VERIFICATION

UDM CHAPTER 2: PASSIVE DISPERSION

DATE: December 2023

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	May 2021	Apply new template	D. Vatier		

Date: December 2023

Prepared by: Digital Solutions at DNV

ABSTRACT

The UDM theory and solution algorithm for passive dispersion have been investigated in detail.

The UDM results are shown to be in close agreement with vertical and crosswind dispersion coefficients and concentrations obtained from an analytical Gaussian passive dispersion formula.

A sensitivity analysis has been carried out for a given base-case problem (passive dispersion of 'air'). Parameter variations have been carried out to the release height, averaging time, surface roughness length, stability class, release rate and wind speed.

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2 PASSIVE-DISPERSION

2.1 Introduction

This report documents the verification and sensitivity analysis of the Unified Dispersion Model (UDM) for the case of continuous isothermal passive dispersion. It accompanies the UDM theory manual.

In Section 2.2 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 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 2.4 a sensitivity analysis is carried out for a given base-case problem (passive dispersion of 'air'). Parameter variations include variations of the release height, averaging time, surface roughness length, stability class, release rate and wind speed.

2.2 UDM equations

2.2.1 Isothermal continuous passive dispersion

The UDM theory manual includes a complete set of dispersion equations. For isothermal, continuous, 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: $I_z = 0$, $u_z = 0$
- 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/area relation $m_{cld} = u_a\rho_a A_{cld}(x)$
- cloud area $A_{cld}(x) = (1+h_d)\,\pi\sigma_y\sigma_z$
- cloud mass entrainment: $dm_{cld}/dx = Ent_{pas} = A_{cld}(x)\, u_a\rho_a[\sigma_y^{-1}d\sigma_{ya}/dx+\sigma_z^{-1}d\sigma_{za}/dx]$
- cloud spreading: $dW_{eff}/dx = 0.5(2\pi)^{0.5}\, d\sigma_y/dx = 2^{0.5}\,C_m\, d\sigma_{ya}/dx(x\text{-}x_0)$, $C_m = 0.5\,\pi^{0.5}$

Thus two equations remain for σ_y, σ_z:

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

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:

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

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 $\sigma_z / z_{cld} <<$ 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}.

2.2.2 Concentration profile

The BWM/TNO passive dispersion profile is given by

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

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

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

Here t_{av} is the averaging time (s), 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

The UDM passive dispersion profile is given by

$$c(x,y,z) = \frac{m_c}{0.5(1+h_d)\pi\, u_a R_y R_z} e^{-\frac{y^2}{R_y^2}} e^{-\frac{(z-z_{cld})^2}{R_z^2}} = \frac{m_c}{(1+h_d)\pi\, u_a \sigma_y \sigma_z} e^{-\frac{y^2}{2\sigma_y^2}} e^{-\frac{(z-z_{cld})^2}{2\sigma_z^2}}$$

with $R_y = 2^{1/2}\sigma_y$, $R_z = 2^{1/2}\sigma_z$. 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

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

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

The following is noted:

- Both profiles conserve the mass flow m_c (kg/s) flowing through a vertical plane at a given downwind distance. This can be verified by means of integration of the profiles over 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. Nevertheless it will be shown in the next Section for an example 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 dispersion formulas (of McMullen and Hosker) and the TNO dispersion formulas (=power-law of HGSYSTEM) are very similar:

- Figure 2.1 shows that the UDM cross-wind dispersion coefficient σ_y is virtually identical for x > 100 m, and slightly smaller for x < 100 m. Note that HGSYSTEM also adopts a modified Briggs formula (in addition to power-law) which leads to smaller values in the far-field. The latter formula may be more accurate.
- Figure 2.2 and Figure 2.3 show that the UDM vertical dispersion coefficient σ_z is virtually identical for 100<x<10000 m. For x< 100 m, the UDM σ_z is smaller (because of linearisation; note that TNO also suggests a linearised formula for x < 100 m, upon which the results would be virtually identical). For x > 10000 m, the UDM values are smaller.

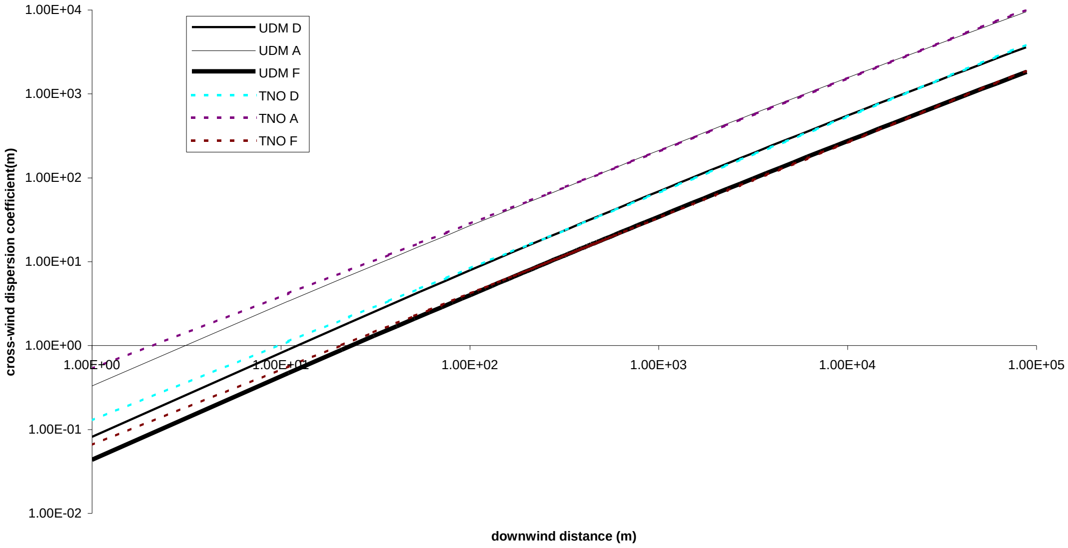


Figure 2.1 TNO and UDM cross-wind dispersion coefficient for stability classes A,D,F

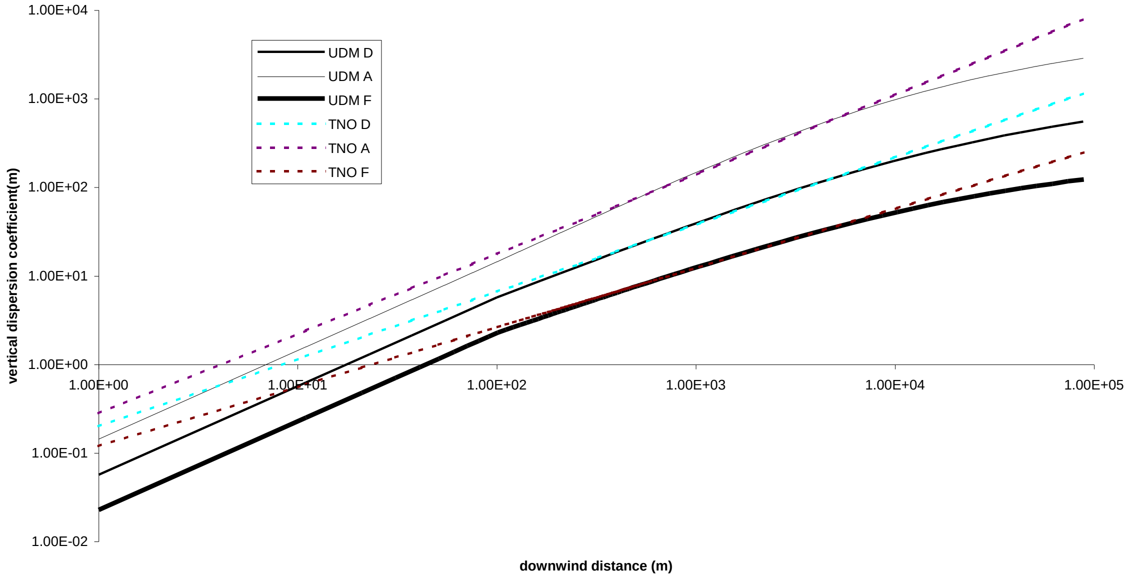


Figure 2.2 TNO and UDM vertical dispersion coefficient (surface roughness z_0=0.1 m) for stability classes A,D,F

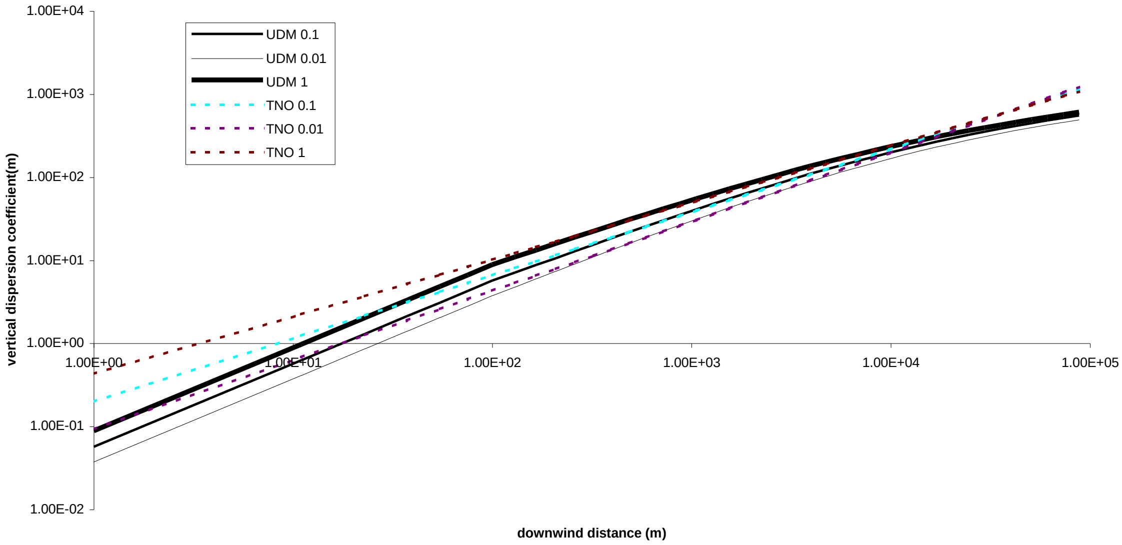


Figure 2.3 **TNO and UDM vertical dispersion coefficient (at stability class D) for surface roughness length z_0=0.01, 0.1, 1 m**

2.3 Basecase

Using the PHAST material database, a new 'pseudo-compound' nitrogen_air (material number –1001) was defined from the 'nitrogen' compound, by modifying the nitrogen mole weight to the air mole weight 28.966[1] . The UDM base-case run was subsequently defined as follows:

- case: continuous (duration 360000 s) 0.05 kg/s release of nitrogen_air at 50 m height with temperature 298K and velocity 5 m/s
- 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 = 600 s
- parameters: maximum distance = 100000, distance multiple for full passive entrainment = 2, dense to passive smoothing transition parameter = 2

For the above base-case problem, the figures below compare the UDM numerical results against the analytical solution for the cross-wind and vertical dispersion coefficients σ_y, σ_z and the centre-line and ground-level concentrations:

- Figure 2.4 shows that the numerical UDM results and results from the analytical McMullen formula for σ_y, are identical if x > L = 11.433. The results are different for x < L since, unlike McMullen, UDM assumes σ_y to vary linearly for x < L (see UDM theory manual).
- Figure 2.5 demonstrates that the UDM value of σ_z is larger further downwind (x>1000m) because of the h_d effect. This effect dies out in the very far field.
- Figure 2.6 depicts centre-line and ground-level concentrations obtained from both the UDM numerical result and the analytical TNO profile. Note that different profiles are used for UDM and analytical TNO formula. Nevertheless results for both centre-line and ground-level concentrations are close.

[1] Defining 'air' as a mixture of N_2 and O_2 did arise in problems.

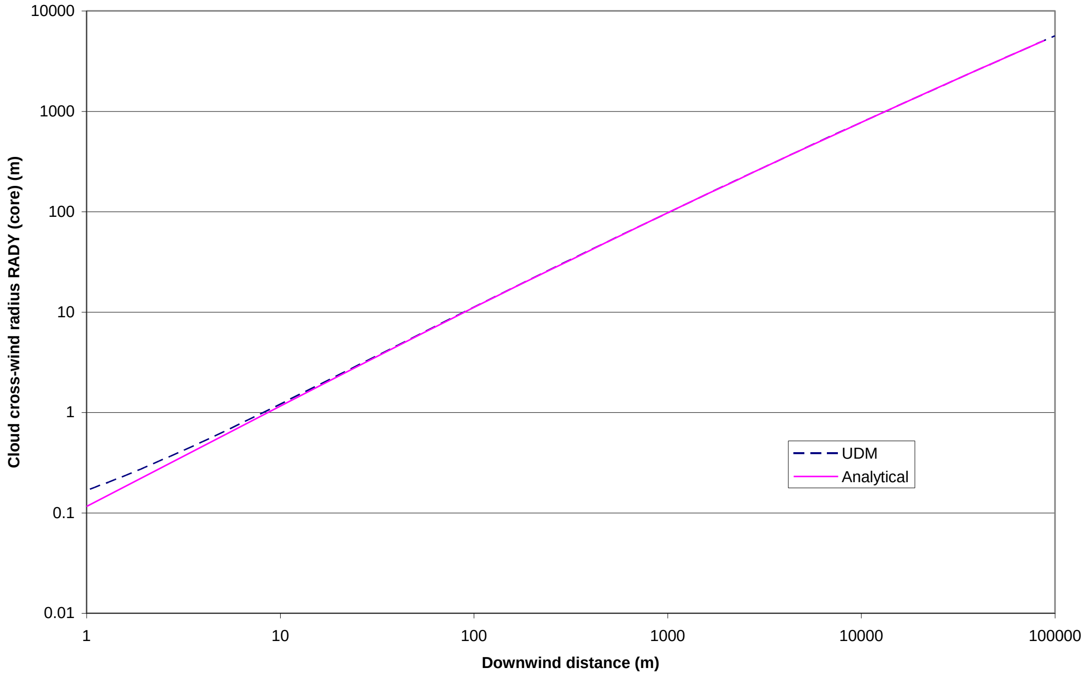


Figure 2.4 **Cross-wind dispersion coefficient: numerical UDM result and analytical formula for ambient dispersion coefficient by McMullen**

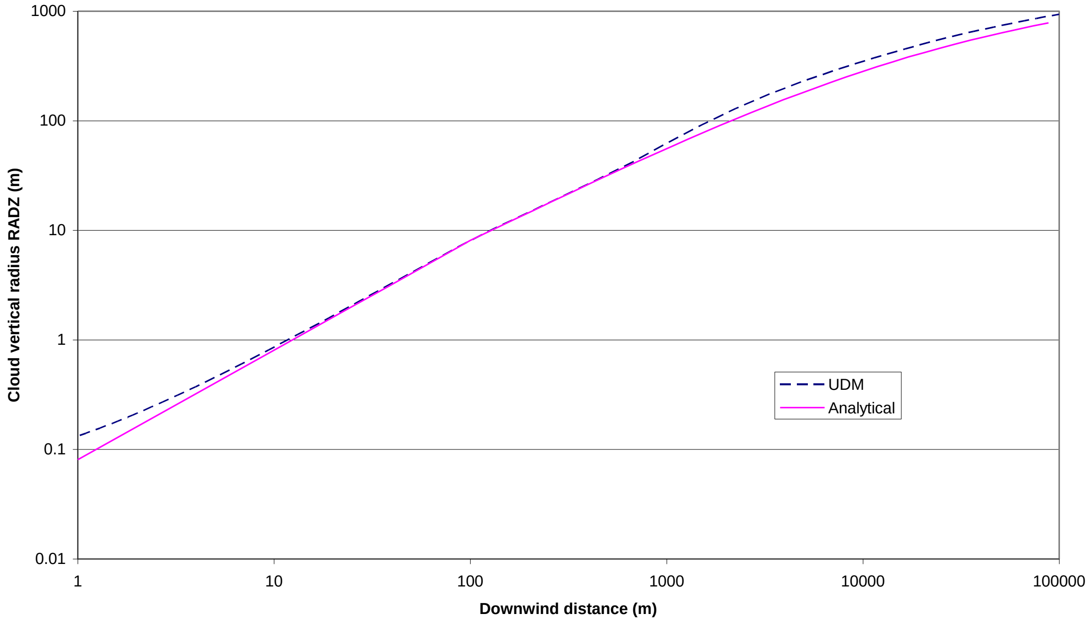


Figure 2.5 **Vertical dispersion coefficient: UDM numerical result and analytical formula for ambient dispersion coefficient by Hosker**

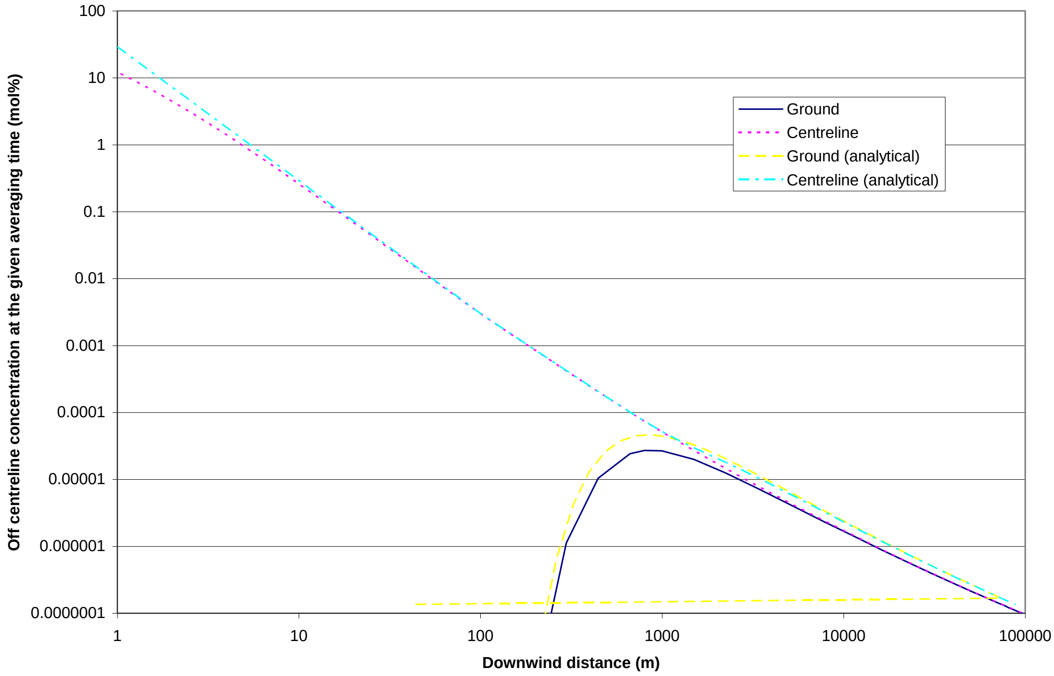


Figure 2.6 **Centre-line and ground-level concentrations: UDM numerical result and analytical TNO profile.**

2.4 Sensitivity analysis

This section reports the sensitivity analysis. The figures below depict results for σ_y, σ_z, the centre-line concentration $c_o(x) = c(x,0,h)$ and the ground-level concentration $c(x,0,0)$. The following conclusions can be drawn.

1. Variation of release height (Figure 2.7): z_R = 0, 0.1, 1, 5, 50, 100, 700 m

    a. The cross-wind dispersion coefficient is always equal to σ_{ya} (apart from small deviation near the source, because of initial non-zero value calculated from the expanded diameter)

    b. In the near-field (where $\sigma_z << z_{cld}$) and in the far field (where $\sigma_z >> z_{cld}$), $\sigma_z \approx \sigma_{za}$ [2]. However deviations from σ_{za} occur as the cloud's vertical dispersion coefficient σ_z approaches the cloud elevation z_{cld} (between near-field and far-field)

    c. As the clouds vertical dispersion coefficient increases the fractional touchdown term, h_d, decreases from 1 to 0. For $\sigma_z >> z_{cld}$, it can be shown from the analytical Gaussian concentration profile that the ground-level concentration is half the centre-line concentration. This can indeed be confirmed from the results depicted in Figure 2.7c,d

2. Variation of averaging time (Figure 2.8) : t_{av} = 18.75, 60, 600, 3600 s

    a. The cross-wind dispersion coefficient is equal to σ_{ya} and increases by a factor, $(t/600)^{0.2}$, for averaging time t_{av} > 18.75 seconds

    b. The vertical dispersion coefficient is independent of averaging time

    c. The centre-line and ground-level concentrations decrease by a factor $(t/600)^{0.2}$, for averaging time t_{av} > 18.75 seconds

3. Variation of surface roughness length (Figure 2.9): z_o = 0.0001,0.001,0.01, 0.1,1,3 m

    a. The cross-wind dispersion coefficient is independent of surface roughness

    b. The vertical dispersion coefficient increases with surface roughness. The comparison of the theoretical values with those obtained with the UDM is good except in the far field. Note that for z_0<0.01 m, the UDM adopts values at z_o = 0.01 m

    c. Since σ_z increases with z_o, the centre-line concentration decreases with z_o. In the near-field the ground-level concentrations are higher (because of larger σ_z) but in the far-field smaller (because of larger overall dilution)

4. Variation of stability class (Figure 2.10): A,B,C,D,E,F (and also intermediate classes and G)

    a. Vertical and horizontal dispersion coefficients decrease with increasing stability (less air entrainment) leading to higher centre-line concentrations. The ground-level concentrations are smaller in the near-field and higher in the far field.

    b. Comparison of the UDM crosswind and vertical dispersion coefficients with theoretical values is good

5. Variation of release rate (Figure 2.11): m_c = 0.005, 0.05, 0.5, 5, 50 kg/s

    a. The plume expanded diameter increases with the release rate. As a result, the initial values of the vertical and crosswind dispersion coefficients (directly set from the expanded diameter) are larger.

    b. The centre-line and ground-level concentrations increase linearly with the release rate (in line with the analytical Gaussian concentration profile)

6. Variation of wind speed (Figure 2.12): u_o = 1, 3, 5, 8, 11 m/s

    a. Concentrations are inversely proportional to wind speed.

    b. The centre-line and ground-level concentration are inversely proportional to the release rate (in line with the analytical Gaussian concentration profile)

[2] The remaining deviation for large heights can be explained because of inaccurate numerical calculations (Runge-Kutta method to be improved)

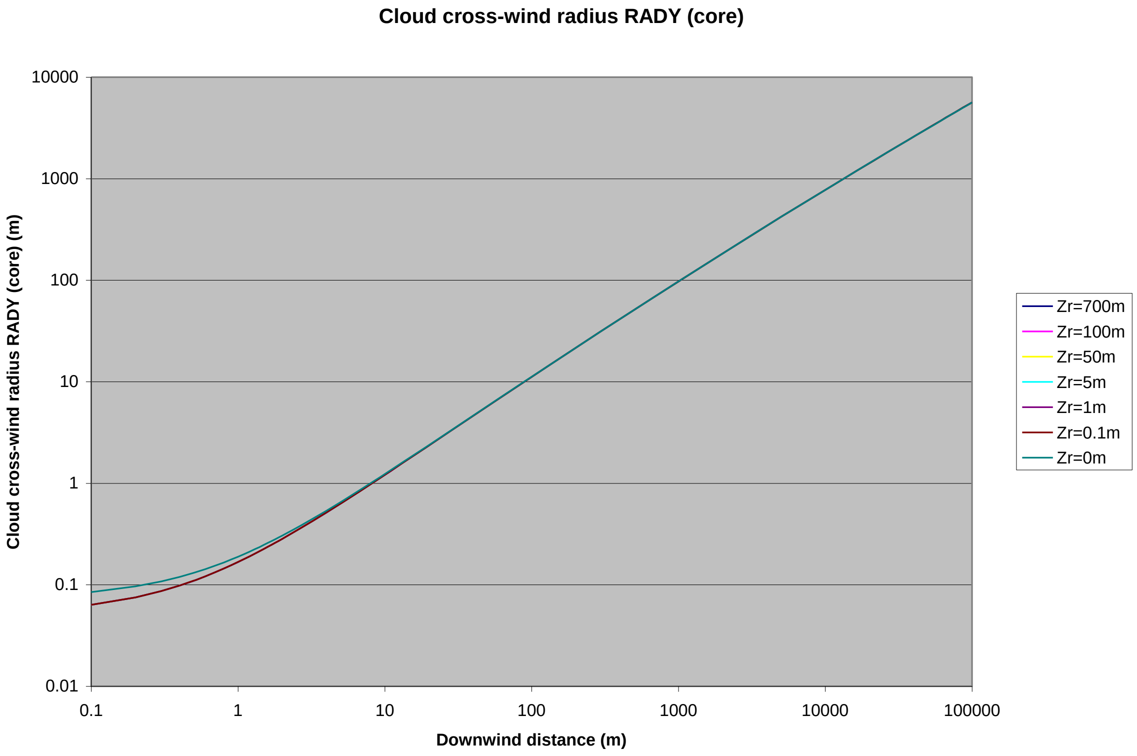


Figure 2.7 (a) cross-wind dispersion coefficient $R_y = 2^{1/2}\sigma_y$

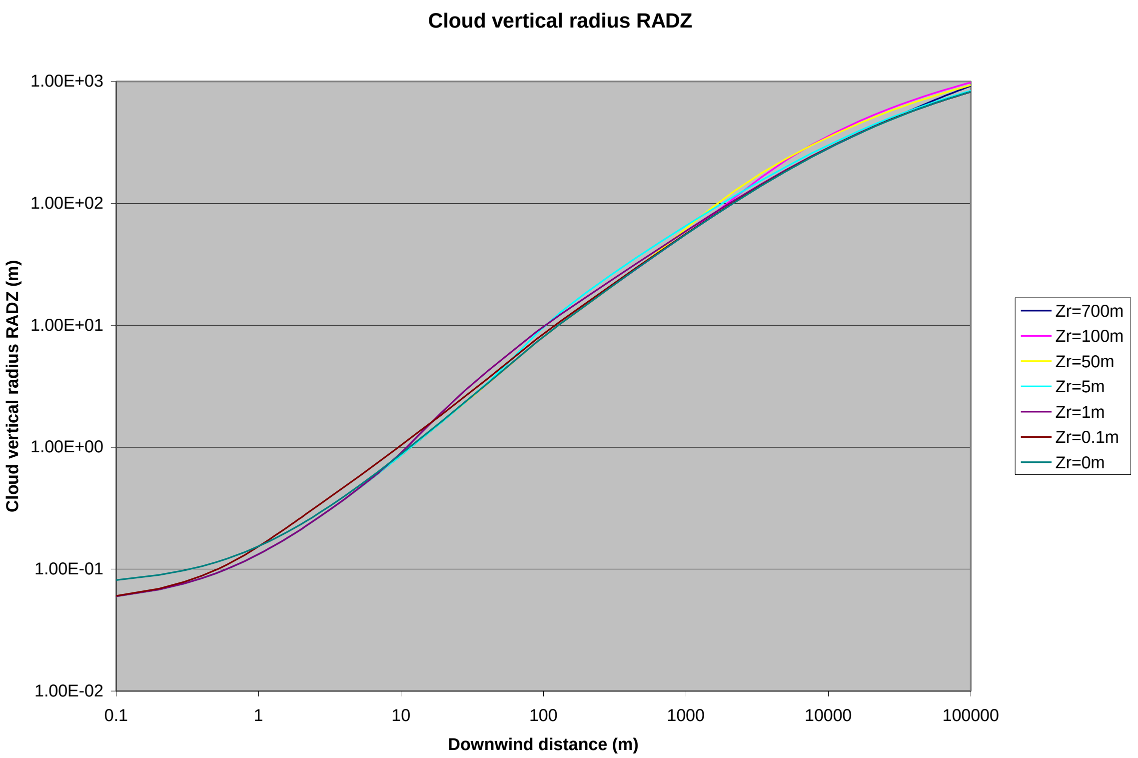
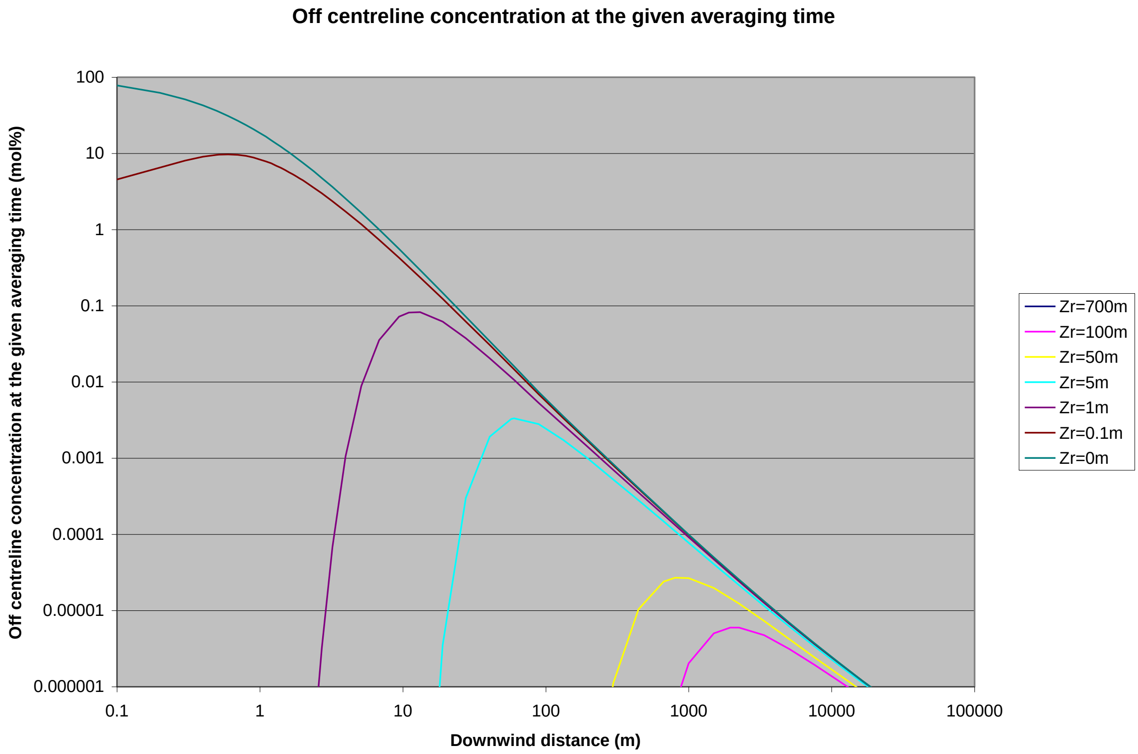
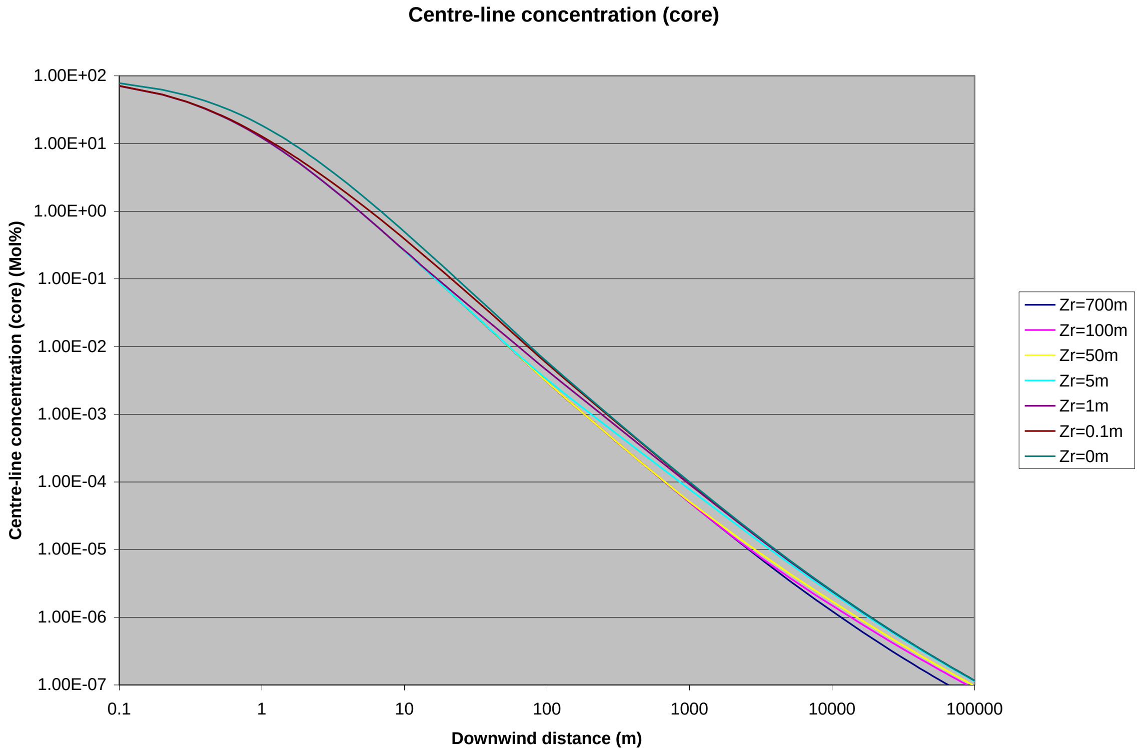


Figure 2.7(b) vertical dispersion coefficient $R_z = 2^{1/2}\sigma_z$



(c) ground-level concentration c(x,0,0)



(d) centre-line concentration $c(x,0,z_{cld}) = c_o(x)$

Figure 2.7 Effect of release height z_R on UDM predictions; z_R = 0, 0.1, 1, 5, 50, 100, 700 m

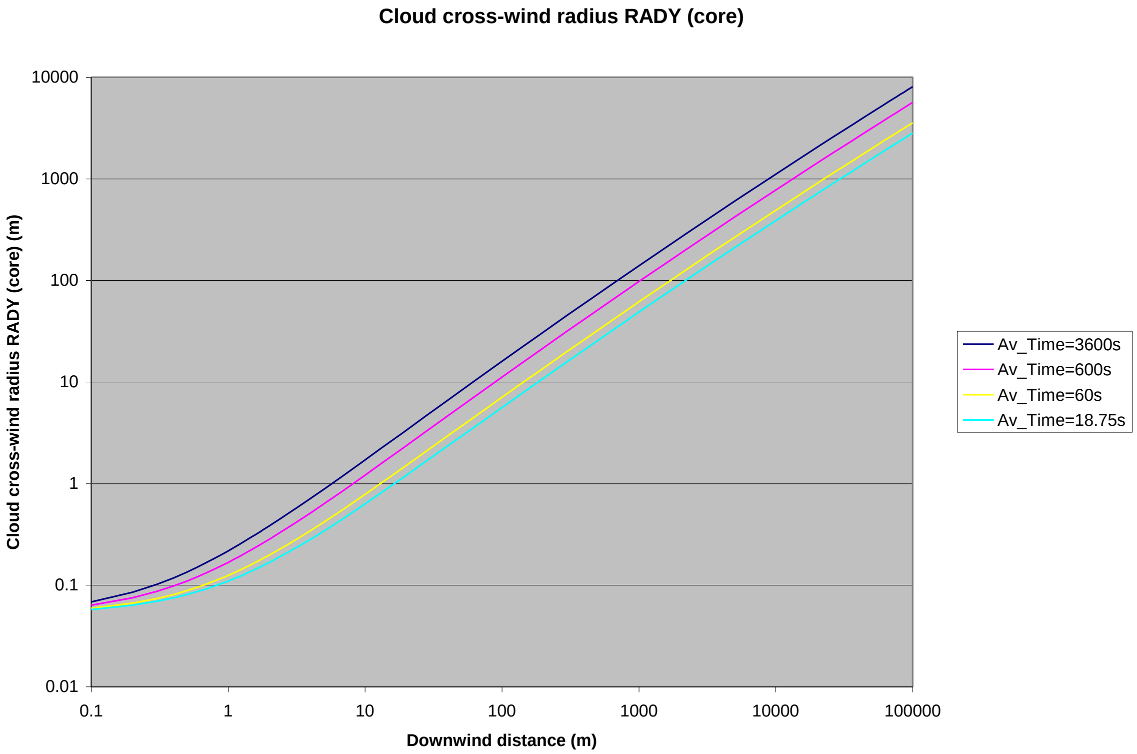


Figure 2.8(a) cross-wind dispersion coefficient $R_y = 2^{1/2}\sigma_y$

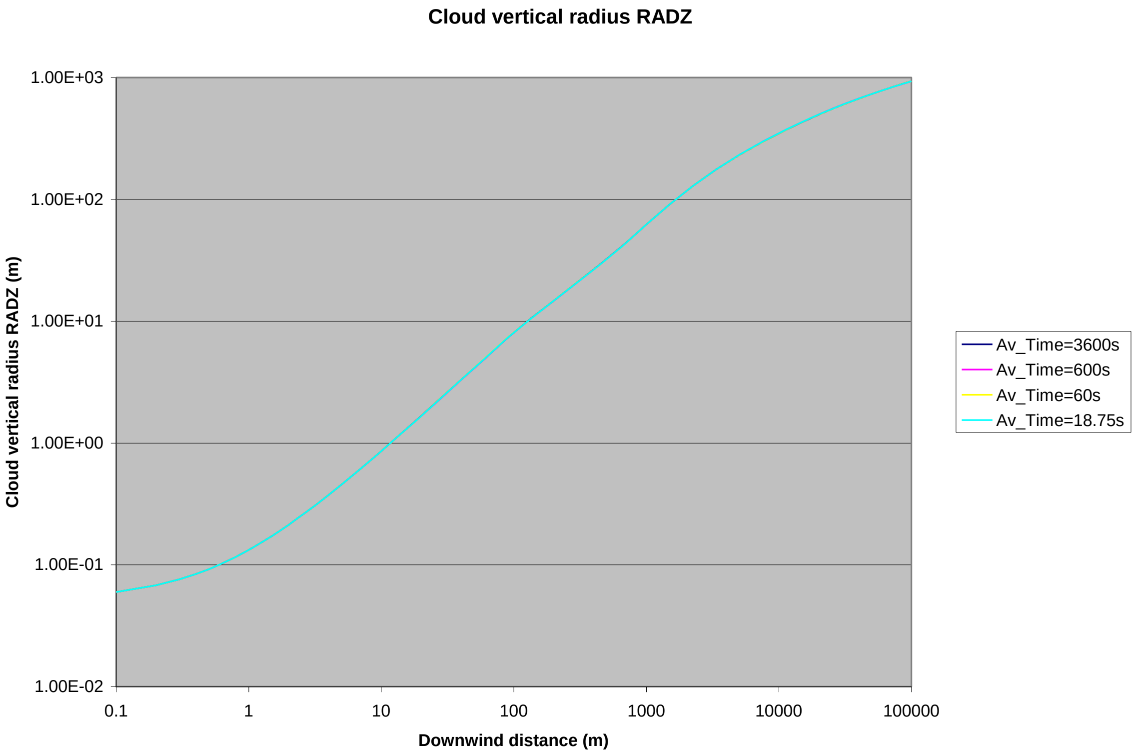
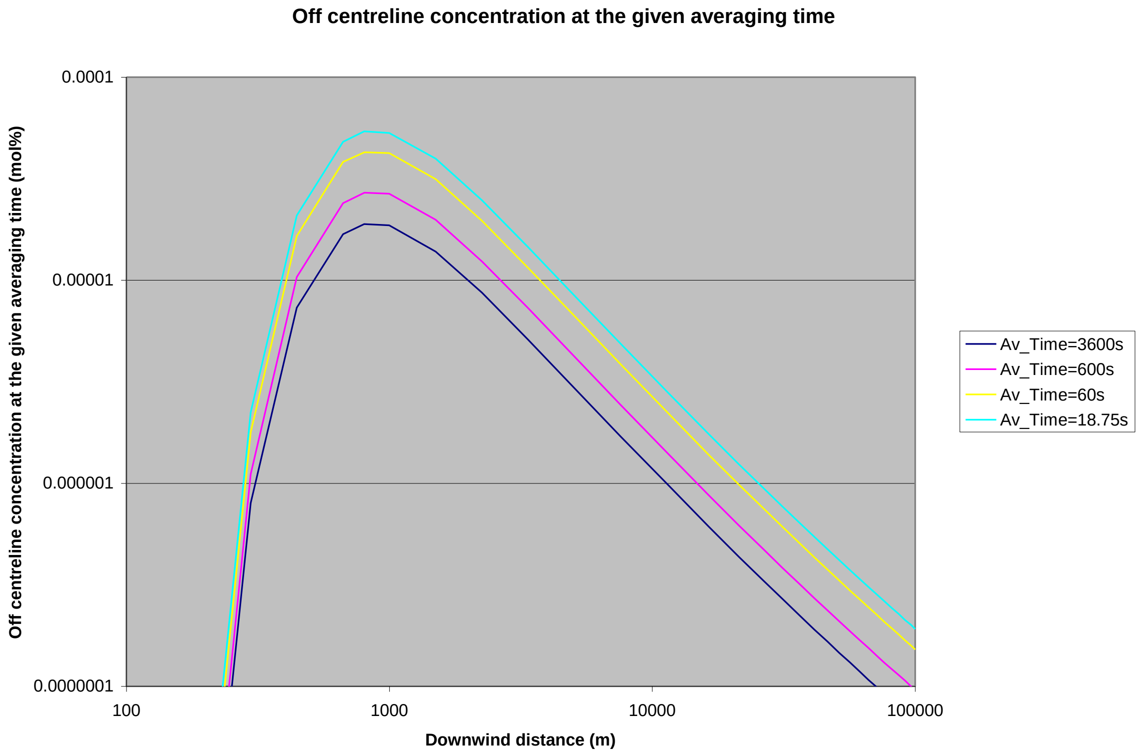
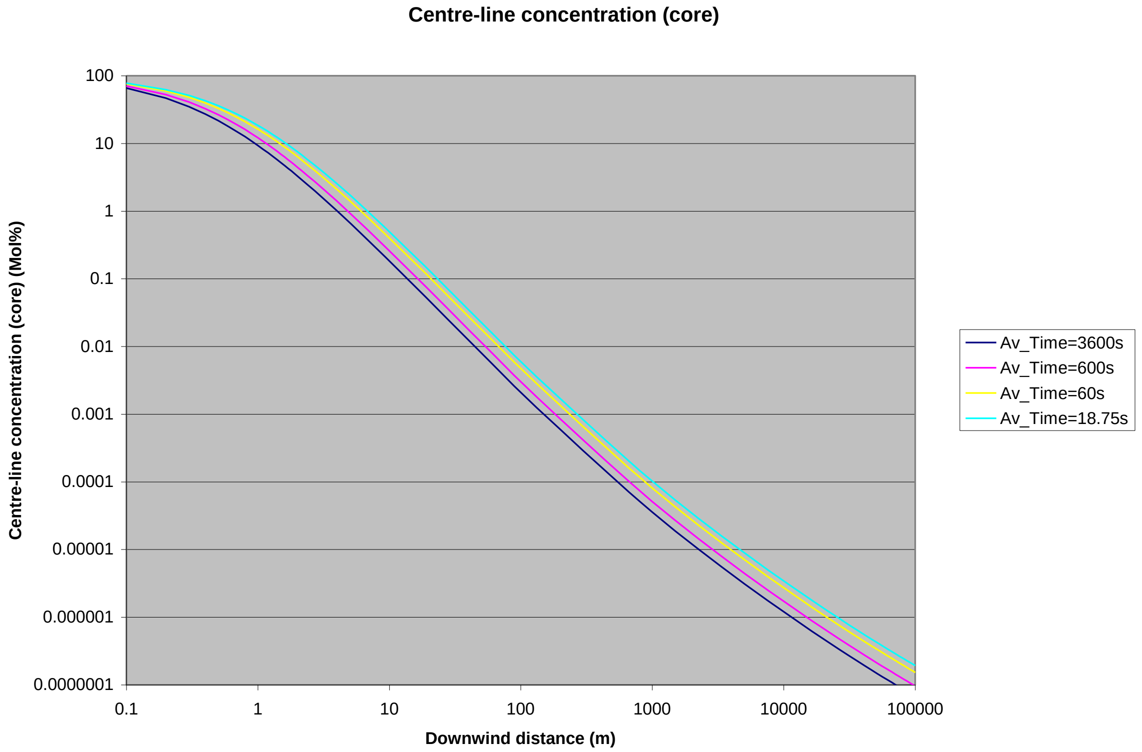


Figure 2.8(b) vertical dispersion coefficient $R_z = 2^{1/2}\sigma_z$

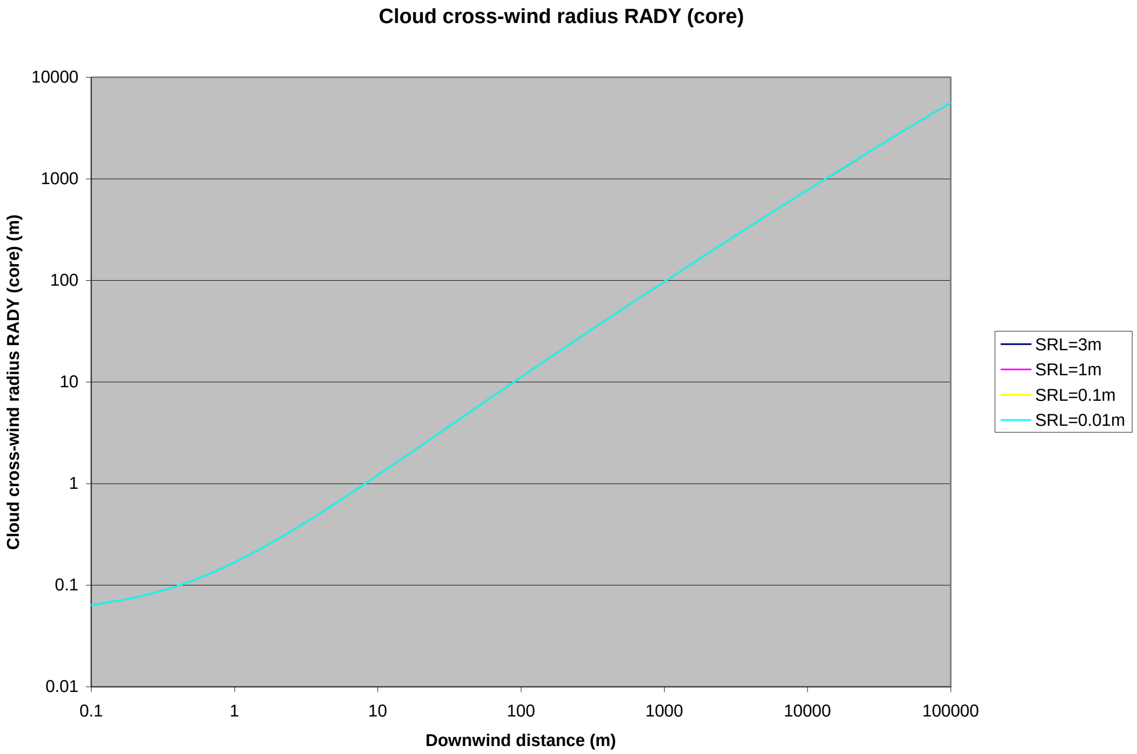


(c) ground-level concentration c(x,0,0)

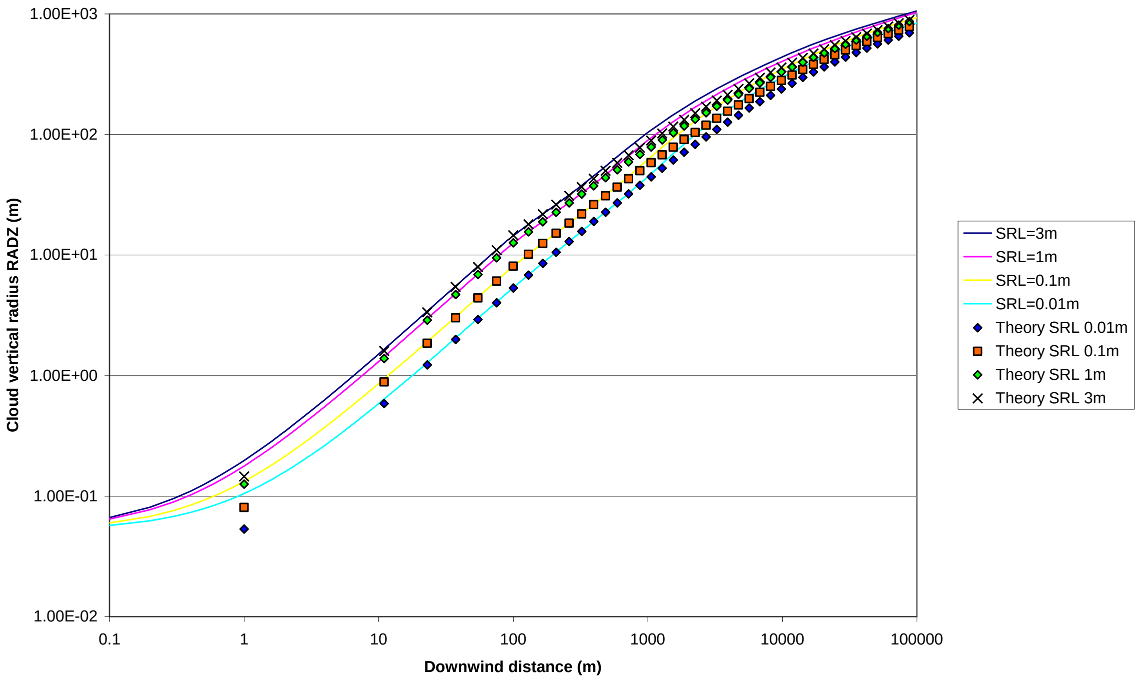


(d) centre-line concentration $c(x,0,z_{cld}) = c_o(x)$

Figure 2.8 **Effect of averaging time t_{av} on UDM predictions; t_{av} = 18.75, 60, 600, 3600 s**

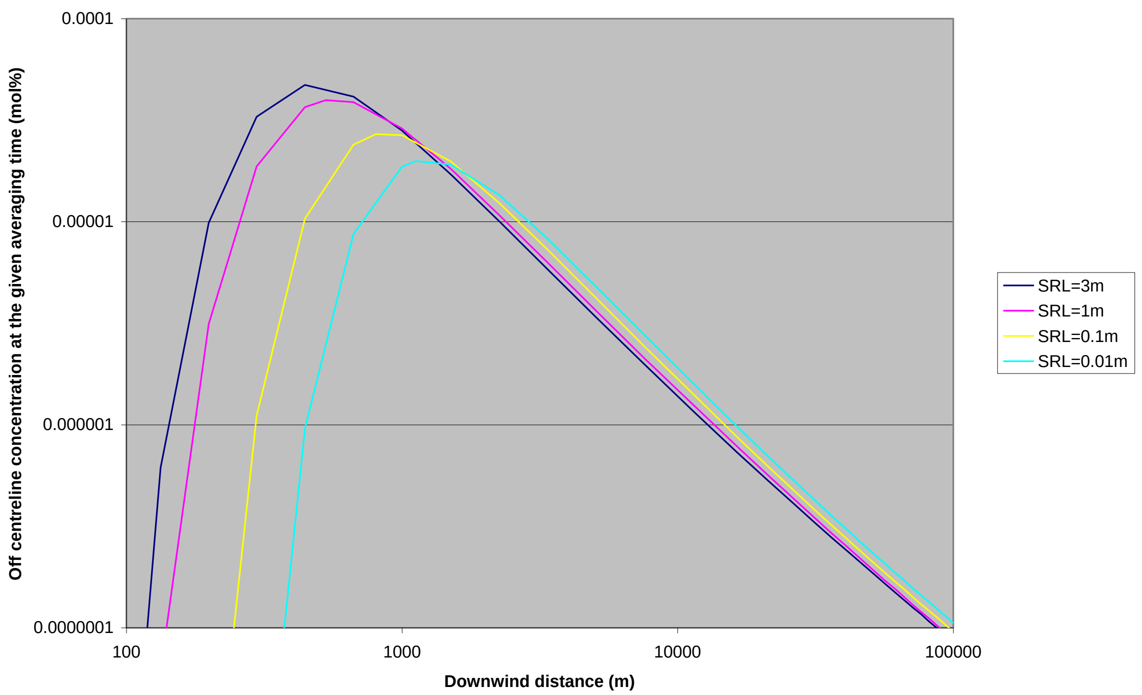


(a) cross-wind dispersion coefficient $R_y = 2^{1/2}\sigma_y$



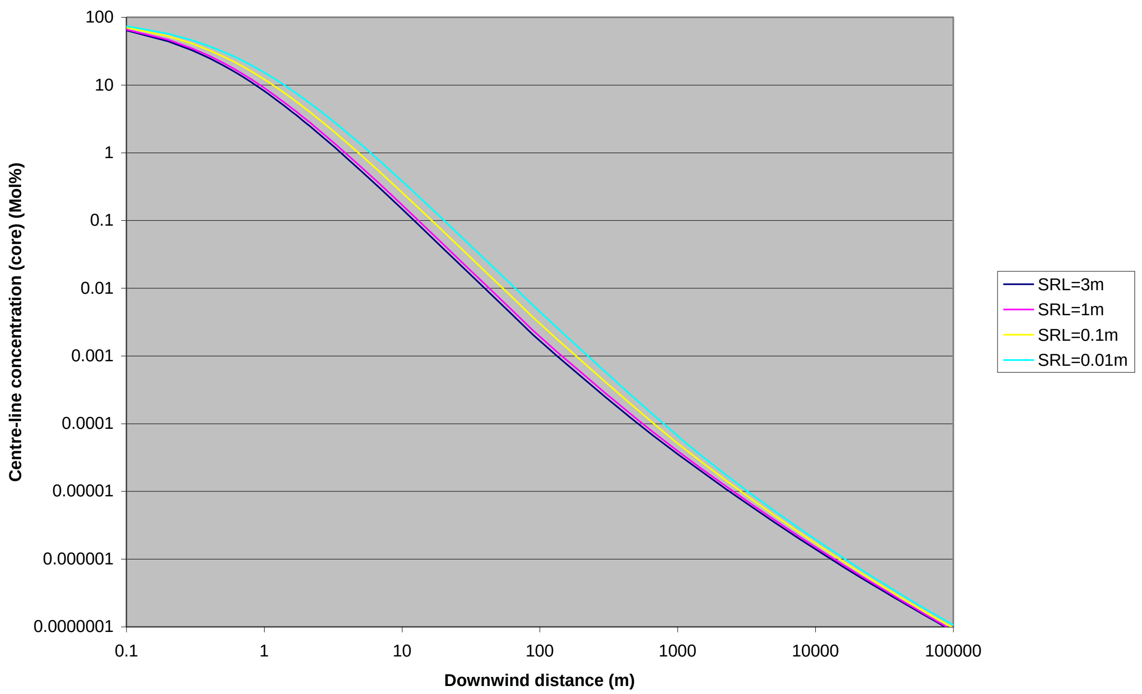
(b) vertical dispersion coefficient $R_z = 2^{1/2}\sigma_z$

Off centreline concentration at the given averaging time



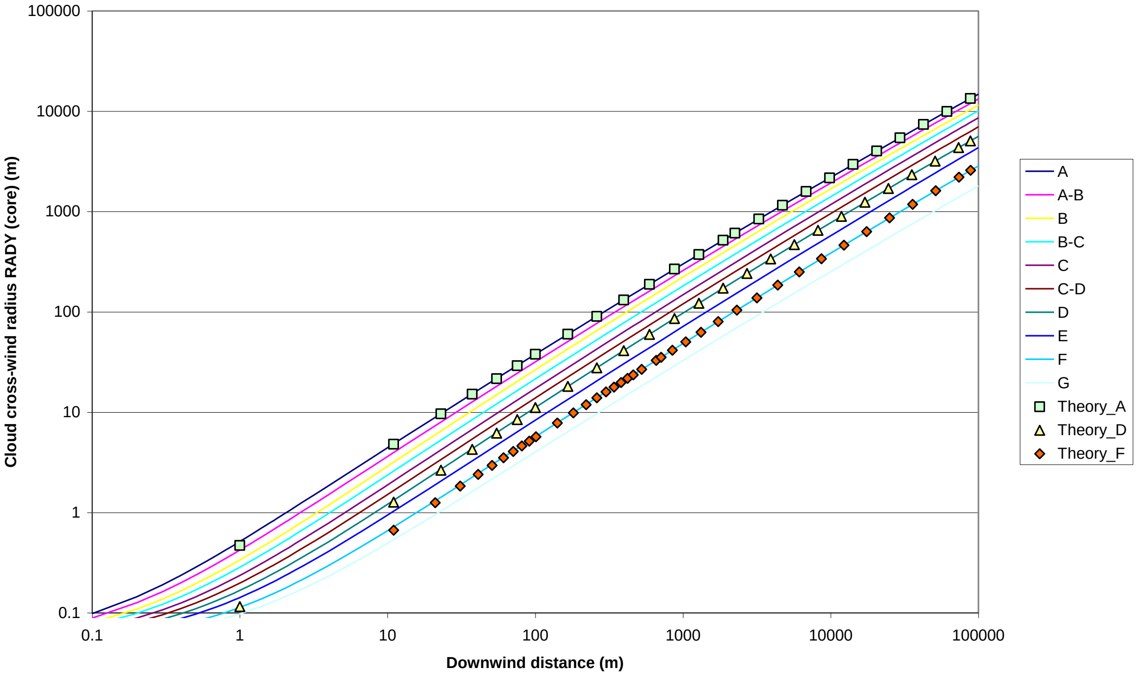
(c) ground-level concentration c(x,0,0)

Centre-line concentration (core)

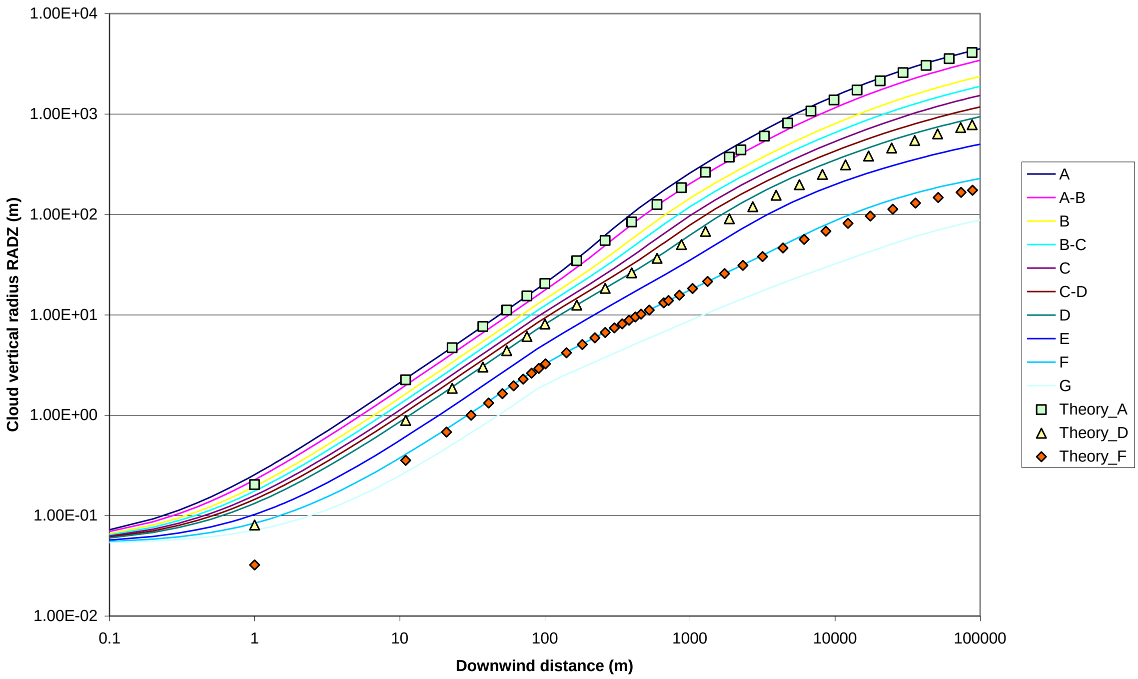


(d) centre-line concentration $c(x,0,z_{cld}) = c_o(x)$

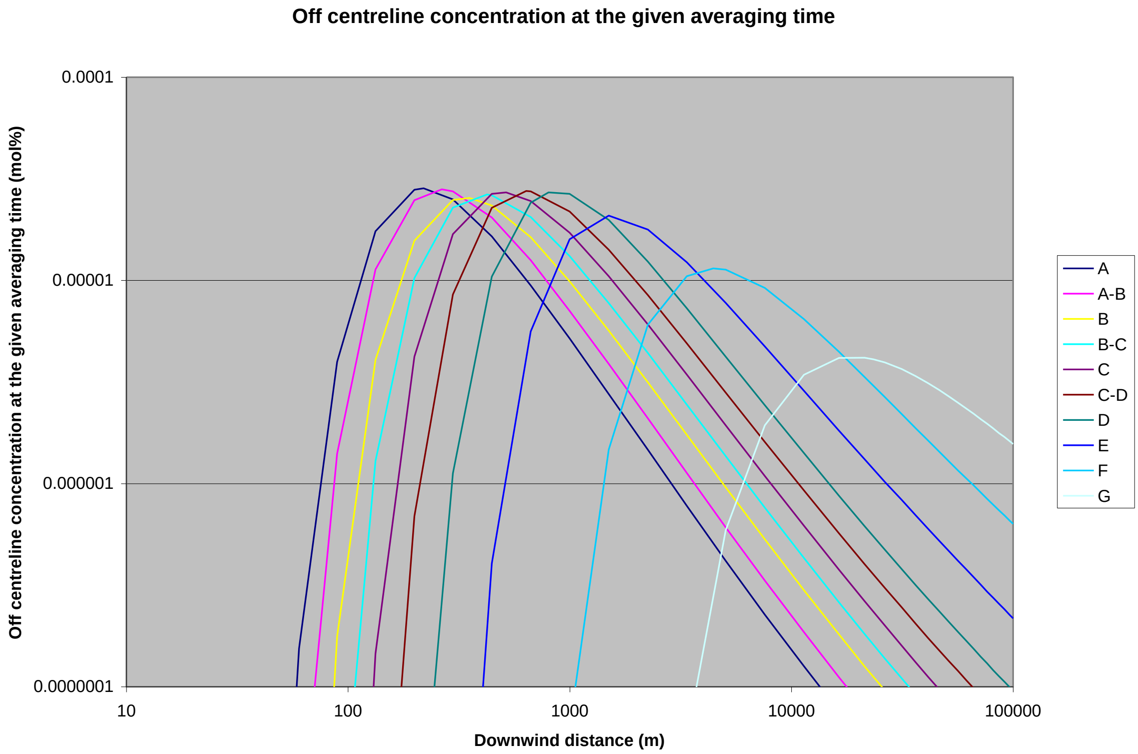
Figure 2.9 Effect of surface roughness length z_o on UDM predictions; z_o = 0.01, 0.1, 1, 3 m



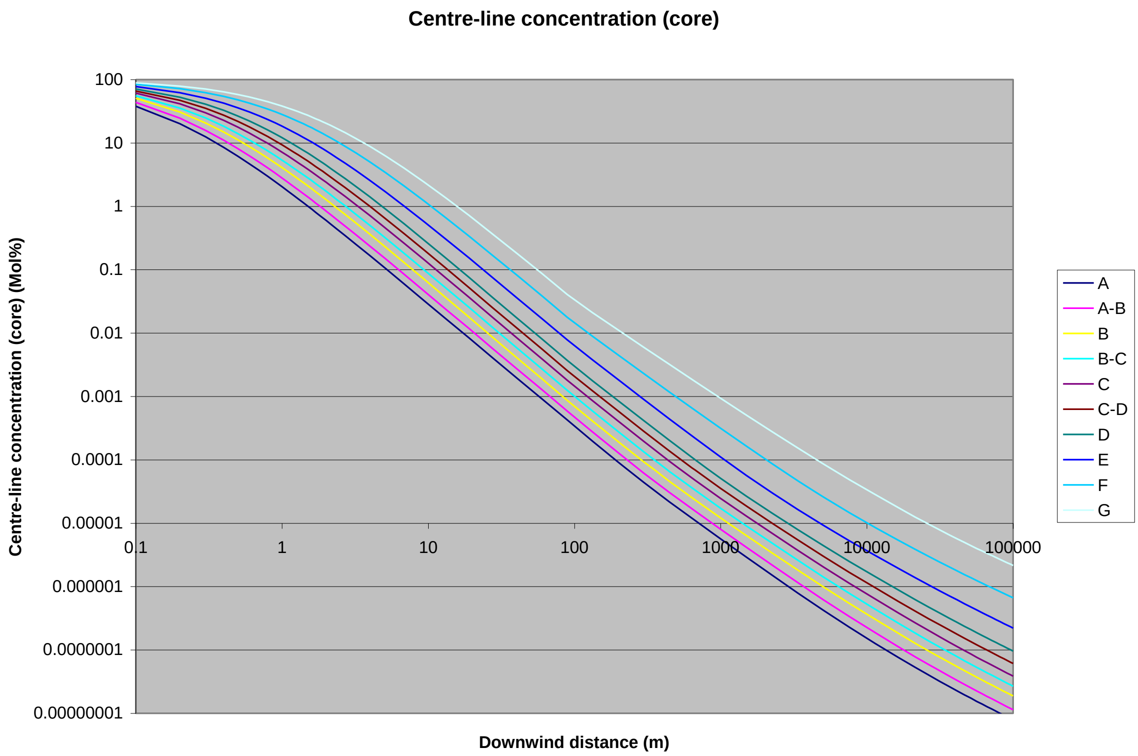
(a) cross-wind dispersion coefficient Ry = $2^{1/2}\sigma_y$



(b) vertical dispersion coefficient $R_z = 2^{1/2}\sigma_z$

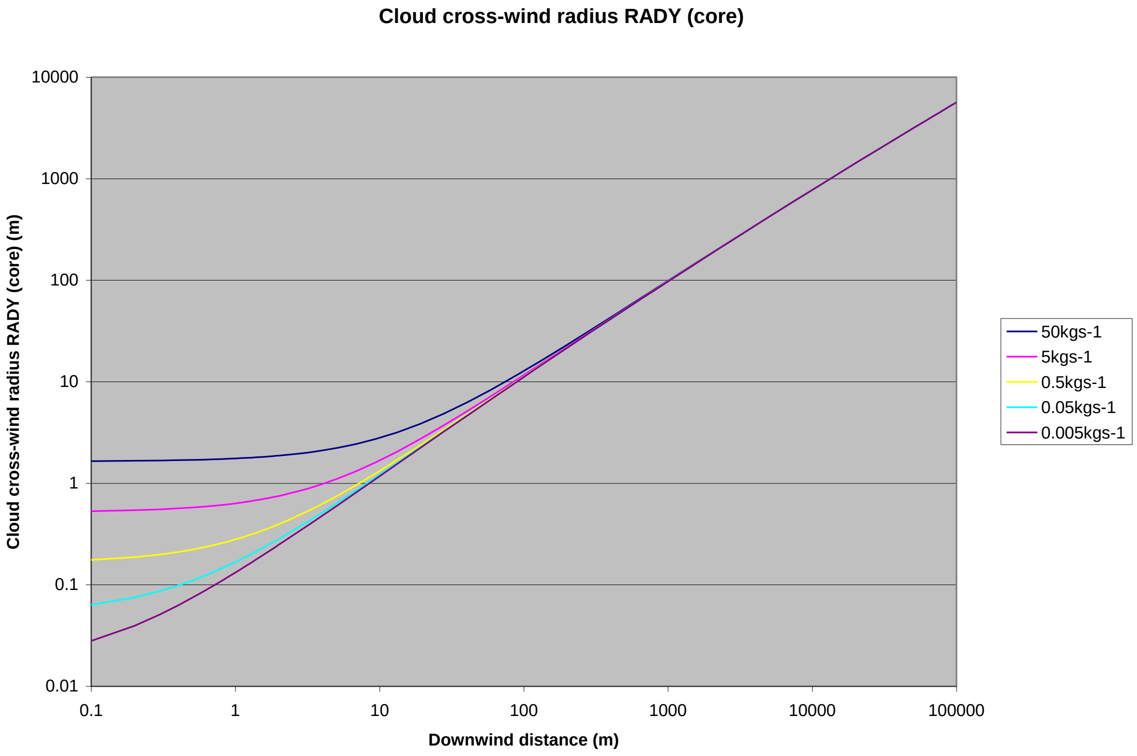


(c) ground-level concentration c(x,0,0)

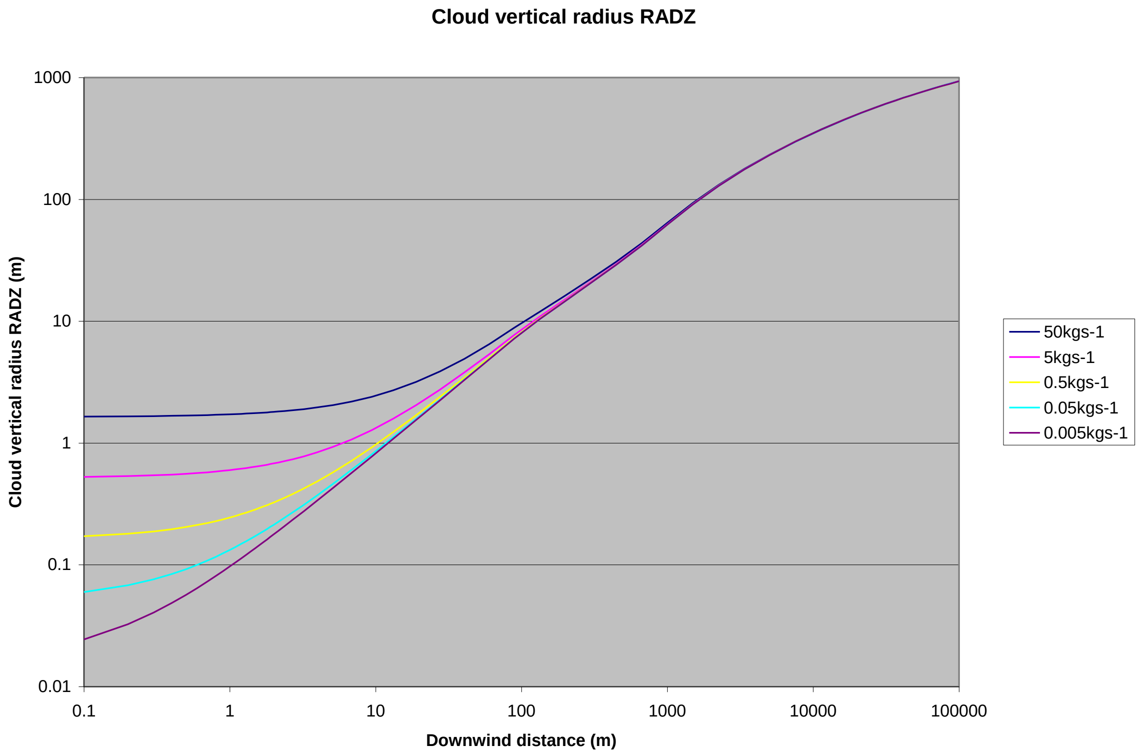


(d) centre-line concentration $c(x,0,z_{cld}) = c_o(x)$

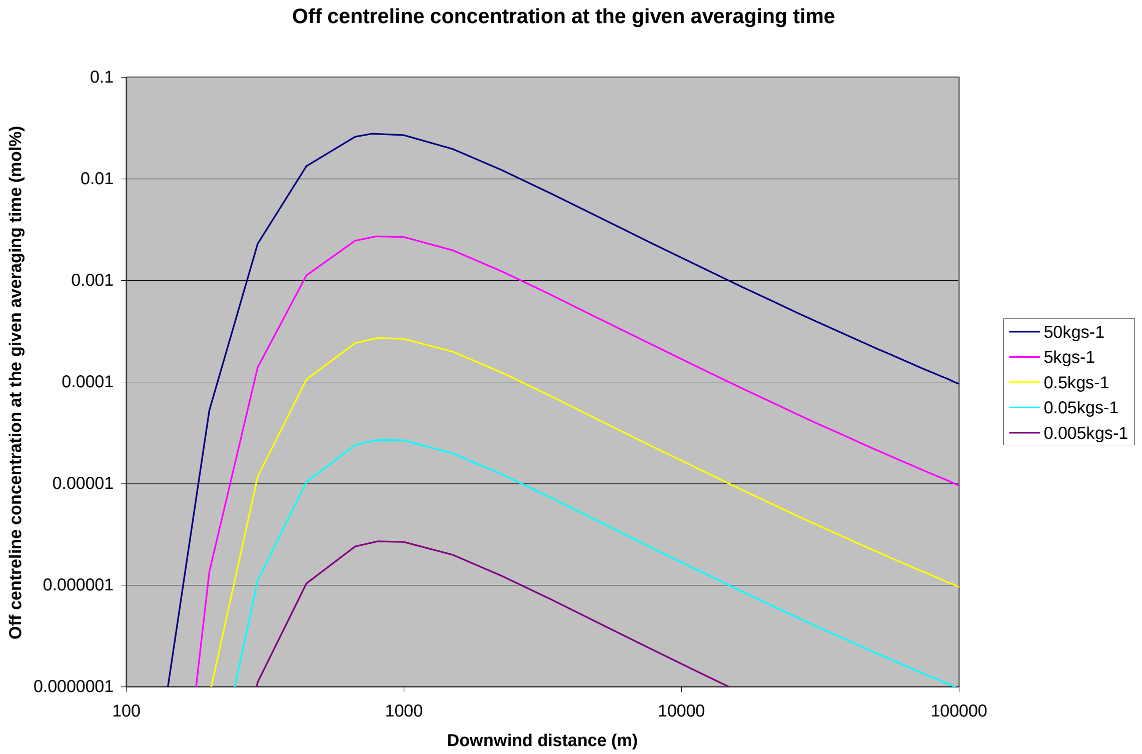
Figure 2.10 **Effect of stability class on UDM prediction; stability class = A, A/B, B, B/C, C, C/D, D, E, F, G, H; Figures (a), (b) illustrate that the UDM predictions are in close agreement with the analytical values for the ambient passive dispersion coefficients σ_{ya}, σ_{za}**



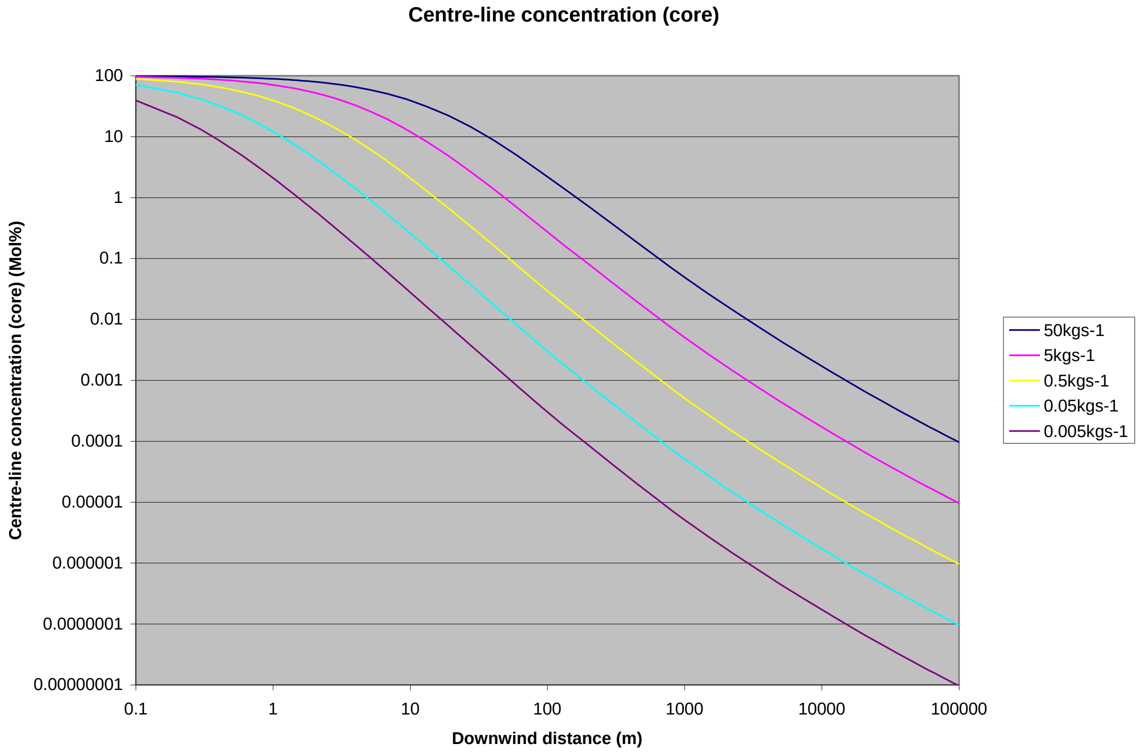
(a) cross-wind dispersion coefficient $R_y = 2^{1/2}\sigma_y$



(b) vertical dispersion coefficient $R_z = 2^{1/2}\sigma_z$

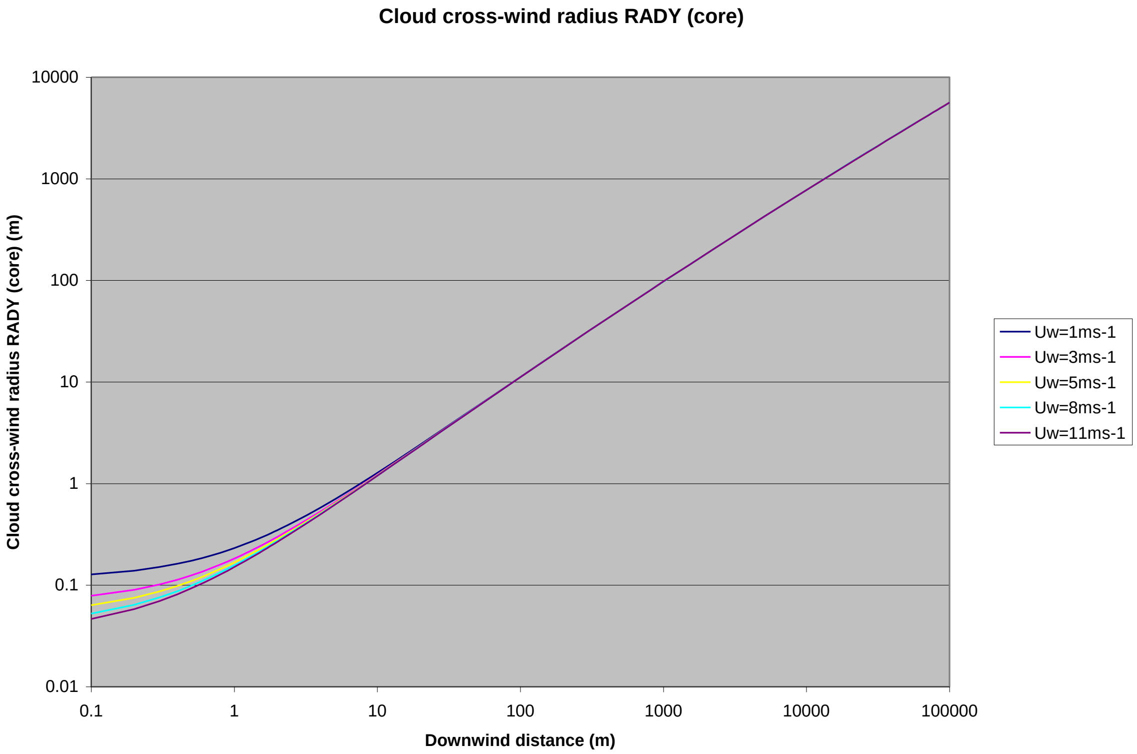


(c) ground-level concentration c(x,0,0)

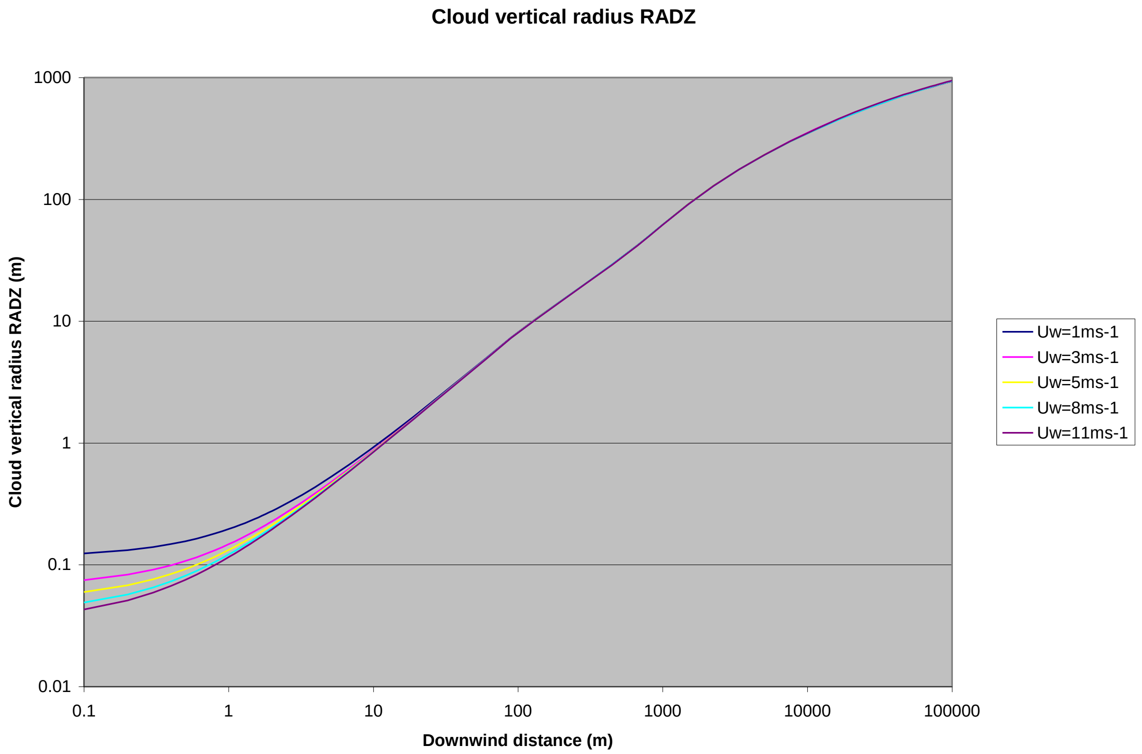


(d) centre-line concentration c(x,0,h) = $c_o(x)$

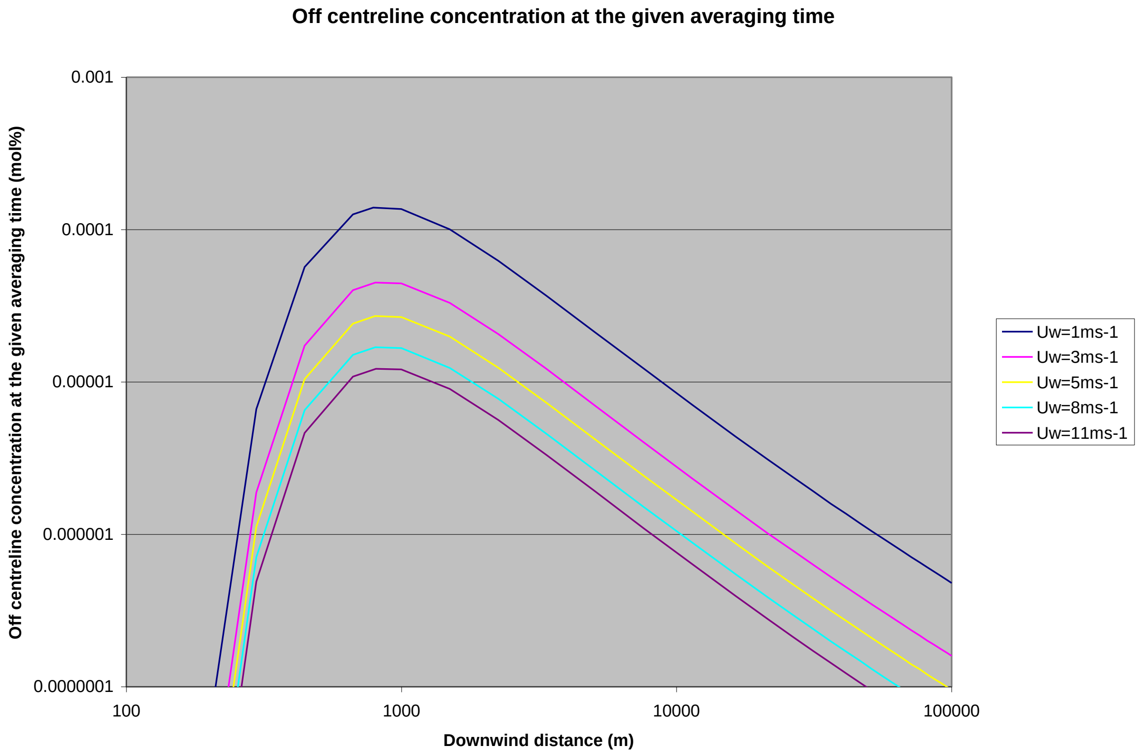
Figure 2.11 Effect of release rate Q on UDM predictions; Q = 0.005, 0.05, 0.5, 5, 50 kg/s



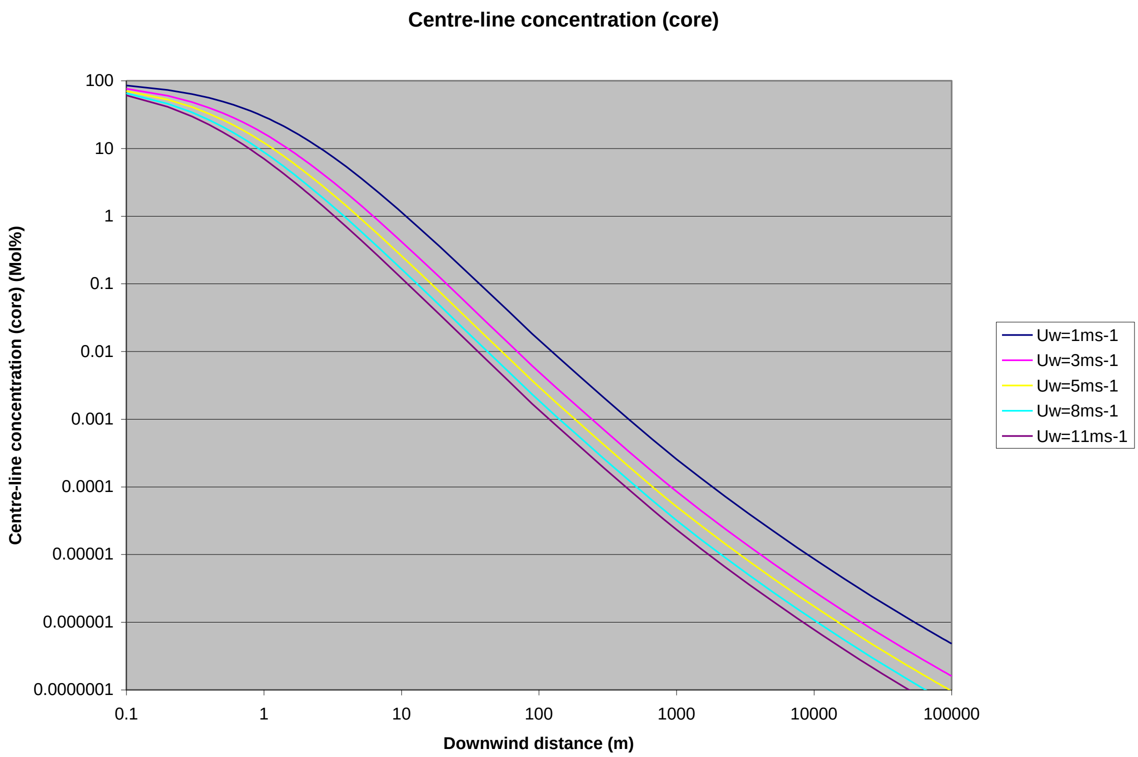
(a) cross-wind dispersion coefficient $R_y = 2^{1/2}\sigma_y$



(b) vertical dispersion coefficient $R_z = 2^{1/2}\sigma_z$



(c) ground-level concentration c(x,0,0)



(d) centre-line concentration $c(x,0,z_{cld}) = c_o(x)$

Figure 2.12 Effect of wind speed u_o on UDM predictions; u_o = 1, 3, 5, 8, 11 m/s

FIGURES

Figure 2.1	BCT4PGSY.xls
Figure 2.2	BCT4PGSZ.xls
Figure 2.3	BCT4ZRSZ.xls
Figure 2.4	BC4_analytical.xls
Figure 2.5	BC4_analytical.xls
Figure 2.6	BC4_analytical.xls
Figure 2.7	BC4_Release_Elevation.xls
Figure 2.8	BC4_Averaging_Time.xls
Figure 2.9	BC4_Surface_Roughness_Length.xls
Figure 2.10	BC4_Stability_Class.xls
Figure 2.11	BC4_Release_Rate.xls
Figure 2.12	BC4_Windspeed.xls

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