

**A UNIFIED MODEL FOR POLLUTANT DISPERSION  
IN ATMOSPHERE AND FOR CONSEQUENCE ASSESSMENT**

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## 1. Introduction

The main objective of an on site emergency plans in case of a chemical accident is to minimise consequences for people and environment by quick undertaking of appropriate emergency action (Borysiewicz M. et al., 2000). This in turn depends strongly on scenarios of the accident. This paper describes the Unified Model of Pollutant Dispersion in Atmospheres (UMPDA) implemented into the MANHAZ software package SWAR. Programs for analysis of accident scenarios implemented in the system SWAR cover a variety of emergency situations related to possible releases of toxic materials, explosions and fires (solid material fires, pool fires etc.). The UMPDA represents unified approach to modelling of pollutant dispersion in atmosphere, for a ground-level or elevated two-phase pressurised or un-pressurised releases both continuous and instantaneous. The model is modification of approach used in the PHAST program, in the model calculating the pollutant dispersion (Witlox, H., 2000). It effectively consists of the following linked modules:

- jet dispersion;
- droplet evaporation and rainout, touchdown;
- pool spread and vaporisation;
- heavy gas dispersion;
- passive dispersion.

A single form of concentration profile is used to cover all stages of a release. This allows for anything from a sharp-edged profile in the initial stages of a jet release through to the diffuse Gaussian profile that would be expected in the final passive stage of spreading.

The UMPDA includes the effects of droplet vaporisation using a non-equilibrium model. Rainout produces a pool which spreads and vaporises. Vapour is added back into the plume and allowance is made for this additional vapour flow to vary with time. In addition to the non-equilibrium model, UMPDA also allows for an equilibrium model.

The UMPDA allows for vertical variation in ambient wind speed, temperature and pressure. Another feature of the UMPDA is possible plume lift-off, where a grounded cloud becomes buoyant and rises into the air. Rising clouds may be constrained to the mixing layer if it is reached. The UMPDA allows for continuous and instantaneous releases.

The model coefficients have been obtained directly from established data in the literature (based on wind-tunnel experiments).

Sections 2 – 8 of this Chapter include a description of the theory, the UMPDA thermodynamics, and the UMPDA pool spreading/evaporation model. In Section 9 the major conclusions are summarised. The reader is referred to the UMPDA Technical Reference Manual for details not included in the present paper.

## 2. Atmospheric profiles

The wind speed varies with height in the atmosphere, as does the atmospheric temperature, pressure, density, humidity, etc. Simple relations are described here which are appropriate to the first few hundred metres of the atmosphere. Three options are provided for the variation of atmospheric temperature and pressure with height:

1. Constant temperature and pressure profiles.
2. Linear temperature and pressure profiles.
3. Logarithmic temperature profile and linear pressure profile.

Two options for the variation of wind speed with height:

1. Constant wind speed profile.
2. Power-law wind profile.

It is recommended that logarithmic temperature, linear pressure, and power-law wind profiles are used since this will give the most realistic modelling.

## 2.1. Temperature

The simplest temperature profile is one where the atmospheric temperature is constant with height. The next most complicated is a linear profile given by:

$$T(z) = T(z_{\text{ref}}) + \alpha (z - z_{\text{ref}}) \quad (2.1)$$

where  $T$  atmospheric temperature, (K);  
 $z$  height, (m);  
 $z_{\text{ref}}$  reference height for temperature, (m);  
 $\alpha$  temperature gradient, (K/m).

Values of  $\alpha$  for the various Pasquill stability classes (Pasquill, F.,1961) are listed in the table below, interpolated for the A/B, B/C and C/D mid-classes (Crutcher, H.L., 1984).

Table 2.1: Values of  $\alpha$  for the various Pasquill stability classes.

Stability Class	$\alpha$ (K/m)
A	-0.020
A/B	-0.019
B	-0.018
B/C	-0.017
C	-0.016
C/D	-0.013
D	-0.010
E	0.005
F	0.028
G	0.040

## 2.2. Pressure

The model offers the choice of two atmospheric pressure profiles. In the simplest, the pressure is constant with height.

In the other profile, the pressure decreases linearly with height, and the pressure gradient is given by:

$$dP/dz = -\rho g \quad (2.2)$$

If it is assumed that  $\rho$  and  $g$  are constants then this can be integrated to give:

$$P(z) = P_0 - \rho_0 g z \quad (2.3)$$

where:  $P_0$  is the atmospheric pressure at ground level, (N/m<sup>2</sup>);  
 $\rho_0$  is the atmospheric density at ground level, (kg/m<sup>3</sup>);  
 $g$  is acceleration due to gravity, 9.81, (m/s<sup>2</sup>);  
 $z$  is the height above ground level, (m).

This is an approximation since  $\rho$  will vary with height as the temperature and pressure change. However this is a second order effect which is not important within the first few hundred metres of the atmosphere.

## 2.3. Vertical wind profiles

The simplest vertical wind profile is one where the wind speed is constant with increasing height in the atmosphere.

To provide more realistic modelling, the program also provides a power law form:

$$u_w(z) = u_w(z_{\text{ref}}) (z/z_{\text{ref}})^p \quad (2.4)$$

where:  $u_w$  wind speed, (m/s);  
 $z$  height above the ground, (m);  
 $z_{ref}$  reference height for measurement of wind speed, (m);  
 $p$  wind profile power, (-).

The power-law exponent  $p$  depends on the stability class and the surface roughness length. It is found that  $p$  is a strong function of stability class for stable conditions (E-G), but is insensitive to stability class for unstable conditions (A-C). Similarly,  $p$  is fairly insensitive to surface roughness length,  $z_0$ , at low values of  $z_0$ , but more sensitive at high values of  $z_0$ .

The illustration shows the variation of the power-law exponent as a function of the surface roughness length and stability class:

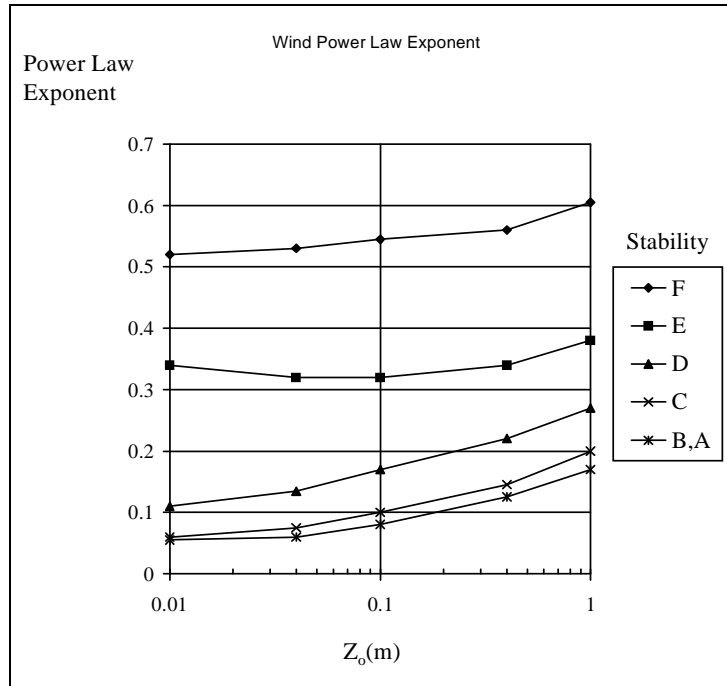


Figure 2.1. Wind power law exponent.

## 2.4. Other atmospheric variables

### Humidity

The relative humidity is assumed to be constant with height.

### Density

The atmospheric density at a height  $z$  is calculated from the atmospheric temperature, pressure and humidity at that height.

### Composition

The composition of the atmosphere is assumed to be constant with height.

## 3. Dispersion models

The main characteristic of dispersion models is that profiles for concentration, velocity, and temperature are assumed. The UMPDA model uses a particularly flexible form, allowing for sharp-edged profiles which become more diffuse downwind. Both instantaneous and continuous releases are treated, for which many model equations are common. The vertical cross section of each is, in general, an ellipse while elevated, and a truncated ellipse while touching the ground (or impinging the mixing height ceiling). A continuous release profile extends from

the source downwind, whereas an instantaneous release profile is a volume defined by revolving the vertical cross section around the vertical axis.

An example of a general case continuous release is shown in the illustration.

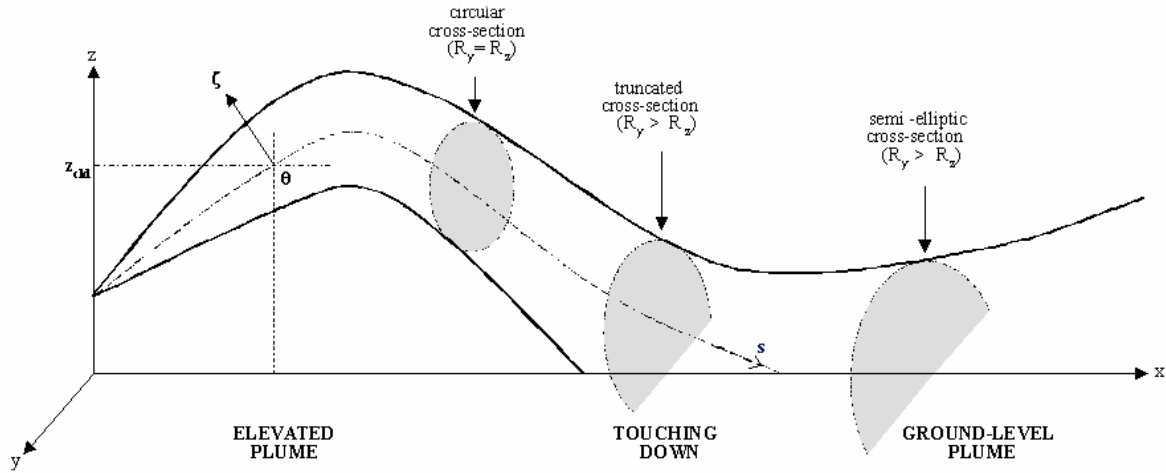


Figure 3.1. Continuous release scheme.

The illustration shows the following aspects of cloud-behaviour:

- An elevated, heavy vapour/aerosol release which starts out with a circular cross section then tends to flatten into an ellipse as the cloud settles.
- Upon touching down, the cross section becomes a truncated ellipse, and the cloud levels off as the vertical component of momentum is dissipated.
- Aerosol droplets may rain out shortly after touchdown. Rainout produces a pool which spreads and vaporises.
- The vapour from the pool is added back to the plume, as a function of time.
- The plume can become buoyant after evaporating all aerosol droplets and picking up heat by ground conduction. A buoyant plume lifts off and rises until constrained by the mixing layer.

An example of a general case instantaneous release is shown in the illustration.

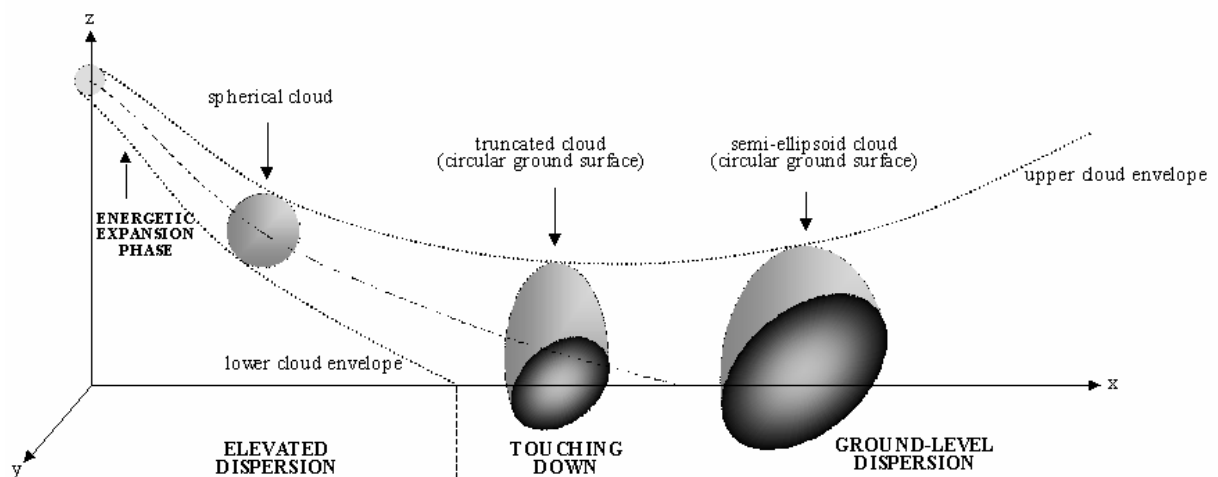


Figure 3.2. Instantaneous release scheme.

### 3.1. Concentration profile and cloud geometry

Figures 3.1 and 3.2 show the movement of the cloud in the downwind direction. The Cartesian co-ordinates x, y, z correspond to the downwind, cross-wind (lateral horizontal) and vertical directions, respectively;  $x = 0$

corresponds to the point of release,  $y = 0$  to the plume centre-line and  $z = 0$  to ground-level. Furthermore  $s$  is the arc length measured along the plume centre,  $\theta = \theta(s)$  the angle between the plume centre-line and the horizontal, and  $\zeta$  the distance from the plume centre-line. In addition, local co-ordinates are used:  $(s, y_0, \zeta)$  for continuous release and  $(x_0, y_0, z_0)$  for instantaneous release.

The concentration  $\rho$  is given by a similarity profile as suggested by Webber et al.

$$\rho(y_0, \zeta, s) = \rho_{\text{clid}}(s) F_v(\zeta, s) F_h(y_0, s) \text{ (continuous)} \quad (3.1)$$

with  $F_v(\zeta, s) = \exp[-(\zeta^2 / a_3^2)]^{m/2}$  and  $F_h(y_0, s) = \exp[-(y_0^2 / a_2^2)]^{n/2}$ ,  $a_2 = a_2(s)$ ,  $a_3 = a_3(s)$ ,

$$\rho(x_0, y_0, z_0, t) = \rho_{\text{clid}}(t) F_v(z_0, t) F_h(r_0, t) \text{ (instantaneous)} \quad (3.2)$$

with  $F_v(z_0, t) = \exp[-(z_0^2 / a_3^2)]^{n/2}$  and  $F_h(r_0, t) = \exp[-(r_0^2 / a_2^2)]^{m/2}$ ,  $a_2 = a_2(t)$ ,  $a_3 = a_3(t)$ ,  $r_0 = \sqrt{(x^2 + y^2)}$ .

Equations (3.1) – (3.2) reduce to the Gaussian form when  $n = m = 2$ . For larger values, say  $m = 50$ , profiles are predicted by Equations (3.1) – (3.2) to be very nearly sharp-edged. This formulation allows modelling of a sharp-edged jet, as occurs from a smooth-edged nozzle, dispersing to a jet with a more nearly Gaussian profile farther downwind.

The exponents  $m$  and  $n$  are correlated as a function of the normalised density difference which goes into the calculation of buoyancy.

In case of steady-state (continuous) dispersion, Equation (3.1) describes exponential decay of the concentration in  $y$  and  $\zeta$  in terms of the cross-wind and vertical dispersion coefficients  $a_2(s)$ ,  $a_3(s)$ . Empirical correlations are adopted for the exponents  $m$ ,  $n$  such that the near-field sharp-edged profile (large value for  $m$ ) develops into a Gaussian profile in the far field ( $m = 2$ ). As shown in Figure 2, the plume cross-section is a circle (radius  $a_2 = a_3$ ) during elevated jet dispersion, a truncated circle during touching down, and a semi-ellipse after touching down. The area of this plume cross-section,  $A(s)$ , is obtained by integration of  $F_v(\zeta, s) F_h(y_0, s)$  over  $\zeta$ ,  $y_0$ . As in many other dispersion models, the cloud is also characterised by an equivalent 'effective cloud' [rectangular cross-section with area  $A$ , effective half-width  $W_{\text{eff}}(x)$ , and effective height  $H_{\text{eff}}(x)(1+h_d)$  with  $h_d = 0$  for grounded plume and  $h_d = 1$  for elevated plume, with centroid cloud speed  $u_{\text{clid}}$ , and equivalent top-hat concentration equal to the centre-line concentration  $\rho_{\text{clid}}(s)$ .

In the case of instantaneous dispersion, the cloud moves in the downwind direction with cloud centre at time  $t$  denoted by  $x = x_{\text{clid}}(t)$ ,  $y = 0$ ,  $z = z_{\text{clid}}(t)$ . Equation (3.2) describes exponential decay of the concentration in  $x_0$ ,  $y_0$ ,  $z_0 = z - z_{\text{clid}}$  in terms of the horizontal and vertical dispersion coefficients  $a_2(t)$ ,  $a_3(t)$ , with downwind spreading assumed to be equal to cross-wind spreading ( $a_2 = a_3$ ). As shown in Figure 3, the cloud is a sphere (radius  $a_2 = a_3$ ) during elevated jet dispersion, a truncated sphere during touching down, and a semi-ellipsoid after touching down. The volume of this cloud,  $V_{\text{clid}}$ , is determined by integration  $F_v(z_0, t) F_h(r_0, t)$  over  $x_0$ ,  $y_0$ ,  $z_0$ . The cloud is also characterised by an equivalent 'effective cloud' [cylindrical shape with volume  $V_{\text{clid}}$ , effective horizontal radius  $W_{\text{eff}}$ , and effective height  $H_{\text{eff}}(1+h_d)$ ] with centroid cloud speed  $u_{\text{clid}}$ , and equivalent top-hat concentration equal to the centre-line concentration  $\rho_{\text{clid}}(t)$ .

The physical interpretation of the effective width and height is that the area under each curve in the illustration above (of the horizontal and vertical concentration profile) to the right of the coefficient  $y = a_2$  or  $z = a_3$  equals the area to the left above the curve and below 1.0. In other words, the concentration profiles are "squared off", so the dimensions  $H_{\text{eff}}$  and  $W_{\text{eff}}$  define an ellipse-shaped cross section of a top hat model which contains all the mass in the cloud having the diffuse concentration profile given by Equations (3.1) – (3.2). This general similarity model, therefore, retains all the simplicity and convenience of a top hat model, but at the same time allows quite general concentration profiles.

### 3.2. Dispersion variables and equations

The UMPDA model is formulated as an integral model. A set of differential equations is integrated to give the key variables as a function of distance or time. A number of algebraic equations are then solved to obtain other variables describing the dispersing cloud. The set of differential equations are basically the same for instantaneous and continuous releases, although they are integrated with respect to time in the first case and with respect to distance in the latter. The same differential equations apply throughout all phases of dispersion (e.g. jet, dense, passive), although the exact terms on the right hand side may vary as the cloud passes from one phase to the next.

The UMPDA model uses the similarity profiles, Equations (3.1) – (3.2). Two sets of ordinary differential equations are integrated separately by a Runge-Kutta-Milne (RKM) integration scheme. The first set, describing the overall cloud behaviour, is described in this section; the second set, describing droplet evaporation and trajectories, is described in the next section. For stability, each integration requires a different step size. The two integrations are kept synchronised in the horizontal direction (i.e. the droplet integration is allowed to catch up to the jet plume integration after each jet plume step).

For each set of equations, we first write the balances as time derivatives, which apply

$$d(\ )/ds = [d(\ )/dt] u_{\text{cld}}^{-1} \quad (3.3)$$

The variables which are integrated are:

- $m_{\text{cld}}$  the mass of the cloud, (kg or kg/s);
- $I_{x2} = I_x - m_{\text{cld}}u_w = m_{\text{cld}}u_x - m_{\text{cld}}u_w$   
the excess horizontal momentum, (kg m/s or kg m/s<sup>2</sup>);
- $I_z = m_{\text{cld}}u_z$  the vertical momentum, (kg m/s or kg m/s<sup>2</sup>);
- $x$  the horizontal position, (m);
- $z$  the vertical position, (m).

The first of the pair of units is for instantaneous releases and the second for continuous releases.

The model equations for the overall behaviour of the dispersing cloud are as follows:

*Conservation of species (air entrainment)*

$$d(\ )/dt = f_{\text{jet}}E_{\text{jet}} + f_{\text{cross}}E_{\text{cross}} + f_{\text{hvy}}E_{\text{hvy}} + f_{\text{pas}}^{\text{nf}}E_{\text{pas}}^{\text{nf}} + f_{\text{pas}}^{\text{ff}}E_{\text{pas}}^{\text{ff}} \quad (3.4)$$

- where  $E_{\text{jet}}$  = jet entrainment rate,
- $E_{\text{cross}}$  = cross entrainment rate,
- $E_{\text{hvy}}$  = heavy gas entrainment rate,
- $E_{\text{pas}}^{\text{nf}}$  = near-field passive entrainment rate,
- $E_{\text{pas}}^{\text{ff}}$  = far-field passive entrainment rate,
- $f$  = coefficients balancing different kinds of entrainment,  $f = (0 \div 1)$ .

Formula for jet entrainment rate has been developed by Morton et al. (1956).

*Conservation of excess horizontal component of momentum*

$$d(I_{x2})/dt = C_{\text{DJ}} S_{\text{abov}} \rho_{\text{air}} u_w^2 |\sin^3 \theta| + S_{\text{gnd}} \rho_{\text{air}} u_w^2 [1 - (u_x/u_w)^2] - S_{\text{gnd}} \rho_{\text{cld}} u_{\text{cld}}^2 \max [0, \sin(-\theta)] \sin \theta \quad (3.5)$$

The last two terms are added only when the cloud is touching the ground, and  $(u_w - u_x) >$  a threshold value.

*Conservation of vertical component of momentum*

$$d(I_z)/dt = -V(t) (\rho_{\text{cld}} - \rho_{\text{air}})g - C_{\text{DJ}} S_{\text{abov}} \rho_{\text{air}} u_w^2 \cos \theta \sin^2 \theta \text{sgn}(\sin \theta) + S_{\text{gnd}} \rho_{\text{cld}} u_{\text{cld}}^2 \max [0, \sin(-\theta)] \cos \theta \quad (3.6)$$

where  $S_{\text{abov}}$  perimeter of the nominal elliptical cross-section of the cloud above the ground.

*Horizontal position*

$$d(x)/dt = u_x = u_{\text{cld}} \cos \theta \quad (3.7)$$

*Vertical position*

$$d(z)/dt = u_z = u_{\text{cld}} \sin \theta \quad (3.8)$$

## 4. Thermodynamics models

UMPDA invokes the thermodynamics module while solving the dispersion equations in the downwind direction. The module describes the mixing of the released component with moist air. The module calculates the phase distribution [component (vapour, liquid), vapour and liquid cloud temperature, and cloud density].

The liquid component in the aerosol is considered to consist of spherical droplets and additional droplet equations may be solved to determine the droplet trajectories, droplet mass and droplet temperature. Rainout of the liquid component occurs if the droplet size is sufficiently large.

The UMPDA includes the following types of thermodynamic models:

- **Equilibrium model.** Thermal equilibrium is assumed, which implies that the same temperature is adopted for all compounds in the cloud (vapour and liquid). The equilibrium model determines the phase distribution and the mixture temperature.
- **Non-equilibrium model.** This model allows the temperature of the droplet (liquid component) to be different of the temperature of the other compounds in the cloud. The non-equilibrium model determines the vapour temperature.

In conjunction with the equilibrium thermodynamics model the droplet model is used to set the droplet trajectories, the droplet mass, and the point of rainout. In conjunction with the non-equilibrium thermodynamics model, it additionally calculates the liquid droplet temperature. The initial drop size is taken as the minimum of the droplet size calculated by mechanical break-up and flashing break-up.

## 5. Pool spreading and vaporisation

If the droplet reaches the ground, rainout occurs, i.e. removal of the liquid component from the cloud. This produces a liquid pool which spreads and vaporises. Vapour is added back into the cloud.

The UMPDA source term model calculates the spreading and vapour flow rate from the pool. The pool spreads until it reaches a bund or a minimum pool thickness. The pool may either boil or evaporate while simultaneously spreading. The model takes into account heat conduction from the ground, ambient convection from the air, radiation and vapour diffusion. These are usually the main mechanisms for boiling and evaporation. These effects are modelled numerically, maintaining mass and heat balances for both boiling and evaporating pools. This allows the pool temperature to vary as heat is either absorbed by the liquid or lost during evaporation.

For a continuous release, the rate of generation of vapour from the spilt liquid is added to the vapour already in the cloud to give a total flow rate for the combined source. When the release stops there may then be a period of vapour generated from the liquid pool alone.

In the case of an instantaneous release the vapour produced by the spilt liquid is added back into the cloud, so long as part of the cloud still covers the point at which the pool was formed by the rained-out liquid. If the spilt liquid all evaporates while covered by the cloud then all that is produced is an instantaneous cloud. If the liquid has not all evaporated then once the upwind edge of the cloud has moved past the pool any remaining liquid is assumed to form a continuous source of vapour.

### 5.1. Droplet evaporation. Equilibrium modelling

This essentially assumes that each increment of added air evaporates the maximum amount of vapour thermodynamically possible. The simplest approach is to assume that the initial flash results in a vapour/liquid aerosol in thermal equilibrium at atmospheric pressure. The mixing process is assumed to be at the saturated condition with respect to the released liquid for as long as there is some proportion of the released material in the liquid phase in the cloud. This may result in low cloud temperatures as air is mixed into the cloud while liquid still remains.

## 5.2. Droplet evaporation. Non-equilibrium modelling

This allows the liquid temperature to decrease as the droplets evaporate, thereby developing a temperature driving force for heat conduction to the drop. The temperature decreases until a balance is achieved between heat gain by convection, conduction, and radiation, and heat loss by evaporation. At the same time, the driving force for mass transfer is decreased by the accumulation of evaporated vapour in the plume, but is increased when air is added by entrainment. In the limit, when either the driving force for mass transfer or the driving force for heat transfer goes to zero, the non-equilibrium model reduces to the special case of the equilibrium model. This is a theoretically more correct approach.

The temperature of the liquid droplets is calculated from a droplet evaporation model, whilst the temperature of the vapour is determined from an enthalpy balance.

## 5.3. Droplet trajectories

With either evaporation model option, the program calculates droplet trajectories. When the droplet trajectories touch the ground, rainout is modelled as occurring, and all remaining liquid in the cloud is assumed to rain out.

The pool is assumed to spread from this point of rain-out.

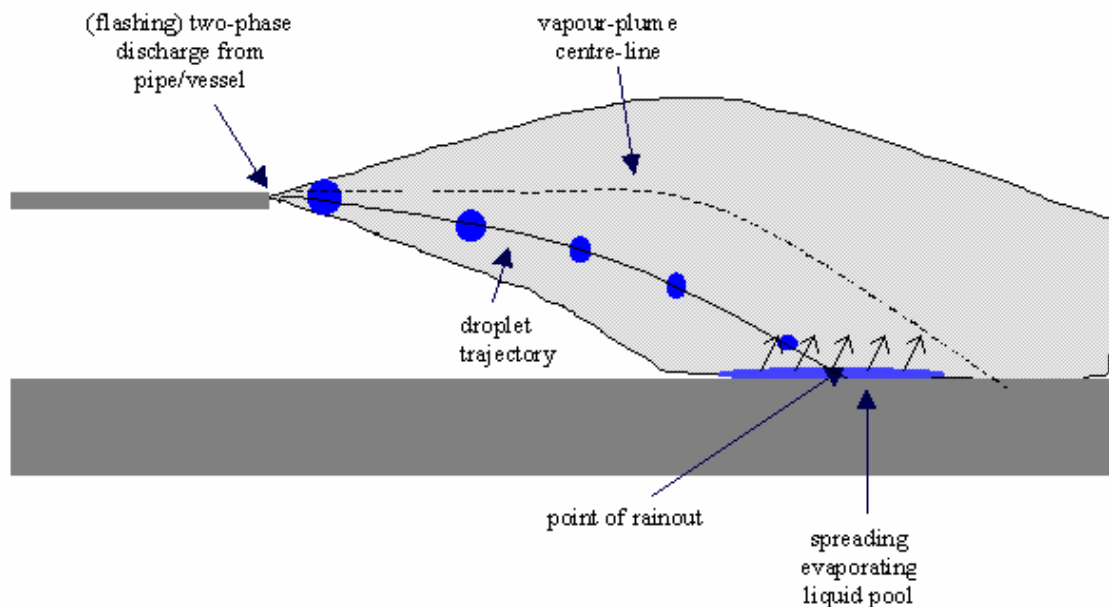


Figure 5.1. Droplet trajectory and liquid pool.

## 5.4. Pool spreading

The fate of the liquid that rains out is determined by using the liquid rate or the total liquid mass removed from the cloud as input to a liquid spill model, and then establishing a vapourisation rate.

The shape of the pool is idealised to be a circular cylinder of radius  $r(t)$  and uniform thickness  $h(t)$ , with a point source located at its centre. The radius of a pool spreading on land is found by numerically integrating the spreading rate equation given by Opschoor (1979):

$$dr/dt = \sqrt{[2g(h-h_{\min})]} \quad (5.1)$$

This assumes that the driving force for the spread is formed by the hydrostatic difference between the thickness of the current liquid layer and a minimum pool thickness characteristic for the substrate. This results in the rate of spreading decreasing as the pool approaches the minimum thickness.

The spreading pool is assumed to grow concentrically until it reaches an obstruction, e.g. a bund, or it attains a minimum thickness. When the pool has reached a bund the pool radius is constrained to be equal to the radius of the bund. Where the pool has spread and vaporised to produce a pool of depth equal to the minimum thickness, the spreading is constrained to be consistent with this thickness. Thereafter the radius will no longer be a simple function of time.

For an instantaneous release, once the minimum thickness has been reached the pool will start to shrink, keeping this thickness. For continuous spills the rate of spread will be constrained once the minimum thickness has been reached but in most cases the pool will continue to grow slowly. Once the release finishes the pool will normally contract as for the instantaneous case.

The minimum thickness depends on the type of surface and is shown in the table below.

Table 5.1. Pool minimum thickness.

Surface Number	Description	Minimum thickness (m)
1	Wet soil	0.03
2	Dry soil	0.05
3	Concrete	0.01
4	Insulating concrete	0.01
5-8	Water	0.001

## 5.5. Pool vaporisation

The liquid spill model can describe the spreading and vaporisation of pools of liquid spilt. For spills on land the model takes into account heat conduction from the ground, ambient convection from the air, radiation and vapour diffusion. These are usually the main mechanisms for boiling and evaporation. These effects are modelled numerically, maintaining mass and heat balances for both boiling and evaporating pools. This allows the pool temperature to vary as heat is either absorbed by the liquid or lost during evaporation.

At each time step in the numerical calculations the heat balance on the pool is evaluated and from this the vaporisation mechanism (i.e., boiling or evaporating), vaporisation rate and pool temperature are determined.

Initially, the temperature of the pool is assumed to be equal to the temperature of the released liquid.

The net rate of heat flow into the pool is calculated from

$$Q_{\text{net}} = Q_{\text{cond}} + Q_{\text{conv}} + Q_{\text{rad}} - Q_{\text{evap}} \quad (5.2)$$

where:  $Q_{\text{cond}}$  is the heat flow rate from conduction, (W);  
 $Q_{\text{conv}}$  is the heat flow rate from convection, (W);  
 $Q_{\text{rad}}$  is the heat flow rate from solar radiation, (W);  
 $Q_{\text{evap}}$  is the heat flow rate from evaporation, (W).

The heat flow rate from conduction is given from formula developed by Shaw and Brisco (1978) while the heat flow rate from convection by Fleisher (Fleischer M. , 1980).

## 5.6. Coupling of pool vaporization and cloud dispersion

The pool-modelling may give the result that there is no vapour generation, because the rate of generation is too low to be of interest.

In the case of an instantaneous release the vapour produced by the spilt liquid is added back into the cloud, so long as the cloud still covers the point at which rain-out occurred. If the spilt liquid all evaporates while covered by the cloud then all that is produced is an instantaneous, circular cloud. If the liquid has not all evaporated then once the upwind edge of the cloud has moved past the spill point any remaining liquid is assumed to form a continuous source of vapour.

For a continuous release, the rate of generation of vapour from the spilt liquid is added to the vapour already in the cloud to give a total flow rate for the combined source. When the release of liquid stops there may then be a period of vapour generated from the liquid pool alone. For both instantaneous and continuous releases this evaporating pool may or may not disappear before the upper limit on release durations prevents further consideration of effects. If it does disappear, it is described as a “cut-off” case while if not then a steadily vaporising pool is left behind. If the release itself is continuous then the “cut-off” vapour generation may give rise to a quasi-instantaneous cloud. It is assumed for simplicity that if the release is instantaneous then if the vaporisation is of such short duration as to give the possibility of quasi-instantaneous behaviour then there will most likely be no liquid pool left behind. To have the original instantaneous puff release and the subsequent quasi-instantaneous vaporised liquid cloud simultaneously would be too complex a situation.

This completes the range of possible behaviour for rained out liquid. While the possible combinations of behaviour give a fairly complex overall picture, each step by itself is relatively straightforward. In the printout for cases where rain-out occurs brief statements are given of how much liquid was removed, at what stage this happened and what the subsequent rates of vaporisation were.

## 6. Source term and release scenarios

### 6.1. Vessel type

With UMPDA one may choose one of the three types of storage vessel:

- A. Unpressurised/refrigerated vessel.
- B. Saturated liquid (the material is stored under its own vapour pressure).
- C. Pressurised gas vessel.

### 6.2. Scenario

One may also choose one of the scenarios. The choice of scenarios available depends on which vessel type has been selected.

1. Catastrophic rupture (for all vessel types). This is an instantaneous release of the entire inventory, either in a spontaneous failure, an internal explosion, or a BLEVE.
2. Line rupture (for all vessel types). This is a full-bore rupture of a length of pipework attached to a vessel (or any kind of pressure reservoir). The discharge modelling calculates the pressure-drop through the line based on the frequency of bends, couplings and junctions and the valve velocity head losses. If the material is a volatile liquid, then flashing may occur in the pipe – equilibrium modelling is used for the change of phase.
3. Leak (for all vessel types). This is a hole in the body of a vessel, or a small hole in a large pipe. The discharge modelling uses a non-equilibrium orifice calculation, which takes no account of friction losses inside the system.

### 6.3. Release parameters

#### *Phase of material to be released*

For some combinations of vessel type and scenario, there is only one possible release-phase e.g. all scenarios for the pressurised gas vessel are “vapour”. For other combinations, there is a choice between vapour and liquid, liquid and two-phase, or vapour and two-phase. The choice depends on the nature of the failure case considered.

#### *Pipe exit diameter*

This is the internal diameter of the process pipework or relief valve tail-pipe.

#### *Hole Diameter*

Leak scenario only. This is the diameter of the equivalent circular orifice with the same area as the area of the leak.

## 6.4. Tank data

### *Temperature/Pressure*

For case which is defined as “Pressurised gas vessel” in the scenario data, both temperature and pressure have to be specified. Check is made that the combination does correspond with the stated storage phase (e.g. that the material is gaseous at those conditions).

For cases which are defined as “Saturated liquid” in the scenario data, one can specify either temperature or pressure, and for “Unpressurised/refrigerated liquid” cases, one specifies only the temperature.

## 7. Discharge calculations: continuous releases

The purpose of the calculations is to predict the condition of the material once it has been discharged and has expanded down to atmospheric pressure, obtaining these conditions for the time of interest. The most important quantities calculated to describe the condition of the material and release are as follows:

- Mass flow rate.
- Phase (vapour, two-phase, liquid).
- Liquid fraction (for two-phase conditions).
- Temperature (for gas or liquid conditions).
- Final velocity.
- Droplet diameter (for liquid or two-phase conditions).
- Duration.

These are the quantities that are passed to the dispersion modelling. The discharge calculations include some additional quantities that are calculated in the course of the modelling and are used to obtain the quantities above, but are not required for the dispersion modelling:

- Discharge velocity.
- Choke pressure.
- Choke temperature.
- Discharge coefficient.

This section describes how these quantities are calculated for the different vessel types and scenarios. The calculations involve the following stages:

1. Establish the initial storage conditions.
2. Calculate the release rate and choke state at the initial storage conditions.
3. Calculate expansion from choke conditions to atmospheric conditions.
4. Calculate droplet size.

### 7.1. Establishing the initial storage conditions

This section covers the types of initial storage condition that can be modelled, introducing some nomenclature, and discussing the modelling requirements for the various conditions.

The material before release is assumed to be stored in a vessel under either pressurised or refrigerated (unpressurised) conditions. The initial conditions are specified by the temperature  $T_i$ , pressure  $P_i$ , phase, and liquid fraction  $F_{L_i}$  (if stored as a saturated mixture of liquid and vapour).

#### *Pressurised storage*

Pressurised storage conditions occur for gases held in pressure vessels containing vapour only, for vessels containing liquid under saturation conditions (i.e. a liquid in equilibrium with its own vapour), or for vessels which contain pressurised liquid with no vapour present. For vessels containing either pressurised gas or liquid it is necessary to define both the temperature  $T_i$  and pressure  $P_i$  to characterise the initial state. The liquid fraction  $F_{L_i}$  is zero for gas vessels, and unity for liquid vessels. For materials which are stored under saturation it is sufficient to define either the temperature (the pressure being determined from the saturation curve at that temperature) and the liquid fraction. Thus a saturated material stored at a temperature  $T_i$  would implicitly be at the pressure  $P_{sat}(T_i)$ .

### Unpressurised storage

The other method of storage which is modelled is refrigerated or unpressurised storage of liquids. There are two types of unpressurised vessel: cooled and saturated. For cooled, unsaturated, storage the temperature  $T_i$  must be specified and the liquid fraction is assumed to be unity. Materials stored under saturation conditions will be at a temperature determined from the saturation curve  $T_i = T_{\text{sat}}(P_a)$  with a specified liquid fraction. For both types of vessel a liquid head  $h_i$  is required.

The liquid head is combined with the ambient pressure  $P_a$  of storage to define an initial pressure:

$$P_i = P_a + \rho_i g h_i \quad (7.1)$$

where:  $\rho_i$  = density of the stored material,  
 $g$  = acceleration due to gravity.

Given the temperature, pressure and liquid fraction, the entropy, enthalpy, and volume of the initial state can be calculated, for use in the discharge modelling:

$$S_i = S(T_i, P_i, F_{Li}) \quad (7.2)$$

$$H_i = H(T_i, P_i, F_{Li}) \quad (7.3)$$

$$V_i = V(T_i, P_i, F_{Li}) \quad (7.4)$$

## 7.2. Discharge modelling for given storage conditions

### Leak scenario

The unimpeded flow through an orifice can be regarded as well approximated by reversible adiabatic expansion, that is isentropic expansion. Only when the kinetic energy of release is converted to heat does irreversibility enter the thermodynamics. The general approach to modelling these flows is then to calculate the mass flux through the orifice as a function of pressure in the plane of the orifice. For choked flows this will have a maximum at some point above atmospheric pressure, while for unchoked flows the pressure in the orifice will be atmospheric. The flow may or may not be in thermodynamic equilibrium; a saturated liquid may not flash until outside the orifice, for example. This can be taken into account by forcing the phase of the flow to remain unchanged when calculating the results of expansion.

The discharge through an orifice can conceptually be considered in two stages; firstly expansion from the initial storage conditions to the conditions in the orifice, followed by an expansion to ambient pressure outside the orifice if the flow is choked. This section describes the expansion to the conditions in the orifice – the expansion from the orifice conditions to atmospheric conditions is described in a later section which covers all scenarios.

The orifice conditions are specified by the temperature  $T_o$ , pressure  $P_o$  and liquid fraction  $F_{Lo}$ . This expansion is assumed to be reversible and adiabatic, that is isentropic. Thus, for a given orifice pressure  $P_o$ , the temperature  $T_o$  and/or liquid fraction  $F_{Lo}$  must be determined such that the entropy at the orifice plane:

$$S_o = S(T_o, P_o, F_{Lo}) \quad (7.5)$$

is equal to that of the initial state  $S_i$  described above. This is achieved by numerically iterating  $T_o$  and/or  $F_{Lo}$  until  $S_o = S_i$ .

In this process the phase, temperature, and liquid fraction of the material in the orifice are determined and from these the enthalpy and volume in the orifice can be calculated:

$$H_o = H(T_o, P_o, F_{Lo}) \quad (7.6)$$

$$V_o = V(T_o, P_o, F_{Lo}) \quad (7.7)$$

The mass flow rate through the orifice at the pressure  $P_o$  is then given by:

$$\dot{m} = C_d A_o \rho_o \sqrt{-2(H_o - H_i)} \quad (7.8)$$

where:  $C_d$  = discharge coefficient,  
 $A_o$  = area of the orifice,

$\rho_o$  = density of the material in the orifice (=  $1/V_o$ ).

The velocity of material flowing through the vena contracta of area  $C_d A_o$  is:

$$u_o = \sqrt{-2(H_o - H_i)} \quad (7.9)$$

For gas flows an estimation of the choke pressure  $P_c$  is made using the ideal gas formula:

$$P_c = P_i \left( \frac{2}{\gamma + 1} \right)^{\gamma/(\gamma-1)} \quad (7.10)$$

where  $\gamma$  = ratio of specific heats.

If the choke pressure  $P_c$  is less than the ambient pressure  $P_a$  then the flow is unchoked. The pressure in the orifice will then be ambient and the calculation described above can be carried out with  $P_o = P_a$ . However if  $P_c$  is greater than  $P_a$  the flow is choked. A calculation of the flow rate is made for an orifice pressure  $P_o$  equal to the choke pressure  $P_c$  calculated from the ideal gas equation. To allow for non-ideality in the actual equation of state the orifice pressure is then varied until the maximum flow rate has been found.

For two-phase flow the orifice discharge calculation described above is first carried out for an orifice pressure equal to the ambient pressure,  $P_o = P_a$ . Another calculation is then carried out at a slightly higher orifice pressure. If there is not an increase in flow rate as the pressure is increased then the flow through the orifice is unchoked. The pressure in the orifice is therefore ambient,  $P_o = P_a$ , and the final state parameters are those equal to the condition of the material in the orifice:  $T_f = T_o$ ,  $F_{Lf} = F_{Lo}$ ,  $u_f = u_o$ . On the other hand, if the flow rate through the orifice increases as the pressure is raised above ambient the flow is choked and has a maximum value at a choke pressure  $P_c$  which is greater than the ambient pressure. This choke pressure is determined by repeating the calculations described above, numerically iterating on the orifice pressure  $P_o$  until the mass flow rate is maximised. It is very unlikely that the flow of a liquid would be choked.

For incompressible fluids, i.e. liquids, a value of 0.6 is used for the discharge coefficient; a value which is well known to be appropriate in this case. For compressible fluids the method described by Bragg (1960) is used to calculate the discharge coefficient, generalised to any equation of state rather than being specific to the ideal gas equation of state.

### ***Line rupture scenario***

For pipes, the equations of flow are solved numerically for a given outlet pressure and a certain mass flux in the pipe. As the pressure drops along the pipe, the state of the material is evaluated from irreversible expansion, conserving the mass flux. For two-phase flows it is assumed that the flow is homogeneous and in thermodynamic equilibrium. The results of this calculation are to give the frictional losses that correspond to a certain outlet pressure and flow rate. For any given pipe the losses from valves, friction along the length of the pipe and miscellaneous other losses are known and so the flow in the pipe is varied until the frictional losses match.

Initially an orifice (or leak scenario) discharge calculation is carried out to obtain a starting value for the mass flow rate in the pipe and the pressure  $P_o$  at the outlet. This is the maximum initial flow rate; the actual flow rate will be lower due to frictional losses in the pipe.

Consider a pipe of length  $L$  and diameter  $d$ . Fluid enters the pipe at a pressure  $P_i$  and exits at a pressure  $P_o$ , flowing down the pipe at a mass flow rate per unit area  $G$ .

Let the fluid have a density  $\rho$  and the pipe a resistance to flow per unit area of surface of  $R$ . Assuming that the pipe is horizontal and that no work is done by the fluid on the pipe, the energy balance equation for a small change in the flowing fluid is:

$$\frac{1}{2}d(u^2) + VdP + dF = 0 \quad (7.11)$$

where:  $u$  = flow velocity,  
 $V$  = specific volume.

The energy lost to friction in the element  $dl$  is:

$$dF = \left( \frac{4R}{\rho d} \right) dl \tag{7.12}$$

Substituting for the flow velocity  $u = GV$  and re-arranging gives:

$$\frac{dV}{V} + \frac{dP}{G^2 V} + \frac{1}{G^2 V^2} \left( \frac{4R}{\rho d} \right) dl = 0 \tag{7.13}$$

Integrating along the length of the pipe then gives the total frictional loss in the pipe as:

$$F_{tot} = \left( \frac{8RL}{\rho u^2 d} \right) = 2 \left[ \ln \left( \frac{V_i}{V_o} \right) - \frac{1}{G^2} \int_{P_i}^{P_o} \frac{dP}{V} \right] \tag{7.14}$$

To calculate  $\int dP/V$  it is assumed that the fluid flow can be modelled as an irreversible adiabatic expansion.

The actual frictional loss in the pipe is determined as follows. The Fanning friction factor is calculated as:

$$f = \left( \frac{2R}{\rho u^2} \right) = \frac{2}{[3.2 - 2.5 \ln(e/d)]^2} \tag{7.15}$$

Where  $e$  = a linear quantity representing the roughness of the pipe surface.

This is modified to account for losses in bends:

$$f' = f[1 + L_{bend} f_{bend}] \tag{7.16}$$

where:  $L_{bend}$  = equivalent length of pipe for a 90° degree bend,  
 $f_{bend}$  = frequency of bends per unit length.

The total frictional loss along the pipe is then:

$$F_{tot} = L \left[ \frac{4f'}{d} + V_{coup} f_{coup} + V_{junc} f_{junc} \right] + \frac{1}{C_d^2} + N_1 K_1 + N_2 K_2 + N_3 K_3 \tag{7.17}$$

where:  $C_d$  - discharge coefficient for a very short length of pipe (0.8 is used),  
 $V_{coup}, V_{junc}$  - velocity head losses for couplings and junctions,  
 $f_{coup}, f_{junc}$  - frequency of occurrence of couplings and junctions,  
 $N_1, N_2, N_3$  - numbers of safety, release and shut-off valves,  
 $K_1, K_2, K_3$  - corresponding losses per valve.

What is now required is the value of the outlet pressure  $P_o$  and the mass flux  $G$  such that the frictional loss implied by these values and found by numerically integrating along the pipe is the same as that determined from the length and type of pipe, and the number of couplings, junctions, and valves placed on it. This would require an iterative calculation to be carried out which is a time-consuming process so instead a logarithmic interpolation of flow against pipe frictional resistance is used to estimate the actual flow. Although this interpolation is usually good it can mean that slightly different results for the same length of pipe can be obtained, depending on how the interpolation is set up.

If the outlet pressure  $P_o$  is the same as the ambient pressure  $P_a$  then the flow is unchoked at the outlet and the thermodynamic state at the outlet and the flow velocity in the pipe become those of the final state.

On the other hand if the flow is choked at the outlet of the pipe – i.e. the outlet pressure  $P_o$  is greater than the ambient pressure  $P_a$  – the material will undergo an additional process of expansion down to atmospheric pressure. This expansion process is described in a later section which covers all scenarios.

For both conditions of outlet pressure, the mass flow rate is given by:

$$\dot{m} = (\pi d^2 / 4)G \tag{7.18}$$

### 7.3. Expansion from choke conditions to atmospheric pressure

If the flow is choked then the pressure in the orifice is above ambient and there will be an expansion of the material outside the orifice to ambient pressure. This is also treated here as an isentropic expansion. The final state now has a pressure  $P_a$  and the temperature  $T_f$  and/or liquid fraction  $F_{Lf}$  are iterated numerically so that the final state entropy  $S_f$  is equal to the initial state entropy  $S_i$  above, where:

$$S_f = S(T_f, P_a, F_{Lf}) \quad (7.19)$$

As before from the results of this expansion the enthalpy of the final state can be calculated:

$$H_f = H(T_f, P_a, F_{Lf}) \quad (7.20)$$

Assuming that all the energy released in the expansion is converted into kinetic energy, the velocity of material at ambient pressure is given by:

$$u_f = \sqrt{-2(H_a - H_i)} \quad (7.21)$$

For choked flows the final velocity  $u_f$  does not correspond to a physically real velocity, and is therefore referred to as the final velocity. It has been developed to be used as a parameter describing the initial kinetic energy in a discharge for input to a dispersion model. These models have been calibrated to produce the correct amount of entrainment when used with this effective velocity. It should be noted that for unchoked flow the orifice and final-velocities are equal.

### 7.4. Calculation of droplet size

If the final state of the released material at ambient pressure contains liquid then the program calculates the size of the liquid droplets. The method used depends on whether or not the liquid flashes.

For non-flashing liquids the calculation is based on the value of the Weber number for the escaping liquid. The Weber number is a dimensionless group representing the ratio of aerodynamic forces on drops to "cohesive" forces holding those drops together.

It is defined as:

$$W = \rho u^2 d / 2 \sigma \quad (7.22)$$

where:  $\rho_{air}$  = density of ambient air,  
 $u^2$  = velocity of the emerging liquid,  
 $d$  = diameter of the drop,  
 $\sigma$  = surface tension of the material.

If the drop has a Weber number which is larger than a critical value  $W_{crit}$  the drop will not be stable and will break up into smaller droplets. The actual value of  $W_{crit}$  depends on several factors such as whether the drop is suddenly exposed to stationary air or whether it falls freely from rest.  $W_{crit}$  can also depend on the type of break-up mechanism involved and even on the viscosity of the material. For the purposes of the present modelling, these complications have been ignored.

Thus if a jet is not liable to flash, the drop size corresponding to  $W_{crit}$  is calculated and if this is smaller than the size of the jet the final droplet size is taken to be this value. Droplet radii are always limited to the jet radius or to a maximum drop size with a typical value of 0.01 m). However, given the range of velocities and length scales found with failure cases, any further increase in this maximum drop size would be unlikely to affect the kinematic behaviour of the drop.

## 8. Discharge calculations: instantaneous releases

This section describes the theory used in the discharge-calculations for the catastrophic rupture scenario. The calculations are much simpler than those for continuous releases.

The catastrophic rupture scenario is designed to model an incident in which a catastrophic failure of a vessel occurs – i.e. the vessel is destroyed by an impact, a crack or some other failure which propagates very quickly, leading to a tank completely losing its integrity. The resulting release is assumed to form a homogeneous mass, expanding rapidly to form a semi-spherical cloud. The assumption is that for a truly instantaneous release, the actual expansion will take place essentially outside the vessel. The expansion of an instantaneous release is, as for continuous releases, taken to be initially a reversible adiabatic expansion.

The most important quantities calculated to describe the condition of the released material are as follows:

- Expansion energy.
- Phase (vapour, two-phase, liquid).
- Liquid fraction (for two-phase conditions).
- Temperature (for gas or liquid conditions).
- Droplet diameter (for liquid or two-phase conditions).

The discharge calculations include some additional quantities that are calculated in the course of the modelling and are used to obtain the quantities above, but are not required for the dispersion modelling:

- Discharge velocity.

**Modelling the expansion**

For a material stored at temperature  $T_i$  and pressure  $P_i$ , and with liquid fraction  $F_{Li}$ , the entropy, enthalpy, and volume under storage-conditions are given by:

$$S_i = S(T_i, P_i, F_{Li}) \tag{8.1}$$

$$H_i = H(T_i, P_i, F_{Li}) \tag{8.2}$$

$$V_i = V(T_i, P_i, F_{Li}) \tag{8.3}$$

Upon release the stored material is assumed to expand reversibly and adiabatically to ambient pressure  $P_a$ . In such an expansion entropy is conserved. Thus the temperature  $T_f$  and/or liquid fraction  $F_{Lf}$  of the final state must be determined such that the entropy of the final state:

$$S_f = S(T_f, P_f, F_{Lf}) \tag{8.4}$$

is equal to that of the initial state  $S_i$ . This is achieved by numerically iterating  $T_f$  and/or  $F_{Lf}$  until  $S_f = S_i$ . In this process the phase, temperature, and liquid fraction of the final state are determined and from these the enthalpy and volume of the final state can be calculated:

$$H_f = H(T_f, P_f, F_{Lf}) \tag{8.5}$$

$$V_f = V(T_f, P_f, F_{Lf}) \tag{8.6}$$

In the adiabatic expansion to atmospheric pressure a certain amount of enthalpy is released. In addition the expanding material has to do work to drive back the atmosphere.

The expansion energy of a release takes both of these quantities into account and is the energy released by adiabatic expansion of the material, minus the work done on the atmosphere:

$$E = -(H_f - H_i) - (P_i - P_a)V_i \tag{8.7}$$

This quantity is used in the correlation from Maurer et al (1977) to describe the initial stages of cloud dilution. The implicit assumption in this is that all the energy released by the reversible expansion goes into the kinetic energy of the release. Even if this is only approximately true, the actual rate of dilution was based on experimental results, correlated against this quantity. Therefore, it is the appropriate physical parameter to describe the state of an instantaneous release.

**Calculation of droplet size**

Just as for continuous releases, instantaneous releases have a drop size estimated. In this case the velocity used in the drop size calculations is determined from the expansion energy on the basis that this is a measure of the kinetic energy in the cloud:

$$u = \sqrt{2E} \tag{8.8}$$

It should be noted that the velocity is only indicative of the actual velocity of droplets in the cloud. In reality there would be a distribution of droplet velocities and sizes.

## 9. Conclusions

The key advantages of the new UMPDA model with respect to other typical dispersion models can be summarised as follows:

- a single model for the entire dispersion regime from the point of release to the far-field dispersion including possible rainout and pool re-evaporation; this eliminates discontinuities and matching problems;
- a very extensive verification and validation to ensure that the model shows the correct behaviour and produces accurate predictions.

The UMPDA is integrated within the user-friendly and well-established SWAR computer network based decision support system for emergency response in case of chemical accidents. This enables plotting, linking with discharge/fire/explosion models, toxic/flammable impact and risk calculations. The results of UMPDA calculations can be used in other modules of the SWAR system both for emergency planning and for supporting emergency response in real-time.

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