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# UNITED KINGDOM ATOMIC ENERGY AUTHORITY SAFETY AND RELIABILITY DIRECTORATE

# Discharge rate calculation methods for use in plant safety assessments

by

P. K. Ramskill

#### SUMMARY

This report reviews the methods which can be used to calculate release rates of fluids (liquid, gas or two-phase) from installations following loss of containment accidents. Such methods are important when a safety assessment of a plant storing hazardous materials is being undertaken.

The subsequent behaviour of the fluid after release is not considered in this report.

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#### 1. INTRODUCTION

When safety studies are carried out on installations handling hazardous materials, failure of plant integrity and the subsequent loss of containment are often important factors to be considered. Possible failure modes need to be identified and material release rates estimated in order to evaluate what the consequences of failure might be.

This report reviews the methods which can be used to evaluate the release rates when loss of containment occurs in certain typical situations. The dispersion and behaviour of the material after the release is not considered here.

Both the state of the contained material and the position of the failure, e.g. pipe break, vessel puncture, are important factors. The methods are thus considered under the following headings:-

- (a) Liquids stored at ambient pressure (including gases held as liquids by refrigeration),
- (b) Gases,
- (c) Superheated liquids stored under pressure (including two-phase discharge).

In practice, there is usually uncertainty about the failure location and conditions, so calculations of release rates cannot be carried out to great precision. By making simplifying assumptions the calculations can be performed manually but care is needed to avoid excessive inaccuracy. A series of worked examples is presented in the text as illustrations of release rate calculations. When doing a safety assessment a range of failure circumstances is generally considered and, after testing the sensitivity of the calculations to these inputs, a set of typical release cases can be derived, which may then form the basis of the assessment.

## 2. LIQUIDS STORED AT AMBIENT PRESSURE (INCLUDING GASES HELD AS LIQUIDS BY REFRIGERATION)

This section details non-flashing liquid flow following a vessel failure. Possible discharge cases are shown in Figs 1-3.

#### Small hole in the liquid space, horizontal or vertical (Fig. 1)

The flow of a liquid is described by incompressible fluid flow theory. This is well covered in many standard texts, e.g. Reference 1. The analysis of the various possible flow cases connected with the incompressible flow of liquid from vessels usually involves the application of Bernoulli's theorem in some form.

The Bernoulli equation, Equation (1), in its general differential form of the energy balance for the flow of unit mass of fluid is:-

$$- dq + dW_s + dH + gdz + d\left(\frac{u^2}{2}\right) = 0$$
 ... (1)

where

g is the acceleration due to gravity

q is the heat absorbed from the surroundings

We is the work done on the surroundings (shaft work)

H is the enthalpy

z is the height above the datum of potential energy

u is the discharge velocity

Equation (1) for finite differences can be shown to be(1):-

$$\int_{1}^{2} v \, dP + F + g\Delta z + \Delta \left(\frac{u^{2}}{2}\right) = 0 \qquad ... (2)$$

where

F is the mechanical energy irreversibly lost by friction

1,2 signify the initial and final states

ν is the specific volume

P is the pressure of the liquid

For a liquid

$$\int_{1}^{2} v \ dP = v \left( P_{2} - P_{1} \right) \qquad ... (3)$$

Assuming negligible frictional loss at the orifice and flow on a horizontal axis, for the flow of non-flashing liquid through a hole which is small compared to the size of the vessel, it can be shown that the mass flow rate is:-

G = Cd Ah 
$$\sqrt{[2 \rho (P_1 - P_2)]}$$
 ... (4)

where

Cd is the discharge coefficient

G is the mass flow rate (kg s-1)

ρ is the liquid density (kg m<sup>-3</sup>)

Ah is the hole area (m3)

The discharge coefficient accounts for friction at the orifice and the reduced cross-sectional area at the vena-contracta. Its value is usually between 0.6 and 1.0.

In the case where the only driving force is the head of liquid in the vessel:-

$$P_1 - P_2 = \rho gh \qquad ... (5)$$

where

h is the head of liquid

g is the acceleration due to gravity

and

$$G = Cd \rho Ah \sqrt{2gh} \qquad ... (6)$$

In the case where a pressurised inert gas, pressure  $P_3$ , is stored above the liquid, the more general form of Equation (6) is:-

$$G = Cd \rho Ah \sqrt{\left[2 \left\{\frac{P_3 - P_2}{\rho} + gh\right\}\right]} \qquad \dots (7)$$

#### 2.2.1 Liquid discharge example

The examples given in this and in following sections use ammonia as the released fluid. To calculate the different discharge rates, thermodynamic properties of ammonia at various temperatures are required. Such data is taken from the thermodynamic tables<sup>(2)</sup> but to allow the reader to clearly follow the worked examples in this report the important properties for ammonia are given in Appendix 1 (Section 6).

Consider ammonia stored under refrigeration at its normal boiling point (- 33°C). If a hole exists in the vessel side below the liquid level, the discharge rate is calculated as follows:-

From thermodynamic tables look up the density of liquid ammonia at - 33°C

$$\rho_{\ell} = 681 \cdot 39 \text{ kg m}^{-3}$$

Take the driving head of liquid ammonia in the tank to be 5 m and the discharge coefficient to be 0.8. Using Equation (6) the discharge rate per unit area is

$$G' = 0.8 \times 681.39 \times \sqrt{2 \times 9.81 \times 5}$$

$$\therefore$$
 G'  $\approx$  5400 kg m<sup>-2</sup> s<sup>-1</sup>

Lewitt<sup>(3)</sup> covers many useful cases of the discharge of liquid from vessels. Derivations of the times to empty a vessel are given in detail. Some useful results are given below but for more detailed discussions the reader is referred to Reference 3.

The time to empty a uniform cross-section tank is:-

$$T = \frac{2 A}{Cd Ah \sqrt{2g}} \sqrt{h} \qquad ... (8)$$

where

A is the cross-sectional area of the tank.

The time to empty a spherical vessel from full is

$$T = \frac{16 \pi r^{\frac{5}{2}}}{15 \text{ Cd Ah } \sqrt{g}} \dots (9)$$

where

r is the vessel radius

### 2.2 Intermediate hole size in vertical side of liquid space (Fig. 2)

If a vertical orifice is large compared to the head of liquid, the velocity of discharge will not be constant over the orifice but will vary due to the change of head at different vertical sections in the orifice. (3) If the breadth of the orifice is B and the height of the liquid level above the top and bottom of the orifice is  $H_1$  and  $H_2$  (respectively) it can be shown that the discharge rate is:-

$$G = \frac{2}{3} \operatorname{Cd} B \sqrt{2 g \rho \left(H_2^{3/2} - H_1^{3/2}\right)} \qquad ... (10)$$

#### 2.3 Discharge from a pipe leading from the liquid space (Fig. 3)

When a break occurs in a pipe leading from the liquid space, energy is dissipated due to frictional losses in the pipe itself and pipe fittings such as bends, valves, contractions, etc.

To calculate the discharge rates in such cases, the usual method<sup>(4)</sup> is to express all the frictional losses in terms of velocity heads. The total head loss is then used to calculate an equivalent discharge coefficient using Equation (11):-

$$Cd = \frac{1}{\sqrt{(1+K)}}$$
 ... (11)

where

K is the total number of velocity head losses.

The frictional head loss due to a straight length of pipe is:-

$$F = \frac{4 f_F L}{D} \qquad \dots (12)$$

where

F is the number of velocity head losses

f<sub>F</sub> is the Fanning friction factor

L is the pipe length

D is the pipe diameter

The friction factor  $f_F$  is a dimensionless quantity and is a function of the Reynolds number (Re) of the flow in the pipe and the relative roughness of the pipe. The relative roughness is defined as the ratio of the surface roughness to the pipe diameter. A widely used correlation for  $f_F$  is that of Moody<sup>(5)</sup> which is given in Reference 6 in graphical form. Also quoted in Reference 6 is a table of surface roughness for various pipe materials and values of head losses for common fittings and valves used in pipes, i.e. head losses at contractions, bends, obstructions, etc.

If the pipe is very long then the loss due to the pipe will be most significant and any other losses can be neglected.

The number of velocity heads lost at the pipe inlet is 0 · 5 and so for a pipe without fittings:-

$$K = F + 0.5$$
 ... (13)

Usually the precise failure location will not be known and the approach adopted is to postulate various failure locations and group those producing similar discharge rates together. In order to avoid underestimating the discharge rate, reliance should not generally be placed in valves being part closed.

Once Cd has been evaluated then the general liquid discharge Equation (7) can be used to evaluate the pipe discharge rate. Because  $f_F$  depends, via the Reynolds number, on the discharge velocity, however, the calculational method must be an iterative one.

An estimate of  $f_F$  is made and the discharge velocity U is calculated. This value of U is then used to recalculate  $f_F$  (using the graph in Reference 6) and the procedure repeated to a satisfactory convergence.

This iterative method of solution can be avoided by using a technique described in Reference (7) in which a series of curves of the dimensionless group ( $f_F/2$ ). Re<sup>2</sup>, which is independent of velocity, are plotted against Reynolds number for fixed values of relative roughness.

It can be shown that:-

$$\left(\frac{f_F}{2}\right)$$
 . Re<sup>2</sup>  $\equiv -\frac{\Delta P_f \cdot D^3 \cdot \rho}{4 \cdot L \cdot \mu^2}$  ... (14)

Hence, if the pressure drop  $\Delta P_f$  down the total length of the pipe is known, then the value of this dimensionless group can be calculated. Using the chart in Reference 7 the corresponding Re value can be found and hence the liquid discharge velocity, since

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$$Re = \rho UD/\mu \qquad ... (15)$$

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#### GASES

#### 3.1 Small hole in vapour space wall

The usual concern is release of gas stored under high pressure through a small hole in the containment (Fig. 4).

A small hole is defined as one where the ratio Ah/A < 0.01.

There are two possible release conditions — adiabatic if the pressure drop between the storage tank and ambient is large, isothermal if the pressure drop is small. The adiabatic case is the most common type occurring in accident situations, the release usually being through a small aperture or crack.

The process is treated as an isentropic free expansion of an ideal gas using the equation of state (1.3):-

$$P\nu^k = constant$$
 ... (16)

where

v is the specific volume of the gas

k is the isentropic expansion factor which is equal to γ, the ratio of the specific heats of the gas, for isentropic expansions; but in practice pure isentropy is not achieved, hence k is less than γ.

Equation (16) is combined with Bernoulli's Equation (2). Assuming flow on a horizontal axis and using a coefficient of discharge to account for friction at the orifice, the mass flow rate of an ideal gas through a hole area Ah is:-

$$G = Cd \rho_2 Ah \sqrt{\left\{\frac{2 P_1}{\rho_1} \frac{k}{(k-1)} \left[1 - \left(\frac{P_2}{P_1}\right)^{\frac{(k-1)}{k}}\right]\right\}} \qquad ... (17)$$

If the pressure ratio  $P_1/P_2$  is above a critical value, given by Equation (18), it is found that the exiting mass flow rate is limited to a critical maximum value, Gmax. This is sonic or choked flow.

$$\left(\frac{\mathsf{P}_1}{\mathsf{P}_2}\right)_{\mathsf{CRIT}} = \left(\frac{2}{\mathsf{k}+1}\right)^{-\frac{\mathsf{k}}{(\mathsf{k}-1)}} \dots (18)$$

and

$$G_{\text{max}} = Cd Ah \sqrt{\left[P_1 \rho_1 k \left(\frac{2}{k+1}\right)^{\frac{(k+1)}{(k-1)}}\right]}$$
 ... (19)

For an ideal gas Equation (19) can be written as:-

$$G_{\text{max}} = Cd \ Ah \ P_1 \left[ \frac{kM}{RT_1} \left( \frac{2}{k+1} \right)^{\frac{(k+1)}{(k-1)}} \right]^{\frac{1}{2}}$$
 ... (20)

where

M is the molecular weight of the gas

T<sub>1</sub> is the temperature of the gas (absolute) K

R is the universal gas constant (8314 · 3 J kg-mole<sup>-1</sup> k<sup>-1</sup>)

Full derivations of these equations can be found in References 1 and 3. Equations (17) to (19) are those normally used for the calculation of high pressure gas discharges from vents, pressure relief valves and ruptures.

The case of isothermal gas flow through an orifice when the pressure difference is very small is covered in Reference 3. It is assumed in this case that the gas density remains constant, i.e. incompressible fluid flow.

The equivalent static head in metres of gas is given by:-

$$h = \frac{(P_1 - P_2)}{g\rho} ... (21)$$

so the velocity of the gas is:-

$$u = \sqrt{2gh} \qquad \dots (22)$$

The mass discharge rate is therefore:-

$$G = Cd \rho_1 u Ah \qquad ... (23)$$

#### 3.1.1 Gas discharge example

To illustrate the calculation of the discharge rate for a gas, consider ammonia stored at a pressure of 728 kPa at 15°C and a small hole forming in the vapour space wall.

From Equation (18) calculate the critical pressure ratio for ammonia, k = 1.31:-

$$\left(\frac{\mathsf{P}_1}{\mathsf{P}_2}\right)_{\mathsf{CRIT}} = \left(\frac{2}{\mathsf{k}+1}\right)^{-\frac{\mathsf{k}}{\mathsf{k}-1}}$$
$$= 1.838$$

In this example  $P_1/P_2 = 7 \cdot 18$ , therefore the outflow of ammonia vapour is sonic and Equation (19) is the relevant one.

From thermodynamic tables (Appendix 1, Section 6) $^{(7)}$  the density of ammonia vapour at 15°C and 728 kPa is  $5 \cdot 174$  kg m<sup>-3</sup>.

Assuming a discharge coefficient of 0.8, the discharge rate per unit area is:-

$$G'_{\text{max}} = 0.8 \sqrt{\left[728 \times 10^3 \cdot 5.174 \cdot 1.31 \cdot \left(\frac{2}{2.31}\right)^{\frac{2.31}{0.31}}\right]}$$
  
 $\approx 1040 \text{ kg m}^{-2} \text{ s}^{-1}$ 

#### 3.2 Break in a vapour space pipe (Fig. 5)

A break may occur in a pipe leading from a high pressure gas vessel<sup>(1)</sup> (Fig. 6).

Energy is lost as the gas flows out due to the resistance of the pipe and any fittings. Charts to facilitate the calculation of discharge rates with differing pipe lengths and reservoir conditions were originally constructed by Lapple (1943) but were corrected by Levenspiel, Figs 7 and 8.<sup>(8)</sup>

Figure 7 can be used to find the allowable length of pipe for a given flow rate, and Fig. 8 for finding the flow rate for a given length of pipe.

Besides the pressures shown in Fig. 8, the other parameters needed in order to use the charts are:-

D the pipe diameter (m)

f<sub>F</sub> the Fanning friction factor

G mass velocity of the gas (kg m<sup>-2</sup> s<sup>-1</sup>)

Gmax critical mass velocity of gas through an adiabatic nozzle (kg m-2 s-1)

k expansion index (ratio of specific heats)

L pipe length (m)

N pipe resistance factor  $\left(\frac{4 f_F L}{d}\right)$ 

# 4. SUPERHEATED LIQUIDS AND LIQUEFIED GASES STORED IN PRESSURISED TANKS

In this section we are concerned with possible release modes from pressurised tanks. Such tanks usually have a vapour space above the liquefied gas itself, the vapour space pressure being much higher than the ambient pressure. Possible release modes are shown in Figs 9 and 10.

#### 4.1 Small hole in vapour space (Fig. 9)

Releases of this type can be dealt with in the same way as for discharges from high pressure gas tanks (see Section 2).

With slow releases of this type from the vapour space, a phenomenon called auto-refrigeration can take place. As vapour is lost from the vapour space so the liquid will vaporize to try and maintain a steady vapour pressure. This vaporization requires latent heat and so this leads to a cooling of the liquid and a gradual reduction in the release rate.

#### 4.2 Catastrophic failure of a pressurised tank (Fig. 10)

If a large hole suddenly forms in a tank containing liquefied gas under pressure, the releases are vastly different from the small hole case. (9) The initial gas release rate is so large that the pressure above the liquid surface will suddenly be released. Flashing of vapour from the bulk liquid occurs as the liquid is at a temperature which is much higher than the saturation temperature corresponding to ambient conditions. It has been suggested (9) that this will occur if the ratio Ah/A is greater than about 0.01.

Under these conditions, vapour will flash off quickly from the liquid until its temperature is reduced to that of the boiling point at the ambient pressure, the amount of vapour flashing off corresponding to the reduction in enthalpy of the remaining liquid. (10)

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All the contents of the tank would be flung into the atmosphere mostly as vapour and liquid droplets. Further heat to vaporize the liquid may be taken from air entrained into the expanding cloud. The amount of air entrainment may be an important feature in determining the cloud density and hence its dispersion characteristics.

#### 4.3 Intermediate hole sizes in the vapour space (Fig. 11)

This covers the range of hole sizes from the very small, when there is no liquid entrainment, up to  $Ah/A \approx 0.01$ , when there is full entrainment of all the liquid contents. Between these extremes a certain fraction of the liquid contents will be lost although knowledge is limited and the exact calculation of the discharge rates is difficult for these intermediate hole sizes. Reference 11 describes experiments carried out for fluids with differing degrees of superheat and for a wide range of hole sizes. A correlation is given which evaluates the mass of liquid remaining in the vessel after the flash off due to loss of containment (Equation (24)).

$$\frac{m'}{m_o} = \frac{1}{k'} \left\{ \frac{m'v}{m_o} \frac{\rho_{\ell}}{\rho_g} + \left( 1 - \frac{m'v}{m_o} \right) \right\}^{-1} \qquad ... (24)$$

where

m' is the mass of liquid remaining (kg)

mo is the original mass of liquid (kg)

m'v is the theoretical flashed off vapour mass (kg) calculated from an energy balance depending on the initial physical conditions

 $\rho_{\ell}$  is the liquid density (kg m<sup>-3</sup>)

 $\rho_q$  is the vapour density (kg m<sup>-3</sup>)

k' is a factor which accounts for venting occurring at intermediate hole sizes.

No method for evaluating the value of k' for a general case is currently available although in Reference 11 it is deduced from the experimental results.

#### 4.4 Releases from the liquid space

When a superheated liquid, i.e. one stored under pressure so that its temperature is above its normal boiling point, is released the discharged material is usually a two-phase mixture of vapour and liquid. The behaviour of such a discharge is difficult to analyse and not fully understood.

If, for example, the superheated liquid discharges down a pipe, there is a pressure loss along the pipe. At some point the pressure will drop below the vapour pressure of the liquid and boiling of the liquid will lead to nucleation of vapour bubbles and the production of a two-phase fluid flow. There are many different types of definite flow patterns into which two-phase flow can be divided depending on the relative flow rates of vapour and liquid and pipe geometry, i.e. annular, bubbly, slug, etc.<sup>(1)</sup>

As with gas flow through an orifice or down a pipe, there is a maximum discharge rate which can exist for a two-phase mixture. This occurs at some critical pressure ratio between the stagnation reservoir pressure and the exit pipe pressure.

#### 4.4.1 Critical flow rate of a single component two-phase flow

Several methods have been proposed in the literature to evaluate the critical discharge rate of a two-phase flow from a pipe. The assumption is made in all the critical, maximum flow models that thermal equilibrium exists in the pipe.

Much work has been done in this area by Fauske. (12) Fauske carried out experiments on the critical discharge of steam-water flows from pipes with different reservoir pressures and L/D ratios,

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although the experiments were only carried out with one value for the pipe diameter, D. It was concluded that for L/D ratios  $\approx 12$  thermodynamic equilibrium could be assumed.

For L/D ratios less than this, however, metastable liquid flows exist without thermodynamic equilibrium. The available critical flow models can therefore only be applied to pipes with L/D > 12. This criterion for the onset of equilibrium flashing flow has been used and generally accepted for many years.

Recent work by Fletcher, (13.14) however, has suggested that it may only be the absolute pipe length, L, and not the ratio L/D which determines whether fully established flashing flow in thermal equilibrium can take place. It would therefore be the time the liquid spends in the pipe which governs to what extent flashing occurs. For pipe lengths up to 75 mm, for a fixed excess pressure, the mass flux drops off rapidly with increasing pipe length but is independent of diameter. The rate of decrease of mass flux becomes much less as pipe lengths increase beyond 75 mm. The 75 mm length appears to be the critical pipe length above which thermodynamic equilibrium flow has become established. It is interesting to note that in Fauske's experiments the critical L/D of 12 corresponded to a pipe length of about 75 mm.

In Reference 12 Fauske suggests limits of L/D within which certain discharge flow rate calculations can be used.

L/D = 0, i.e. hole in vessel side. The critical flow data for the release of saturated liquid is well correlated using the standard liquid flow equation

$$G_{max} = 0.61 \cdot Ah \cdot \sqrt{(2\rho (P_0 - P_b))}$$
 ... (25)

where

P<sub>o</sub> = upstream pressure

P<sub>b</sub> = atmospheric pressure

 $0 \le L/D \le 3$  The critical mass flow rate is predicted by using Equation (25) but replacing  $P_b$  by the critical exit pressure  $P_c$ .

$$G_{\text{max}} = 0.61 \cdot Ah \cdot \sqrt{(2\rho (P_0 - P_c))}$$
 ... (26)

and

$$P_c = 0.55 \cdot P_o (1 - \exp(-L/3D))$$
 ... (27)

 $3 \le L/D \le 12$  is a transition region corresponding to pipe lengths of up to 75 mm for Fletcher. Towards the higher ratios the effect of L/D on  $G_{max}$  is reduced suggesting that metastable flow conditions are giving way to thermodynamic equilibrium flow.

 $12 \le L/D \le 40$  The critical mass flow rate can be calculated using a two-phase equilibrium flow model (see below). This region corresponds to Fletcher's pipe lengths of above 75 mm.

An important point to be borne in mind is that, when calculating discharge rates for superheated liquid releases, using Fauske's L/D limits would generally tend to lead to an over-prediction of the mass flow rate, particularly for pipes longer than 75 mm, but with L/D ratios less than 12, i.e. it would produce conservative release rate estimates.

One of the most widely used thermodynamic equilibrium methods  $^{(4.15.16)}$  based on Fauske's  $^{(12)}$  conclusions for long pipes (L/D  $\geqslant$  12) is the Homogeneous Equilibrium Model (HEM):-

(i) Calculate the critical pressure at the pipe exit. For long pipes Fauske proposed(12)

$$\frac{P_c}{P_o} = 0.55 \qquad \dots (28)$$

Some assessments<sup>(4)</sup> have used this ratio in the general case, but others<sup>(15)</sup> have used the single phase gas formula

$$\frac{P_c}{P_o} = \left(\frac{2}{\gamma + 1}\right)^{\frac{\gamma}{\gamma - 1}} \dots (29)$$

This gives very similar critical pressures, e.g. for  $\gamma=1\cdot 1$ ,  $P_c/P_o=0\cdot 58$  and for  $\gamma=1\cdot 4$ ,  $P_c/P_o=0\cdot 53$ .

- (ii) The temperature corresponding to the saturated choke pressure, T<sub>c</sub>, is then found using vapour pressure data.
- (iii) Assuming thermodynamic equilibrium the vapour mass fraction which would flash off from the liquid is calculated:-

$$m_v = 1 - \exp\left\{-\frac{c}{\lambda} \left(T_i - T_c\right)\right\} \qquad \dots (30)$$

where

my = vapour mass fraction or quality

c = specific heat capacity of liquid (J kg<sup>-1</sup> k<sup>-1</sup>)

 $\lambda$  = latent heat of vaporization of liquid (J kg<sup>-1</sup>)

T<sub>1</sub> = reservoir storage temperature (k)

(iv) Assuming homogeneous mixing and no slip between the phases, the mixture density is calculated at the choke conditions

$$\rho_{c} = \left\{ \frac{m_{v}}{\rho_{g}} + \frac{1 - m_{v}}{\rho_{\ell}} \right\}^{-1} \qquad ... (31)$$

where

 $\rho_g$  is the vapour density at  $T_c$  and  $P_c$ 

 $\rho_{\ell}$  is the liquid density at T<sub>c</sub> and P<sub>c</sub>

(v) The standard discharge formula is then used to calculate the critical flow rate:-

$$G_{\text{max}} = Cd Ah \sqrt{2 \rho_c (P_o - P_c)} \qquad ... (32)$$

where

Cd is the discharge coefficient

Gmax is the maximum discharge rate (kgs-1)

To illustrate the calculation of the critical discharge rate for a two-phase mixture, consider ammonia stored at 728 kPa at 15°C.

(i) Calculate the critical pressure at the pipe exit (y = 1.31)

$$\frac{P_c}{P_0} = \left(\frac{2}{\gamma + 1}\right)^{\frac{\gamma}{\gamma - 1}}$$

$$P_c = 728 \times 10^3 \left(\frac{2}{2 \cdot 31}\right)^{\frac{1 \cdot 31}{0 \cdot 31}}$$
  
= 396 x 10<sup>3</sup> Pa

(ii) The temperature corresponding to this pressure under saturated conditions can be found using the thermodynamic tables.

$$T_c = -2 \cdot 23^{\circ}C$$

(iii) Using Equation (30) calculate the vapour flash fraction

$$m_v = 1 - \exp \left\{ -\frac{4 \cdot 57 \times 10^3}{1294 \times 10^3} \left( 15 - \left( -2 \cdot 23 \right) \right) \right\}$$
  
= 0.0590

(iv) Look up in Appendix 1  $\rho_g$  and  $\rho_\ell$  corresponding to a pressure of 396 kPa and temperature of  $-2\,^{\circ}\text{C}$  ( $\rho_g = 3\cdot 1759\,\text{kg}\,\text{m}^{-3}$ ,  $\rho_\ell = 640\cdot 58\,\text{kg}\,\text{m}^{-3}$ . If tables are not available  $\rho_g$  is usually estimated from the gas molecular weight, assuming ideal gas behaviour).

Calculate the mixture density:-

$$\rho_{c} = \left\{ \frac{m_{v}}{\rho_{g}} + \frac{1 - m_{v}}{\rho_{\ell}} \right\}^{-1}$$

$$= \left\{ \frac{0.0590}{3.1759} + \frac{0.941}{640.58} \right\}^{-1}$$

$$= 49.85 \, \text{kg} \cdot \text{m}^{-3}$$

(v) The critical discharge rate can now be calculated from Equation (32):-

$$G_{\text{max}} = Cd \cdot \sqrt{2 \cdot \rho_c (P_o - P_c)}$$

for a discharge coefficient of 0.8

$$G_{max} = 4600 \, kg \cdot m^{-2} \cdot s^{-1}$$

Fauske, (17) Moody, (18) and Levy (19) also propose methods for calculating maximum flow rate for a two-phase mixture. The main difference between these methods and the simple model described above is that slip between the phases, i.e. vapour phase travelling faster than the liquid phase is taken into account. These do not therefore assume a homogeneous mixing model. As an example of these models Fauske (17) assumes annular flow of the mixture, i.e. a core of gas with liquid flowing along the inner perimeter of the pipe, one-dimensional steady flow, slip flow with uniform linear velocities of each phase and accounts for frictional forces applied to the fluid in the pipe. Equation (33) is derived in Reference 17 by Fauske to calculate the maximum two-phase discharge rate:

$$G_{\text{max}} = \left[ \frac{-k}{\left[ (1 + kx - x) x \right] \frac{d\nu_g}{dp} + \left[ \nu_g (1 + 2kx - 2x) + \nu_f (2kx - 2k - 2xk^2 + k^2) \right] \frac{dx}{dp}} \right]^{\frac{1}{2}} + \left\{ k \left[ 1 + x (k - 2) - x^2 (k - 1) \right] \right\} \frac{d\nu_f}{dp} \qquad ... (33)$$

where

k is the critical slip ratio = 
$$\left(\frac{v_g}{v_f}\right)^{1/2}$$
 ... (34)

x is the exit quality

 $\nu_{\alpha}$  is the specific volume of the vapour at the exit

 $v_{\ell}$  is the specific volume of the liquid at the exit

By specifying the critical outlet pressure and quality at the pipe exit, Equation (33) can be used to calculate the maximum flow rate.

The derivative terms in Equation (33) can be approximated by finite difference equations calculated under isenthalpic conditions:-

$$\frac{d\nu_g}{dp} \approx \left(\frac{\Delta\nu_g}{\Delta p}\right)_H \qquad ... (35)$$

$$\frac{d\nu_{\ell}}{dp} \approx \left(\frac{\Delta\nu_{\ell}}{\Delta p}\right)_{H} \qquad ... (36)$$

$$\frac{dx}{dp} \approx -\frac{1}{hf_g} \left( \frac{\Delta h_f}{\Delta p} + x \frac{\Delta hf_g}{\Delta p} \right) \qquad ... (37)$$

where

h<sub>f</sub> is the specific enthalpy of the liquid at the choke conditions

hf<sub>a</sub> is the latent heat of vaporization

The finite differences are calculated by straddling the critical outlet pressure, in the thermodynamic tables, by one point below it and one above. The relevant quantities can then be found at these two points, i.e.  $h_f$ ,  $hf_g$ , P, etc. and then the differences evaluated and substituted into Equations (35) to (37). Hence, knowing the critical outlet pressure and quality,  $G_{max}$  can be found.

The example previously quoted for a two-phase release was recalculated using the Fauske method. The result was  $6600 \, \text{kg m}^{-2} \, \text{s}^{-1}$  compared with  $4600 \, \text{kg m}^{-2} \, \text{s}^{-1}$  by the homogeneous method. These values are in the ratio of  $1 \cdot 4$ .

On comparing the mathematical computation involved in the two methods, the similar results and bearing in mind the uncertainty over the exact conditions, position of the containment failure, and the accuracy to which the calculations are needed, the more straightforward method would generally appear to be adequate.

Homogeneous equilibrium critical two-phase discharge can be estimated by solving the appropriate thermodynamic and flow equations, as for example in the computer programs developed by Hall<sup>(20)</sup> for single and multicomponent systems. It is usually necessary to make a number of simplifying assumptions in order to obtain a solution, and data, particularly for multicomponent systems, is often scarce.

#### 5. REFERENCES

- LEES, Frank P. Loss prevention in the process industries, Vol. 1, Butterworth & Co (Publishers) Ltd (1980)
- HAYWOOD, R. W. Thermodynamic tables in SI (metric) units, Cambridge at the University Press (1968)
- 3. LEWITT, E. Hydraulics, Sir Isaac Pitman & Sons Ltd (1943)
- 4. Risk analysis of six potentially hazardous industrial objects in the Rijnmond Area. A pilot study, Reidel (1982)
- 5. MOODY, L. F. Transactions of the American Society of Mechanical Engineers, 66, 671 (1944)
- 6. PERRY, John H. Chemical Engineers Handbook, McGraw-Hill (1974)
- COULSON, J. M. and RICHARDSON, J. F. Chemical Engineering, Vol. 1, 3rd Edition (SI units), Pergamon Press (1977)
- 8. LEVENSPIEL, O. The discharge of gases from a reservoir through a pipe. AIChEJ, 23, 402 (1977)
- FRYER, L. S. and KAISER, G. D. DENZ A computer program for the calculation of the dispersion of dense toxic or explosive gases in the atmosphere, UKAEA Report SRD R152 (1979)
- JENNINGS, A. J. D. The physical chemistry of safety. The Chemical Engineer, No. 290, October 1974
- 11. FLETCHER, B. Sudden discharge of a superheated fluid to atmosphere, I. Chem. E. Symposium Series, No. 71, p 25
- FAUSKE, H. K. The discharge of saturated water through tubes, CEP Symposium Series 59, pp 210 et seq (1965)
- FLETCHER, B. and JOHNSON, A. E. The discharge of superheated liquids from pipes. I. Chem. E. Symposium Series, No. 85. The Protection of Exothermic Reactors and Pressurised Storage Vessels Conference, Chester, 25-27 April 1984
- FLETCHER, B. Flashing through orifices and pipes, AICHE Loss Prevention Symposium, Denver, August 1983
- Canvey, a Second Report. A review of potential hazards from operations in the Canvey Island/Thurock area three years after publication of the Canvey report
- CUDE, A. L. The generation spread and decay of flammable vapour clouds. I. Chem. E. course "Process Safety – theory and practice", Teeside Polytechnic, Middlesborough, 7-10 July 1975
- FAUSKE, H. K. Contribution to the theory of two-phase, one-component critical flow, ANL-6633
- MOODY, F. J. Maximum flow rate of a single-component, two-phase mixture. Transactions of the ASME, February 1975
- 19. LEVY, S. Journal of heat transfer, 87c, 53 (1965)
- HALL, S. F. A simple homogeneous equilibrium critical discharge model applied to multicomponent, two-phase systems – the computer programs CRITS and CRITTER, UKAEA Report SRD R127 (1978).

Thermodynamic properties of ammonia (7)

| Saturation temperature | Pressure<br>MN/m² | Specific volume<br>m³ kg-1 |         | Density<br>kg m <sup>-3</sup> |        | Specific enthalpy kJ . kg <sup>-1</sup> |        | Latent heat of vaporization |
|------------------------|-------------------|----------------------------|---------|-------------------------------|--------|---|--------|-----------------------------|
| (°C)                   |                   | Liquid                     | Vapour  | Liquid                        | Vapour | Liquid                                  | Vapour | kJ . kg <sup>-1</sup>       |
| -40                    | 0.0718            | 0.00145                    | 1 · 552 | 689 · 66                      | 0.644  | 0.0                                     | 1390   | 1390                        |
| -35                    | 0.0932            | 0.00146                    | 1.216   | 684.93                        | 0.822  | 22.3                                    | 1398   | 1375.7                      |
| - 30                   | 0.1196            | 0.00148                    | 0.963   | 675.67                        | 1.038  | 44.7                                    | 1406   | 1361.3                      |
| -25                    | 0.1516            | 0.00149                    | 0.772   | 671.14                        | 1.295  | 67.2                                    | 1413   | 1345.8                      |
| -20                    | 0.190             | 0.0015                     | 0.624   | 666.66                        | 1.602  | 89.8                                    | 1420   | 1330.2                      |
| - 15                   | 0.236             | 0.00152                    | 0.509   | 657.89                        | 1.965  | 112.3                                   | 1426   | 1313.7                      |
| -10                    | 0.291             | 0.00153                    | 0.418   | 653.59                        | 2.392  | 135.4                                   | 1433   | 1297.6                      |
| - 5                    | 0.355             | 0.00155                    | 0.347   | 645.16                        | 2.882  | 158.2                                   | 1439   | 1280.8                      |
| 0                      | 0.429             | 0.00157                    | 0.289   | 636.94                        | 3.460  | 181.2                                   | 1444   | 1262.8                      |
| 5                      | 0.516             | 0.00158                    | 0.243   | 632.91                        | 4.115  | 204.5                                   | 1450   | 1245.5                      |
| 10                     | 0.615             | 0.00160                    | 0.206   | 625.00                        | 4.854  | 227.7                                   | 1454   | 1226.3                      |
| 15                     | 0.728             | 0.00162                    | 0.175   | 617.28                        | 5.714  | 251.4                                   | 1459   | 1207.6                      |
| 20                     | 0.857             | 0.00164                    | 0.149   | 609.76                        | 6.711  | 275.2                                   | 1463   | 1187.8                      |
| 25                     | 1.001             | 0.00166                    | 0.128   | 602.40                        | 7.812  | 298.9                                   | 1466   | 1167.1                      |
| 30                     | 1.167             | 0.00168                    | 0.111   | 595.24                        | 9.009  | 323.1                                   | 1469   | 1145.9                      |
| 35                     | 1.350             | 0.00170                    | 0.096   | 588.24                        | 10.417 | 347.5                                   | 1471   | 1123.5                      |
| 40                     | 1.554             | 0.00173                    | 0.083   | 578.03                        | 12.048 | 371.5                                   | 1473   | 1101.5                      |
| 45                     | 1.782             | 0.00175                    | 0.073   | 571.43                        | 13.698 | 396.8                                   | 1474   | 1077.2                      |
| 50                     | 2.033             | 0.00178                    | 0.063   | 561.79                        | 15.873 | 421.9                                   | 1475   | 1053.1                      |

### 7. APPENDIX 2

### List of symbols

| Α                | Top section area of the vessel  | (m²)                                  |
|------------------|---|---------------------------------------|
| Ah               | Hole area   | (m²)                                  |
| В                | Breadth of the orifice  | (m)                                   |
| Cd               | Discharge coefficient   |                                       |
| C                | Specific heat capacity of the liquid  | $(J kg^{-1} k^{-1})$                  |
| D                | Diameter of the pipe/hole   | (m)                                   |
| F                | Number of velocity heads lost as friction   |                                       |
| f <sub>F</sub>   | Fanning friction factor   |                                       |
| g                | Acceleration due to gravity   | (m s <sup>-2</sup> )                  |
| G                | Mass discharge rate   | (kg s <sup>-1</sup> )                 |
| G'               | Mass discharge rate/unit area   | (kg s <sup>-1</sup> m <sup>-2</sup> ) |
| $G_{\text{max}}$ | Critical discharge rate/unit area   | (kg m <sup>-2</sup> s <sup>-1</sup> ) |
| $G'_{max}$       | Critical discharge rate/unit area   | (kg m <sup>-2</sup> s <sup>-1</sup> ) |
| Н                | Enthalpy  | (J kg <sup>-1</sup> )                 |
| H <sub>2</sub>   | Height of the liquid level above the bottom of the orifice                          | (m)                                   |
| H <sub>1</sub>   | Height of the liquid level above the top of the orifice                             | (m)                                   |
| h                | Head of liquid/gas  | (m)                                   |
| h <sub>f</sub>   | Specific enthalpy of the liquid   | (J kg <sup>-1</sup> )                 |
| hf <sub>g</sub>  | Latent head of vaporization of the liquid   | (J kg <sup>-1</sup> )                 |
| К                | Total number of velocity head losses  |                                       |
| k'               | Factor to account for venting through an intermediate size hole in the vapour space |                                       |
| k                | Isentropic expansion factor   |                                       |
| L                | Pipe length   | (m)                                   |
| М                | Molecular weight of the gas   |                                       |
| m'               | Mass of liquid remaining  | (kg)                                  |
| $m_o$            | Original mass of liquid   | (kg)                                  |
| m'v              | Theoretical flashed off vapour mass   | (kg)                                  |
| $m_v$            | % of vapour flashed off   |                                       |
| P                | Pressure  | (N m <sup>-2</sup> )                  |
| P <sub>3</sub>   | Gas pressure stored above liquid  | (N m <sup>-2</sup> )                  |
| $P_b$            | Atmospheric pressure  | (N m <sup>-2</sup> )                  |
| $P_c$            | Critical exit pressure  | (N m <sup>-2</sup> )                  |
| Po               | Reservoir pressure  | (N m <sup>-2</sup> )                  |
| q                | Heat absorbed from the surroundings   | (J kg <sup>-1</sup> )                 |
| r                | Vessel radius   | (m)                                   |
|                  |   |                                       |

| R          | Universal gas constant, 8 · 314 x 10³      | (J kg-mole <sup>-1</sup> k <sup>-1</sup> ) |
|------------|--|--|
| Re         | Reynolds number                            | $ ho_{ m g}$ uD/ $\mu$                     |
| T          | Time to empty a vessel                     | (s)  |
| Tı         | Gas temperature                            | (k)  |
| u          | Discharge velocity                         | (ms <sup>-1</sup> )                        |
| ν          | Specific volume                            | (m³ kg-1)                                  |
| $W_s$      | Work done by the fluid on the surroundings | (J kg <sup>-1</sup> )                      |
| x          | Quality of the two-phase mixture           |  |
| Z          | Height above the potential energy datum    | (m)  |
| ρ          | Density                                    | (kg m <sup>-3</sup> )                      |
| γ          | Ratio of specific heat capacities          |  |
| λ          | Latent heat of vaporization of the liquid  | (J kg <sup>-1</sup> )                      |
| μ          | Dynamic viscosity of the liquid            | (N s m <sup>-2</sup> )                     |
| Subscripts |  |  |
| С          | Refers to critical flow conditions         |  |
| e          | Refers to liquid properties                |  |

c Refers to critical flow conditions
 ℓ Refers to liquid properties
 g Refers to vapour properties
 1,2 are initial and final states

Fig.1 Small hole in liquid space

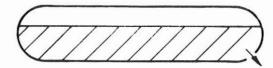


Fig.2 Intermediate size hole in liquid space

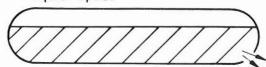


Fig. 3 Failure in liquid pipe

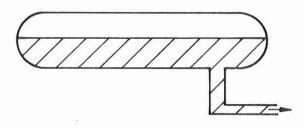


Fig. 4 Small hole in gas storage vessel

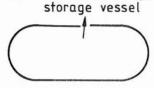


Fig.5 Failure in gas pipe

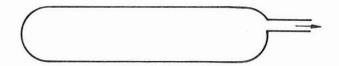


Fig.9 Small hole in vapour space

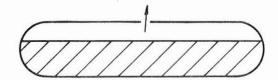


Fig. 10 Large hole in vapour space

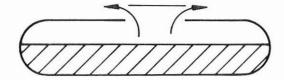


Fig. 11 Intermediate size hole in vapour space

