VERIFICATION

UDM CHAPTER 6: UNPRESSURISED INSTANTANEOUS DISPERSION

DATE: December 2023

Reference to part of this report which may lead to misinterpretation is not permissible.

No.	Date	Reason for Issue	Prepared by	Verified by	Approved by
1	1999	PHAST 6.0	Witlox and Holt		
2	Oct 2005	SAFETI 6.5	Witlox and Harper		
3	May 2011	Phast 6.7; UDM v2	Harper		
4	Sep 2017	Phast 8.0; UDM v3	Witlox		
5	May 2021	Apply new template	D. Vatier		

Date: December 2023

Prepared by: Digital Solutions at DNV

ABSTRACT

The UDM theory and solution algorithm for an unpressurised instantaneous release has been investigated in detail. Several improvements have been applied. These include:

- consistent assumptions for the cloud shape (concentration profile, effective cloud dimensions)
- improved calculation of the cloud surface area above the ground, and the cloud footprint area
- improved criterion for onset of touchdown
- more physically well-based calculation of near-field dispersion. This includes new formulas for jet entrainment, crosswind entrainment and airborne drag force (proportional to the cloud surface area above the cloud). Moreover near-field passive dispersion has now been included.
- more physically well-based calculation of interaction with the ground. This includes new formulas for ground drag force, ground heat transfer and ground water-vapour transfer (proportional to the cloud footprint area).

For purely passive dispersion, the UDM results are shown to be in close a close agreement with vertical and crosswind dispersion coefficients and concentrations obtained from an analytical Gaussian passive dispersion formula. For ground-level heavy dispersion, good results have been obtained for validation against the Thorney Island experiments.

As part of further work, the UDM instantaneous model should be extended to allow for along-wind diffusion to be different from cross-wind diffusion. This could involve the instantaneous DRIFT approach and/or the more general HEGADAS-T time-dependent approach. The current approach lead to inaccurate results for [a] unstable conditions in conjunction with large averaging times (too large σ_x, too low maximum concentrations) and [b] stable conditions in conjunction with small averaging times (too small σ_x, too large maximum concentrations).

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6 UNPRESSURISED INSTANTANEOUS DISPERSION

6.1 Introduction

This report documents the verification and sensitivity analysis of the Unified Dispersion Model (UDM) for the case of an unpressurised instantaneous release. It accompanies the UDM theory manual.

In Section 6.2 far-field and near-field instantaneous passive dispersion are considered. In Section 6.3 a literature review is carried out for ground-level heavy gas dispersion (side entrainment, crosswind spreading). Effects of jet entrainment and ground heat transfer are tested in Section 6.4.

6.2 Passive dispersion

This section considers instantaneous passive dispersion, in an analogous fashion to continuous passive dispersion (see Chapter 2).

In Section 6.2.1 the UDM equations are given for isothermal continuous passive dispersion. A reduced set of two equations for the crosswind and vertical dispersion coefficients is derived. In Section 6.2.2 the UDM concentration profile is compared against the usually adopted analytical passive dispersion profile.

In Section 6.2.3 a base-case problem is defined. It is shown for this base case that the UDM numerical results correspond to the analytical results for the ambient passive dispersion coefficients, and that the UDM concentration profile is consistent with the analytical passive-dispersion profile.

In Section 6.2.5 the near-field passive dispersion formulation is compared against the far-field passive dispersion formulation.

6.2.1 UDM equations and analytical solution

The UDM theory manual includes a complete set of dispersion equations. For isothermal, instantaneous, horizontal passive dispersion these equations simplify as follows:

- zero water-vapour transfer from ground: $m_{wv}^{gnd} = 0$
- no heat transfer from ground: $q_{gnd} = 0$
- horizontal momentum = ambient momentum: $u_{cld}=u_a$, $I_x=m_{cld}u_a$, $I_{x2}=0$
- zero vertical momentum: $I_z = 0$, $u_z = 0$
- cloud position: $\theta=0$, $x_{cld} = u_a t$
- enthalpy equation: $T_{cld}=T_a$ → density $\rho=\rho_a$ → concentration profile m=n=2 [note n> 2 for non neutral]
- cloud mass/volume relation $m_{cld} = \rho_{cld}V_{cld}(x)$
- cloud volume $V_{cld}(x) = 0.5(1+h_d)\,(2\pi)^{3/2}\,\sigma_y^2\sigma_z$
- cloud mass entrainment: $dm_{cld}/dt = Ent_{pas} = V_{cld}(x)\,u_a\rho_a[2\sigma_y^{-1}d\sigma_{ya}/dx+\sigma_z^{-1}d\sigma_{za}/dx]$
- cloud spreading: $dR_y/dx = 2^{0.5}\,d\sigma_y/dx = 2^{0.5}\,d\sigma_{ya}/dx(x-x_0)$

Thus two equations remain for σ_y, σ_z:

$$d/dx\,[(1+h_d)\sigma_y^2\sigma_z] = (1+h_d)\sigma_y^2\sigma_z[2\sigma_y^{-1}d\sigma_{ya}/dx+\sigma_z^{-1}d\sigma_{za}/dx],\quad d\sigma_y/dx = d\sigma_{ya}/dx(x-x_0)$$

Using virtual-source distance x_o=0, initial σ_y=0 (true for small release rate), the solution to the second equation equals: $\sigma_y=\sigma_{ya}$. Thus one equation remains for σ_z:

$$d/dx\,[(1+h_d)\sigma_{ya}^2\sigma_z] = (1+h_d)\sigma_{ya}^2\sigma_z[2\sigma_{ya}^{-1}d\sigma_{ya}/dx+\sigma_z^{-1}d\sigma_{za}/dx]$$

which can be simplified to

$$d/dx\,[(1+h_d)\,\sigma_z] = (1+h_d)\,d\sigma_{za}/dx \quad \text{or} \quad d\sigma_z/dx = d\sigma_{za}/dx - (1+h_d)^{-1}[dh_d/dx]\,\sigma_z$$

where

$$h_d = \mathrm{erf}(z_{cld}/\sigma_z)$$
$$dh_d/dx = -\,[2/\pi]^{0.5}\,[z_{cld}\,\sigma_z^2\,d\sigma_z/dx]\ /\ (\exp[z_{cld}^{\,2}/(2\sigma_z^2)] < 0$$

Thus $\sigma_z > \sigma_{za}$. Note that for $\sigma_z / z_{cld} << 1$ (in near-field, h_d=1) applies $dh_d/dx << 1$ and therefore $\sigma_z \cong \sigma_{za}$. When σ_z / z_{cld} << 1 approaches 1 (i.e. cloud depth comparable to cloud height, h_d reducing from 1 to 0), σ_z starts to become larger than σ_{za}.

Note that the above differential equation for σ_z is identical to that derived for the continuous case.

6.2.2 Concentration profile

BWM/TNO profile

The BWM/TNO instantaneous passive dispersion profile (beyond the initial spherical expansion zone) is given by

$$c(x,y,z) = \frac{m_c}{(2\pi)^{3/2}\,\sigma_{xa}\,\sigma_{ya}\,\sigma_{za}} e^{-\frac{(x-u_a t)^2}{2\sigma_{xa}^2}} e^{-\frac{y^2}{2\sigma_{ya}^2}} \left\{ e^{-\frac{(z-z_{cld})^2}{2\sigma_{za}^2}} + e^{-\frac{(z+z_{cld})^2}{2\sigma_{za}^2}} \right\} \quad (1)$$

with dispersion coefficients σ_{za} and σ_{ya} (at 600sec) from TNO formulas (see Duijm[i], or TNO yellow book[ii])

$$\sigma_{xa}(x) = 0.13x \;\; , \sigma_{ya}(x) = \left(\frac{t_{av}}{600}\right)^{0.2} a\,x^b \;\; , \sigma_{za}(x) = C_{ZR}\, c\, x^d \,, C_{ZR} = (10 z_R)^{0.53x^{-0.22}} \quad (2)$$

Here the averaging time t_{av} (s) is taken to be t_{av} = 18.75 s (i.e. no time averaging is applied for instantaneous dispersion), and $C_{ZR} = C_{ZR}(x;z_R)$ is the correction factor for the influence of the surface roughness z_R [$C_{ZR}(x;0.1)=1$]. The parameters a, b, c, d are given as a function of stability class in the table below.

stability class	a (m)	b (-)	c (m)	d (-)
A	0.527	0.865	0.28	0.90
B	0.371	0.866	0.23	0.85
C	0.209	0.897	0.22	0.80
D	0.128	0.905	0.20	0.76
E	0.098	0.902	0.15	0.73
F	0.065	0.902	0.12	0.67

UDM profile

The un-averaged UDM instantaneous passive dispersion profile is given by

$$c(x,y,z,t) = \frac{m_c}{V_{cld}(t)} e^{-\frac{[x-x_{cld}(t)]^2}{R_x^2}} e^{-\frac{y^2}{R_y^2}} e^{-\frac{(z-z_{cld})^2}{R_z^2}} = \frac{m_c}{\frac{1}{2}(1+h_d)(2\pi)^{3/2}\,\sigma_x\sigma_y\sigma_z} e^{-\frac{[x-x_{cld}(t)]^2}{2\sigma_x^2}} e^{-\frac{y^2}{2\sigma_y^2}} e^{-\frac{(z-z_{cld})^2}{2\sigma_z^2}} \quad (3)$$

with $R_y = 2^{1/2}\sigma_y = 2^{1/2}(t_{av}/t_{av}^{core})^{0.2}\,\sigma_y(t_{av}^{core})$, $R_z = 2^{1/2}\sigma_z$, $R_x = 2^{1/2}\sigma_y(t_{av}^{core})$, $x_{cld} = u_a t$. Furthermore $h_d = \mathrm{erf}(z_{cld}/R_z)$, with erf the error function. Note that h_d = 0 for a ground-level plume (z_{cld}=0) or $z_{cld} << \sigma_z$, and that h_d = 1 for $z_{cld} >> \sigma_z$. According to the preceding section, the dispersion coefficients σ_y and σ_z are given by

$$d\sigma_z/dx = d\sigma_{za}/dx - (1+h_d)^{-1}[dh_d/dx]\,\sigma_z \;\; , \;\; \sigma_y=\sigma_{ya}.$$

where σ_{ya}, σ_{za} are taken from the McMullen and Hosker formulas, respectively (see UDM theory manual).

Comparison of profiles
The following is noted by comparing the TNO profile (1) and the UDM profile (3):

- Both profiles conserve the mass m_c (kg). This can be verified by means of integration of the profiles over x,y,z.
- Both profiles exhibit the same cross-wind dependency, since $\sigma_y=\sigma_{ya}$.
- For a ground-level plume (z_{cld} = 0) or for $z_{cld} << \sigma_z$, $\sigma_z = \sigma_{za}$ and both profiles are identical.
- For the extreme case of $z_{cld} >> \sigma_z$, the profiles are somewhat different. However, similarly as shown for continuous passive dispersion (see Chapter 2), it can be shown that both profiles still lead to close results. The difference between σ_z and σ_{za} will compensate for the difference in the form of the profiles.
- The UDM adopts the simplifying assumption of $\sigma_x = \sigma_y$, unlike the TNO model.
- The UDM dispersion formulas (of McMullen and Hosker) and the TNO dispersion formulas (=power-law of HGSYSTEM) for $\sigma_{y,}$ σ_z are very similar (see Chapter 2).

6.2.3 Base case

The UDM base-case run for instantaneous passive dispersion was defined similarly to continuous passive dispersion:

- basecase: instantaneous release of 0.05 kg release of nitrogen_air at 50 m height with temperature 298K and velocity 5 m/s[1]

- ambient: logarithmic temperature and linear pressure profile, D5 and 298K at 50 m (cut-off for wind = 1 m), solar flux = 500 W/m^2, air mole weight = 28.966

- substrate: dispersion over land – dry soil (temperature = 298K), surface roughness = 0.1m

- averaging time = 18.75 s

- parameters: maximum distance = 100000, distance multiple for full passive entrainment = 2, dense to passive smoothing transition parameter = 2, core averaging time = 18.75 s

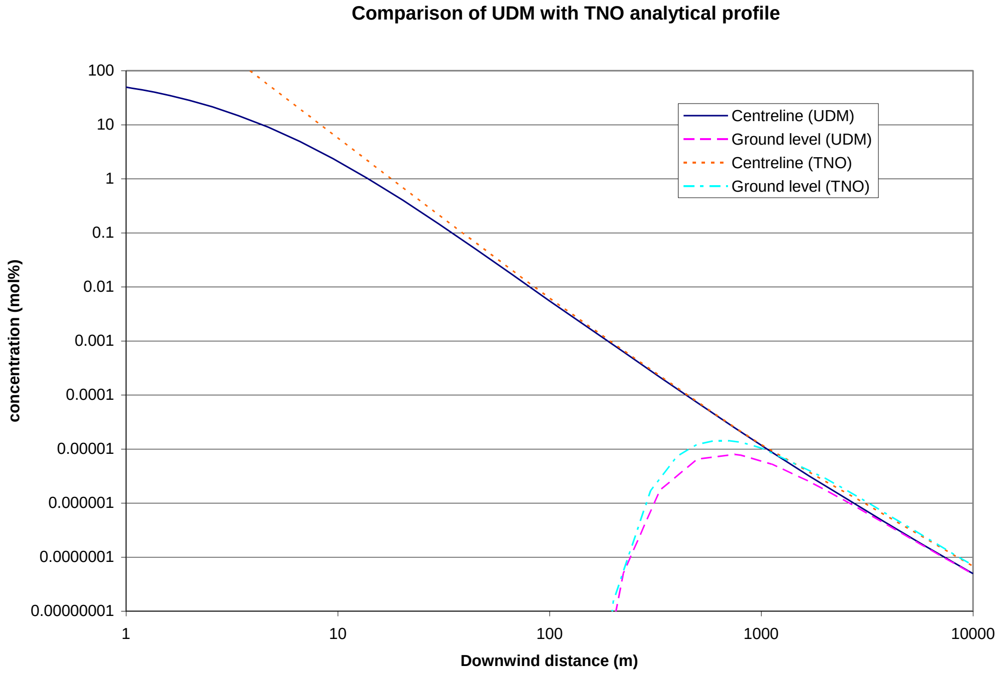
For the above base-case problem, the UDM numerical results have been compared against the analytical solution for the cross-wind and vertical dispersion coefficients σ_y, σ_z and the centre-line and ground-level concentrations. In addition they have been compared against the corresponding runs carried out for continuous dispersion (see Section 2.3). The conclusions are as follows:

- In Section 6.2.1 it was derived theoretically that the 'passive instantaneous dispersion' differential equations for σ_y, σ_z are identical to those for 'passive continuous dispersion'. It was indeed confirmed that the UDM numerical results were virtually identical; see Section 2.3 (Figures 2.4, 2.5) for further details of comparison against analytical results. Note that different profiles are used for the UDM and the analytical TNO formula:

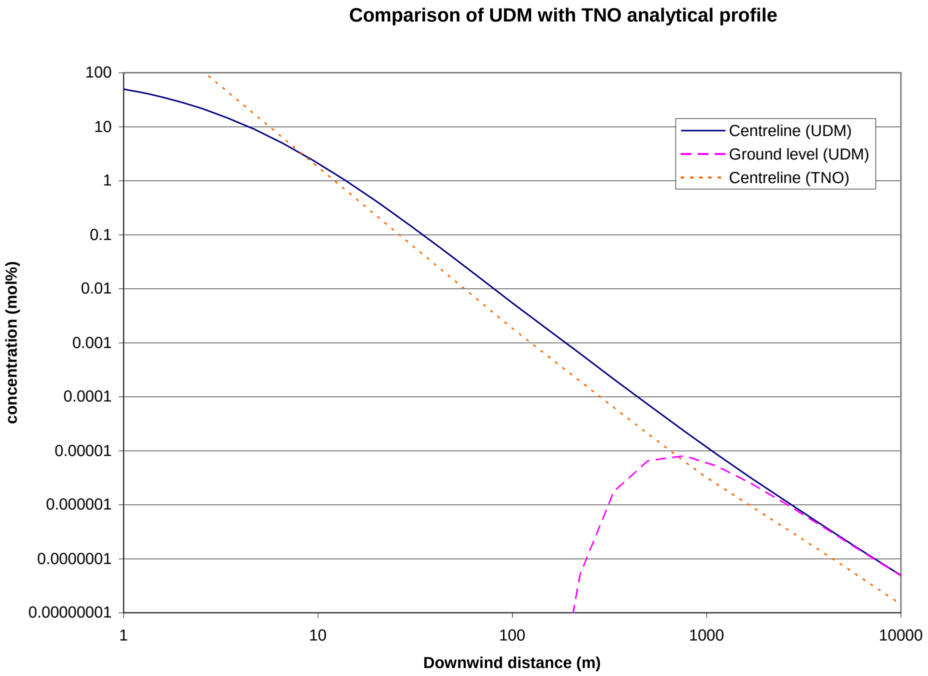
    * Figure 6.1a adopts a modification from the TNO profile (1), i.e it applies $\sigma_{xa} = \sigma_{ya} = 0.5\ a\ x^b = 0.5 * 0.128\ x^{0.905}$ instead of $\sigma_{xa} = 0.13x$. As for continuous passive dispersion (see Chapter 2), it is seen that the results for the centre-line concentrations are very close. Also ground-level concentrations are reasonable close.
    * Figure 6.1b adopts the original TNO profile (1), with $\sigma_{xa} = 0.13x$. It is seen that this results in significant larger UDM centre-line concentrations. This is because the UDM applies $\sigma_{xa} = \sigma_{ya} = a\ x^b = 0.5 * 0.128\ x^{0.905}$, which is significantly smaller than the TNO value $\sigma_{xa} = 0.13x$. This confirms the observation in the preceding section, and a large core averaging time (e.g. 600 seconds) would be more appropriate for this case. This would ensure that the cylindrical shape of the instantaneous cloud is more justified for the core calculations.

- It was confirmed that following equation (3), the maximum concentration is independent of the ambient wind speed. However the received dose reduces with increasing wind speed (cloud passes a given point more quickly).

[1] Release velocity of 5 m/s imposed by setting minimum velocity to 5 m/s



(a) use of $\sigma_{xa} = \sigma_{ya}$ in both UDM and 'TNO' profiles (t_{av}^{core}=18.75s)



(b) use of TNO value σ_{xa} = 0.13x for 'TNO' profile (t_{av}^{core} = 18.75s)

Figure 6.1 Centre-line and ground-level concentrations: UDM numerical result and analytical TNO profile

6.2.4 Along-wind diffusion and choice of core averaging time

UDM assumption for along-wind diffusion

As described in the UDM theory manual, a circular horizontal cross-section is always assumed (R_x=R_y) for the UDM calculations in the case of instantaneous dispersion. Thus the downwind passive dispersion coefficient σ_{xa}(x) is assumed to be equal to the crosswind passive dispersion coefficient $\sigma_{ya}(x;t_{av})$ at the averaging time t_{av}. The crosswind dispersion coefficient σ_{ya} increases with averaging time, $\sigma_{ya}(x;t_{av}) = (t_{av}/ t_{av}^{core})^{0.2} \sigma_{ya}(x;t_{av}^{core})$, where t_{av}^{core} is the core averaging time

The UDM assumption $R_x=R_y$ implies that the passive downwind dispersion coefficient σ_{xa} also increases with averaging time, $\sigma_{xa}(x;t_{av}) = (t_{av}/ t_{av}^{core})^{0.2} \sigma_{ya}(x;t_{av}^{core})$.

However it would be more accurate to assume that σ_{xa} is NOT a function of averaging time, and the following discussion relates to the assumption that $\sigma_{xa} = \sigma_{xa}(x)$ is a function of x only.

<u>Formula for along-wind diffusion from literature</u>

Passive along-wind diffusion (σ_{xs}) is caused by both wind shear (σ_{xs}) and turbulent spread (σ_{xt}), while passive cross-wind diffusion is caused by turbulent spread only (see the description of the finite-duration correction method in the UDM theory manual):

$$\sigma_{xa}(x) = \sqrt{\sigma_{xs}^2(x) + \sigma_{xt}^2(x)} \qquad (4)$$

with $\sigma_{xt} = \sigma_{yt} = \sigma_{ya}(x;18.75)$ and

$$\sigma_{xs}(x) = a_{xs}\, x \;, \qquad with \;\; a_{xs} = 0.6\, p \left[\frac{0.48}{\gamma}\right]^p, \gamma = \sqrt{2}\left\{\frac{(1-p\,d)\,\Gamma(\frac{1}{2}p+\frac{1}{2})}{\sqrt{\pi}}\right\}^{1/p} \qquad (5)$$

Furthermore $d = d_{sc} + d_{zo}$ is the exponent in the approximate power-law fit $\sigma_z(x) = (c\,x^d)$. Here c and d_{sc} are a function of stability class, and d_{zo} a function of surface roughness.

Thus for no time averaging (t_{av} = 18.75s) the instantaneous passive plume will be longer in the downwind direction than in the cross-wind direction, i.e. $\sigma_{xa} > \sigma_{ya}(t_{av}=18.75)$. With increasing averaging time σ_{ya} increases.

<u>Validity of UDM assumption for along-wind diffusion (at core averaging time)</u>

To validate the assumption $R_x=R_y$ at the core averaging time t_{av}^{core}, t_{av}^{core} could be chosen such that $\sigma_{xa}(x) \approx \sigma_{ya}(t_{av}^{core})$, i.e.

$$\sigma_{xa}(x) = \sqrt{\sigma_{xs}^2(x) + \sigma_{ya}^2(x;18.75)} = \sigma_{ya}(x;t_{av}^{core}) = \left(\frac{t_{av}^{core}}{18.75}\right)^{0.2} \sigma_{ya}(x;18.75) \qquad (6)$$

The table below includes the results for the required core averaging time for surface roughness z_o=0.1 m. Note that the wind-shear diffusion σ_{xs} increases with stability, while turbulent diffusion $\sigma_{xt}=\sigma_{yt}$ decreases with stability. As a result the averaging time needed for $\sigma_{xa} \approx \sigma_{ya}(t_{av}^{core})$ increases significantly with stability class. Note that the TNO value σ_x = 0.13 x is comparable to the value of 0.113 x calculated in the table.

Table 6.1. Evaluation of $\sigma_{xa}(x)$ from Equation (6), and core averaging time needed for $\sigma_{ya}(x;t_{av}^{core}) = \sigma_{xa}(x)$

[value of wind-speed exponent from Irwin[iii], value of d from power-law fit to Hosker σ_z formula, formula for γ from UDM theory manual, formula for σ_{xs} from Ermak, formula for σ_{ya} from Briggs[iv]], and core averaging time needed for $\sigma_{xa} = \sigma_{ya}$; surface roughness = 0.1 m]

stability class	p (Erwin)	d	γ	σ_{xs}/x (Ermak)	$\sigma_{ya}(x;18.75)/x = \sigma_{xt}/x$ (Briggs)	σ_{xa}/x	core averaging time (s) needed for $\sigma_{ya}=\sigma_{xa}$
A	0.08	0.9021	0.218	0.051	0.11	0.121	31
B	0.09	0.8354	0.235	0.058	0.08	0.099	54
C	0.11	0.8031	0.244	0.071	0.055	0.090	218
D	0.16	0.7614	0.258	0.106	0.04	0.113	3418
E	0.32	0.7322	0.272	0.23	0.03	0.232	$5.18*10^5$
F	0.54	0.669	0.299	0.418	0.02	0.418	$7.52*10^7$

From the table it follows that using a core averaging time of t_{av}^{core} = 18.75 seconds, will always produce a too low value for $\sigma_{xa}(x;t_{av}^{core})$, i.e. too conservative (too high) predictions for the maximum concentration. Using t_{av}^{core} = 600 seconds, will produce un-conservative predictions for A,B,C and conservative predictions for D,E,F.

Following the above the following observations are made.

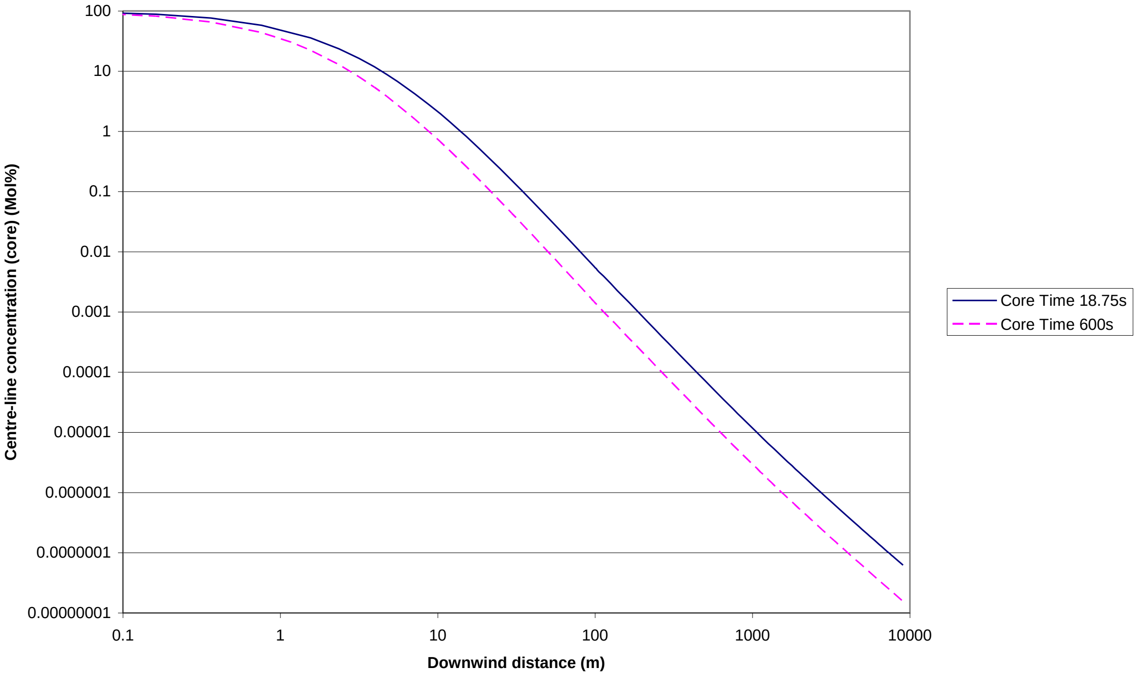
1. In case of a fixed core averaging time, the choice t_{av}^{core} = 18.75 seconds is recommended to produce always conservative predictions for all stability classes. The under-prediction of σ_x will be more severe for increasing stability.
2. The choice of a fixed core averaging time t_{av}^{core} = 600 seconds provides better predictions for stability class D. This choice will involve unconservative predictions for unstable conditions and conservative predictions for stable conditions.
3. Using $t_{av} = t_{av}^{core}$ (variable core averaging time) would lead to the following:
   - for flammable releases usually $t_{av} = t_{av}^{core}$ = 18.75 seconds would lead to conservative predictions for passive along-wind diffusion, but passive diffusion would often not effect flammability zones
   - for toxic releases, $t_{av} = t_{av}^{core}$ = 600 seconds would lead to unconservative predictions for unstable conditions and conservative predictions for stable conditions
   - using $t_{av} = t_{av}^{core}$ is the most appropriate choice for continuous releases, and following quasi-instantaneous transition the choice $t_{av} = t_{av}^{core}$ for instantaneous dispersion would be compatible.
4. Note that the above observations are applicable for ground-level dispersion. For elevated dispersion the windshear is smaller and therefore σ_{xs} smaller. Therefore for large heights $\sigma_x \approx \sigma_{xs} = \sigma_{yt}(18.75s)$. Thus for this case a core averaging time of 18.75 seconds would be appropriate
5. Note that the UDM currently takes into account effects of time averaging for wind meander only [except for finite-duration correction and duration adjustment]. Time averaging because of time-varying concentrations due to limited duration is not taken into account.

As a result the following recommendations are made.

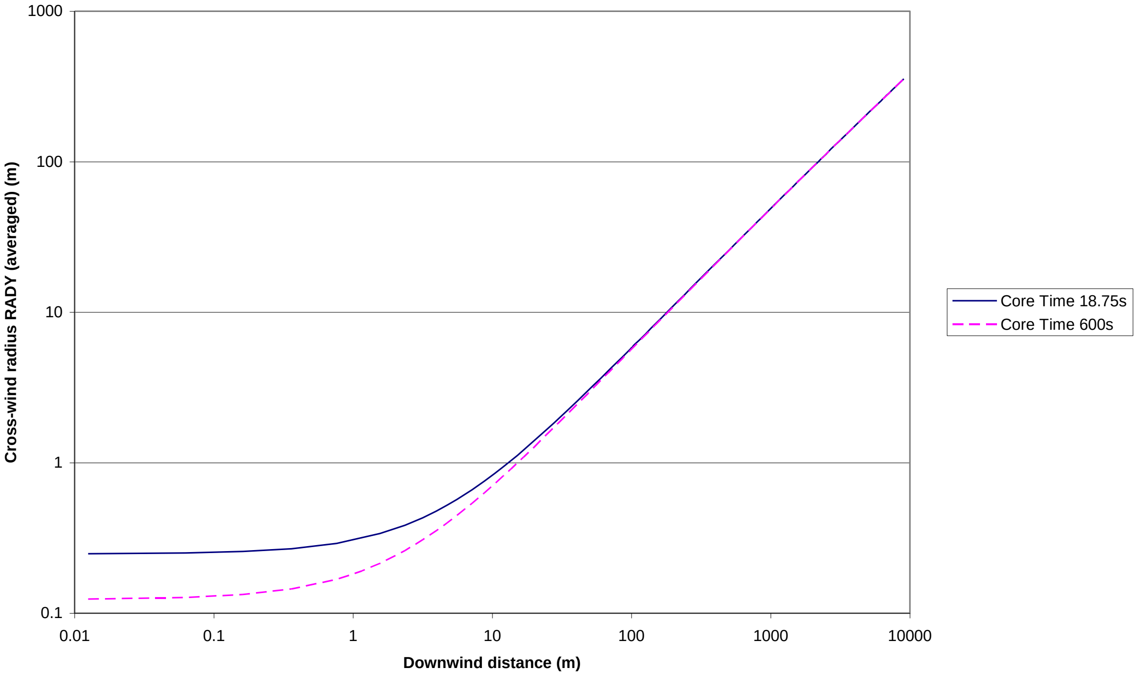
1. For current implementation $t_{av} = t_{av}^{core}$ (variable core averaging time) is recommended for both continuous and instantaneous dispersion , with default values for t_{av} = 18.75,600 for flammable and toxic releases. This choice may lead to inaccurate results for [a] unstable conditions in conjunction with large averaging times (too large σ_x, too low maximum concentrations) and [b] stable conditions in conjunction with small averaging times (too small σ_x, too large maximum concentrations). However it leads to most smooth results.
2. Alternatively, to ensure always conservative predictions (and when CPU times are important), the choice t_{av}^{core} = 18.75 seconds is recommended. This option is chosen as the **default** option in Phast.
3. As further work the UDM should be extended to allow for R_x different from R_y, and effects of along wind diffusion should be included in a more rigorous manner. This could involve the DRIFT approach and/or the HEGADAS-T approach. The current simplistic modelling of along-wind diffusion (R_x=R_y for **all** averaging times) may lead to large inaccuracies for some cases.

Following the above observations, a brief sensitivity analysis is carried out for a range of averaging times and core averaging times. Figure 6.2, Figure 6.3 and Figure 6.4 include results for averaging times of 18.75, 600 and 3600 seconds, respectively. Note that in these simulations the along-wind diffusion σ_x is taken to be independent of the averaging time (unlike for the standard UDM), i.e. $R_x(x;t_{av}) = R_y(x;t_{av}^{core})$. The case is considered of an elevated instantaneous passive release of air. The following points should be noted:

- Concentrations for one given averaging time decrease with increasing core averaging time. This is due to the fact that for the instantaneous cloud $\sigma_x = \sigma_y(x;t_{av}^{core})$ increases with increasing core averaging time. Note however that this is not the case for the standard UDM in which $R_x(x;t_{av}) = R_y(x;t_{av})$.
- Cloud σ_y values are identical except near the source. This is due to the fact that the initial cloud size does not match the ambient σ_{ya} values causing the effect of the averaging time correction to be more pronounced.
- Near the source, concentrations for a core averaging time of 600s and averaging time of 18.75 s can exceed 100 %. This is clearly not desired!

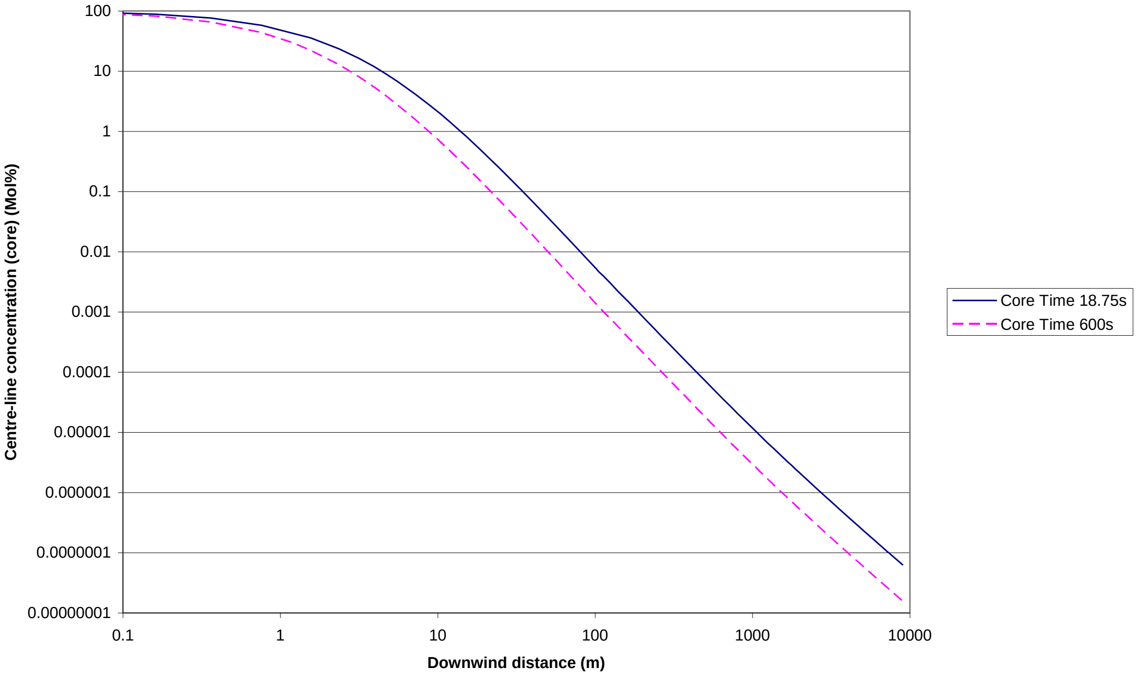


(a) centre-line concentration (mol %)

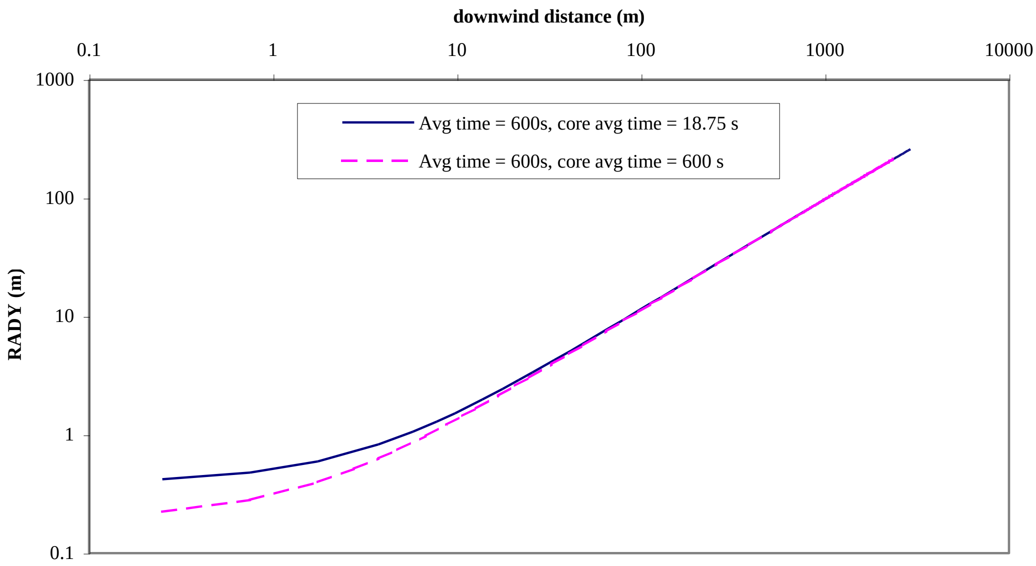


(b) cloud half-width R_y

Figure 6.2. Elevated instantaneous passive release of air (averaging time = 18.75 seconds) [non-standard UDM option $R_x(x;t_{av}) = R_y(x;t_{av}^{core})$ instead of normal UDM assumption $R_x(x;t_{av}) = R_y(x;t_{av})$]

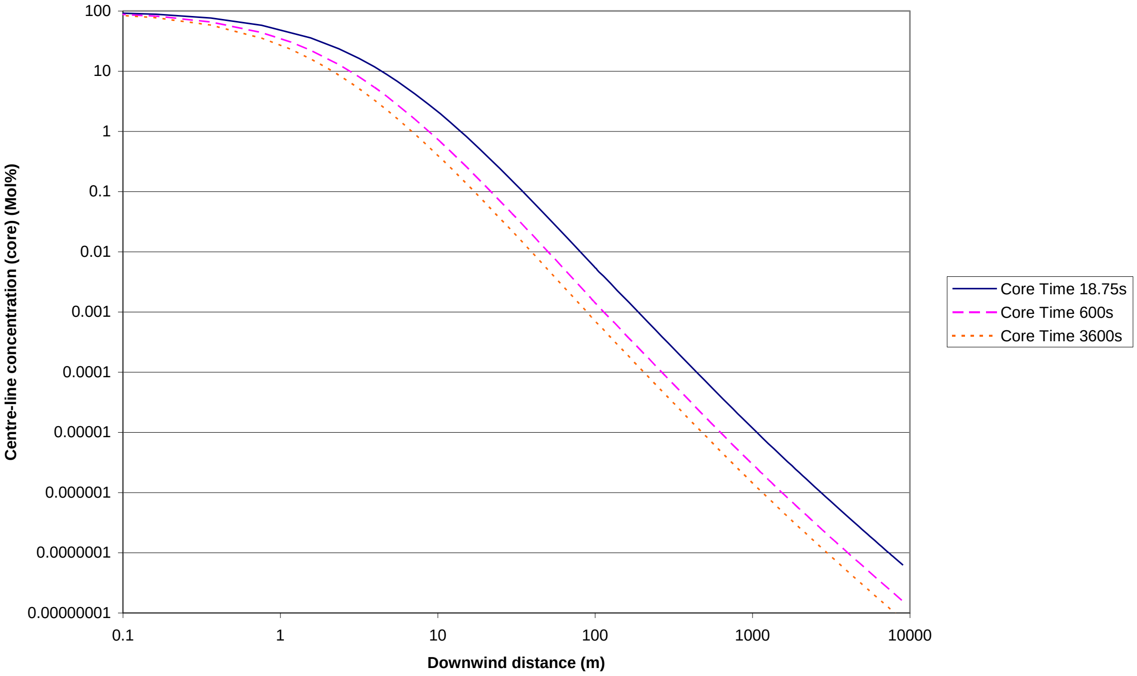


(a) centre-line concentration (mol %)

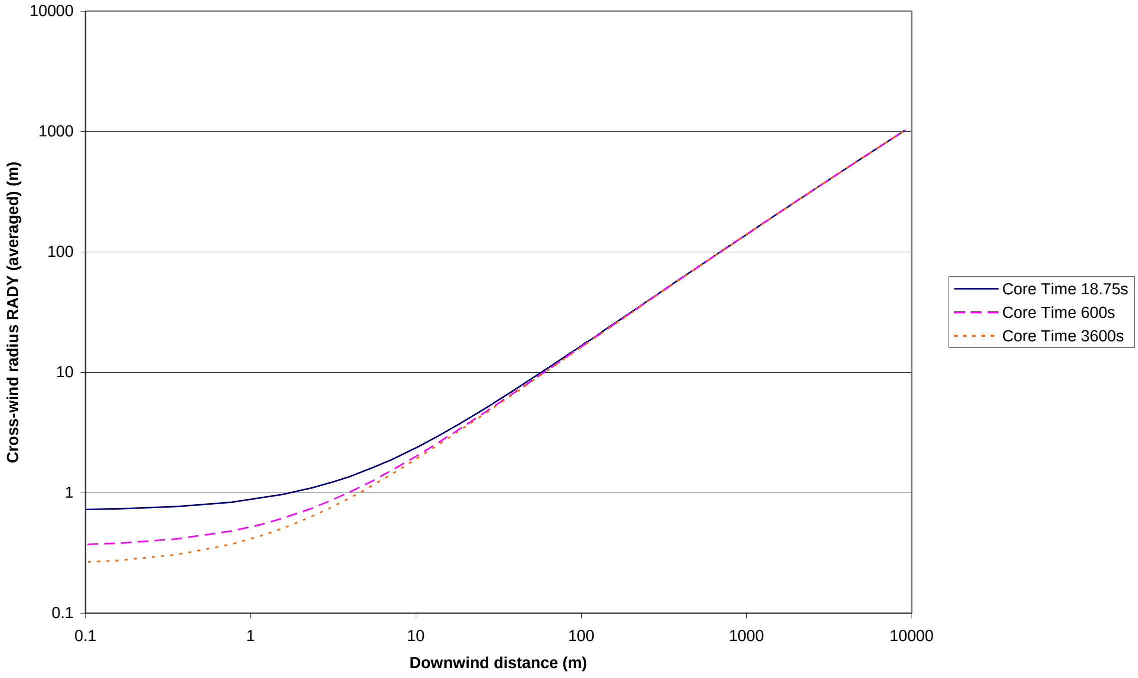


(b) cloud half-width R_y

Figure 6.3. Elevated instantaneous passive release of air (averaging time = 600 seconds) [non-standard UDM option $R_x(x;t_{av}) = R_y(x;t_{av}^{core})$ instead of normal UDM assumption $R_x(x;t_{av}) = R_y(x;t_{av})$]



(a) centre-line concentration (mol %)



(b) cloud half-width R_y

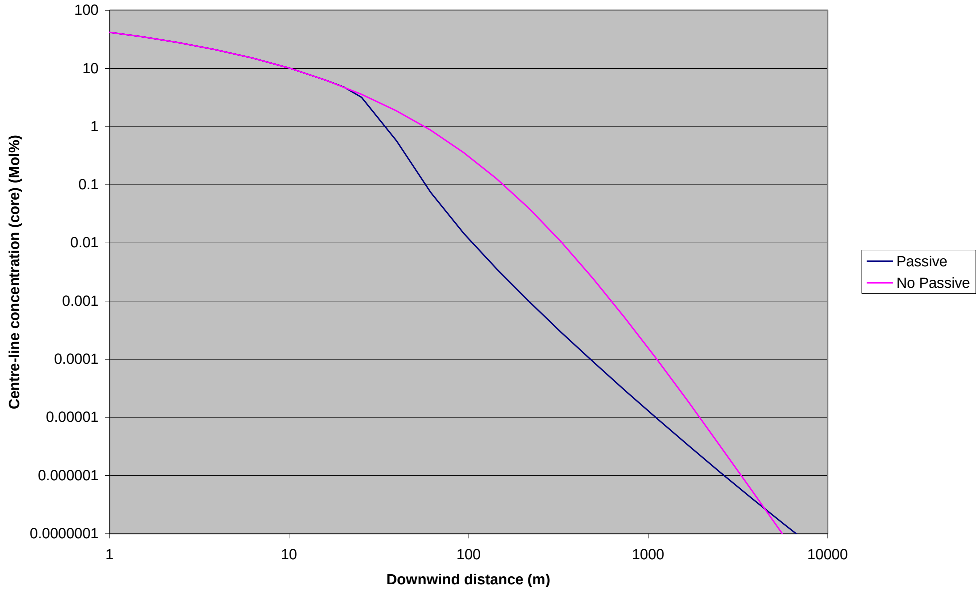
Figure 6.4. **Elevated instantaneous passive release of air (averaging time = 3600 seconds)** [non-standard UDM option $R_x(x;t_{av}) = R_y(x;t_{av}^{core})$ instead of normal UDM assumption $R_x(x;t_{av}) = R_y(x;t_{av})$]

6.2.5 Near-field passive formulation versus far-field passive formulation

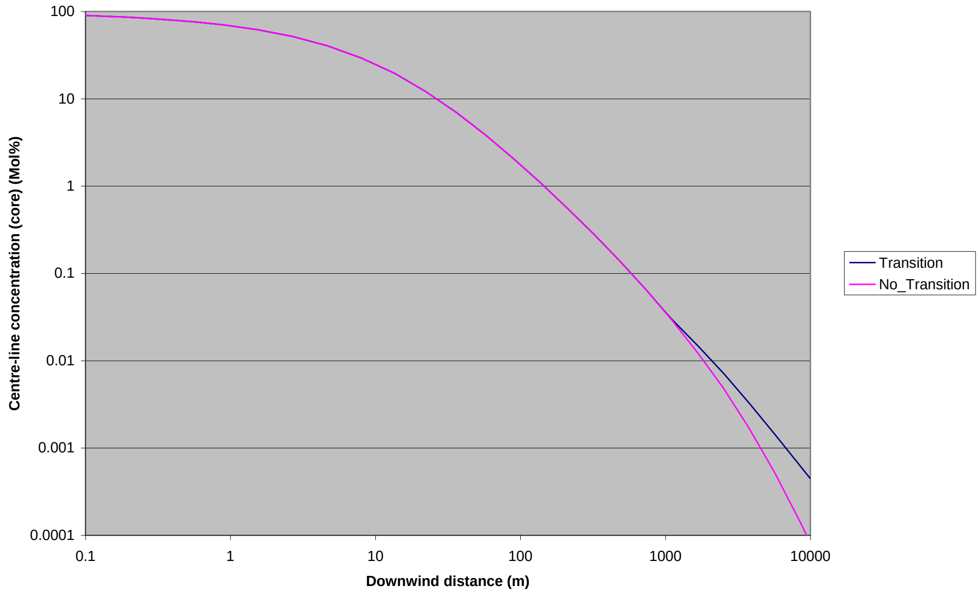
In Figure 6.5 the above basecase of an elevated instantaneous plume is considered, with a release velocity of 0.1 m/s, an ambient velocity of 5 m/s, and a release height of 600 m. Results of two UDM analyses are included i.e. with passive transition from near-field to far-field dispersion and without transition to far-field dispersion.

- For release of ‘air’ (Figure 6.5a), it is seen that in the near-field the near-field passive dispersion formulation leads to less entrainment than the far-field passive dispersion formulation ($E_{pas}^{nf}<E_{pas}^{ff}$) , while in the far-field it leads to more entrainment ($E_{pas}^{nf}>E_{pas}^{ff}$). Note however that the discrepancy for the old UDM 5.2 formulation was even larger.
- For release of ‘methane’ (Figure 6.5b), the plume is not horizontal but buoyancy induces plume rise. As a result, the passive transition is considerably later (due to initial plume rise), and only the effect of $E_{pas}^{nf}>E_{pas}^{ff}$ in the far-field is visible.

Centre-line concentration (core)



(a) air (horizontal plume)



(b) methane (plume rise delays passive transition)

Figure 6.5 **Elevated instantaneous 0.1 m/s release (600 m) at 5 m/s wind speed; results of simulations with and without passive transition to far-field passive dispersion.**

6.3 Ground-level heavy dispersion

This section discusses the results of a literature review on side-entrainment and cross-wind spreading formulations for unpressurised heavy-gas instantaneous dispersion (see Section 3 in the UDM theory manual). The UDM adopts the value γ=0.3 for the side entrainment coefficient and the value C_E=1.15 for the spreading coefficient.

The Special November 1987 issue of Journal of Hazardous material on the Thorney Island dispersion trials contains a range of proposed formulations and associated values for the side-entrainment coefficient γ and the spreading coefficient C_E:

1. The formulation in the HGSYSTEM model HEGABOX by Puttock[v] for instantaneous releases assumes the following:

    - the cloud is treated as a cylinder of uniform gas concentration, which is in line with the UDM assumption of an effective cylindrical cloud with top-hat concentration c_o; however c_o is the maximum concentration
    - the radius of the cloud is given by $dR/dt = 1.15(g'H)^{0.5}$ which is in line with the UDM assumption $dW_{eff}/dt = 1.15(g'H_{eff})^{0.5}$. However HEGABOX adopts $g' = g[\rho_{cld}-\rho_a]/\rho_a$ [larger value ➔ more spreading] instead of $g' = g[\rho_{cld}-\rho_a]/\rho_{cld}$
    - it adopts the same side-entrainment formulation $u_{side} = \gamma\ dW_{eff}/dt$, but with γ = 0.85 to fit data by Spicer and Havens [although it is stated in the HGSYSTEM manual that this value may be significantly smaller]
    - top entrainment is defined via a Richardson number entrainment function, in line with the UDM model [although different formulations are adopted!]
    - A transition is made to HEGADAS-T if the Richardson number drops to 10 (assuming a uniform HEGADAS cross-wind profile of width the cloud width at that distance, and the maximum concentration being the top-hat concentration). Thus in the near-field HEGABOX and the UDM would be more equivalent if $m=n=\infty$.

2. Carpenter, Cleaver, Waite, and English[vi] adopt the same type of model, but with a different top entrainment term, C_E=1.15, γ = 0.65±0.05.

3. Van Ulden[vii] argues that using concentration data from 0.4 m elevation sensors may lead to too large value of γ being deduced, owing to a non-uniform vertical concentration gradient. He neglects side entrainment. He adopts the cross-wind spreading law $dR/dt = C_E(g'H)^{0.5}$, with C_E = 1.15 from Thorney Island or C_E=1.2 from Haven and Spicer experiments.

4. Deaves[viii] investigates both options of the spreading law $dR/dt = C_E\{[(\rho_{cld}-\rho_a)/\rho_r]\ gH]^{0.5}$ with $\rho_r=\rho_a$ or ρ_{cld}. According to Webber $\rho_r=\rho_a$ is superior, since it enables analytical similarity solutions. By means of comparison against Thorney Island Trials, Deaves showed that $\rho_r=\rho_{cld}$ gave slightly less scatter (with value $C_E=2^{0.5}$), than $\rho_r=\rho_a$ (with C_E=1.15).

5. Britter indicated that vortices observed for Thorney Island don't make this representative to set γ. Laboratory experiments by Simpson and Britter[ix] suggest lower values.

6. Figure 6.6 presents results for a UDM sensitivity analysis for Thorney Island run 8. Values for the side entrainment coefficient, γ, of 0.3, 0.5, 0.6 and 0.7 were used. The influence of this parameter is greatest in the near field where the default UDM value for γ = 0.3 gives the closest comparison to the experimental data.

<u>Summary of conclusions:</u>

1. Most standard approach would be to adopt γ = 0.7 and $dW_{eff}/dt = 1.15(g'H_{eff})^{0.5}$ with $g' = g[\rho_{cld}-\rho_a]/\rho_a$ (see e.g. overview paper by Brighton[x]). However these are used in top-hat models, which would be only approximate to the UDM model adopting equivalent cylindrical effective cloud with uniform maximum concentration. The current UDM model adopts γ = 0.3, which leads to the most accurate results for Thorney Island experiment 8.

2. Deaves suggests the alternative $g' = g[\rho_{cld}-\rho_a]/\rho_{cld}$ with associated $C_E = 2^{0.5}$.

3. The evaluation of the heavy-gas top entrainment may need to be further checked against observations in the overview paper by Brighton[x].

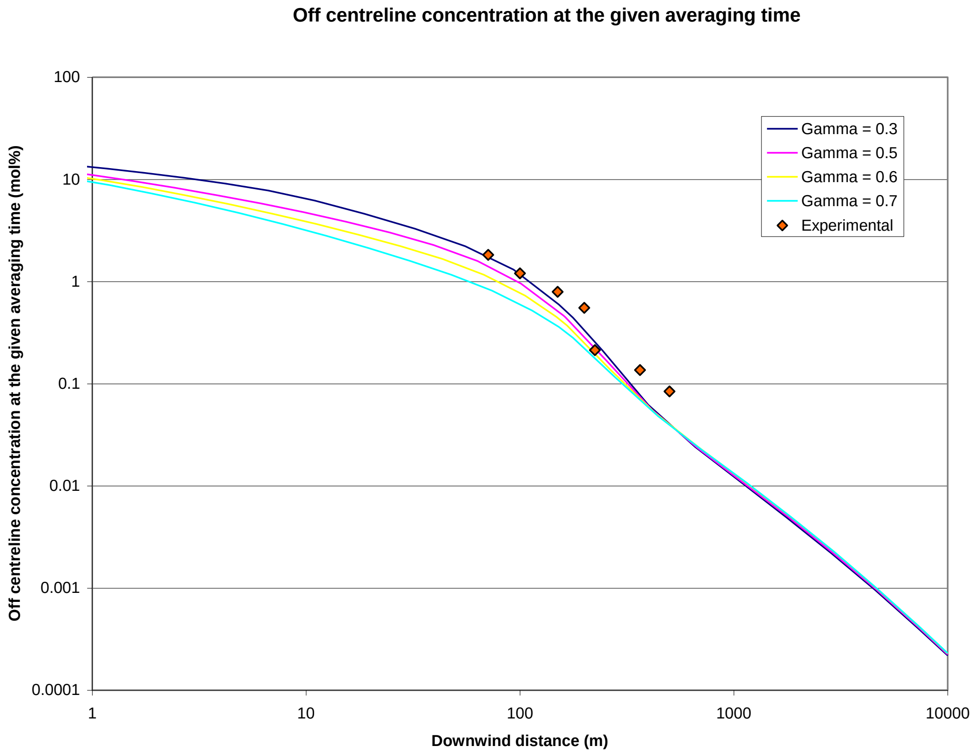


Figure 6.6. Comparison of experimental data from Thorney Island 8 against UDM predictions using values of the side entrainment coefficient γ = 0.3, 0.5, 0.6 and 0.7.

6.4 Effect of jet entrainment and heat transfer

In Figure 6.7 the above basecase of a ground-level instantaneous plume is considered, with a release velocity of 0.1 or 5 m/s, an ambient velocity of 5 m/s. Results of UDM analyses are included with and without heat transfer from the ground. It is concluded that in the case of a release velocity of 0.1 m/s, the additional 'jet' entrainment (resulting from the difference between cloud and ambient speeds) results in smaller concentrations.

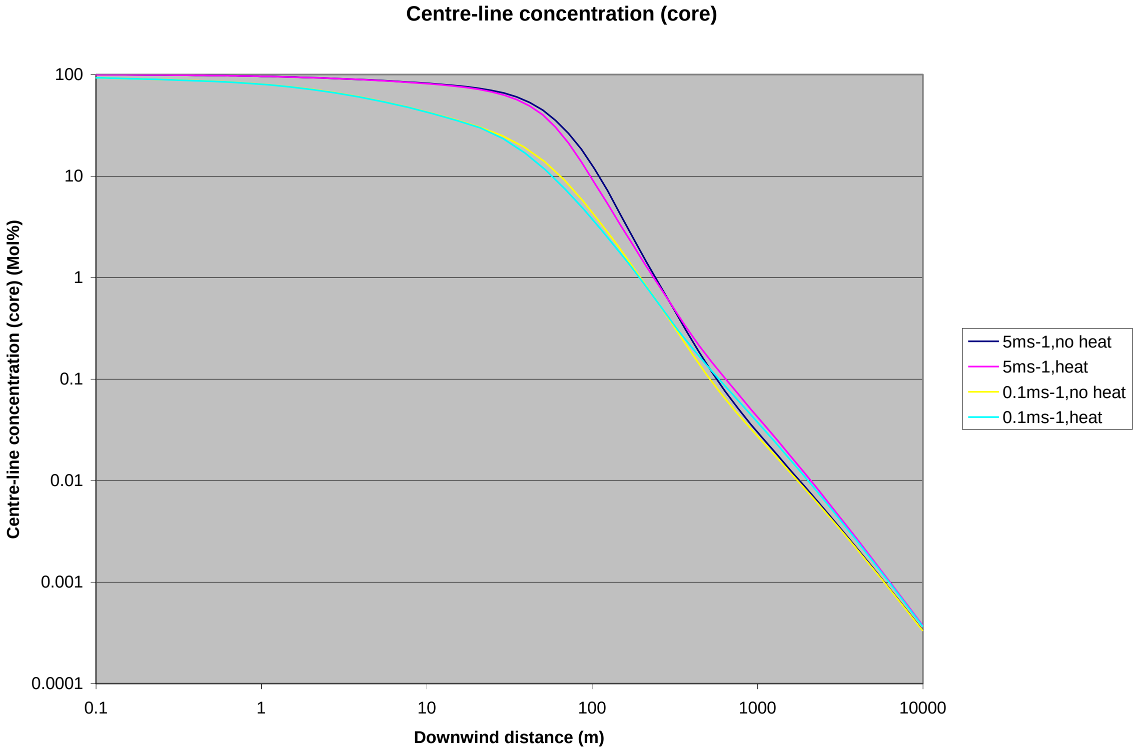


Figure 6.7. Ground-level release of propane at 5 m/s wind speed; effect of release speed (0.1 or 5 m/s) and heat transfer)

6.5 Further work

1. Allow for different values for cross-wind width and cloud width of instantaneous cloud, i.e. $R_x \neq R_y$, e.g. by adopting logic from the model DRIFT[xi]. This should allow σ_x to be evaluated in line with logic of HGSYSTEM heavy-gas dispersion program HEGADAS-T[xii,xiii].

2. More detailed sensitivity analysis (particularly for ground-level dispersion?)

3. Validation against more instantaneous experiments

4. Additional verification may be carried out by means of comparison against Shell HEGABOX program.

SPREADSHEETS

Figure 6.1	inst_Passive_Analytical.xls
Figure 6.2	inst_Average_Time18.75.xls (non-standard UDM)
Figure 6.3	inst_Average_Time600.xls (non-standard UDM)
Figure 6.4	inst_Average_Time3600.xls (non-standard UDM)
Figure 6.5a	inst_Air_Passive_Transition.xls,
Figure 6.5b	inst_Methane_Passive_Transition.xls
Figure 6.6	thorney_8.xls
Figure 6.7	inst_propane_jet_heat.xls

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