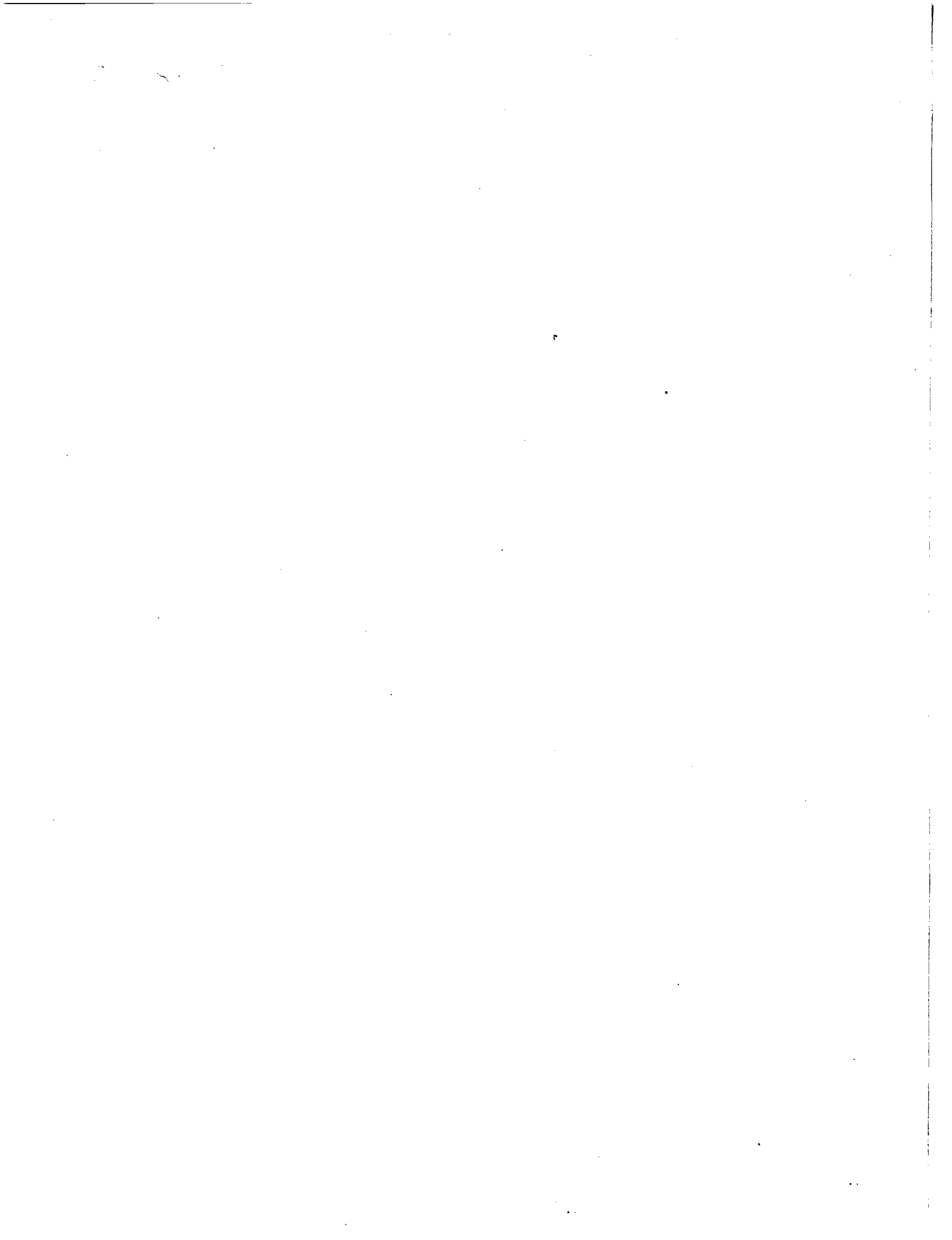
MW = Molecular weight	(grams/mole)
BP = Normal boiling point	(degrees centigrade)
VD = Relative vapor density	(air = 1)
SG = Specific gravity	(grams/cubic centimeter)
CP = Heat capacity of liquid	(calories/gram-degree centigrade)
HV = Heat of vaporization of liquid	(calories/gram)
VP = Vapor pressure at 40 degrees centigrade	(millimeters of mercury)
D = Diffusion coefficient	(centimeter squares/second)

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