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"Source Models"

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Please note: These notes are intended for internal distribution only.

SOURCE MODELS

Introduction

To predict the consequences of accidents we predominantly use three main types of models:

source models,
dispersion models, and
physical effects models.

The source models determine what is released and the dispersion models calculate where it goes to.

The physical effects models refer to the calculation of, for example, toxicity effects thermal radiation levels or significant overpressures.

An important aspect of consequence modelling involves estimating the volume or mass flow rate of material which is likely to be released during an envisaged scenario. In addition the state (liquid, gas, suspended aerosol etc.) of the material after release and its thermodynamic description are required.

Figure 1, from Fryer and Kaiser (1979), shows the many diverse release scenarios. Most of these relate to storage vessels. A further set of scenarios are required for piping arrangements.

Despite the range of scenarios, there are only three basic models required. They are:

mass flow rate from a liquid storage vessel or pipeline
mass flow rate from a gas storage vessel or pipeline
mass flow rate from a boiling or evaporating pool.

Chemical, thermodynamic and fluid flow concepts are used in the development of the models.

It is useful to consider source models in two parts:

(i) a rupture model, and

(ii) a vessel or pipeline response model.

The rupture model typically takes the form of an orifice equation. The response model reflects how conditions change as the vessel or pipeline loses mass.

It is frequently the case that the model required may not be obvious and some intelligent assessment of the problem is required to ensure correct source model selection.

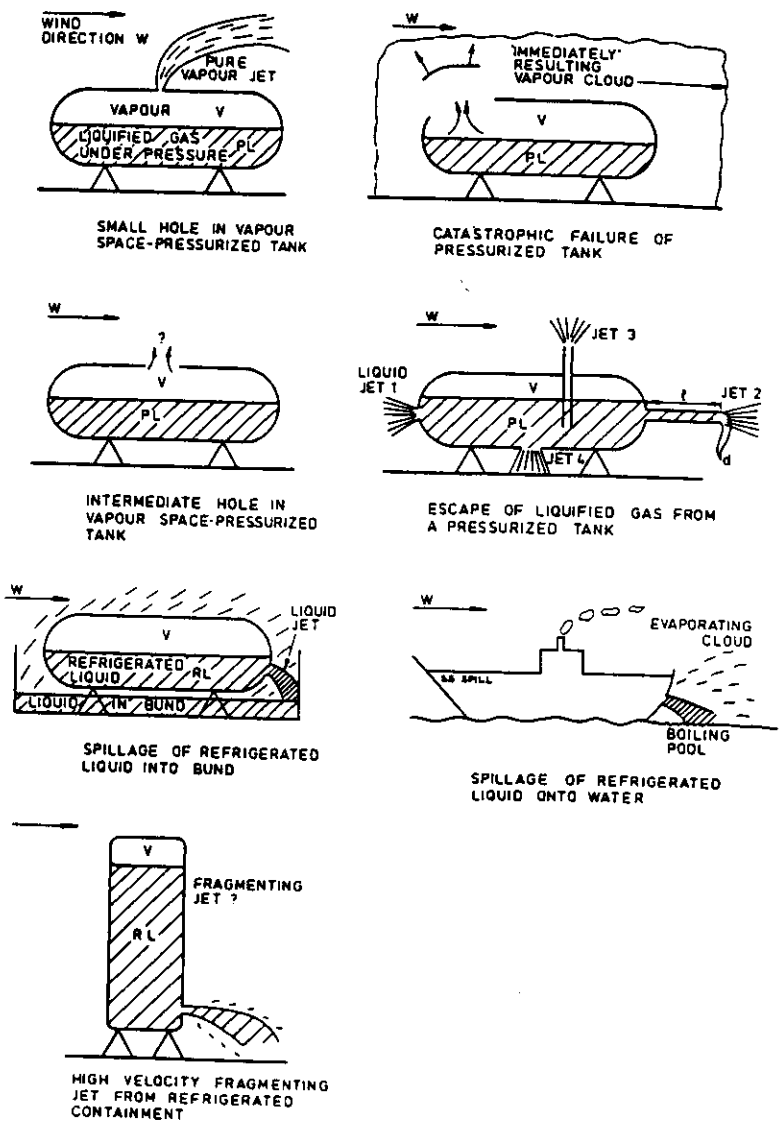


Figure 1 Some conceivable release mechanisms

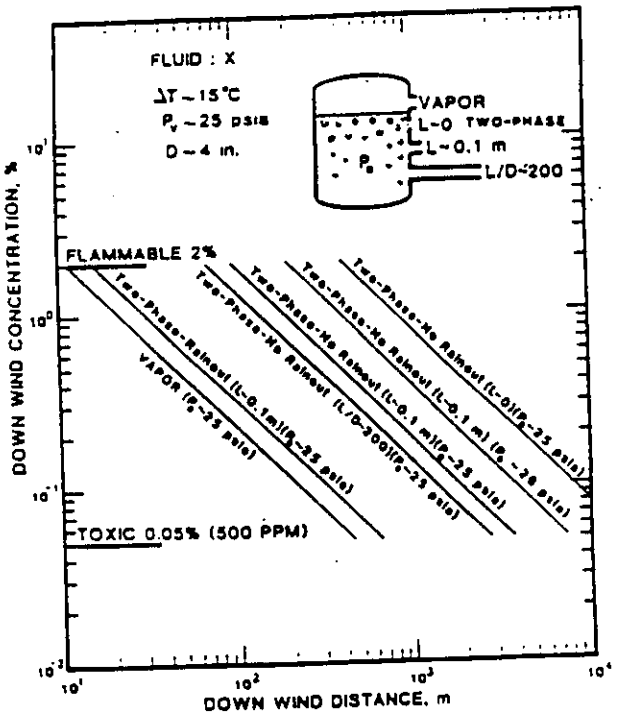


Illustration of source term sensitivity and hazard evaluation.

Figure 2. From Fauske and Epstein (1989)

The importance of correct model selection is shown in Figure 2 where the down-wind concentration (using a simple dispersion model) varies by a factor of 30 between a gas only and a liquid only release.

1. Material is liquid under storage and released (atmospheric) conditions

In the absence of any frictional effects, and assuming quasi-steady flow, Bernoulli's equation may be applied to this incompressible fluid problem.

The exit velocity of the liquid will be given by

$$U = \left(\frac{2(P_1 - P_3)}{\rho_\ell} + 2gH \right)^{\frac{1}{2}}$$

where P_1 is the pressure in the reservoir above the liquid, P_3 is the atmospheric pressure, and H is the height of the free surface above the rupture as shown in Figure 3.

The exit velocity U is the velocity where the streamlines emitted from the rupture are straight and parallel.

The volume flow rate will be

$$Q_\ell = A_{\text{jet}} U,$$

and the mass flow rate

$$\dot{m} = \rho_\ell A_{\text{jet}} U.$$

Due to streamline contraction, A_{jet} can be smaller than the rupture area A and

$$Q_\ell = C_c A U$$

where C_c is a contraction coefficient equal to about 0.6 for a sharp-edged circular rupture and 1.0 for emission from a pipe where there is no contraction.

Additionally there may be some local frictional effects, for example when a short length of pipe (greater than 3 diameters) is attached to a sharp-edged hole. In this case the velocity U is reduced by a factor of about 0.8.

This latter effect and the contraction coefficient are frequently combined to form a discharge coefficient so that

$$Q_\ell = C_D A \left(\frac{2P_1 - P_3}{\rho_\ell} + 2gH \right)^{\frac{1}{2}}$$

where $C_D = 0.6$ for a sharp-edged circular rupture, $C_D = 0.8$ for a small length of pipe attached to a sharp-edged hole, $C_D = 1.0$ for a well-rounded nozzle. The mass flow rate is still given by

$$\dot{m} = \rho_\ell Q_\ell.$$

If there is extensive pipework between the vessel and the rupture the resulting frictional pressure losses may be included in the calculation. These result in a reduced mass flow rate.

The vessel response may be determined by considering how H drops as the liquid is removed and, if appropriate, how the pressure above the liquid responds as the volume there increases. If the rupture is large enough the possibility exists for an exchange flow of liquid and ambient air through the rupture.

Similar calculations may be performed for a rupture at the end of a pipe or in the side of a pipe. Here the pressure and velocity of the flowing liquid need to be considered, as does the pipeline response. For ruptures in the side of pipes, the liquid momentum in the pipe produces a liquid jet which is not normal to the pipe axis.

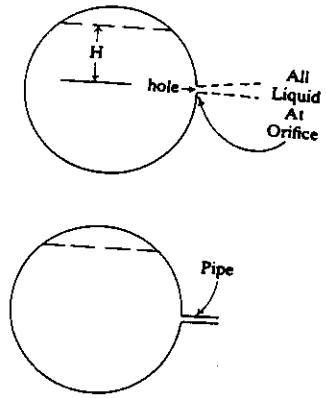


Figure 3

2. Material is gas under storage and released conditions

If the storage or reservoir pressure is quite low, such that the emission velocity is less than about 0.3 times the speed of sound, the gas may be considered incompressible and the results of the previous section are applicable. However, more generally the compressibility of the gas must be taken into account.

We restrict the argument here to perfect gases in the absence of significant frictional and external heating effects and expanding through an orifice from a reservoir whose contents are at rest.

Initially consider the equation for flow through the rupture (orifice). Application of Euler's equation

$$UdU + \frac{dP}{\rho} = 0$$

and the continuity equation

$$\rho AU = \text{constant}$$

will produce a solution for the exit velocity U if the term dP/ρ can be evaluated. The assumption of a reversible (frictionless) adiabatic expansion leads to the flow being isontropic for which the fluid pressure and density are related by

$$P/\rho^\gamma = \text{constant}$$

where γ is the ratio of the fluid specific heats

$$\gamma = C_p/C_v.$$

This result may be combined with the equation of state for a perfect gas

$$P/\rho = \frac{R}{M}T$$

where R is the universal gas constant = 8314 $J/\text{kmole}K$ and M is the molecular weight, to produce the following results. The subscripts 1, 2, 3 used in the following are specifically for different positions:

'1' refers to storage, reservoir or stagnation conditions

'2' refers to conditions just at the orifice

'3' refers to ambient conditions.

Obviously P_1, the reservoir pressure, is larger than P_3, and our interest is in what mass flow rate can be driven through the orifice by the pressure difference between P_1 and P_3.

For a fixed P_1 the mass flow rate increases as P_3 is reduced until a maximum flow rate is achieved. After this no further increase in mass flow rate is experienced as the pressure P_3 is further reduced. This phenomenon is called 'choking'.

Analysis shows that if

$$\frac{P_1}{P_3} < \left(\frac{\gamma+1}{2}\right)^{\gamma/\gamma-1}$$

then the flow is not choked and the pressure at the orifice P_2 equals the ambient pressure P_3. Note that $\left(\frac{\gamma+1}{2}\right)^{\frac{\gamma}{\gamma-1}}$ is typically about 2. If

$$\frac{P_1}{P_3} \geq \left(\frac{\gamma+1}{2}\right)^{\frac{\gamma}{\gamma-1}}$$

then the flow is choked, a maximum mass flow rate is achieved and the pressure at the orifice P_2 is given by

$$P_2 = P_1\left(\frac{2}{\gamma+2}\right)^{\frac{\gamma}{\gamma-1}}.$$

For both cases,

$$\rho_1 = \frac{P_1}{\left(\frac{R}{M}\right)T_1}$$

$$T_2 = T_1(P_2/P_1)^{\frac{\gamma-1}{\gamma}}$$

$$\rho_2 = \rho_1(P_2/P_1)^{1/\gamma}.$$

The resulting velocities at the orifice plane appear in many forms, which can be confusing. One form is

$$\dot{m} = A\rho U$$

$$= A\left(2P_1\rho_1\frac{\gamma}{\gamma-1}\left(\frac{P_3}{P_1}\right)^{2/\gamma}\left(1-\left(\frac{P_3}{P_1}\right)^{\frac{\gamma-1}{\gamma}}\right)\right)^{\frac{1}{2}}$$

for unchoked flow

and

$$\dot{m} = A\left(P_1\rho_1\gamma\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{\gamma-1}}\right)$$

for choked flow.

A somewhat more obvious form is

$$\dot{m} = A\rho_2(2C_p(T_1 - T_2))^{0.5}$$

where T_2 and ρ_2 may be calculated from T_1, ρ_1 and P_2/P_1 from previously.

These results were based on several assumptions and we consider them again.

The frictionless assumption should be applicable for an orifice flow. However, if extensive pipework separates the reservoir from the orifice further, more complex calculations are required of both a fluid mechanical and thermodynamic nature. However the frictionless result will produce the largest mass flow rate.

Some of the thermodynamic aspects of the calculation may be approached by replacing the isentropic expansion coefficient γ with a smaller coefficient k. In a similar way some aspects of non-ideal fluid behaviour can be accounted for by the use of a $k \neq \gamma$.

For gases at very high pressures modifications to the equation of state by inclusion of the compressibility Z may be made.

Finally a discharge coefficient, combining a contraction coefficient and local frictional losses, can be incorporated so that

$$\dot{m} = C_D A\rho_2(2C_p(T_1 - T_2))^{0.5}$$

where a value of $C_D = 0.8$ is frequently used for choked flow.

Further complications will arise when the rupture is from a pipe carrying gas with significant velocity rather than from a reservoir.

The vessel response to the mass efflux will depend upon the heat transferred to the vessel as it cools due to expansion of the contents.

Two limiting cases might be considered. If the expansion is rapid and the vessel is well insulated it will cool, reduce the pressure of the contents and further reduce the mass flow rate. A different view might allow enough heat transfer to maintain the vessel temperature at its initial value. This isothermal case would produce a smaller reduction in the mass flow rate.

This analysis may also be extended to consider a liquid-containing vessel with a vapour space above and with the rupture in the vapour space. Under these conditions the rupture equations are as described earlier, but a more complex analysis is required to consider the boil-off of the vessel contents. Note that under rapid depressurisation the material within the vessel will not remain quiescent but may vigorously boil and foam, leading to liquid ejection even when the liquid is well below the rupture position.

3. Material is liquid under storage conditions and gas under released (atmospheric) conditions

The model required here is one for a rupture within the liquid space but with the possibility of a phase change and a two-phase release: partly liquid, partly gas. Fauske and Epstein (1989) provide correlations for this two-phase flashing release problem (Table 1). G is the mass flux per unit area.

Table 1. Summary of discharge rates and exit conditions
(from Fauske and Epstein 1989)

Flow condition	G	U_2	P_2
Non-equilibrium $L \sim 0$	$\sqrt{2(P_1 - P_3)\rho_\ell}$	G/ρ_ℓ	$P_v(T_1)$
Subcooled $L \sim 0.1$m	$\sqrt{2(P_1 - P_v(T_1)\rho_f}$	G/ρ_ℓ	$P_v(T_1)$
Saturated, no friction $L \sim 0.1$m	$h_{fg}\rho_\ell \left(\frac{1}{TC}\right)^{\frac{1}{2}}$	G/ρ_ℓ	$P_v(T_1)$
Saturated, friction*	$Fh_{f_g\rho_g} \left(\frac{1}{TC}\right)^{\frac{1}{2}}$	$\frac{G}{(\rho_g/x)}$	$FP_v(T_1)$

*F is *flow reduction factor* and *critical pressure ratio* (homogeneous flow)

L/D	F
0	1
50	0.8
100	0.7
200	0.6
400	0.5

The function F can be approximated by $(1 + 4 \times 0.0015 \times L/D)^{-0.5}$.

In the absence of significant frictional losses, the flashing flow through pipes and orifices are generally choked. For two-phase flows the velocity of sound is quite low because the compressibility is linked to the gas properties and the density to the liquid properties. Consequently quite low mass flow rates correspond to choked conditions.

In many cases the pressure at the choke (the rupture position) can be approximated by the vapour pressure corresponding to the reservoir temperature. Fauske and Epstein (1989) adopt this approach for all cases other than when the storage is at saturated conditions and the effects of friction are significant. That is, apart from this last case, the exit pressure is given by $P_v(T_1)$.

For sub-cooled reservoir conditions the mass flow rate is given by one of two formulae.

Under non-equilibrium conditions, when the duct or orifice *length* is approximately zero,

$$\dot{m} = C_D A[2(P_1 + \rho_\ell g H - P_3)\rho_\ell]^{0.5}$$

where H is the distance between the interface and the release height. This result is valid for saturated as well as sub-cooled reservoir conditions.

Under equilibrium conditions, when the duct or orifice length is at least 0.1m, then

$$\dot{m} = C_D A[2(P_1 + \rho_\ell g H - P_v(T_1))\rho_\ell]^{0.5}.$$

For saturated storage conditions with friction but $L \gtrsim 0.1$m the mass flow rate is given by

$$\dot{m} = C_D A \left[F \frac{h_{fg}}{v_{fg}} \left[\frac{1}{T_1 C_{p\ell}}\right]^{0.5}\right]$$

where the properties can be evaluated at the reservoir conditions and $F = (1 + 4 \times 0.0015 \times L/d)^{-0.5}$. This result is invalid if the mass fraction of vapour

$$x > \frac{P_1 v_{fg}}{h_{fg}^2} T_1 C_{p\ell}$$

that is

$$x > \frac{P_1}{v_{fg}} \frac{(C_D A F)^2}{\dot{m}^2}.$$

However, this flow rate determination will be conservative so we may use the result for $\dot{m}$.

The liquid upon release to the atmosphere will flash, i.e. adopt ambient pressure which will be below the saturated vapour pressure. Part of the liquid will change phase to a gas reducing the gas and liquid to the boiling temperature at ambient pressure, that is adopt a temperature such that the saturated vapour pressure at this temperature equals the ambient pressure.

Application of the steady flow energy equation produces the result that the mass fraction of the vapour at exit will be

$$x = \frac{C_{p\ell}(T_1 - T_b)}{h_{fg}}$$

where $C_{p\ell}$ is the specific heat of the liquid, T_1 is the storage temperature, T_b is the temperature at which the saturated vapour pressure is the ambient pressure, and h_{fg} is the latent heat of vaporisation at the ambient pressure.

Of considerable importance here is whether the liquid released 'rains out' or becomes a suspended aerosol. The later consequences of these alternatives is quite profound in determining hazard zones. The flashing can be a very vigorous process which leads to the break up of the liquid into fine liquid droplets that can remain in suspension, evaporating as air is entrained into the two-phase jet. Estimating the fraction of liquid entrained as an aerosol is very uncertain.

4. Material is a liquid spilling onto a surface and then changing phase

There are two limiting cases that can be considered separately. The first is a slowly evaporating pool applicable when the boiling point of the liquid is above the ambient or surface temperatures. Under these circumstances heat transfer will bring the pool to the ambient temperature and there are then light to moderate evaporation rates dependent strongly on the wind blowing over the pool.

For example, the SPILLS model uses conventional chemical engineering correlations to produce

$$\dot{m} = Ak_g \cdot \frac{P_v}{(R/M)T_p}$$

where P_v is the vapour pressure at the pool temperature T_p and R/M is the gas constant. k_g is the mass transfer coefficient whose non-dimensional form is the Sherwood number

$$Sh = \frac{k_g D}{D_m}$$

where D is the pool diameter and D_m is the molecular diffusivity of the vapour in air. The Sherwood number is given by

$$Sh = 0.037 \left(\frac{\nu}{D_m}\right)^{\frac{1}{3}} \left[\left(\frac{UD}{\nu}\right)^{0.8} - 15,200\right]$$

where U is the wind speed and ν the kinematic viscosity of air. Similar correlations are to be found in other models.

The other limiting case is for a boiling cryogen where the boiling point of the liquid is well below the ambient or surface temperature.

Under these conditions, and for a quasi steady-state, the gas evolution rate is directly dependent upon the heat flux into the pool from the surface below, or from any other sources such as solar radiation. Thus

$$\dot{m} = \frac{Q}{\rho_\ell h_{fg}}$$

where Q is the heat input to the pool, ρ_ℓ the liquid density and h_{fg} the latent heat of vaporisation at the boiling temperature. The pool rapidly adopts the boiling temperature (the temperature at which the saturation vapour pressure equals ambient pressure). The heat input to the pool is typically dominated from the surface below and we note that

(i) the area of the pool will greatly influence the gas evolution rate and therefore bunded containers are wise;

(ii) as heat is extracted from the underlying surface it will cool cown and thereby decrease the heat transfer from the surface to the pool. An insulated solid surface will reduce the gas evolution rate markedly. For a spill onto a water surface the motion within the water will always ensure that the heat transfer and consequent gas evolution rates are high.

Where the release produces an intermediate case in which the boiling point of the spill material is about ambient temperature a considerably more complex analysis is required in which the pool temperature is the principal variable. Here the pool adopts a temperature influenced by the heat transfer to the pool and the mass transfer from the pool with a feedback where the transfer rates depend upon the pool temperature. As mentioned earlier, the pool area is of considerable importance in determining the gas evolution rate.

To a first approximation the pool may be treated as a right circular cylinder of changing radius and hieght. The constraints on the flow are that the change of mass of the cylinder is the result of an increase from the source and a decrease due to the gas evolution from the liquid. The problem is closed by specifying a radial velocity of the leading edge of the pool.

For a spill onto a liquid the leading edge velocity is proportional to

$$\left(g\left(\frac{\rho_w - \rho_\ell}{\rho_w}\right)H\right)^{\frac{1}{2}}$$

where ρ_w, ρ_ℓ are the densities of the water and the spilled pool and H is the pool depth. The coefficient of proportionality is normally taken as unity.

For a spill onto land one approach is to take the leading edge velocity proportional to $(gH)^{\frac{1}{2}}$. However this approach is not rigorous and a more complete analysis or situation-specific correlations should be used for the spill onto land. One appropriate, more rigorous approach is to use the shallow-layer equation technique.

Complications arise if the surface is rough (for both land and water waves), when the flow may be surface tension limited and when ice layers may form beneath a cryogenic spill over water. The influences of slopes, porous ground, mixtures of substances, and whether the evolving gas above the liquid pool may inhibit further evaluation also require more specific treatment.

5. The linking of jet source models to jet dispersion models

Jet dispersion models in use for consequence modelling are usually constant pressure models, that is the fluid within the jet is at a constant pressure, the ambient pressure.

However in two of the previous cases studied the mass flow rate exits the rupture at a pressure in excess of the ambient pressure:

(i) for a sonic jet from a choked flow;

(ii) for a liquid release which is at the saturated vapour pressure corresponding to storage conditions but which subsequently flashes.

Consider the first case. There are available in the literature many analyses of the sonic jet as it relaxes back to ambient pressure. The flow is complex and involves shock waves. The results of the analyses differ, sometimes considerably and consequentially.

The following analysis is typical as it attempts to keep the depressurisation of the jet distinct from subsequent entrainment. It assumes perfect gas behaviour (and allows no Joule–Thompson nor vena contracta effects). Application of

the steady flow mass equation
the steady flow momentum equation, and
the steady flow energy equation

produces a depressurised jet velocity (Figure 4)

$$U_3 = U_2 + \frac{P_2 - P_3}{\dot{m}/A}$$
$$T_3 = T_1 - U_3^2/2C_p$$
$$\rho_3 = \frac{P_3}{\left(\frac{R}{M}\right)T_3}$$

and an exit area of the jet

$$A_3 = \frac{\dot{m}}{\rho_3 U_3} = \pi R_3^2$$

where R_3 is the pseudo-diameter.

A difficulty arises in this analysis in that quite low temperatures may be experienced, low enough for the released gas to condense.

For the two-phase release the exit pressure is

$$P_2 = P_v(T_1)$$

where $P_v(T_1)$ is the saturated vapour pressure at the storage temperature, and

$$U_2 = \frac{\dot{m}}{\rho_\ell A_2} .$$

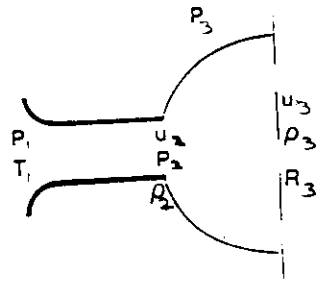
After jet depressurisation

$$U_3 = U_2 + \frac{P_2 - P_3}{\dot{m}/A_2} .$$

The flashing calculation in which the final temperature is the boiling point, T_b, provides the mass fraction of vapour as

$$x = \frac{C_{p\ell}(T_1 - T_b)}{h_{fg}} .$$

Subsequent calculation of the density allows the relevant pseudo-diameter to be calculated for input to a jet dispersion calculation.



Summary of jet expansion model.

Figure 4

where $C_D = 0.6$ for a sharp-edged circular rupture, $C_D = 0.8$ for a small length of pipe attached to a sharp-edged hole, $C_D = 1.0$ for a well-rounded nozzle. The mass flow rate is still given by

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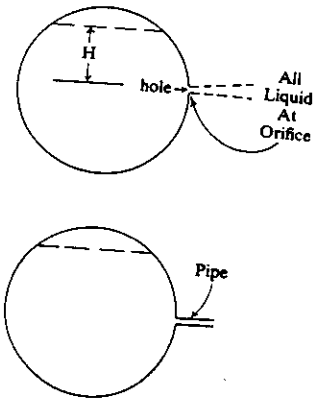
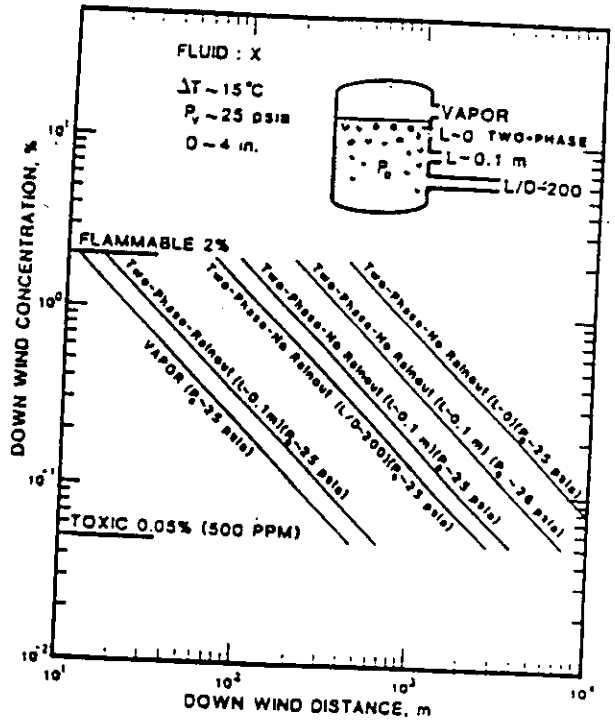


Figure 3



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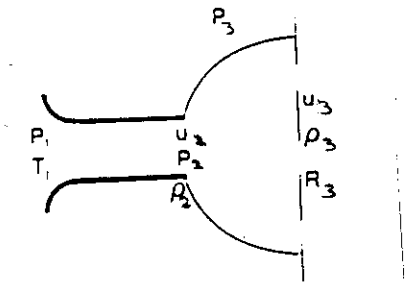

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